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# SU(mn)⊃SU(m)×SU(n) isoscalar factors and S($f_1+f_2$)⊃S($f_1$)×S($f_2$) isoscalar factors

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A simple relation is found between the isoscalar factor (ISF) of the unitary group and those of the permutation group, i.e. the SU($mn$)⊂SU($m$)×SU($n$)ISF is equal to the S($f_1+f_2$)⊂S($f_1$)×S($f_2$) ISF. Since the values of $S(f_1+f_2)\subset S(f_1)\times S(f_2)$ISF are independent of $m$ and $n$, one arrives at an important conclusion that the values of SU($mn$)⊂SU($m$)×SU($n$) ISF are also independent of $m$ and $n$. Therefore they can be calculated for all $m$ and $n$ by a single stroke instead of one $m$ and one $n$ at a time. An eigenfunction metho for evaluating the SU($mn$)⊂SU($m$)×SU($n$)ISF is given which can be easily translated into a computer program.

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## 1. INTRODUCTION

With the development of the particle physics and hyper-nuclear physics, one has to extend the Wigner supermultiplet theory of SU(4)⊃SU(2)×SU(2) to the more general case of SU($mn$)⊃SU($m$)×SU($n$) and face the problem of evaluating the SU($mn$)⊃SU($m$)×SU($n$) isoscalar factor (ISF) with $m$ and/or $n$ larger than two. Up to now, only some results of the SU(6)⊃SU(3)×SU(2) ISF can be found in Refs. 1–3. It is currently believed that there are at least five and probably six flavor quarks, therefore, one needs SU(10)⊃SU(5)×SU(2) or SU(12)⊃SU(6)×SU(2) ISF. However, in the methods[1–3] traditionally used for calculating the SU($mn$)⊃SU($m$)×SU($n$) ISF, the labor involved in such calculation increases drastically as $m$ or $n$ increases. From our earlier work[4] it is known that the SU($n$) ⊃SU($n-1$) ISF are independent of $n$. Any SU($n$) ⊃SU($n-1$) ISF belongs either to the derivable type [i.e. it is equal to SU($n-1$)⊃SU($n-2$) ISF] or the underivable type (i.e. it must be calculated directly). Therefore the calculation of any SU($n$)⊃SU($n-1$) ISF is reduced to the calculation of a few underivable ones. In this paper, we want to generalize this result. We identify the SU($mn$)⊃SU($m$)×SU($n$) ISF with $S(f_1+f_2)\supset S(f_1)\times S(f_2)$ ISF [$S(f_1)$ etc. stand for the permutation groups], therefore the values of the SU($mn$)⊃SU($m$)×SU($n$) ISF are independent of $m$ and $n$.

In a series of papers,[5–6] we proposed a new approach to the group representation theory. Three kinds of complete sets of commuting operators, denoted as CSCO-I, II and III, were introduced. The basic problems encountered in the group representation theory such as the finding of (I) characters, (II) irreducible bases, the Clebsch–Gordan coefficients and (III) irreducible matrix elements, etc., are all simplified to the solving of eigenequations of the CSCO-I, II, and III, respectively. Therefore, we call it the Eigenfunction Method. The CSCO-I, denoted as $C$, of a group $G$ is a set of operators which commutes with any element of $G$, and is a complete set of commuting operators in the class space of the group $G$. For finite groups, CSCO-I consists of a few class operators of the group. The CSCO-I for commonly used finite groups are listed in Ref. 6. For the permutation group S($f$) the CSCO-I is $C_{(2)}(f)$ for $f\leqslant 5$ and $f=7$ or $(C_{(2)}(f), C_{(3)}(f))$, for $f=6$ and $8\leqslant f\leqslant 14$, where $C_{(i)}(f)$ is the $i$-cycle class operator of S($f$).

Suppose $G\supset G(s)$ is a canonical subgroup chain of $G$ and $C(s)$ is a set of operators which consist of the CSCO-I of all the subgroups contained in the subgroup chain $G(s)$. Then the set $(C,C(s))$ is called the CSCO-II of the group $G$. It was proved that a necessary and sufficient condition for $\psi_m^{(\nu)}$ to belong to the basis in the $G\supset G(s)$ classification is that $\psi_m^{(\nu)}$ is the eigenfunction of the CSCO-II of $G$, i.e.

$$\begin{pmatrix} C \\ C(s) \end{pmatrix} \psi_m^{(\nu)} = \begin{pmatrix} \nu \\ m \end{pmatrix} \psi_m^{(\nu)}. \tag{1a}$$

It was proved[6] that $(f-1)$ operators

$$(C\,C(s)) = (C_{(2)}(f), C_{(2)}(f-1),\ldots, C_{(2)}(2)), \tag{1b}$$

constitute the CSCO-II of the permutation group $S(f)$, whose simultaneous eigenfunctions give the Yamanouchi bases.

Since the Eigenfunction Method proves to be very successful for calculating the Clebsch–Gordan coefficients and the outer-product reduction coefficients of the permutation group,[7] this method is now used to calculate the S($f+f_2$)⊃S($f_1$)×S($f_2$) ISF, namely the SU($mn$)⊃SU($m$) ×SU($n$) ISF. The merit of this method is that it is independent of $m$ and $n$ and can be easily implemented on a computer. Expressions of SU($mn$)⊃SU($m$)×SU($n$) ISF in terms of the Clebsch–Gordan coefficients of the permutation group and the transformation coefficients from the standard (i.e. Yamanouchi) basis to the nonstandard basis of the permutation group are also given.

## 2. $S(f)\supset S(f-1)\times S(1)$ ISF

Suppose the coordinate $q$ of a particle is divided into two parts, $\chi$ and $\xi$, and $q=(\chi,\xi)$. For example, $\chi$ may represent the orbital coordinates and $\xi$ may represent the spin-isospin coordinates, or $\chi$ represents the isospin coordinate and $\xi$ represents the spin coordinate. Thus for a system with $f$ particles we hae three realizations of the permutation group $S(f)$ i.e. $S^{\chi}(f), S^{\xi}(f)$ and $S^{q}(f)$ which permute the indices of

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TABLE I. Notation for the irreducible bases of $S^{\nu}(l)$, $S^{\xi}(l)$ and $S^{q}(l)$, $l=f, f-1$.

| $S^{\nu}(f)$ | $S^{\nu}(f-1)$ | $S^{\xi}(f)$ | $S^{\xi}(f-1)$ | $S^{q}(f)$ | $S^{q}(f-1)$ |
|---|---|---|---|---|---|
| $\left\vert \begin{matrix}[\sigma] \\ m_1\end{matrix} \right\rangle = \left\vert \begin{matrix}[\sigma] \\ [\sigma']m_1'\end{matrix} \right\rangle$ | $\left\vert \begin{matrix}[\sigma'] \\ m_1'\end{matrix} \right\rangle$ | $\left\vert \begin{matrix}[\mu] \\ m_2\end{matrix} \right\rangle = \left\vert \begin{matrix}[\mu] \\ [\mu']m_2'\end{matrix} \right\rangle$ | $\left\vert \begin{matrix}[\mu'] \\ m_2'\end{matrix} \right\rangle$ | $\left\vert \begin{matrix}[\nu] \\ m\end{matrix} \right\rangle = \left\vert \begin{matrix}[\nu] \\ [\nu']m'\end{matrix} \right\rangle$ | $\left\vert \begin{matrix}[\nu'] \\ m'\end{matrix} \right\rangle$ |

$\chi_i$'s, $\xi_i$'s and $q_i$'s respectively. Let us first introduce notations. The labeling of the irreducible bases of the three groups and their subgroups is listed in Table I, where $m_1$, $m_1'$, $m_2$, etc. may be understood as the indices specifying the given Yamanouchi symbols with the convention in decreasing page order.[8] Let $Y^{[\sigma']}_{m_1'}$, $Y^{[\mu']}_{m_2'}$ and $Y^{[\nu']}_{m_1'}$ be the Young tableaux after dropping the last box (containing the number $f$) on the Young tableaux $Y^{[\sigma]}_{m_1}$, $Y^{[\mu]}_{m_2}$ and $Y^{[\nu]}_{m}$ respectively. According to the branching law[8] of the permuation group one has

$$\begin{aligned}&[\sigma]m_1 = [\sigma]\,[\sigma']\,m_1',\\ &[\mu]m_2 = [\mu][\mu']\,m_2',\\ &[\nu]m = [\nu][\nu']m'.\end{aligned} \tag{2}$$

For example,

$$\left\vert \begin{matrix}[42] \\ 9\end{matrix} \right\rangle = \left\vert \begin{matrix}1\ 3\ 5\ 6 \\ 2\ 4\end{matrix} \right\rangle = \left\vert \begin{matrix}[42] \\ [32]5\end{matrix} \right\rangle .$$

Due to Racah's factorization lemma[9], the Clebsch–Gordan coefficients of the permutation group S($f$) can be written

$$C^{[\nu]\beta,m}_{[\sigma]m_1,[\mu]m_2} = \sum_{\beta'} C^{[\nu]\beta,\,[\nu']\beta'}_{\sigma\sigma',\mu\mu'}\, C^{[\nu']\beta',m'}_{[\sigma']m_1',\,[\mu']\,m_2'}, \tag{3}$$

where the first factor in the right-hand side is the $S(f)\supset S(f-1)\times S(1)$ ISF (or shortened as $S(f)\supset S(f-1)$ ISF), the second one is the Clebsch–Gordan coefficient of the group $S(f-1)$, and $\beta, \beta'$ are the multiplicity labels. From Eq. (3), the $S(f)\supset S(f-1)$ ISF can be expressed in terms of the Clebsch–Gordan coefficients

$$C^{[\nu]\,\beta,[\nu']\,\beta'}_{\sigma\sigma',\mu\mu'} = \sum_{m_1'm_2'} C^{[\nu]\beta,m}_{\sigma m_1,\,\mu\,m_2}\, C^{[\nu']\,\beta',m'}_{\sigma' m_1',\,\mu'\,m_2'}. \tag{4}$$

In the case when the multiplicity label $\beta'$ is redundant, one gets a simpler expression for $S(f)\supset S(f-1)$ ISF:

$$C^{[\nu]\,\beta,[\nu']}_{\sigma\sigma',\,\mu\,\mu'} = C^{[\nu]\beta,m}_{\sigma m_1,\,\mu\,m_2}\quad C^{[\nu']\,m'}_{\sigma' m_1',\,\mu'\,m_2'}. \tag{5}$$

The $S(f)\supset S(f-1)$ ISF satisfy the unitarity condition

$$\sum_{\sigma'\mu'\beta'} C^{[\bar\nu]\,\bar\beta,[\nu']\,\beta'}_{\sigma\sigma',\,\mu\,\mu'}\, C^{[\nu]\,\beta,[\nu]\,\beta'}_{\sigma\sigma',\,\mu\,\mu'} = \delta_{\nu\bar\nu}\,\delta_{\bar\beta\beta}, \tag{6a}$$

$$\sum_{\nu\beta} C^{[\nu]\,\beta,[\nu']\,\bar\beta'}_{\sigma\bar\sigma',\,\mu\,\bar\mu'}\, C^{[\nu]\,\beta,[\nu']\,\beta'}_{\sigma\sigma',\,\mu\,\mu'} = \delta_{\bar\sigma'\sigma}\,\delta_{\bar\mu'\mu}\,\delta_{\bar\beta'\beta}. \tag{6b}$$

We now proceed to derive the eigenequations to be satisfied by the $S(f)\supset S(f-1)$ ISF. From Eq. (3) one has

$$\begin{aligned}\left\vert \begin{matrix}[\nu]\,\beta \\ m\end{matrix} \right\rangle &= \left\vert \begin{matrix}[\nu]\,\beta \\ [\nu']m'\end{matrix} \right\rangle = \sum_{\sigma'\mu'\beta'} C^{[\nu]\,\beta,[\nu']\,\beta'}_{\sigma\sigma',\,\mu\mu'}\\ &\times \left[\left\vert \begin{matrix}[\sigma] \\ [\sigma']\end{matrix} \right\rangle \left\vert \begin{matrix}[\mu] \\ [\mu']\end{matrix} \right\rangle\right]^{[\nu']\,\beta'}_{m'},\end{aligned} \tag{7}$$

$$\left[\left\vert \begin{matrix}[\sigma] \\ [\sigma']\end{matrix} \right\rangle \left\vert \begin{matrix}[\mu] \\ [\mu']\end{matrix} \right\rangle\right]^{[\nu']\,\beta'}_{m'} \equiv \left\vert (\sigma'\mu')\beta' \right\rangle$$

$$= \sum_{m_1'm_2'} C^{[\nu']\,\beta',m}_{\sigma' m_1',\,\mu' m_2'} \left\vert \begin{matrix}[\sigma] \\ [\sigma']\ m_1'\end{matrix} \right\rangle \left\vert \begin{matrix}[\mu] \\ [\mu']\ m_2'\end{matrix} \right\rangle . \tag{8}$$

According to the definition, Eq. (7) is already the Yamanouchi basis $[\nu']m'$ of the permutation group $S(f-1)$. The requirement for Eq. (7) to be a Yamanouchi basis $[\nu]m$ of $S(f)$ is thus equivalent to the requirement that it must satisfy the eigenequations

$$C_{(2)}(f) \left\vert \begin{matrix}[\nu] \\ [\nu']m'\end{matrix} \right\rangle = \lambda^{(\nu)}_f \left\vert \begin{matrix}[\nu] \\ [\nu']m'\end{matrix} \right\rangle \tag{9}$$

from (1b), where the eigenvalue $\lambda^{(\nu)}_f$ is related to the partition $[\nu]=[\nu_1\nu_2\ldots]$ through[6]

$$\lambda^{(\nu)}_f = \tfrac{1}{2}f + \frac{1}{2}\sum_l \nu_l(\nu_l - 2l). \tag{10}$$

Using the relation

$$C_{(2)}(f) = C_{(2)}(f-1) + \sum_{i=1}^{f-1}(if), \tag{11}$$

Eq. (9) can be rewritten

$$\sum_{i=1}^{f-1}(if) \left\vert \begin{matrix}[\nu]\,\beta \\ [\nu']m'\end{matrix} \right\rangle = (\lambda^{(\nu)}_f - \lambda^{(\nu)}_{f-1}) \left\vert \begin{matrix}[\nu]\,\beta \\ [\nu']\ m'\end{matrix} \right\rangle . \tag{12}$$

Thus to get $S(f)\supset S(f-1)$ ISF one only needs to diagonalize the operator $\sum_{i=1}^{f-1}(if)$ in the basis $|(\sigma'\mu')\beta'\rangle$ of Eq. (8), i.e.,

$$\begin{aligned}\sum_{\sigma'\mu'\beta'}\sum_{i=1}^{f-1} &(\langle(\bar\sigma'\bar\mu')\bar\beta'|(if)|(\sigma'\mu')\beta'\rangle\\ &- (\lambda^{(\nu)}_f - \lambda^{(\nu')}_{f-1})\delta_{\bar\beta'\beta'}\,\delta_{\bar\sigma'\sigma'}\delta_{\bar\mu'\mu'})\\ &\times C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} = 0.\end{aligned} \tag{13}$$

With the help of Eq. (8), the matrix element in the above equation can be expressed in terms of the Clebsch–Gordan coefficients and the irreducible matrix elements of the permutation group $S(f)$,

$$\begin{aligned}&\langle\bar\sigma'\,\bar\mu')\bar\beta'|(if)|(\sigma'\mu')\beta'\rangle\\ &\quad= \sum_{\bar m_1'\bar m_2' m_1' m_2'} C^{[\nu']\,\bar\beta',m'}_{\bar\sigma'\bar m_1',\bar\mu'\,\bar m_2'}\, C^{[\nu']\,\beta',m'}_{\sigma' m_1',\mu'\,m_2'}\\ &\qquad\times D^{[\sigma]}_{\bar m_1 m_1}(if)\, D^{[\mu]}_{\bar m_2 m_2}(if).\end{aligned} \tag{14}$$

If for a given eigenvalue $\lambda^{(\nu)}_f$, Eq. (13) has $(\sigma\mu\nu)$ independent eigensolutions, it means (irreducible representation) irrep $[\nu]$ occurs $(\sigma\mu\nu)$ times in the representation $[\sigma]\times[\mu]$ of the permutation group. We can choose the eigensolutions in such a way that the $S(f)\supset S(f-1)$ ISF satisfy the orthogonality condition on index $\beta$ [see Eq. (6b)]. If the Clebsch–Gordan coefficients of both $S(f)$ and $S(f-1)$ are known, one can get $S(f)\supset S(f-1)$ ISF by means of Eq. (4) or (5). If only the Clebsch–Gordan coefficients of $S(f-1)$ are known, one can get $S(f)\supset S(f-1)$ ISF by solving the eigenequation (13). For large $f$, it is preferable to use Eq. (13), since compared with the eigenequation satisfied by the Clebsch–Gordan coefficients of $S(f)$, it is a lower order eigenequation.

### 3. $S(f)\supset S(f_1)\times S(f_2)$ ISF

Let $S(f_1)$ and $S(f_2)$ be the permutation groups for particles $1,2..,f_1$ and $f_1+1, f_1+2..f_1+f_2$, respectively, with $f=f_1+f_2$. Use the following notation to designate the irreps of the nine groups $S^{\chi}(f_1)...S^{q}(f)$

$$\begin{pmatrix}\sigma' & \mu' & \nu'\\ \sigma'' & \mu'' & \nu''\\ \sigma & \mu & \nu\end{pmatrix}\begin{pmatrix}S^{\chi}(f_1) & S^{\xi}(f_1) & S^{q}(f_1)\\ S^{\chi}(f_2) & S^{\xi}(f_2) & S^{q}(f_2)\\ S^{\chi}(f) & S^{\xi}(f) & S^{q}(f)\end{pmatrix}. \tag{15}$$

For example, $[\mu'']$ and $[\sigma]$ are the irreps of $S^{\xi}(f_2)$ and $S^{\chi}(f)$ respectively. The irreducible bases classified according to the irreps of the group chain $S(f)\supset S(f_1)\times S(f_2)$ in the $\chi$, $\xi$ and $q$ space are denoted by

$$\left|\begin{matrix}[\sigma]\\ \theta\,[\sigma']m_1'\,[\sigma'']\,m_1''\end{matrix}\right\rangle,\quad \left|\begin{matrix}[\mu]\\ \phi\,[\mu']m_2'\,[\mu'']m_2''\end{matrix}\right\rangle,$$

$$\theta=1,2,...\{\sigma'\sigma''\sigma\},\quad \phi=1,2,...\{\mu'\mu''\mu\},$$

$$\left|\begin{matrix}[\nu]\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle,$$

$$\tau=1,2...\{\nu'\nu''\nu\}, \tag{16}$$

where $\theta,\phi$ and $\tau$ are multiplicity labels, and the multiplicities $\{\sigma'\sigma''\sigma\}$, $\{\mu'\mu''\mu\}$ and $\{\nu'\nu''\nu\}$ are determined by the Littlewood rule.[8] For example $|_{\theta\,[\sigma']m_1'[\sigma'']m_1''}^{[\sigma]}\rangle$ belongs to the irrep $[\sigma]$ of $S^{\chi}(f)$ and at the same time it is the Yamanouchi basis $[\sigma']m_1'$ and $[\sigma'']m_1''$ of the group $S^{\chi}(f_1)$ and $S^{\chi}(f_2)$ respectively.

The former two in Eq. (16) can be linearly combined into the third one through the following two steps:

(1). Use the Clebsch–Gordan coefficient of $S(f_1)$ and $S(f_2)$ to combine them into irreducible basis $[\nu']m'$ and $[\nu'']m''$ of $S^{q}(f_1)$ and $S^{q}(f_2)$ respectively,

$$\begin{aligned}&|(\sigma'\sigma'')\theta(\mu'\mu'')\phi\beta'\beta''\rangle\\ &\equiv\left[\left|\begin{matrix}[\sigma]\\ \theta\,[\sigma'][\sigma'']\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \phi\,[\mu'][\mu'']\end{matrix}\right\rangle\right]\begin{matrix}[\nu']_{\beta'}\,[\nu'']_{\beta''}\\ m'\qquad m''\end{matrix}\\ &=\sum_{m_1'm_2'm_1''m_2''}C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2'}\,C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2''}\\ &\times\left|\begin{matrix}[\sigma]\\ \theta\,[\sigma']m_1'\,[\sigma'']m_1''\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \phi\,[\mu']m_2'\,[\mu'']m_2''\end{matrix}\right\rangle.\end{aligned} \tag{17a}$$

(2). Use $S(f)\supset(f_1)\times S(f_2)$ ISF to combine Eq. (17a) into a basis belonging to the irrep $[\nu]$ of $S^{q}(f)$

$$\begin{aligned}\left|\begin{matrix}[\nu]\,\beta\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle&=\sum_{\substack{\sigma'\sigma''\theta\beta'\\ \mu'\mu''\phi\beta''}}C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}\\ &\times\left[\left|\begin{matrix}[\sigma]\\ \theta\,[\sigma'][\sigma'']\end{matrix}\right\rangle\left|\begin{matrix}[\mu]\\ \phi\,[\mu'][\mu'']\end{matrix}\right\rangle\right]\begin{matrix}[\nu']_{\beta'}\,[\nu'']_{\beta''}\\ m'\qquad m''\end{matrix}.\end{aligned} \tag{17b}$$

The $S(f)\supset S(f_1)\times S(f_2)$ ISF $C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}$ satisfy the unitarity condition:

$$\sum_{\substack{\beta'\sigma'\mu'\theta\\ \beta''\sigma''\mu''\phi}}C^{[\bar\nu]\bar\beta,\bar\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}\,C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}=\delta_{\bar\nu\nu}\,\delta_{\bar\tau\tau}\,\delta_{\bar\beta\beta}, \tag{18a}$$

$$\sum_{\nu\tau\beta}C^{[\nu]\beta,\tau[\nu']\bar\beta'[\nu'']\bar\beta''}_{[\sigma]\theta\bar\sigma'\bar\sigma'',[\mu]\phi\bar\mu'\bar\mu''}\,C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}=\delta_{\bar\kappa\kappa}, \tag{18b}$$

$$\delta_{\bar\kappa\kappa}\equiv\delta_{\bar\beta'\beta'}\,\delta_{\bar\beta''\beta''}\delta_{\bar\sigma'\sigma'}\delta_{\bar\mu'\mu'}\delta_{\bar\sigma''\sigma''}\delta_{\bar\mu''\mu''}\delta_{\bar\theta\theta}\delta_{\bar\phi\phi}. \tag{18c}$$

Corresponding to E. (9) has

$$C(f)\left|\begin{matrix}[\nu]\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle=\lambda^{(\nu)}\left|\begin{matrix}[\nu]\\ \tau[\nu']m'[\nu'']m''\end{matrix}\right\rangle. \tag{19}$$

It should be emphasized that there is a significant difference between Eq. (9) and (19). $C(f)$ here is the CSCO-I of $S^{q}(f)$ rather than the 2-cycle class operator $C_{(2)}(f)$ of $S^{q}(f)$.

The $S(f)\supset S(f_1)\times S(f_2)$ ISF satisfy the eigenequation

$$\begin{aligned}&\sum_{\substack{\sigma'\sigma''\theta\beta'\\ \mu'\mu''\phi\beta''}}(\langle(\bar\sigma'\bar\sigma'')\bar\theta(\bar\mu'\bar\mu'')\bar\phi\bar\beta'\bar\beta''|C(f)|\\ &(\sigma'\sigma'')\theta(\mu'\mu'')\phi\beta'\beta''\rangle-\lambda^{(\nu)}\delta_{\bar\kappa\kappa})\\ &\times C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}=0,\end{aligned} \tag{20}$$

where the symbol $\delta_{\bar\kappa\kappa}$ is the same as that in Eq. (18c). The $S^{\chi}(f)\supset S^{\chi}(f_1)\times S^{\chi}(f_2)$ and $S^{\xi}(f)\supset S^{\xi}(f_1)\times S^{\xi}(f_2)$ basis in Eq. (17a) can be transformed into the Yamanouchi basis of $S^{\chi}(f)$ and $S^{\xi}(f)$, respectively, by means of the transformation coefficients of the permutation group.[10]

For example

$$\left|\begin{matrix}[\sigma]\\ \theta\,[\sigma']m'[\sigma'']m_1''\end{matrix}\right\rangle=\sum_m\left(\begin{matrix}[\sigma]\\ m\end{matrix}\middle|[\sigma],\begin{matrix}\theta\,[\sigma'][\sigma'']\\ m_1'm_1''\end{matrix}\middle|\begin{matrix}[\sigma]\\ m\end{matrix}\right\rangle. \tag{21}$$

From Eq.(17a) and (21), one gets the expression for the matrix element of any permutation $P$ in the $q$-space between states (17a):

$$\begin{aligned}&\langle\bar\sigma'\bar\sigma'')\bar\theta(\bar\mu'\bar\mu'')\bar\phi\bar\beta'\bar\beta''|P|(\sigma'\sigma'')\theta(\mu'\mu'')\phi\beta'\beta''\rangle\\ &=\sum D^{[\sigma]}_{\bar m_1m_1}(P)\,D^{[\mu]}_{\bar m_2m_2}(P)\,C^{[\nu']\bar\beta',m'}_{\bar\sigma'\bar m_1',\bar\mu'\bar m_2'}\,C^{[\nu'']\bar\beta'',m''}_{\bar\sigma''\bar m_1'',\bar\mu''\bar m_2''}\\ &\times C^{[\nu']\beta,m'}_{\sigma m_1',\bar\mu'm_2'}\,C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2''}\\ &\times\left(\begin{matrix}[\sigma]\\ \bar m_1\end{matrix}\middle|[\sigma],\begin{matrix}\bar\theta\,[\bar\sigma'][\bar\sigma'']\\ m_1'\bar m_1''\end{matrix}\right)\left(\begin{matrix}[\mu]\\ \bar m_2\end{matrix}\middle|[\mu],\bar\phi\begin{matrix}[\bar\mu'][\bar\mu]\\ \bar m_2'\quad\bar m_2''\end{matrix}\right)\\ &\times\left(\begin{matrix}[\sigma]\\ m_1\end{matrix}\middle|[\sigma],\begin{matrix}\theta\,[\sigma'][\sigma'']\\ m_1'\quad m_1''\end{matrix}\right)\\ &\times\left(\begin{matrix}[\mu]\\ m_2\end{matrix}\middle|[\mu],\phi\begin{matrix}[\mu'][\mu'']\\ m_2'\quad m_2''\end{matrix}\right),\end{aligned} \tag{22}$$

where the sum is over $\bar m_1'\bar m_2'\bar m_1''\bar m_2''m_1'm_2'm_1''\bar m_2''\bar m_1m_1\bar m_2$ and $m_2$.

With the help of Eq. (22), one can calculate the matrix elements of the CSCO-I of the permutation groups $S^{q}(f)$. Therefore from the Clebsch–Gordan coefficients of $S(f_1)$ and $S(f_2)$ and the transformation coefficients of Eq. (21) which can also be evaluated by the Eigenfunction Method, one obtains the matrix elements occurring in Eq. (20). Solving the eigenequation (20), one gets the $S(f)\supset S(f_1)\times S(f_2)$ ISF. Again, if the eigenvalue $\lambda^{(\nu)}$ is degenerate [the degeneracy equals to $N=\{\nu'\nu''\nu\}\times(\sigma\mu\nu)$], through a proper choice of the $N$ linearly independent eigensolutions belonging to the same $\lambda^{(\nu)}$, one can make the $S(f)\supset S(f_1)\times S(f_2)$ ISF to be orthogonal on indices $\beta$ and $\tau$ [see Eq. (18a)].

A computer program has already been set up [7] for calculating the Clebsch–Gordan coefficients of the permutation group by the Eigenfunction Method. It is straightforward to transplant this program to the case of eigenequation (20) for the $S(f)\supset S(f_1)\times S(f_2)$ ISF.

## 4. SU(*mn*)⊃(*m*)×SU(*n*) ISF

In analogy to Eq. (15), we introduce the following symbols to denote the irreps of SU(*m*), SU(*n*) *and* SU(*mn*)

$$\begin{pmatrix} \sigma' & \mu' & \nu' \\ \sigma'' & \mu'' & \nu'' \\ \sigma & \mu & \nu \end{pmatrix} \begin{pmatrix} \mathrm{SU}(m), & \mathrm{SU}(n), & \mathrm{SU}(mn) \\ \mathrm{SU}(m), & \mathrm{SU}(n), & \mathrm{SU}(mn) \\ \mathrm{SU}(m), & \mathrm{SU}(n), & \mathrm{SU}(mn) \end{pmatrix} \tag{23a}$$

Let

$$\left|\begin{matrix}[\nu'] \\ \beta'[\sigma']W_1'[\mu']W_2'\end{matrix}\right\rangle, \quad \left|\begin{matrix}[\nu''] \\ \beta''[\sigma'']W_1''[\mu'']W_2''\end{matrix}\right\rangle, \quad \left|\begin{matrix}[\nu] \\ \beta[\sigma]W_1[\mu]W_2\end{matrix}\right\rangle, \tag{23b}$$

be the SU(*mn*)⊃SU(*m*)×SU(*n*) irreducible bases in the *q*-space for particles (1,2...,$f_1$), ($f_1+1$,..,$f$) and (1,2...,$f$) respectively, and $W_1'(W_2')$ etc. are the component indices of the irreps of SU(*m*)(SU(*n*)). The SU(*mn*)⊃SU(*m*)×SU(*n*) ISF are defined as the coefficients in the following expansion:

$$\left|\begin{matrix}[\nu]\tau \\ \beta[\sigma]W_1[\mu]W_2\end{matrix}\right\rangle = \sum_{\substack{\beta'\sigma'\mu'\theta \\ \beta''\sigma''\mu''\phi}} C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} \times \left[\left|\begin{matrix}[\nu'] \\ \beta'[\sigma'][\mu']\end{matrix}\right\rangle \left|\begin{matrix}[\nu''] \\ \beta''[\sigma''][\mu'']\end{matrix}\right\rangle\right]^{[\sigma]_\theta[\mu]_\phi}_{W_1 \quad W_2}, \tag{24}$$

where $\tau = 1,2,\ldots\{\nu'\nu''\nu\}$ is the multiplicity label, and the square bracket indicates that the bases are to be combined into the irreducible basis $[\sigma_1]W_1$ and $[\sigma_2]W_2$ of SU(*m*) and SU(*n*) in terms of the Clebsch–Gordan coefficients of SU(*m*) and SU(*n*), respectively, i.e.

$$\begin{aligned} &\left[\left|\begin{matrix}[\nu'] \\ \beta'[\sigma'][\mu']\end{matrix}\right\rangle \left|\begin{matrix}[\nu''] \\ \beta''[\sigma''][\mu'']\end{matrix}\right\rangle\right]^{[\sigma]_\theta[\mu]_\phi}_{W_1 \quad W_2} \\ &= \sum_{W_1'W_2'W_1''W_2''} C^{[\sigma]\theta,W_1}_{\sigma'W_1',\sigma''W_1''} C^{[\mu]\phi,W_2}_{[\mu']W_2',[\mu'']W_2''} \times \left|\begin{matrix}[\nu'] \\ \beta'[\sigma']W_1'[\mu']W_2''\end{matrix}\right\rangle \left|\begin{matrix}[\nu''] \\ \beta''[\sigma'']W_1''[\mu'']W_2''\end{matrix}\right\rangle. \end{aligned} \tag{25}$$

The inverse expansion of Eq. (24) is

$$\begin{aligned} &\left[\left|\begin{matrix}[\nu'] \\ \beta'[\sigma'][\mu']\end{matrix}\right\rangle \left|\begin{matrix}[\nu''] \\ \beta''[\sigma''][\mu'']\end{matrix}\right\rangle\right]^{[\sigma]_\theta[\mu]_\phi}_{W_1 \quad W_2} \\ &= \sum_{\nu\tau\beta} C^{[\nu]\tau'\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\mu''} \left|\begin{matrix}[\nu] \\ \beta[\sigma]W_1[\mu]W_2\end{matrix}\right\rangle. \end{aligned} \tag{26}$$

Attaching the Young tableaux $Y^{[\nu']}_{m'}(\omega_1^0)$ and $Y^{[\nu'']}_{m''}(\omega_2^0)$ with $(\omega_1^0) = (1,2,..f_1)$ and $(\omega_2^0) + (f_1+1,..,f)$ to the two irreducible bases in the right-hand side of Eq. (24), it reads

$$\begin{aligned} &\left|\begin{matrix}[\nu] \\ \tau[\nu']m'[\nu'']m'',\beta[\sigma]W_1[\mu]W_2\end{matrix}\right\rangle \\ &= \sum_{\substack{\beta'\sigma'\mu'\theta \\ \beta''\sigma''\mu''\phi}} C^{[\nu]\tau'\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} \times \left[\left|\begin{matrix}[\nu'] \\ m'\omega_1^0,\beta'[\sigma'][\mu']\end{matrix}\right\rangle \times \left|\begin{matrix}[\nu''] \\ m''\omega_2^0,\beta''[\sigma''][\mu'']\end{matrix}\right\rangle\right]^{[\sigma]_\theta[\mu]_\phi}_{W_1 \quad W_2}. \end{aligned} \tag{27a}$$

The left-hand side of Eq. (27a) is still the SU(*mn*)⊃SU(*m*)×SU(*n*) basis. It belongs to the irrep [$\nu$] of SU(*mn*), therefore it must also belong to the irrep [$\nu$] of the permutation group $S^q(f)$[11]. In other words it is also a $S^q(f)\supset S^q(f_1)\times S^q(f_2)$ basis.

The Clebsch–Gordan coefficients of the permutation group are known[11] as the coupling coefficients which couple the irreducible basis of SU(*m*) and SU(*n*) into those of SU(*mn*). For example

$$\left|\begin{matrix}[\nu'] \\ m',\beta'[\sigma']W_1'[\mu']W_2'\end{matrix}\right\rangle = \sum_{m_1'm_2'} C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2'} \left|\begin{matrix}[\sigma'] \\ m_1' \quad W_1'\end{matrix}\right\rangle \left|\begin{matrix}[\mu'] \\ m_2' \quad W_2'\end{matrix}\right\rangle. \tag{28}$$

On the other hand the Clebsch–Gordan coefficients of the unitary group are the coupling coefficients which couple the irreducible basis of $S(f_1)$ and $S(f_2)$ into those of $S(f)$. For example

$$\left|\begin{matrix}[\sigma] \\ \theta[\sigma']m_1'[\sigma'']m_2'',W_1\end{matrix}\right\rangle = \sum_{W_1'W_2''} C^{[\sigma]\theta,W_1}_{[\sigma']W_1',[\sigma'']W_2''} \left|\begin{matrix}[\sigma'] \\ m_1' \quad W_1'\end{matrix}\right\rangle \left|\begin{matrix}[\sigma''] \\ m_1'' \quad W_1''\end{matrix}\right\rangle. \tag{29}$$

With the help of Eqs. (25) (28) and (29), the last factor in Eq. (27a) can be put into the form

$$\begin{aligned} &\left[\left|\begin{matrix}[\nu'] \\ m'\omega_1^0,\beta'[\sigma'][\mu']\end{matrix}\right\rangle \left|\begin{matrix}[\nu''] \\ m''\omega_2^0,\beta''[\sigma''][\mu'']\end{matrix}\right\rangle\right]^{[\sigma]_\theta[\mu]_\phi}_{W_1 \quad W_2} \\ &= \sum_{m_1'm_2'm_1''m_2''} C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2'} C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2''} \left|\begin{matrix}[\sigma] \\ \theta[\sigma']m_1'[\sigma'']m_1'',W_1\end{matrix}\right\rangle \left|\begin{matrix}[\mu] \\ \phi[\mu']m_2'[\mu'']m_2'',W_2\end{matrix}\right\rangle. \end{aligned} \tag{27b}$$

Comparing Eq. (27) with Eq. (17) one gets an important relation

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = C^{[\nu]\beta,\tau[\nu']\beta'[\nu'']\beta''}_{[\sigma]\theta\sigma'\sigma'',[\mu]\phi\mu'\mu''}. \tag{30}$$

Or, expressed in the form of an overlap integral,

$$\begin{aligned} &\left\langle\begin{matrix}[\nu] \\ \tau\nu'm'\nu''m'',\beta\sigma W_1\mu W_2\end{matrix}\right| \left[\begin{pmatrix}[\sigma] \\ \theta\sigma'\sigma'' W_1\end{pmatrix}\times\begin{pmatrix}[\mu] \\ \varphi\mu'\mu'', W_2\end{pmatrix}\right]^{[\nu]_{\beta'}[\nu'']_{\beta''}}_{m'm''} \Bigg\rangle \\ &= \left\langle\begin{matrix}[\nu] \\ \tau\nu'm'\nu''m'',\beta\sigma W_1\mu W_2\end{matrix}\right| \left[\begin{pmatrix}[\nu'] \\ m',\beta'\sigma'\mu'\end{pmatrix}\times\begin{pmatrix}[\nu''] \\ m'',\beta''\sigma''\mu''\end{pmatrix}\right]^{[\sigma]_\theta[\mu]_\varphi}_{W_1W_2} \Bigg\rangle \end{aligned} \tag{31}$$

namely the SU(*mn*)⊃SU(*m*)×SU(*n*) ISF [or the $f_2$ particle CFP (coefficients of fractional parentage)] are equal to the $S(f_1+f_2)\supset S(f_1)\times S(f_2)$ ISF.

Furthermore, since the value of $S(f_1+f_2)\supset S(f_1)\times S(f_2)$ ISF is independent of *m* and *n*, one arrives at the conclusion that the value of SU(*mn*)⊃SU(*m*)×SU(*n*) ISF is independent of *m* and *n*. The reason we failed to realize this obvious fact for so long is because we usually use concrete

TABLE II. $SU(mn)\supset SU(m)\times SU(n)$ ISF $C^{[2111],\,[32]\,[32]}_{[211][\sigma'][\mu'],\,[1][1][1]}$.

| $[\nu][\sigma][\mu]$ / $[\nu]^{2T+1\,2S+1}\Gamma$ / $[\nu](\lambda\mu)S$ | $[\sigma'][\mu']$ $2T'+1, 2S'+1\Gamma$ $(\lambda'\mu')S'$ | $[22]\,[31]$ $^{13}\Gamma$ (02)1 | $[31]\,[22]$ $^{31}\Gamma$ (21)0 | $[31]\,[31]$ $^{33}\Gamma$ (21)1 |
|---|---|---|---|---|
| $[21^3]\,[32]\,[32]$ | | | | |
| $[21^3]\,{}^{22}\Gamma$ | | $-\sqrt{\frac{1}{5}}$ | $-\sqrt{\frac{1}{5}}$ | $-\sqrt{\frac{3}{5}}$ |
| $[21^3]\,(12)\,1/2$ | | | | |

quantum number for a given $m$ and $n$ rather than the partitions to represent the irreps of $SU(m)$ and $SU(n)$. For example, in the case of SU(3), we use $(\lambda\mu)$ (corresponding to the partition $[\lambda+\mu,\mu]$) or the dimension of the irrep; for SU(2) we use the quantum number $S$ or $T$. As a test of the above conclusion, in Table II we list the $SU(6)\supset SU(3)\times SU(2)$ ISF for $[\nu]=[21^3]$, $(\lambda\,\mu)=(12)$, $S=1/2$ calculated by Zhang *et al.*[2] and the $SU(4)\supset SU(2)\times SU(2)$ ISF for $[\nu]=[21^3]$, $S=T=1/2$ given by Jahn.[12] They are exatly the same. (See Table II).

Therefore, every $SU(mn)\supset SU(m)\times SU(n)$ ISF with a particular $m$ and $n$ gives an infinite number of $SU(m'n')\supset SU(m')\times SU(n')$ ISF with $m'=m, m+1,\ldots$ and $n'=n, n+1,\ldots$

Another point worth mentioning is that not every $SU(mn)\supset SU(m)\times SU(n)$ ISF can be deduced from the $SU((m-1)n)\supset SU(m-1)\times SU(n)$ ISF or the $SU(m(n-1))\supset SU(m)\times SU(n-1)$ ISF. The reason is that the Young diagrams $[\sigma']$, $[\sigma'']$ and $[\sigma]$ of $SU(m-1)$ can have at most $m-1$ rows, therefore the $SU(mn)\supset SU(m)\times SU(n)$ ISF with the Young diagrams $[\sigma']$, $[\sigma'']$ and $[\sigma]$ of $m$ rows can not be deduced from the $SU((m-1)n)\supset SU(m-1)\times SU(n)$ ISF.

## 5. $SU(mn)\supset SU(m)\times SU(n)$ ISF AND CLEBSCH–GORDAN COEFFICIENTS OF PERMUTATION GROUP

Putting $[\nu'']=[\sigma'']=[\mu'']=[1]$ in Eq. (30), using Eq. (4), and omitting redundant indices $\tau,\theta,\phi,\beta''$, one gets a relation between the single particle CFP in the group chain $SU(mn)\supset SU(m)\times SU(n)$ and the Clebsch–Gordan coefficients of $S(f)$ and $S(f-1)$:

$$C^{[\nu]\beta[\sigma][\mu]}_{[\nu']\beta'[\sigma'][\mu'],[1][1][1]} = C^{[\nu]\beta,[\nu']\beta'}_{\sigma\sigma',\mu\mu'} = \sum_{m_1'm_2'} C^{[\nu]\beta m}_{\sigma m_1,\mu m_2}\, C^{[\nu']\beta' m'}_{\sigma' m_1',\mu' m_2'}. \tag{32}$$

In the case when $\beta'$ is redundant, Eq. (32) reduces to Eq. (5).

Now we turn to derive a similar expression for $f_2$-particle CFP. The $SU(mn)\supset SU(m)\times SU(n)$ basis and the Yamanouchi basis of $S(f)\big|^{[\nu]}_{m,\beta[\sigma]W_1[\mu]W_2}\rangle$, can be expanded in the following two ways:

(1). Transform the Yamanouchi basis of $S(f)$ into the $S(f)\supset S(f_1)\times S(f_2)$ basis

$$\left|{}^{[\nu]}_{m,\beta[\sigma]W_1[\mu]W_2}\right\rangle = \sum_{\nu''m''\tau}\begin{pmatrix}[\nu]\\ m\end{pmatrix}\begin{matrix}[\nu],\\ \end{matrix}\begin{matrix}\tau[\nu'][\nu'']\\ m'\quad m''\end{matrix}\Bigg)\times\left|{}^{[\nu]}_{\tau[\nu']m'[\nu'']m'',\beta[\sigma]W_1[\mu]W_2}\right\rangle \tag{33}$$

Using Eqs. (27), and (29) this becomes

$$\left|{}^{[\nu]}_{m,\beta[\sigma]W_1[\mu]W_2}\right\rangle = \sum\begin{pmatrix}[\nu]\\ m\end{pmatrix}\begin{matrix}[\nu],\\ \end{matrix}\begin{matrix}\tau[\nu'][\nu'']\\ m'\quad m''\end{matrix}\Bigg) \times C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''}\, C^{[\sigma]\theta,W_1}_{\sigma'W_1',\sigma''W_1''}\, C^{[\mu]\phi,W_2}_{\mu'W_2',\mu''W_2''} \times C^{[\nu']\beta',m'}_{\sigma'm_1',\mu'm_2'} C^{[\nu'']\beta'',m''}_{\sigma''m_1'',\mu''m_2''} \times\left|{}^{[\sigma]}_{m_1'\omega_1^0,W_1'}\right\rangle\left|{}^{[\mu']}_{m_2'\omega_2^0,W_2'}\right\rangle\left|{}^{[\sigma'']}_{m_1''\omega_2^0,W_1''}\right\rangle \times\left|{}^{[\mu'']}_{m_2''\omega_2^0,W_2''}\right\rangle. \tag{34}$$

The sum is over $\nu''m''\tau\beta\sigma'\mu'\beta''\sigma''\mu''\theta\phi W_1'W_2'W_1''W_2''m_1'm_2'm_1''$ and $m_2''$.

(2). In analogy with Eq. (28) one has

$$\left|{}^{[\nu]}_{m,\beta[\sigma]W_1[\mu]W_2}\right\rangle = \sum_{m_1m_2} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2}\left|{}^{[\sigma]}_{m_1\,W_1}\right\rangle\left|{}^{[\mu]}_{m_2\,W_2}\right\rangle. \tag{35}$$

By means of the expansion

$$\left|{}^{[\sigma]}_{m_1W_1}\right\rangle = \sum_{\substack{\theta\sigma''m_1''\\ W_1'W_1''}}\begin{pmatrix}[\sigma]\\ m_1\end{pmatrix}\begin{matrix}[\sigma],\\ \end{matrix}\begin{matrix}\theta[\sigma'][\sigma'']\\ m_1'\quad m_1''\end{matrix}\Bigg) \times C^{[\sigma]\theta,W_1}_{\sigma'W_1',\sigma''W_1''}\left|{}^{[\sigma']}_{m_1'\omega_1^0,W_1'}\right\rangle\left|{}^{[\sigma'']}_{m_1'\omega_2^0,W_2'}\right\rangle \tag{36}$$

and a similar equation for $|{}^{[\sigma]}_{m_2W_2}\rangle$, Eq. (35) becomes

$$\left|{}^{[\nu]}_{m,\beta[\sigma]W_1[\mu]W_2}\right\rangle = \sum C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} \times\begin{pmatrix}[\sigma]\\ m_1\end{pmatrix}\begin{matrix}[\sigma],\\ \end{matrix}\begin{matrix}\theta[\sigma'][\sigma'']\\ m_1'\quad m_1''\end{matrix}\Bigg)\begin{pmatrix}[\mu]\\ m_2\end{pmatrix}\begin{matrix}[\mu],\\ \end{matrix}\begin{matrix}\phi[\mu'][\mu'']\\ m_2'm_2''\end{matrix}\Bigg) \times C^{[\sigma]\theta,W_1}_{\sigma'W_1',\sigma''W_1''}\, C^{[\mu]\phi,W_2}_{\mu'W_2',\mu''W_2''}\left|{}^{[\sigma']}_{m_1'\omega_1^0,W_1'}\right\rangle\left|{}^{[\sigma'']}_{m_1''\omega_2^0,W_1''}\right\rangle \times\left|{}^{[\mu']}_{m_2'\omega_2^0,W_2'}\right\rangle\left|{}^{[\mu'']}_{m_2''\omega_2^0,W_2''}\right\rangle \tag{37}$$

The sum is over $m_1m_2\sigma''\ m_1''\mu''m_2''\theta\phi W_1'W_2'W_1''$ and $W_2''$.

Comparing Eqs. (34) and (37) one gets

$$\sum_{\nu' m''} \sum_{\tau \beta' \beta''} \begin{pmatrix} [\nu] \\ m \end{pmatrix} [\nu], \begin{matrix} \tau [\nu'][\nu''] \\ m' \; m'' \end{matrix} \Big) \times C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''}$$

$$= \sum_{m_1 m_2}^{\text{fix } m_1' m_2'} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} \times \begin{pmatrix} [\sigma] \\ m_1 \end{pmatrix} [\sigma], \begin{matrix} \theta [\sigma'][\sigma''] \\ m_1' \; m_1'' \end{matrix} \Big) \begin{pmatrix} [\mu] \\ m_2 \end{pmatrix} [\mu], \begin{matrix} \phi [\mu'][\mu''] \\ m_2' \; m_2'' \end{matrix} \Big), \tag{38}$$

where the sum over $m_1$ and $m_2$ is carried out with fixed $m_1'$ and $m_2'$. Utilizing the unitarity property property of the Clebsch–Gordan coefficients and of the transformation coefficients $\left(\begin{smallmatrix} [\nu] \\ m \end{smallmatrix}\right| [\nu], \begin{smallmatrix} \tau[\nu'][\nu''] \\ m' \; m'' \end{smallmatrix})$, we finally get an expression for the $SU(mn) \supset SU(m) \times SU(n)$ ISF

$$C^{[\nu]\tau,\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''}$$

$$= \sum_{m}^{\text{fix } m'} \sum_{m_1 m_2 m_1'' m_2''} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2} C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2'} \times C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''} \begin{pmatrix} [\nu] \\ m \end{pmatrix} [\nu], \begin{matrix} \tau [\nu'][\nu''] \\ m' \; m'' \end{matrix} \Big) \times \begin{pmatrix} [\sigma] \\ m_1 \end{pmatrix} [\sigma], \begin{matrix} \theta [\sigma'][\sigma''] \\ m_1' \; m_1'' \end{matrix} \Big) \begin{pmatrix} [\mu] \\ m_2 \end{pmatrix} [\mu], \begin{matrix} \phi [\mu'][\mu''] \\ m_2' \; m_2'' \end{matrix} \Big). \tag{39}$$

In the case when any of the multiplicity labels $\tau, \beta'$ and $\beta''$ is redundant, Eq. (39) can be simplified. For example, if $\tau$ is redundant, one gets

$$C^{[\nu],\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu',[\nu'']\beta''\sigma''\mu''} = \begin{pmatrix} [\nu] \\ m \end{pmatrix} [\nu], \begin{matrix} [\nu'][\nu''] \\ m' \; m'' \end{matrix} \Big)^{-1} \sum_{m_1 m_2} \sum_{m_1'' m_2''} C^{[\nu]\beta,m}_{\sigma m_1,\mu m_2}$$

$$C^{[\nu']\beta',m'}_{\sigma' m_1',\mu' m_2'} C^{[\nu'']\beta'',m''}_{\sigma'' m_1'',\mu'' m_2''} \times \begin{pmatrix} [\sigma] \\ m_1 \end{pmatrix} [\sigma], \begin{matrix} \theta [\sigma'][\sigma''] \\ m_1' \; m_1'' \end{matrix} \Big) \begin{pmatrix} [\mu] \\ m_2 \end{pmatrix} [\mu], \begin{matrix} \phi [\mu'][\mu''] \\ m_2' \; m_2'' \end{matrix} \Big). \tag{40}$$

For the totally antisymmetric irreps $[\nu'] = [1^{f_1}]$, $[\nu''] = [1^{f_2}]$, $[\nu] = [1^f]$, Eq. (40) reduces to

$$C^{[1^f],[\sigma]\theta[\mu]\phi}_{[1^{f_1}][\sigma'][\mu'],[1^{f_2}][\sigma''][\mu'']} = \delta_{\bar{\sigma}\mu} \delta_{\bar{\sigma}'\mu'} \delta_{\bar{\sigma}''\mu''} \frac{1}{(h_\sigma h_{\sigma'} h_{\sigma''})^{1/2}}$$

$$\sum_{m_1' m_1''} \sum_{m_1} \begin{pmatrix} [\sigma] \\ m_1 \end{pmatrix} [\sigma], \begin{matrix} \theta [\sigma'][\sigma''] \\ m_1' \; m_1'' \end{matrix} \Big) \times \begin{pmatrix} [\sigma] \\ m_1 \end{pmatrix} [\sigma], \begin{matrix} \phi [\sigma'][\sigma''] \\ m_1' \; m_1'' \end{matrix} \Big) = \delta_{\bar{\sigma}\mu} \delta_{\bar{\sigma}'\mu'} \delta_{\bar{\sigma}''\mu''} \delta_{\theta\phi} \left( \frac{h_{\sigma'} h_{\sigma''}}{h_\sigma} \right)^{1/2}, \tag{41}$$

where $h_{\sigma'}$, $h_{\sigma''}$ and $h_\sigma$ are the dimensions of irreps $[\sigma']$, $[\sigma'']$ and $[\sigma]$ of the permutation groups $S(f_1)$, $S(f_2)$ and $S(f)$, respectively.

We know that the total CFP in the shell model can be factorized as

$$(l^{f_1}[\nu']\alpha_1\beta_1 L_1 S_1 T_1, l^{f_2}[\nu'']\alpha_2\beta_2 L_2 S_2 T_2 | \} l^f [\nu]\alpha\beta LST)$$

$$= \sum_{\tau} \left( \frac{h_{\nu'} h_{\nu''}}{h_\nu} \right)^{1/2} C^{[\nu]\tau,\alpha L}_{[\nu']\alpha_1 L_1,[\nu'']\alpha_2 L_2} \times C^{[\tilde{\nu}]\tau,\beta ST}_{[\tilde{\nu}']\beta_1 S_1 T_1,[\tilde{\nu}'']\beta_2 S_2 T_2}. \tag{42}$$

The factor $(h_{\nu'} h_{\nu''}/h_\nu)^{1/2}$ is called the weight factor. Now we know it is a $SU(4(2l+1)) \supset SU(2l+1) \times SU(4)$ ISF for the totally antisymmetric states, and the total CFP of Eq. (42) is nothing else but the $SU(4(2l+1)) \supset (SU(2l+1) \supset SO(3)) \times (SU(4) \supset SU(2) \times SU(2))$ ISF.

By using the symmetries of the transformation coefficients[13] and those of the Clebsch–Gordan coefficients[8] of the permutation group, from Eq. (39) we get another symmetry of $SU(mn) \supset SU(m) \times SU(n)$ ISF

$$C^{[\nu],\beta[\sigma]\theta[\mu]\phi}_{[\nu']\beta'\sigma'\mu'[\nu'']\beta''\sigma''\mu''} = \epsilon C^{[\nu],\beta[\bar{\sigma}]\theta[\bar{\mu}]\phi}_{[\nu']\beta'\bar{\sigma}'\bar{\mu}'[\nu'']\beta''\bar{\sigma}''\bar{\mu}''},$$

where $\epsilon = \pm 1$ is a phase factor depending on phase conventions and the tildes represent the conjugate irreps (interchange rows and columns in Young diagrams).

The relations between the $SU(m+n) \supset SU(m) \times SU(n)$ ISF and the outer-product reduction coefficients are very similar to those between the $SU(mn) \supset SU(m) \times SU(n)$ ISF and the Clebsch–Gordan coefficients of the permutation group, which will be the subject of our next paper.

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# On the existence of real Clebsch–Gordan coefficients

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The question of the possible general existence of real Clebsch–Gordan coefficients (coupling coefficients) for compact groups is considered. Criteria are established for a group to be susceptible to the classical rotation group approach in which a choice of standard irreducible matrix representations is made such that there is a fixed inner automorphism of the group carrying all standard representations into their complex conjugate. In connection with a generalization of this approach the concept of quasi-ambivalence of a group is shown to be relevant.

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## I. INTRODUCTION

In his review[1] of coupling and recoupling theory for compact groups, Butler raised the question of the possible general existence of real Clebsch–Gordan (C–G) coefficients (coupling coefficients). After noting the lack of an answer to this problem he stated in a footnote[2] that the tetrahedral group requires nonreal coefficients. It will be shown below, however, that this is not the case (Sec. VI). In fact, there do not seem to be examples in the literature contradicting a "reality conjecture." In the present paper we consider the general problem and establish *sufficient* conditions for a compact group to allow a choice of real C–G coefficients.

As is well known, C–G coefficients for a compact group $G$ are elements of unitary matrices intertwining tensor products of unitary irreducible matrix representations of $G$ with matrix direct sums of unitary irreducible representations of $G$. More specifically, if $\Gamma_1$ and $\Gamma_2$ are unitary irreducible matrix representations $R\to\Gamma_i(R)$, $R\in G$, of $G$, any unitary matrix $\mathbf{C}$ with the property that the representation $R\to\mathbf{C}^{-1}(\Gamma_1(R)\otimes\Gamma_2(R))\,\mathbf{C}$ of $G$ is a matrix direct sum of unitary irreducible representations of $G$ will be called *a matrix of* C–G *coefficients for* $\Gamma_1\otimes\Gamma_2$. Here $\otimes$ denotes tensor (or Kronecker or direct) product of matrices.

By *a system of standard representations for a compact group* $G$ we shall mean a system of continuous unitary irreducible matrix representations of $G$ containing one irreducible representation from each equivalence class and with the property that if a matrix representation $\Gamma$ of $G$ is among the standard representations and $\Gamma$ is *not* equivalent to its complex conjugate representation $\overline{\Gamma}$, then $\overline{\Gamma}$ is also among the standard representations. In connection with systems of standard representations we shall understand matrices of C–G coefficients to transform tensor products of standard representations into direct sums of *standard* representations.

Now, the precise problem which we wish to consider is the following one:

(A) *Given a compact group* G, *is it possible to find a system of standard representations of* $G$ *such that for any two standard representations* $\Gamma_1$ *and* $\Gamma_2$ *there exists a* real *matrix of* C–G *coefficients for* $\Gamma_1\otimes\Gamma_2$?

We shall start by formulating the problem a little differently in order to make it easier to attack. To this end, we introduce a concept closely related to C–G coefficients, namely that of *triple coefficients*. Given an ordered triple $\Gamma_1\Gamma_2\Gamma_3$ of matrix representations of a group $G$, we define *a set of triple coefficients for* $\Gamma_1\Gamma_2\Gamma_3$ to be a column vector $\mathbf{c}$ satisfying

$$[\overline{\Gamma}_1(R)\otimes\overline{\Gamma}_2(R)\otimes\overline{\Gamma}_3(R)]\,\mathbf{c}=\mathbf{c}\quad\text{for all } R\in G. \tag{I.1}$$

In (I.1) $\mathbf{c}$ is a joint *fix-vector* (i.e., eigenvector with eigenvalue 1) for the matrices $\overline{\Gamma}_1(R)\otimes\overline{\Gamma}_2(R)\otimes\overline{\Gamma}_3(R)$, $R\in G$. Thus the set of all $\mathbf{c}$ satisfying (I.1) forms a linear space which we shall denote $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$. The dimension $\dim\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ of this space is equal to the number of times the trivial one-dimensional representation of $G$ occurs in $\overline{\Gamma}_1\otimes\overline{\Gamma}_2\otimes\overline{\Gamma}_3$. Denoting the elements of $\mathbf{c}$ by $\binom{\Gamma_1\Gamma_2\Gamma_3}{\gamma_1\gamma_2\gamma_3}$, where the $\gamma_i$ are component designations for the $\Gamma_i$, Eq. (I.1) may be written

$$\sum_{\gamma_1'\gamma_2'\gamma_3'}\overline{\Gamma}_1(R)_{\gamma_1\gamma_1'}\overline{\Gamma}_2(R)_{\gamma_2\gamma_2'}\overline{\Gamma}_3(R)_{\gamma_3\gamma_3'}\binom{\Gamma_1\ \Gamma_2\ \Gamma_3}{\gamma_1'\ \gamma_2'\ \gamma_3'}=\binom{\Gamma_1\ \Gamma_2\ \Gamma_3}{\gamma_1\ \gamma_2\ \gamma_3}\quad\text{for all }\gamma_1,\gamma_2,\gamma_3\text{ and all }R\in G. \tag{I.2}$$

Equation (I.2) will be recognized to be an identity satisfied by the general 3-$j$ symbols defined by Wigner[3] [and in particular, the famous 3-$j$ symbols for the special case of $G=\mathrm{SU}(2)$, the rotation group, when the $\Gamma_i$ are chosen as the conventional irreducible matrix representations of SU(2)]. The concept of triple coefficients is a slight generalization of that of 3-$j$ symbols; it was introduced in Ref. 4 in connection with a discussion of the Wigner–Eckart theorem [cf. Eq. (I.3) below].

The problem posed in (A) above now turns out to be equivalent to that of the existence of real triple coefficients, the latter being precisely formulated as follows:

(B) *Given a compact group* G, *is it possible to find a system of standard representations of* G *such that for any ordered triple* $\Gamma_1\Gamma_2\Gamma_3$ *of three standard representations there is a basis* $(\mathbf{c}_1,\ldots,\mathbf{c}_N)$ *for* $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ *consisting of* real *column vectors*?

It requires a series of arguments of a rather detailed and nonfundamental nature to demonstrate the equivalence of the reality problems (A) and (B). We therefore defer this discussion to Appendix A. Before attacking problem (B) in Sec.

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II, then, we want to observe the following reasons for being interested in an answer to it:

(i) The well-known *Wigner–Eckart theorem* in our notation[4] reads

$$\langle \psi^{\Gamma_1}_{\gamma_1} | \mathcal{O}^{\Gamma_2}_{\gamma_2} | \varphi^{\Gamma_3}_{\gamma_3} \rangle = \sum_{\beta=1}^{N} \langle \psi^{\Gamma_1} \| \mathcal{O}^{\Gamma_2} \| \varphi^{\Gamma_3} \rangle_\beta \begin{pmatrix} \overline{\Gamma}_1 & \Gamma_2 & \Gamma_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix}_\beta . \tag{I.3}$$

One usually thinks of this formula for matrix elements of a tensor operator $\mathcal{O}^{\Gamma_2}_{\gamma_2}$ between symmetry-adapted basis vectors as giving a factorization into quantities (the triple coefficients) expressing the "symmetry" or "geometry" of the operator and quantities carrying the "physical" content of it (the numbers $\langle \varphi^{\Gamma_1} \| \mathcal{O}^{\Gamma_2} \| \varphi^{\Gamma_3} \rangle_\beta$, the so-called reduced matrix elements). It would be nice to know to what extent any "nonreality" of the operator $\mathcal{O}^{\Gamma_2}_{\gamma_2}$ can be attributed to the reduced matrix element (by choosing real triple coefficients) and thus be regarded as an aspect of its physical nature.

(ii) For *practical calculations*, real numbers are usually preferable to nonreal complex numbers.

(iii) A theorem proved in Feit's book[5] (but apparently otherwise not much recognized in the literature) asserts that C–G coefficients of a finite group—nonunique as they are—in a certain sense characterize the group up to isomorphism. Thus, these coefficients might also be of a more fundamental *mathematical* interest.

## II. THE REPRESENTATION TRIPLE PROJECTION MATRIX

Let $G$ be a compact group ($G$ may, in particular, be finite) and let $dR$ be normalized Haar measure on $G$ [if $G$ is finite of order $|G|$, this means that $\int_G f(R)\,dR = |G|^{-1} \sum_{R\in G} f(R)$ for any function $f$ on $G$]. If $\Gamma_1, \Gamma_2, \Gamma_3$ are continuous unitary (irreducible) matrix representations of $G$, the matrix

$$\Gamma_{123} = \int_G [\overline{\Gamma}_1(R) \otimes \overline{\Gamma}_2(R) \otimes \overline{\Gamma}_3(R)]\, dR$$

has the following properties:

(i) $\Gamma_{123}{}^2 = \Gamma_{123}$,

(ii) $\Gamma_{123} = \Gamma_{123}{}^\dagger$ (the adjoint matrix)

(iii) a column vector $\mathbf{c}$ is a fix-vector for $\Gamma_{123}$ if and only if $\mathbf{c}$ satisfies (I.1).

*Sketch of proof*: Property (i) is immediate from the translational invariance of integration over $G$. Property (ii) follows from the unitarity of the $\Gamma_i$ and the unimodularity of $G$, i.e., the fact[6] that $\int_G f(R^{-1})\,dR = \int_G f(R)\,dR$ for any continuous function $f$ on $G$. As for (iii), "if" is trivial; "only if" follows from the observation that $\mathbf{c} = \Gamma_{123}\mathbf{c}$ implies that for all $R\in G$,

$$[\overline{\Gamma}_1(R) \otimes \overline{\Gamma}_2(R) \otimes \overline{\Gamma}_3(R)]\,\mathbf{c} = [\overline{\Gamma}_1(R) \otimes \overline{\Gamma}_2(R) \otimes \overline{\Gamma}_3(R)]\,\Gamma_{123}\,\mathbf{c} = \Gamma_{123}\mathbf{c} = \mathbf{c},$$

again because of the translational invariance of integration.

Thus $\Gamma_{123}$ is the matrix for the orthogonal *projection onto* $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$, a fact which has also been noted by Wigner.[7] (This projection property is well known in general representation theory.[8]) This means that $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ is spanned by the columns of $\Gamma_{123}$. In particular, a basis for $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ may be selected from the columns of $\Gamma_{123}$. Therefore, *if* $\Gamma_{123}$ *is a real matrix for all triples* $\Gamma_1\Gamma_2\Gamma_3$ of standard representations, we can answer question (B) from Sec. I. in the affirmative.

One way in which $\Gamma_{123}$ may become real for all standard triples is through the existence of a continuous mapping $\tau$ of $G$ into itself and a choice of standard representations such that the following conditions are satisfied:

(a) Haar measure on $G$ is invariant with respect to $\tau$, that is,

$$\int_G f(\tau(R))\,dR = \int_G f(R)\,dR$$

for any continuous function $f$ on $G$.

(b) For any standard representation $\Gamma$ we have

$$\Gamma(\tau(R)) = \overline{\Gamma}(R) \quad \text{for all } R\in G.$$

Indeed, in this situation we have

$$\begin{aligned}\Gamma_{123} &= \int_G [\overline{\Gamma}_1(R) \otimes \overline{\Gamma}_2(R) \otimes \overline{\Gamma}_3(R)]\,dR \\ &= \int_G [\Gamma_1(\tau(R)) \otimes \Gamma_2(\tau(R)) \otimes \Gamma_3(\tau(R))]\,dR \\ &= \int_G [\Gamma_1(R) \otimes \Gamma_2(R) \otimes \Gamma_3(R)]\,dR = \overline{\Gamma}_{123}.\end{aligned}$$

We now point out some consequences of having a situation with (a) and (b) fulfilled.

Note first that (b) implies that for any standard $\Gamma$ we have

$$\Gamma(\tau^2(R)) = \Gamma(\tau(\tau(R))) = \overline{\Gamma}(\tau(R)) = \overline{\overline{\Gamma}}(R) = \Gamma(R) \quad \text{for all } R\in G.$$

This shows, by the Gel'fand–Raĭkov theorem,[9] that $\tau^2(R) = R$ for all $R$, that is, $\tau$ is an *involution* and thus, in particular, a bijection of $G$. This is immediate if $G$, as is often the case in practice, has a faithful irreducible representation. *phism* of $G$ since any standard representation composed with $\tau$ gives a representation (the complex conjugate representation).

Thus, the mapping $\tau$ is necessarily *an involutory automorphism of* $G$. In Sec. IV we investigate to what extent the above situation may be realized with $\tau$ being an *inner* automorphism of $G$, i.e., a mapping of the form $R\to R_0 R R_0^{-1}$, $R\in G$, where $R_0$ is a fixed element of $G$. For inner automorphism (a) is automatically satisfied because of the translational invariance of integration over $G$. [Actually, (a) is satisfied for any continuous involutory automorphism.[10]] Since the investigation of (b) in the case of inner automorphisms falls into two parts, according to the Frobenius–Schur classification of irreducible representations, we discuss this classification briefly in Sec. III.

## III. THE FROBENIUS–SCHUR CLASSIFICATION

We start by introducing the following auxiliary concept:

If $R\to\Gamma(R)$, $R\in G$, is a unitary matrix representation of a group $G$, a *conjugating matrix* for $\Gamma$ is a unitary matrix $\mathbf{U}$ intertwining $\Gamma$ and $\overline{\Gamma}$ (the complex conjugate representation):

$$\mathbf{U}\Gamma(R)\,\mathbf{U}^{-1} = \bar{\Gamma}(R) \quad \text{for all } R\in G. \tag{III.1}$$

If $\Gamma$ and $\bar{\Gamma}$ are equivalent [meaning that there is a nonsingular $\mathbf{U}$ satisfying (III.1)], it can easily be shown that $\Gamma$ has a conjugating matrix (see Ref. 4, Sec. 5.2 or refer to the well-known fact that equivalent *unitary* irreducible matrix representations are *unitarily* equivalent[11]).

Using the unitarity of the matrices $\Gamma(R)$, $R\in G$, we see that (III.1) is equivalent to

$$\Gamma(R)^{\mathrm{T}}\ \ \mathbf{U}\Gamma(R) = \mathbf{U} \quad \text{for all } R\in G, \tag{III.2}$$

where T denotes transposition of a matrix. Now suppose that $\Gamma$ is irreducible. From the form of the left-hand side of (III.2) the linear space of *all* (for the moment not necessarily unitary) matrices $\mathbf{U}$ satisfying (III.2) is stable under transposition of matrices and is therefore the direct sum of two subspaces consisting of symmetric matrices and antisymmetric matrices, respectively. On the other hand, by Schur's lemma, this space is of dimension at most 1, since $\Gamma$ and $\bar{\Gamma}$ are irreducible. Thus, given $\Gamma$, either all matrices $\mathbf{U}$ satisfying (III.2) are symmetric or all such matrices are antisymmetric. This observation forms the basis for the Frobenius–Schur classification:

*Definition*: A unitary irreducible matrix representation is of the *first kind* if it has a *symmetric* conjugating matrix. A unitary irreducible matrix representation is of the *second kind* if it has an *antisymmetric* conjugating matrix. A unitary irreducible matrix representation is of the *third kind* if it is not equivalent to its complex conjugate representation.

Suppose $\Gamma$ is a unitary matrix representation and $\mathbf{U}$ a conjugating matrix for $\Gamma$. Let $\mathbf{A}$ be any unitary matrix. Then it is immediately verified that $\bar{\mathbf{A}}\mathbf{U}\mathbf{A}^{-1}$ is a conjugating matrix for the representation $R\to\mathbf{A}\Gamma(R)\,\mathbf{A}^{-1}$, $R\in G$. Since the transformation

$$\mathbf{U}\to\bar{\mathbf{A}}\mathbf{U}\mathbf{A}^{-1} = (\mathbf{A}^{-1})^{\mathrm{T}}\ \ \mathbf{U}\mathbf{A}^{-1} \tag{III.3}$$

evidently preserves symmetry/anitsymmetry of $\mathbf{U}$, we see that *equivalent matrix representations are of the same kind.*

*Note*: This classification was introduced first by Frobenius and Schur in a slightly different way[12] (cf. the remark following Theorem 1 below). Various alternative descriptions of the classification exist, including a simple character test for classifying an irreducible representation, but as we shall not need these we refer the reader to some relevant literature[13–17] and to the more detailed treatment in Ref. 18.

The entries of conjugating matrices are what Wigner[3] and several subsequent authors have named 1-*j* symbols and for which Butler[1] has suggested the name 2-*jm* symbols.

## IV. COMPLEX CONJUGATION OF MATRIX REPRESENTATIONS BY INNER AUTOMORPHISMS

We now turn to the subject of complex conjugation of matrix representations by inner automorphisms announced in Sec. II. Suppose a choice of standard representations can be made for a compact group $G$ such that there is an inner automorphism $R\to R_0RR_0^{-1}$, $R\in G$, taking each of these representations into its complex conjugate. Since we then have

$$\bar{\Gamma}(R) = \Gamma(R_0RR_0^{-1}) = \Gamma(R_0)\Gamma(R)\,\Gamma(R_0)^{-1} \quad \text{for all } R\in G \tag{IV.1}$$

for any standard representation $\Gamma$, we see that all standard representations of $G$ must be equivalent to their complex conjugate and thus be of the first or the second kind (i.e., $G$ must be *ambivalent*). Some further necessary conditions for the desired situation to be attainable may be noted immediately.

Firstly, by inserting $R = R_0$ in (IV.1), we see that for every $\Gamma$ the matrix $\Gamma(R_0)$ is *necessarily real.*

Secondly, the statement (IV.1) is equivalent to saying that $\Gamma(R_0)$ *is a conjugating matrix for* $\Gamma$ for every $\Gamma$. Thus, if $\Gamma$ is of *the first kind*, $\Gamma(R_0)$ is *necessarily symmetric*; if $\Gamma$ is of *the second kind*, $\Gamma(R_0)$ is *necessarily antisymmetric.*

Combining these observations on $\Gamma(R_0)$, we see that if $\Gamma$ is of the first kind we have

$$\begin{aligned}\Gamma(R_0^2) &= \Gamma(R_0)^{\mathrm{T}}\,\Gamma(R_0) = \Gamma(R_0)^{\mathrm{T}}\,\Gamma(R_0)\\ &= \bar{\Gamma}(R_0)^{\mathrm{T}}\ \ \Gamma(R_0) = \mathbf{1},\end{aligned} \tag{IV.2}$$

where $\mathbf{1}$ is the unit matrix.

If $\Gamma$ is of the second kind we have

$$\begin{aligned}\Gamma(R_0^2) &= \Gamma(R_0)\,\Gamma(R_0) = -\Gamma(R_0)^{\mathrm{T}}\ \ \Gamma(R_0)\\ &= -\bar{\Gamma}(R_0)^{\mathrm{T}}\ \ \Gamma(R_0) = -\mathbf{1}.\end{aligned} \tag{IV.3}$$

From (IV.2) and (IV.3), we have $\Gamma((R_0^2)^2) = \mathbf{1}$ for all standard $\Gamma$. This implies (by the Gel'fand–Raĭkov theorem[9]) that $(R_0^2)^2 = 1$ (the identity element in $G$). Thus $R_0^2$ is an involution in $G$. In Sec. II we noted that $R\to R_0RR_0^{-1}$ is an involutory mapping of $G$ into itself; this means that $R_0^2RR_0^{-2} = R$ for all $R\in G$ or that $R_0^2$ commutes with all $R\in G$. Thus, $R_0^2$ is a *central involution* in $G$.

Summarizing, *the inner automorphism approach requires G to be ambivalent and to have a central involution which is a square and which is mapped to* $\mathbf{1}$ *by all irreducible representations of the first kind and to* $-\mathbf{1}$ *by all irreducible representations of the second kind.*

When the approach is actually realized the standard irreducible matrix representations of $G$ necessarily have *real* conjugating matrices.

(We note that for a finite ambivalent group the explicit assumption of the existence of a square root of the central involution is unnecessary since the remaining assumptions and the Frobenius–Schur square-root count[12,19,20] there are $\Sigma\,\dim\Gamma$ such elements, where the sum is over all standard irreducible representations.)

The *necessary* conditions thus established turn out as well to be *sufficient* for the inner automorphism method to be applicable. This follows from Theorems 1 and 2, which we state below. These theorems have been proved in Ref. 18. Note the large degree of freedom which one has in prescribing the actual form of the conjugating matrices of the standard representations. This is of importance in establishing a convenient Wigner–Racah algebra for the group. Examples of groups satisfying the above necessary and sufficient conditions are SU(2), the icosahedral double group $I^*$, the octahedral double group $O^*$, and the dihedral double groups $D_2^*$, $D_4^*$, and $D_6^*$. The conventional treatment of the rotation group, SU(2), uses standard irreducible matrix representations $\mathscr{D}^{[j]}$ all having $\mathscr{D}^{[j]}(C_2^Y)$ as a conjugating matrix.[21] The inner automorphism approach has been used in the con-

struction of a Wigner–Racah algebra involving real C–G coefficient for $O^*$ in Ref. 22 and for $I^*$ in Ref. 4. See the general discussion in Sec. 5.4 of Ref. 4.

Not all ambivalent groups satisfy the above conditions; see Sec. V and Appendix B.

*Theorem* 1: Let $G$ be a group and $\Gamma$ an equivalence class of unitary irreducible matrix representations of $G$ of the first kind. Suppose $R_0 \in G$ is an element with $\Gamma(R_0^2) = \mathbf{1}$ for any matrix representation $\Gamma$ in $\Gamma$. Let $\mathbf{P}$ be any symmetric real orthogonal matrix with $\mathrm{Tr}\mathbf{P} = \chi_\Gamma(R_0)$ [Tr$\mathbf{P}$ is the trace of $\mathbf{P}$; $\chi_\Gamma(R_0)$ is the character of $\Gamma$ at $R_0$]. Then there exists a matrix representation $\Gamma$ in $\Gamma$ with the following properties:

(i) $\Gamma(R_0) = \mathbf{P}$,

(ii) $\mathbf{P}\Gamma(R)\mathbf{P}^{-1} = \overline{\Gamma}(R)$ for all $R \in G$.

*Remark*: Taking $R_0 = 1$ and $\mathbf{P} = \mathbf{1}$, we see that there is in particular a *real* matrix form $\Gamma$ of $\Gamma$. This was actually the criterion for a representation to be of the first kind in the paper by Frobenius and Schur.[12] The choice of real matrix representations is of course a rather natural one for irreducibles of the first kind and such a choice ensures the existence of real C–G coefficients (if no irreducibles of the second kind are involved). However, in certain cases, e.g., when adaptation of the standard representations of a group to specific group-subgroup hierarchies is desired, it may be necessary to have $\mathbf{P} \neq \mathbf{1}$ (for several examples of this see Ref. 4).

*Theorem* 2: Let $G$ be a group and $\Gamma$ an equivalence class of unitary irreducible matrix representations of $G$ of the second kind. Suppose $R_0 \in G$ is an element with $\Gamma(R_0^2) = -\mathbf{1}$ for any matrix representation $\Gamma$ in $\Gamma$. Let $\mathbf{P}$ be any antisymmetrix real orthogonal matrix. Then there exists a matrix representation $\Gamma$ in $\Gamma$ with the following properties:

(i) $\Gamma(R_0) = \mathbf{P}$,

(ii) $\mathbf{P}\Gamma(R)\mathbf{P}^{-1} = \overline{\Gamma}(R)$ for all $R \in G$.

*Remark*: It may be seen from the treatment in Ref. 18 that the assumptions of Theorem 2 imply that $\mathbf{P}$ and $\Gamma(R_0)$ both have trace zero. This is why the assumptions in Theorem 2 do not include, as do those of Theorem 1, a condition on the trace of $\mathbf{P}$.

If one has established a matrix form of an irreducible representation which is brought into its complex conjugate by a certain inner automorphism it may be useful to know to what extent this matrix form may be changed by similarity transformations without destroying the inner automorphism property. This is answered by the following proposition.

*Proposition*: Suppose $\Gamma$ is an *irreducible* matrix representation of a group $G$ and $R_0 \in G$ is an element such that

$$\Gamma(R_0 R R_0^{-1}) = \overline{\Gamma}(R) \quad \text{for all } R \in G.$$

Then, if $\Gamma'$ is unitarily equivalent to $\Gamma$, $\Gamma'$ is brought into its complex conjugate by the inner automorphism $R \to R_0 R R_0^{-1}$ if and only if there is a *real orthogonal* matrix $\mathbf{A}$ such that

$$\mathbf{A}\Gamma(R)\mathbf{A}^{-1} = \Gamma'(R) \quad \text{for all } R \in G.$$

*Proof*: "If" is easily checked. To see "only if," let $\mathbf{B}$ be a unitary matrix such that $\Gamma'(R) = \mathbf{B}\Gamma(R)\mathbf{B}^{-1}$ for $R \in G$. Now $\Gamma(R_0)$ is a conjugating matrix for $\Gamma$ and $\Gamma'(R_0)$ is a conjugating matrix for $\Gamma'$. Remembering the transformation rule (III.3) for conjugating matrices and noting that all conjugating matrices for $\Gamma'$ are proportional (because $\Gamma'$ is irreducible), we see that there is a complex number $\lambda$ with $|\lambda| = 1$ such that $\mathbf{B}\Gamma(R_0)\mathbf{B}^{-1} = \Gamma'(R_0) = \lambda\bar{\mathbf{B}}\Gamma(R_0)\mathbf{B}^{-1}$, i.e., such that $\mathbf{B} = \lambda\bar{\mathbf{B}}$. Choosing $\mu$ such that $\overline{\mu^2} = \lambda$ and putting $\mathbf{A} = \mu\mathbf{B}$ gives the desired conclusion. Q.E.D.

Fano and Racah in their argumentation[23] for the reality of SU(2) coupling coefficients use the "only if" part of this proposition for *reducible* representations without any comment. The line of argument in the present paper circumvents this inconvenient point.

## V. FURTHER REMARKS ON THE APPLICABILITY OF THE INNER AUTOMORPHISM APPROACH

There is an immediate consequence for the "representation algebra" of an ambivalent compact group $G$—that is, the way the tensor products of irreducible representations of $G$ decompose into irreducibles—of the group being susceptible to the inner automorphism approach. Suppose that $R_0 \in G$ with $\Gamma(R_0^2) = \mathbf{1}$ for all irreducible representations $\Gamma$ of $G$ of the first kind and $\Gamma(R_0^2) = -\mathbf{1}$ for all irreducible representations of the second kind. Then, given a triple $\Gamma_1\Gamma_2\Gamma_3$ of irreducible representations and a fix-vector $\mathbf{c}$ [that is, a solution to (I.1)], we have

$$\begin{aligned}\mathbf{c} &= [\overline{\Gamma}_1(R_0^2) \otimes \overline{\Gamma}_2(R_0^2) \otimes \overline{\Gamma}_3(R_0^2)]\,\mathbf{c} \\ &= [(\pm\mathbf{1}_1) \otimes (\pm\mathbf{1}_2) \otimes (\pm\mathbf{1}_3)]\,\mathbf{c} = \pm\mathbf{c}, \end{aligned} \tag{V.1}$$

where $\mathbf{1}_i$ is the unit matrix of the same dimension as $\Gamma_i$; $i = 1,2,3$. Equation (V.1) shows that if nonzero fix-vectors exist, i.e., if $\dim\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3) > 0$, an *even* number of the $\Gamma_i$ are of the second kind (either two of them or none of them). Now, it is easily seen, for example by the use of characters, that $\dim\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$, the number of occurrences of the trivial one-dimensional representation of $G$ in $\overline{\Gamma}_1 \otimes \overline{\Gamma}_2 \otimes \overline{\Gamma}_3$, is equal to the number of times any one of the $\Gamma_i$ occurs in the tensor product of the remaining two (since $G$ is ambivalent, the complex conjugations may be dropped here). Thus, the property of triple tensor products deduced above from (V.1) may be translated into the following property of the representation algebra: *the product of two irreducible representations of the same Frobenius–Schur kind always decomposes into a direct sum of irreducible representations of the first kind.* For the purpose of the present discussion we shall express this property by saying that "the representation algebra of $G$ is *regular* with respect to the Frobenius–Schur classification." [Butler[24] uses the term "quasi-ambivalent" for this property; this is unfortunate for the following two reasons: (1) this term has already been used in the literature for a different property (see Sec. VI); (2) an ambivalent group does not necessarily have the property, as we point out below.]

Wigner[20] noted that multiplicity-free ambivalent groups [ambivalent groups with $\dim\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3) \leqslant 1$ for all triples, so-called *simply reducible* groups] have a regular re-

presentation algebra. (His proof was actually slightly incomplete; a full proof was given by Mackey.[17]) The property of being multiplicity free is not necessary for the representation algebra to be regular; this is demonstrated by the examples of the octahedral and icosahedral double groups referred to in Sec. IV. The question arises whether all ambivalent groups have a regular representation algebra. Butler and King[25] examined various groups and came up with an example (due to J.S. Frame) of a group, ${}^2F_4(2)$, of very large order featuring a triple of *two* first-kind irreducible representations and *one* of the second kind having nonzero fix-vectors; however, this group is not ambivalent.[26] Here we demonstrate that the above question must be answered in the negative. Indeed, there is an ambivalent group of order only 72 which has a nonregular representation algbebra. Because of its fundamental interest we describe this example briefly in Appendix B.

It still remains to be investigated to what extent it is possible and desirable to apply the inner automorphism approach to groups of practical importance other than the subgroups of SU(2) mentioned in Sec. IV. We stress, though, that even if the group satisfies the necessary and sufficient conditions of Sec. IV there may not exist matrix forms of the irreducible representations compatible with the inner automorphism *and* which have *additional* desirable properties. Thus, for example, it is demonstrated in Ref. 4 that a choice of standard representations with the inner automorphism property allows for an adaptation to the icosahedral group–subgroup hierarchy $I^* \supset C_5^*$ (in the usual Schoenflies notation) but does *not* allow for adaptation to $I^* \supset D_5^* \supset C_5^*$ or $I^* \supset T_2^* \supset C_2^*$.

## VI. QUASI-AMBIVALENT GROUPS

Referring to the discussion in Sec. II, we note that a consequence of condition (b) is that for every irreducible character $\chi$ of $G$ we have

$$\chi(\tau(R)) = \overline{\chi(R)} = \chi(R^{-1}) \quad \text{for all } R \in G.$$

If $G$ finite, this means that for any $R$ the elements $\tau(R)$ and $R^{-1}$ belong to the same conjugacy class (since the irreducible characters of $G$ separate its conjugacy classes[27]). Groups admitting an involutory automorphism $\tau$ with the property that $\tau(R)$ and $R^{-1}$ are conjugate for all $R \in G$ have been called *quasi-ambivalent*.[28] (Note that an ambivalent group is quasi-ambivalent; indeed, in this case $\tau$ may be taken to be the identity.) Thus, *a finite group to which the automorphism approach expressed by* (a) *and* (b) *may be applied is necessarily quasi-ambivalent.*

Conversely, one may ask if the automorphism approach may be applied to any quasi-ambivalent group. We do not have an answer to this, but we give an example of a more restricted result which still indicates the relevance of quasi-ambivalence to the problem we are studying.

*Proposition.* The automorphism approach may be applied to any quasi-ambivalent compact group $G$ having no irreducible representations of even dimension.

*Proof.* Let $\tau$ be a (continuous) conjugacy class-inverting involutory automorphism of $G$. It will be sufficient to show that given an equivalence class $\Gamma$ of unitary irreducible matrix representations of $G$ we may find a $\mathbf{\Gamma}$ in $\Gamma$ such that

$$\mathbf{\Gamma}(\tau(R)) = \overline{\mathbf{\Gamma}}(R) \quad \text{for all } R \in G. \tag{VI.1}$$

Now, if $\chi$ is the character of the representation $\Gamma$ and $\chi_\tau$ is the character of the representation $R \to \Gamma(\tau(R))$, $R \in G$, we have

$$\chi_\tau(R) = \chi(\tau(R)) = \chi(R^{-1}) = \overline{\chi(R)} \quad \text{for all } R \in G \tag{VI.2}$$

from the assumptions on $\tau$. Let $\mathbf{\Gamma}'$ be any matrix representation in $\Gamma$. From (VI.2) the representations $\overline{\mathbf{\Gamma}}'$ and $R \to \mathbf{\Gamma}'(\tau(R))$ are equivalent (they have the same character). Thus there is a unitary matrix $\mathbf{V}$ such that

$$\mathbf{\Gamma}'(\tau(R)) = \mathbf{V}^{-1}\,\overline{\mathbf{\Gamma}}'(R)\,\mathbf{V} \quad \text{for all } R \in G. \tag{VI.3}$$

Rewriting—as was done in obtaining (III.2)—we get

$$\mathbf{\Gamma}'(R)^{\mathrm{T}}\ \mathbf{V}\mathbf{\Gamma}'(\tau(R)) = \mathbf{V} \quad \text{for all } R \in G. \tag{VI.4}$$

Using that $\tau$ is involutory one now shows that $\mathbf{V}$ satisfies (VI.4) if and only if $\mathbf{V}^{\mathrm{T}}$ does. As in the discussion following (III.2), this leads to the conclusion that $\mathbf{V}$ is symmetric or antisymmetric. Since it is of odd dimension, it must be symmetric. This means[29] that there is a unitary matrix $\mathbf{Q}$ such that $\mathbf{V} = \bar{\mathbf{Q}}\mathbf{Q}^{-1}$. Putting

$$\mathbf{\Gamma}(R) = \mathbf{Q}^{-1}\mathbf{\Gamma}'(R)\,\mathbf{Q} \quad \text{for all } R \in G$$

gives a matrix representation with the desired properties. Q.E.D.

An example of a group satisfying the conditions in the proposition is the tetrahedral group $T$ (isomorphic to the alternating group $A_4$). This group is not ambivalent since it has nonreal irreducible characters, but it is quasi-ambivalent[28] and has only irreducible representations of dimensions one and three. Thus, real Clebsch–Gordan coefficients may be chosen for $T$ (cf. Sec. I). In fact, in Ref. 30, we have even given real coefficients for the two *double*-group hierarchies $T^* \supset C_3^*$ and $T^* \supset C_2^*$.

## APPENDIX A

In this appendix we shall demonstrate the equivalence of the reality problems (A) and (B) of Sec. I. Some of the material needed for this demonstration has been given in the thorough treatment of triple coefficients in Ref. 4. We shall not repeat all of that here but instead give references to the appropriate parts of Ref. 4.

We start with an important remark concerning problem (B). In practice—and partly in the arguments to follow—one requires more than just *some* basis for $\mathcal{F}(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Gamma}_3)$. Firstly, the basis may be required to be *orthonormal*, and secondly, when two or three of the $\mathbf{\Gamma}_i$ are identical, leading to a partial or full permutational symmetry of $\mathbf{\Gamma}_1 \otimes \mathbf{\Gamma}_2 \otimes \mathbf{\Gamma}_3$, one may require the basis vectors to be adapted to irreducible representations of the relevant permutation group ($S_2$ or $S_3$; see Sec. 3.2 of Ref. 4). These additional requirements, however, raise no difficulties in the present context since the group-theoretical projection operators of $S_2$ and $S_3$, as well as the

Gram-Schmidt orthonormalization procedure, applied to a set of real columns will lead again to a set of real columns.

We next need to introduce some notation. The matrix direct sum $\mathbf{C}^{-1}(\mathbf{\Gamma}_1 \otimes \mathbf{\Gamma}_2)\,\mathbf{C}$ of representations of $G$ referred to in connection with formulation (A) is of the form

$$\mathbf{C}^{-1}(\mathbf{\Gamma}_1 \otimes \mathbf{\Gamma}_2)\,\mathbf{C} = \begin{pmatrix} \mathbf{\Delta}_1 & & & 0 \\ & \mathbf{\Delta}_2 & & \\ & & \ddots & \\ 0 & & & \mathbf{\Delta}_p \end{pmatrix}, \tag{A.1}$$

where the $\mathbf{\Delta}_i$ are standard matrix representations of $G$. If any two of the $\mathbf{\Delta}_i$ are *equivalent* they are *identical* because they all are standard. Suppose now that $\mathbf{\Delta}$ is a matrix representation of $G$ appearing among the $\mathbf{\Delta}_i$ in (A.1). If $\gamma_1$ is a component of $\mathbf{\Gamma}_1$, $\gamma_2$ is a component of $\mathbf{\Gamma}_2$, and $\delta$ a component of $\mathbf{\Delta}$, we shall designate the element of $\mathbf{C}$ corresponding to these components as

$$\langle \mathbf{\Gamma}_1\gamma_1\, \mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle\,. \tag{A.2}$$

This is the conventional coupling coefficient notation. The index $\beta$ is needed to indicate the position of $\mathbf{\Delta}$ in the block diagonal matrix representation in (A.1) when several of the $\mathbf{\Delta}_i$ are identical to $\mathbf{\Delta}$. Thus the pairs $\gamma_1\gamma_2$ serve as row indices in $\mathbf{C}$ and the triples $\beta\,\mathbf{\Delta}\delta$ as column indices in $\mathbf{C}$.

Furthermore, if $(\mathbf{c}_1,\ldots,\mathbf{c}_N)$ is a basis for $\mathscr{F}(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta})$, where $\mathbf{\Gamma}_1$, $\mathbf{\Gamma}_2$, and $\mathbf{\Delta}$ are unitary irreducible matrix representations of $G$ (not necessarily standard), we shall denote the element of a basis column $\mathbf{c}_\beta$ corresponding to the components $\gamma_1$ of $\mathbf{\Gamma}_1$, $\gamma_2$ of $\mathbf{\Gamma}_2$, and $\delta$ of $\mathbf{\Delta}$ by the symbol

$$\begin{pmatrix} \mathbf{\Gamma}_1 & \mathbf{\Gamma}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta. \tag{A.3}$$

The connection between C-G coefficients and triple coefficients may now be stated compactly in the following formula:

$$\langle \mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle = \varphi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)(\dim\mathbf{\Delta})^{1/2} \begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta. \tag{A.4}$$

Here the triple coefficients are assumed to come from an *orthonormal* basis $(\mathbf{c}_1,\ldots,\mathbf{c}_N)$ for $\mathscr{F}(\overline{\mathbf{\Gamma}}_1\overline{\mathbf{\Gamma}}_2\mathbf{\Delta})$; $\varphi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)$ is a phase factor (complex number with modulus 1) and $\dim\mathbf{\Delta}$ is the dimension of $\mathbf{\Delta}$. The formula is to be interpreted in the following way:

*Given* triple coefficients

$$\begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta$$

for each distinct $\mathbf{\Delta}$ occurring in (A.1) and a choice of $\phi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)$ for every pair $\mathbf{\Delta}\beta$, the numbers $\langle \mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle$ defined by (A.4) will form a matrix of C–G coefficients for $\mathbf{\Gamma}_1 \otimes \mathbf{\Gamma}_2$. [The number of times a given $\mathbf{\Delta}$ occurs in (A.1) is equal to the dimension of $\mathscr{F}(\overline{\mathbf{\Gamma}}_1\overline{\mathbf{\Gamma}}_2\mathbf{\Delta})$, cf. Appendix of Ref. 4.] *Conversely, given* a matrix of C–G coefficients $\langle \mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle$ for $\mathbf{\Gamma}_1 \otimes \mathbf{\Gamma}_2$ and a choice of $\varphi(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Delta}\beta)$ for every $\mathbf{\Delta}\beta$, the numbers

$$\begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta$$

defined by (A.4) will form sets of triple coefficients for the ordered triples $\overline{\mathbf{\Gamma}}_1\overline{\mathbf{\Gamma}}_2\mathbf{\Delta}$. (See Sec. 5.4 of Ref. 4 for the specific phase conventions relevant to groups susceptible to the inner automorphism approach.) The proof of these assertions runs along the following lines:

(1) One shows that triple coefficients of the form

$$\begin{pmatrix} \overline{\mathbf{\Gamma}} & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta$$

couple $\mathbf{\Gamma}_1$ with $\mathbf{\Gamma}_2$ to give $\mathbf{\Delta}$: rearranging

$$\sum_{\gamma_1'\gamma_2'\delta'} \mathbf{\Gamma}_1(R)_{\gamma_1\gamma_1'}\, \mathbf{\Gamma}_2(R)_{\gamma_2\gamma_2'}\, \overline{\mathbf{\Delta}}(R)_{\delta\delta'} \times \begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1' & \gamma_2' & \delta' \end{pmatrix}_\beta = \begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta \tag{A.5}$$

for all $\gamma_1$, $\gamma_2$, $\delta$ and all $R\in G$,

using the unitarity of $\mathbf{\Delta}$, gives

$$\sum_{\gamma_1',\gamma_2'} [\mathbf{\Gamma}_1(R)_{\gamma_1\gamma_1'}\, \mathbf{\Gamma}_2(R)_{\gamma_2\gamma_2'}] \times \begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1' & \gamma_2' & \delta \end{pmatrix}_\beta = \sum_{\delta'} \begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta' \end{pmatrix}_\beta \mathbf{\Delta}(R)_{\delta'\delta}$$

for all $\gamma_1$, $\gamma_2$, $\delta$ and all $R\in G$, (A.6)

which is that part of the matrix equation obtained from (A.1) by multiplying by $\mathbf{C}$ from the left which pertains to the particular copy of $\mathbf{\Delta}$ distinguished by $\beta$.

(2) One shows that the coefficients $\langle \mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle$ defined from triple coefficients by (A.4) form a unitary matrix $\mathbf{C}$. This is the least trivial part of the proof; it requires Schur's lemma (see Sec. 3.3 and Appendix of Ref. 4).

(3) Conversely, one shows that C-G coefficients $\langle \mathbf{\Gamma}_1\gamma_1\mathbf{\Gamma}_2\gamma_2 |\, \beta\, \mathbf{\Delta}\delta \rangle$ are triple coefficients of the type

$$\begin{pmatrix} \overline{\mathbf{\Gamma}}_1 & \overline{\mathbf{\Gamma}}_2 & \mathbf{\Delta} \\ \gamma_1 & \gamma_2 & \delta \end{pmatrix}_\beta;$$

this is just a reversal of the argument in (1). The unitarity of the C–G coefficient matrix assures that an *orthonormal* basis for $\mathscr{F}(\overline{\mathbf{\Gamma}}_1\overline{\mathbf{\Gamma}}_2\mathbf{\Delta})$ is, in fact, obtained if (A.4) is used to define the triple coefficients.

Thus, having established (A.4), we see that we shall be satisfied to show the equivalence of the reality problem (B) and the corresponding one "with two conjugations", i.e., the one obtained from (B) by replacing $\mathscr{F}(\mathbf{\Gamma}_1\mathbf{\Gamma}_2\mathbf{\Gamma}_3)$ by $\mathscr{F}(\overline{\mathbf{\Gamma}}_1\overline{\mathbf{\Gamma}}_2\mathbf{\Gamma}_3)$. Let us call this one (B'). We proceed as follows:

First note that if $\mathbf{\Gamma}$ is a unitary irreducible matrix representation of $G$ and we have a nonzero set of triple coefficients

$$\begin{pmatrix} \mathbf{\Gamma} & \mathbf{\Gamma} & 1_G \\ \gamma & \gamma' & 0 \end{pmatrix}$$

for the triple $\mathbf{\Gamma}\mathbf{\Gamma}1_G$ (where $1_G$ denotes the trivial one-dimensional representation of $G$ and 0 its component), then for a suitably chosen real number $n(\mathbf{\Gamma})$ the matrix $\mathbf{U}$ with elements

$$u_{\gamma\gamma'} = n(\mathbf{\Gamma}) \begin{pmatrix} \mathbf{\Gamma} & \mathbf{\Gamma} & 1_G \\ \gamma & \gamma' & 0 \end{pmatrix} \tag{A.7}$$

will be a conjugating matrix for $\Gamma$. This follows by observing that the equation

$$\sum_{\gamma_1,\gamma_1'} \overline{\Gamma}(R)_{\gamma\gamma_1}\,\overline{\Gamma}(R)_{\gamma'\gamma_1'}\,u_{\gamma_1\gamma_1'} = u_{\gamma\gamma'} \quad \text{for all } R\in G, \tag{A.8}$$

satisfied by the $u_{\gamma\gamma'}$, if rewritten as

$$\sum_{\gamma_1,\gamma_1'} \Gamma(R)_{\gamma_1\gamma}\,u_{\gamma_1\gamma_1'}\Gamma(R)_{\gamma_1'\gamma'} = u_{\gamma\gamma'} \quad \text{for all } R\in G, \tag{A.9}$$

demonstrates that $\Gamma(R)^{\dagger}\mathbf{U}\Gamma(R) = \mathbf{U}$. Compare Eq. (III.2). From the discussion in Sec. III we now see that $\mathbf{U}$ is proportional to a conjugating matrix for $\Gamma$. Obviously, $\Gamma$ is of the first or second Frobenius–Schur kind if and only if nonzero triple coefficients of the type (A.7) exist.

Suppose now that (B) can be answered in the affirmative. We want to show that then (B′) can as well, i.e., that for any three standard matrix irreps $\Gamma_1$, $\Gamma_2$, and $\Gamma_3$ of $G$ there is a real basis for $\mathcal{F}(\overline{\Gamma}_1\overline{\Gamma}_2\Gamma_3)$. We distinguish four cases:

(i) If $\Gamma_1$ and $\Gamma_2$ are both of the third kind, their complex conjugates are, according to the definition of a system of standard representations in Sec. I, both standard representations themselves and there is nothing to show.

(ii) If $\Gamma_1$ is of the first or second kind and $\Gamma_2$ is of the third kind, we argue as follows: define a matrix $\mathbf{U}_1$ by (A.7), with $\Gamma_1$ taking the place of $\Gamma$, so that $\mathbf{U}_1$ becomes a conjugating matrix for $\Gamma_1$. In doing this, use real triple coefficients [this is possible because there is a real basis for $\mathcal{F}(\Gamma_1\Gamma_1 1_G)$ by assumption] and a real number $n(\Gamma_1)$; then $\mathbf{U}_1$ will be a *real* matrix. Since $\overline{\Gamma}_2$ is itself a standard matrix representation, there is by assumption a real basis $(\mathbf{c}_1,\ldots,\mathbf{c}_N)$ for $\mathcal{F}(\Gamma_1\overline{\Gamma}_2\Gamma_3)$. Put $\mathbf{U} = \mathbf{U}_1^{-1}\otimes\mathbf{1}_2\otimes\mathbf{1}_3$, where $\mathbf{1}_i$ is the unit matrix of the same dimension as $\Gamma_i$; $i = 2,3$. It is then seen by direct verification that $(\mathbf{Uc}_1,\ldots,\mathbf{Uc}_N)$ is a real basis for $\mathcal{F}(\overline{\Gamma}_1\overline{\Gamma}_2\Gamma_3)$.

(iii) If $\Gamma_2$ is of the first or second kind and $\Gamma_1$ is of the third kind, the argument is completely analogous to the one in (ii).

(iv) If neither $\Gamma_1$ nor $\Gamma_2$ is of the third kind, the argument is as in (ii) except that now *two* real conjugating matrices $\mathbf{U}_1$ and $\mathbf{U}_2$ enter, the matrix $\mathbf{U}$ turning a real basis for $\mathcal{F}(\Gamma_1\Gamma_2\Gamma_3)$ into a real basis for $\mathcal{F}(\overline{\Gamma}_1\overline{\Gamma}_2\Gamma_3)$ being then defined by $\mathbf{U} = \mathbf{U}_1^{-1}\otimes\mathbf{U}_2^{-1}\otimes\mathbf{1}_3$.

If, conversely, we assume that (B′) can be answered in the affirmative, we get to (B) by using conjugating matrices for the conjugates of standard representations, using then (A.7) with $\overline{\Gamma}$ instead of $\Gamma$.

The desired proof is hereby completed: formula (A.4) and the discussion following it showed the equivalence of (A) and (B′), and we have just shown (B′) to be equivalent to (B).

## APPENDIX B

Here we describe the example alluded to in Sec. V, namely a group of order 72 which is ambivalent and the representation algebra of which is *not* regular with respect to the Frobenius–Schur classification. The inner automorphism approach is not applicable to such a group (see Secs. IV and V). P. Landrock constructed this example[31] when asked by the author if all ambivalenty groups have the central involution property derived in Sec. IV.

The group in question is a semidirect product[32] $G = (C_3\times C_3)\mathrm{O}D_2^*$ of the direct product $C_3\times C_3$ of the cyclic group of order three with itself and the dihedral double group $D_2^*$, the latter being isomorphic to the quaternion group. This semidirect product is constructed in such a way[33] that it has six conjugacy classes: $\mathscr{C}_1 = \{E\}$; $\mathscr{C}_8$, which is all of $C_3\times C_3$ except $E$ and thus contains eight elements of order 3; $\mathscr{C}_9$, which consists of nine (noncentral!) involutions, among which is the involution of $D_2^*$ (the element usually described as the rotation of 360°); and three classes $\mathscr{C}_{18}^1$, $\mathscr{C}_{18}^2$, and $\mathscr{C}_{18}^3$, each consisting of 18 elements of order 4 and each intersecting $D_2^*$ in two elements. The group therefore has six irreducible characters, and the character table is

| | $\mathscr{C}_1$ | $\mathscr{C}_8$ | $\mathscr{C}_9$ | $\mathscr{C}_{18}^1$ | $\mathscr{C}_{18}^2$ | $\mathscr{C}_{18}^3$ | |
|---|---|---|---|---|---|---|---|
| $\chi_{11}$ | 1 | 1 | 1 | 1 | 1 | 1 | |
| $\chi_{12}$ | 1 | 1 | 1 | 1 | −1 | −1 | |
| $\chi_{13}$ | 1 | 1 | 1 | −1 | 1 | −1 | first kind |
| $\chi_{14}$ | 1 | 1 | 1 | −1 | −1 | +1 | |
| $\chi_2$ | 2 | 2 | −2 | 0 | 0 | 0 | second kind |
| $\chi_8$ | 8 | −1 | 0 | 0 | 0 | 0 | first kind |

The characters $\chi_{11}$, $\chi_{12}$, $\chi_{13}$, $\chi_{14}$, and $\chi_2$ will be recognized each to yield one of the five irreducible characters of $D_2^*$ when restricted to (subduced to) $D_2^*$. The sixth character is easily found by the orthogonality relations. The Frobenius–Schur classification of the irreducible representations may be found using the character test referred to in Sec. III.

Since all characters are real, the group is ambivalent. Furthermore, it is readily verified that the tensor product $\chi_8\otimes\chi_8$ decomposes according to

$$\chi_8\otimes\chi_8 = \chi_{11}+\chi_{12}+\chi_{13}+\chi_{14}+2\chi_2+7\chi_8,$$

from which it is apparent that the representation algebra of $G$ is *not* regular.


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of *any* group, the product of $M$ and its adjoint matrix can be shown from Schur's lemma to be a scalar matrix. Since this product matrix obviously can have only positive real eigenvalues we conclude that it is a positive real multiple of the unit matrix, so that $M$ itself is proportional to a unitary matrix.]


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[33]Specifically, the quaternion group is embedded in the automorphism group of $C_3 \times C_3$ by assigning to any two fourth-order elements which are not mutually inverse the GL(2,3)-matrices $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, respectively, and letting GL(2,3)-matrices operate on $C_3 \times C_3$ in the natural way ($C_3 \times C_3$ is viewed as a vector space over the finite field of order 3). By this construction the quaternion group acts transitively on $(C_3 \times C_3) \setminus \{E\}$.

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# On the matrix elements of the U($n$) generators

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A straightforward derivation of the matrix elements of the U($n$) generators is presented using algebraic infinitesimal techniques. An expression for the general fundamental Wigner coefficients of the group is obtained as a polynomial in the group generators. This enables generalized matrix elements to be defined without explicit reference to basis states. Such considerations are important for treating groups such as Sp($2n$) whose basis states are not known.

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## 1. INTRODUCTION

It was shown in a previous publication[1] (herein referred to as I) that the polynomial identities satisfied by the infinitesimal generators of a semisimple Lie group may be applied to give a simple determination of the (multiplicity-free) Wigner coefficients of the group. In this paper we shall extend some of the techniques presented in I to give a simple self-contained derivation of the matrix elements of the U($n$) generators.

An orthonormal basis for the finite dimensional irreducible representations of U($n$) was first constructed by Gel'fand and Zetlin.[2] The matrix elements of the U($n$) generators in this basis were first derived by Gel'fand and Zetlin[2] and rederived using boson-calculus techniques by Baird and Biedenharn.[3] In their discussion of the Gel'fand–Zetlin results Baird and Biedenharn made an important contribution by explicitly expressing the general matrix element as a product of a reduced matrix element and a Wigner coefficient. As a result the fundamental Wigner coefficients of U($n$), for general $n$, were given for the first time. It is our principal aim to obtain these results using algebraic infinitesimal techniques in contrast to the integral techniques of Gel'fand and Zetlin and Baird and Biedenharn.

The relationship between our approach and that employed by Biedenharn *et al.*[3-5] has been discussed in I. Although the two approaches are closely related we feel that our approach offers some novel features. In the literature it is customary to obtain the matrix elements of generators of the form $a^m_{m+1}$ and $a^{m+1}_m$ $(m<n)$ first and to obtain the matrix elements of the remaining generators by repeated commutation. Making use of the concept of simultaneous shift operators which shift the representation labels of U($n$) and each of its canonical subgroups in a certain prescribed way, we shall present an alternative derivation where the matrix elements of all generators are obtained just as easily as those of the form $a^m_{m+1}$ and $a^{m+1}_m$. An expression for the general fundamental Wigner coefficients of U($n$) is also given in terms of polynomials in the group generators constructed using the characteristic identities of U($n$) and each of its canonical subgroups. The expressions obtained are clearly generalizable to more general groups.

We shall also obtain an expression for the U($n$) : U($n-1$) reduced Wigner coefficients (or isoscalar factors) as a polynomial in the group generators. The simultaneous shift operators used in this paper are obviously related to the pattern calculus of Biedenharn *et al.*[5] and their concept of Wigner operator. The exact relationship between them will be discussed in a forthcoming publication.

The extension of this work to the discrete series of representations of the noncompact groups U($n$,1) and the orthogonal groups O($n$) and O($n$,1) is evident.

## 2. WIGNER COEFFICIENTS AND REDUCED MATRIX ELEMENTS

The generators $a^i_j (i,j=1,\ldots,n)$ of the Lie group U($n$) satisfy the commutation relations

$$[a^i_j, a^k_l] = \delta^k_j a^i_l - \delta^i_l a^k_j$$

and the Hermiticity property

$$(a^i_j)^\dagger = a^j_i.$$

These generators may be assembled into a square matrix $a$ whose $(i,j)$ entry is the generator $a^i_j$. Polynomials in $a$ may be defined recursively by the formula

$$(a^{m+1})^i_j = (a^m)^i_k a^k_j = a^i_k (a^m)^k_j.$$

Associated with the matrix $a$ is its adjoint $\bar{a}$ with entries $\bar{a}^i_j = -a^i_j$. Polynomials in $\bar{a}$ may be defined by

$$(\bar{a}^{m+1})^i_j = (\bar{a}^m)^k_j \bar{a}^i_k = \bar{a}^k_j (\bar{a}^m)^i_k.$$

It has been shown[5] on a finite dimensional irreducible representation of U($n$) with highest weight $\lambda = (\lambda_1,\ldots,\lambda_n)$ that the matrices $a$ and $\bar{a}$ satisfy the polynomial identities

$$\prod_{r=1}^{n} (a - \alpha_r) = 0, \quad \prod_{r=1}^{n} (\bar{a} - \bar{\alpha}_r) = 0, \tag{1}$$

where the roots $\alpha_r$ and $\bar{\alpha}_r$ are given by

$$\alpha_r = \lambda_r + n - r = n - 1 - \bar{\alpha}_r.$$

By virtue of the identities (1), projection operators $P[r]$ and $\bar{P}[r]$ may be constructed by setting

$$P[r] = \prod_{l \neq r} \left( \frac{a - \alpha_l}{\alpha_r - \alpha_l} \right),$$

$$\bar{P}[r] = \prod_{l \neq r} \left( \frac{\bar{a} - \bar{\alpha}_l}{\bar{\alpha}_r - \bar{\alpha}_l} \right).$$

The matrix elements of such projectors in unitary represen-

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tations of the group were shown in I to be bilinear combinations of Wigner coefficients. To be more explicit let $V(\lambda)$ be a finite dimensional irreducible representation with highest weight $\lambda$ and let $|{}^{\lambda}_{(\nu)}\rangle$ and $|{}^{\lambda}_{(\nu')}\rangle$ be Gel'fand basis states in the space $V(\lambda)$. According to I we have

$$\left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}\middle| P[r]^i_j \middle| \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle = \sum_{(\mu)} \left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}; \begin{matrix}\overline{1\dot{0}}\\ i\end{matrix}\middle| \begin{matrix}\lambda-\Delta_r\\(\mu)\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda-\Delta_r\\(\mu)\end{matrix}\middle| \begin{matrix}\overline{1\dot{0}}\\ j\end{matrix}; \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle, \tag{2}$$

where $|{}^{\overline{10}}_{i}\rangle$ constitutes an orthonormal basis for the contragredient vector representation and where $|{}^{\overline{10},\lambda}_{i,(\nu)}\rangle$ denotes the product state $|{}^{\overline{10}}_{i}\rangle \otimes |{}^{\lambda}_{(\nu)}\rangle$. Similarly, we have

$$\left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}\middle| \bar{P}[r]^i_j \middle| \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle = \sum_{(\mu)} \left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}; \begin{matrix}1\dot{0}\\ j\end{matrix}\middle| \begin{matrix}\lambda+\Delta_r\\(\mu)\end{matrix}\right\rangle \left\langle \begin{matrix}\lambda+\Delta_r\\(\mu)\end{matrix}\middle| \begin{matrix}1\dot{0}\\ i\end{matrix}; \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle, \tag{3}$$

where $|{}^{1\dot{0}}_{i}\rangle$ forms the usual basis for the fundamental vector representation. Substituting $i=j=n$ into Eqs. (2) and (3) we obtain

$$\left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}\middle| P[r]^n_n \middle| \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle = \delta_{(\nu),(\nu')} \left| \left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}; \begin{matrix}\overline{1\dot{0}}\\ n\end{matrix}\middle| \begin{matrix}\lambda-\Delta_r\\(\nu)\end{matrix}\right\rangle \right|^2,$$

$$\left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}\middle| \bar{P}[r]^n_n \middle| \begin{matrix}\lambda\\(\nu')\end{matrix}\right\rangle = \delta_{(\nu),(\nu')} \left| \left\langle \begin{matrix}\lambda\\(\nu)\end{matrix}; \begin{matrix}1\dot{0}\\ n\end{matrix}\middle| \begin{matrix}\lambda+\Delta_r\\(\nu)\end{matrix}\right\rangle \right|^2. \tag{4}$$

It is our aim now to apply the U($n$) characteristic identities (1) to evaluate the operators $P[r]^n_n$ and $\bar{P}[r]^n_n$ which, by Eqs. (4), are essentially squares of Wigner coefficients.

We now turn our attention to the group U($n+1$) whose generators $a^i_j$ ($i,j=1,\ldots,n+1$) may be assembled into a matrix $b$ whose $(i,j)$ entry is the generator $a^i_j$. The matarix $b$ satisfies an $n+1$ degree polynomial identity analogous to the U($n$) matrix $a$:

$$\prod_{k=1}^{n+1}(b-\beta_k)=0,$$

where the $\beta_k$ take constant values on an irreducible representation with highest weight $\lambda=(\lambda_1,\ldots,\lambda_{n+1})$ given by $\beta_k=\lambda_k+n+1-k$. In a similar way we define the adjoint matrix $\bar{b}$ whose roots $\bar{\beta}_k$ are given by $\bar{\beta}_k=n-\beta_k$.

As for U($n$) we may construct the U($n+1$) projection operators

$$Q[k]=\prod_{\substack{l=1\\ \neq k}}^{n+1}\left(\frac{b-\beta_l}{\beta_k-\beta_l}\right),$$

$$\bar{Q}[k]=\prod_{\substack{l=1\\ \neq k}}^{n+1}\left(\frac{\bar{b}-\bar{\beta}_l}{\bar{\beta}_k-\bar{\beta}_l}\right).$$

Also, according to I, if $p(x)$ is any polynomial we may write

$$P(b)=\sum_{k=1}^{n+1}P(\beta_k)Q[k]. \tag{5}$$

From the U($n+1$) identity we have

$$bQ[k]=\beta_k Q[k].$$

Taking the $(i,n+1)$ entry of this matrix equation we may write

$$\sum_{l=1}^{n+1} a^i_l Q[k]^l_{n+1} = \beta_k Q[k]^i_{n+1}, \quad i=1,\ldots,n.$$

Rearranging this expression we obtain

$$a^i_{n+1}\,Q[k]^{n+1}_{n+1} = (\beta_k-a)^i_l Q[k]^l_{n+1}. \tag{6}$$

Similarly, we may write

$$Q[k]^{n+1}_{n+1}\,a^{n+1}_i = Q[k]^{n+1}_l(\beta_k-a)^l_i. \tag{7}$$

For simplicity let us for the moment denote the U($n$) invariant $Q[k]^{n+1}_{n+1}$ by $C_k$. Clearly, the $C_k$ are U($n+1$) analogs of the operators $P[r]^n_n$ whose matrix elements are squares of Wigner coefficients. It is our aim to express $C_k$ as a function of the $\beta_k$ and $\alpha_r$. Note that Eq. (5) implies

$$P(b)^{n+1}_{n+1}=\sum_{k=1}^{n+1}P(\beta_k)C_k,$$

which enables a systematic evaluation of U($n$) invariants of the form $P(b)^{n+1}_{n+1}$ once the $C_k$ have been determined.

We may invert Eqs. (6) and (7) by writing

$$Q[k]^i_{n+1} = [(\beta_k-a)^{-1}]^i_j a^j_{n+1}\,C_k,$$

$$Q[k]^{n+1}_i = C_k a^{n+1}_j[(\beta_k-a)^{-1}]^j_i, \tag{8}$$

where $(\beta_k-a)^{-1}$ denotes the matrix

$$(\beta_k-a)^{-1}=\sum_{r=1}^{n}(\beta_k-\alpha_r)^{-1}P[r].$$

Throughout the remainder of this section let $\psi$ denote the U($n$) vector operator with components $\psi^i=a^i_{n+1}$, $i=1,\ldots,n$, with adjoint $\psi^\dagger$ whose components are given by $\psi^\dagger_j=a^{n+1}_j$. Following Green and Bracken,[6] the vector operator $\psi$ and its contragredient $\psi^\dagger$ may be resolved into a sum of shift vectors

$$\psi=\sum_{r=1}^{n}\psi[r],\quad \psi^\dagger=\sum_{r=1}^{n}\psi^\dagger[r]$$

which alter the U($n$) representation labels according to

$$\lambda_k\psi[r]=\psi[r](\lambda_k+\delta_{kr}),$$

$$\lambda_k\psi^\dagger[r]=\psi^\dagger[r](\lambda_k-\delta_{kr}).$$

Such shift vectors may be constructed by application of the U($n$) projectors $P[r]$ and $\bar{P}[r]$ as follows:

$$\psi[r]=P[r]\psi=\psi\bar{P}[r],$$

$$\psi^\dagger[r]=\bar{P}[r]\psi^\dagger=\psi^\dagger P[r].$$

Decomposing the U($n$) vector $\psi$ into its shift components allows us to write Eqs. (8) in the form

$$Q[k]^i_{n+1} = \sum_{r=1}^{n}\psi[r]^i(\beta_k-\alpha_r-1)^{-1}\,C_k,$$

$$Q[k]^{n+1}_i = \sum_{r=1}^{n}C_k(\beta_k-\alpha_r-1)^{-1}\,\psi^\dagger[r]_i. \tag{9}$$

However, from Eq. (5), we have

$$\sum_{k=1}^{n+1}Q[k]^i_{n+1}=\delta^i_{n+1}=0,\quad \text{for } i=1,\ldots,n.$$

Hence, summing Eqs. (9) over $k$ from 1 to $n+1$, we obtain

$$\sum_{r=1}^{n}\psi[r]\left(\sum_{k=1}^{n+1}(\beta_k-\alpha_r-1)^{-1}\,C_k\right)=0.$$

However, the shift vectors $\psi[r]$ form a linearly independent

set since they effect different shifts. This implies that

$$\sum_{k=1}^{n+1} (\beta_k - \alpha_r - 1)^{-1} C_k = 0, \quad r = 1,...,n. \tag{10}$$

This set of equations together with the condition

$$\sum_{k=1}^{n+1} C_k = 1 \left( \sum_{k=1}^{n+1} Q[k]_{n+1}^{n+1} = \delta_{n+1}^{n+1} \right)$$

uniquely determine the $C_k$. These equations are easily solved (using Cramer's rule for example) and yield the solution

$$C_k = \prod_{\substack{p=1 \\ \neq k}}^{n+1} (\beta_k - \beta_p)^{-1} \prod_{l=1}^{n} (\beta_k - \alpha_l - 1). \tag{11}$$

Similarly, using the adjoint projectors $\bar{Q}[k]$, one may deduce the equations

$$\begin{aligned} \bar{Q}[k]_{n+1}^{i} &= \sum_{r=1}^{n} \bar{C}_k (\beta_k - \alpha_r)^{-1} \psi[r]^i, \\ \bar{Q}[k]_i^{n+1} &= \sum_{r=1}^{n} \psi^\dagger[r]_i (\beta_k - \alpha_r)^{-1} \bar{C}_k, \end{aligned} \tag{12}$$

where $\bar{C}_k$ is shorthand notation for $\bar{Q}[k]_{n+1}^{n+1}$ which may be expressed in terms of the $\beta$'s and $\alpha$'s according to

$$\bar{C}_k = \prod_{\substack{p=1 \\ \neq k}}^{n+1} (\beta_k - \beta_p)^{-1} \prod_{l=1}^{n} (\beta_k - \alpha_l). \tag{13}$$

The U($n$) invariants $C_k$ and $\bar{C}_k$ are the $U(n+1)$ analogs of the operators $P[r]_n^n$ and $\bar{P}[r]_n^n$ which may likewise be expressed in terms of the roots in the U($n$) and U($n-1$) identities. This then enables us to evaluate the fundamental Wigner coefficients (4) as required. However, in order to determine the matrix elements of the group generators we must also determine the reduced matrix elements of $\psi$ and $\psi^\dagger$.

Since the matrix elements of the projectors $P[r]$ and $\bar{P}[r]$ are bilinear combinations of Wigner coefficients, the Wigner–Eckart theorem allows us to write

$$\begin{aligned} \psi[r]\psi^\dagger[r] &= \bar{M}_r P[r], \\ \psi^\dagger[r]\psi[r] &= M_r \bar{P}[r], \end{aligned} \tag{14}$$

where the $M_r$ ($\bar{M}_r$) are U($n$) invariants whose eigenvalues determine the squares of the reduced matrix elements of $\psi$ ($\psi^\dagger$). Equation (14) is clearly an operator generalization of the Wigner–Eckart theorem and may be derived using purely algebraic techniques as demonstrated in Ref. 7. By taking the traces of Eqs. (14) we obtain the result

$$\begin{aligned} \bar{M}_r &= \frac{\psi[r]^i \psi^\dagger[r]_i}{t_r(P[r])}, \\ M_r &= \frac{\psi^\dagger[r]_i \psi[r]^i}{t_r(\bar{P}[r])}, \end{aligned} \tag{15}$$

which enables the invariants $\bar{M}_r$ and $M_r$ to be expressed as a function of the $\beta_k$ and $\alpha_r$ using techniques similar to those used in the derivation of the $C_k$ and $\bar{C}_k$ (see Ref. 7 for further details). We obtain

$$\bar{M}_r = (-1)^n \prod_{p=1}^{n+1} (\beta_p - \alpha_r) \prod_{l \neq r} (\alpha_r - \alpha_l - 1)^{-1}, \tag{16}$$

$$M_r = (-1)^n \prod_{p=1}^{n+1} (\beta_p - \alpha_r - 1) \prod_{l \neq r} (\alpha_r - \alpha_l + 1)^{-1}. \tag{17}$$

One may check directly from Eq. (15) and the Wigner–Eckart theorem that the $\bar{M}_r$ and $M_r$ in fact determine the reduced matrix elements as required.

Taking the $(n,n)$ entries of Eqs. (14), we obtain

$$\begin{aligned} \psi[r]^n \psi^\dagger[r]_n &= \bar{M}_r P[r]_n^n, \\ \psi^\dagger[r]_n \psi[r]^n &= M_r \bar{P}[r]_n^n, \end{aligned} \tag{18}$$

which, using formulas (11), (13), (16), and (17), enables us immediately to write down the matrix elements of the generators $a_{n+1}^n$ and $a_n^{n+1}$. However, in order to obtain the matrix elements of the remaining generators we need more information. To this end we obtain a relationship between the U($n+1$) and U($n$) projection operators which, as we shall later see, reflects the properties of U($n+1$) : U($n$) reduced Wigner operators.

First of all it is easily seen, as a trivial property of Wigner coefficients and Eqs. (2) and (3), that the following relations holds:

$$\begin{aligned} Q[k]_{n+1}^{i} (C_k)^{-1} Q[k]_j^{n+1} &= Q[k]_j^i, \\ \bar{Q}[k]_i^{n+1} (\bar{C}_k)^{-1} \bar{Q}[k]_{n+1}^{j} &= \bar{Q}[k]_i^j. \end{aligned}$$

A proof of this result which exploits only the Lie algebra commutation relations is presented in Ref. 7 (see also Green[8]). By applying the U($n$) projectors $P[r]$ ($\bar{P}[r]$) to both sides of the above equations, we obtain, by virtue of Eqs. (9) and (12), the result

$$\begin{aligned} &\sum_{l,m=1}^{n} P[r]_l^i Q[k]_m^l P[r]_j^m \\ &\quad = \psi[r]^i C_k (\beta_k - \alpha_r - 1)^{-2} \psi^\dagger[r]_j. \end{aligned}$$

We now note, from the form of $C_k$ given by Eq. (11), that $C_k(\beta_k - \alpha_r - 1)^{-1}$ is independent of $\alpha_r$ and hence commutes with $\psi[r]$. We therefore obtain

$$\begin{aligned} &P[r]_l^i Q[k]_m^l P[r]_j^m \\ &\quad = C_k (\beta_k - \alpha_r - 1)^{-1} (\beta_k - \alpha_r)^{-1} \psi[r]^i \psi^\dagger[r]_j. \end{aligned}$$

Using Eqs. (14) this in turn may be written

$$\begin{aligned} &P[r]_l^i Q[k]_m^l P[r]_j^m \\ &\quad = C_k \bar{M}_r (\beta_k - \alpha_r - 1)^{-1} (\beta_k - \alpha_r)^{-1} P[r]_j^i. \end{aligned} \tag{19}$$

Similarly, we obtain

$$\begin{aligned} &\bar{P}[r]_i^l \bar{Q}[k]_l^m \bar{P}[r]_m^j \\ &\quad = \bar{C}_k M_r (\beta_k - \alpha_r - 1)^{-1} (\beta_k - \alpha_r)^{-1} \bar{P}[r]_i^j. \end{aligned} \tag{20}$$

As we shall see Eqs. (19) and (20) are essentially all we need to determine the matrix elements of the U($n$) generators.

## 3. SIMULTANEOUS SHIFTS

The Lie group U($n$) admits the canonical[9] chain of subgroups

$$U(n) \supset U(n-1) \supset \cdots \supset U(1), \tag{21}$$

where each group U($m$) occurring in this chain has infinites-

imal generators consisting of the U($n$) generators $a^i_j$ for values of $i$ and $j$ in the range 1,...,$m$. Before proceeding we establish some notation. We denote the U($m$) matrix whose $(i,j)$ entry is the U($m$) generator $a^i_j$ $(i,j=1,...,m)$ simply by $a_m$. We denote the characteristic roots of $a_m$ by $\alpha_{r,m}$ $(r=1,...,m)$. They take constant values on a finite dimensional irreducible representation of U($m$) with highest weight $(\lambda_{1m},...,\lambda_{mm})$ given by $\alpha_{r,m}=\lambda_{r,m}+m-r$. We denote the corresponding U($m$) projectors simply by $P\binom{m}{r}$ and $\bar{P}\binom{m}{r}$:

$$P\binom{m}{r}=\prod_{l\neq r}\left(\frac{a_m-\alpha_{l,m}}{\alpha_{r,m}-\alpha_{l,m}}\right),$$

$$\bar{P}\binom{m}{r}=\prod_{l\neq r}\left(\frac{\bar{a}_m-\bar{\alpha}_{l,m}}{\bar{\alpha}_{r,m}-\bar{\alpha}_{l,m}}\right),$$

where $\bar{a}_m$ is the U($m$) adjoint matrix whose roots $\bar{\alpha}_{l,m}$ are given by $\bar{\alpha}_{l,m}=m-1-\alpha_{l,m}$. We denote the $(m,m)$ entries of these projectors by $C_{r,m}$ and $\bar{C}_{r,m}$, respectively. From the previous section we know that these operators are essentially squares of Wigner coefficients whose eigenvalues are given by [cf. Eqs. (11) and (13)]

$$\begin{aligned}C_{r,m}&=\prod_{\substack{k=1\\ \neq r}}^{m}(\alpha_{r,m}-\alpha_{k,m})^{-1}\prod_{l=1}^{m-1}(\alpha_{r,m}-\alpha_{l,m-1}-1),\\ \bar{C}_{r,m}&=\prod_{\substack{k=1\\ \neq r}}^{m}(\alpha_{r,m}-\alpha_{k,m})^{-1}\prod_{l=1}^{m-1}(\alpha_{r,m}-\alpha_{l,m-1}).\end{aligned}\tag{22}$$

Finally we denote the U($m$) vector operator $\{a^i_{m+1}\}$ $(i=1,...,m)$ simply by $\psi(m)$. Its Hermitian conjugate $\psi^\dagger(m)$ constitutes a contragredient vector operator with components $\psi^\dagger(m)_i=a^{m+1}_i$. We denote the shift components of these operators by $\psi\binom{m}{r}$ and $\psi^\dagger\binom{m}{r}$, respectively. According to Eqs. (14) we may write

$$\begin{aligned}\psi\binom{m}{r}\psi^\dagger\binom{m}{r}&=\bar{M}_{r,m}P\binom{m}{r},\\ \psi^\dagger\binom{m}{r}\psi\binom{m}{r}&=M_{r,m}\bar{P}\binom{m}{r},\end{aligned}\tag{23}$$

where the U($m$) invariants $\bar{M}_{r,m}$ and $M_{r,m}$ (the squared reduced matrix elements) are given by

$$\begin{aligned}M_{r,m}&=(-1)^m\prod_{k=1}^{m+1}(\alpha_{k,m+1}-\alpha_{r,m}-1)\\ &\quad\times\prod_{l\neq r}(\alpha_{r,m}-\alpha_{l,m}+1)^{-1},\\ \bar{M}_{r,m}&=(-1)^m\prod_{k=1}^{m+1}(\alpha_{k,m+1}-\alpha_{r,m})\\ &\quad\times\prod_{l\neq r}(\alpha_{r,m}-\alpha_{l,m}-1)^{-1}.\end{aligned}\tag{24}$$

The $(m,m)$ entries of Eqs. (23) yield the relations

$$\begin{aligned}\psi\binom{m}{r}^m\psi^\dagger\binom{m}{r}_m&=\bar{M}_{r,m}C_{r,m},\\ \psi^\dagger\binom{m}{r}_m\psi\binom{m}{r}^m&=M_{r,m}\bar{C}_{r,m},\end{aligned}\tag{25}$$

which determines the matrix elements of the generators $a^m_{m+1}$ and $a^{m+1}_m$.

If U($m+1$) and U($m$) are two canonical subgroups of U($n$), we have already remarked that the operator $\psi(m)$ with components $\psi(m)^l=a^l_{m+1}$ constitutes a U($m$) vector operator. Hence, each operator $a^l_{m+1}$ may be written as a sum of shift components $\psi\binom{m}{r}$ which alter the representation labels of the group U($m$). However, if $k$ is a positive integer less than $m$, then the components $\psi(m)^i$ $(i=1,...,k)$ also constitute a vector operator with respect to the subgroup U($k$). Hence, any given operator of the form $a^l_{m+1}$ $(l<m+1)$ transforms as a component of a vector operator with respect to the subgroups U($m$), U($m-1$),...,U($l$).

In the limiting case when $l=m$ we see that $a^m_{m+1}$ can only be a component of a vector operator with respect to the subgroup U($m$). In this case $a^m_{m+1}$ can only alter the representation labels of the subgroup U($m$) and we may resolve $a^m_{m+1}$ into its U($m$) shift components according to

$$a^m_{m+1}=\sum_{r=1}^{m}\psi\binom{m}{r}^m.$$

Suppose now we consider a generator of the form $a^{m-1}_{m+1}$ which transforms as a component of a vector with respect to the subgroups U($m-1$) and U($m$). Firstly, $a^{m-1}_{m+1}$ must alter the representation labels of the subgroup U($m$) and we obtain a primary decomposition into U($m$) shift components

$$a^{m-1}_{m+1}=\sum_{r=1}^{m}\psi\binom{m}{r}^{m-1},$$

where

$$\psi\binom{m}{r}^i=P\binom{m}{r}^i_j a^j_{m+1}=a^j_{m+1}\bar{P}\binom{m}{r}^i_j.$$

Now each $\psi\binom{m}{r}^{m-1}$ is also a component of a vector operator with respect to U($m-1$). Hence, we may further decompose $\psi\binom{m}{r}^{m-1}$ into its U($m-1$) shift components according to

$$\psi\binom{m}{r}^{m-1}=\sum_{l=1}^{m-1}\psi\binom{m\quad m-1}{r\qquad l}^{m-1},$$

where

$$\begin{aligned}\psi\binom{m\quad m-1}{r\qquad l}^{m-1}&=P\binom{m-1}{l}^{m-1}_i\psi\binom{m}{r}^i\\ &=\psi\binom{m}{r}^i\bar{P}\binom{m-1}{l}^{m-1}_i.\end{aligned}$$

Hence, we obtain the resolution

$$a^{m-1}_{m+1}=\sum_{r=1}^{m}\sum_{l=1}^{m-1}\psi\binom{m\quad m-1}{r\qquad l}^{m-1},$$

where each component $\psi\binom{m\ m-1}{r\ l}$ simultaneously alters the representation labels of $U(m)$ and its subgroup $U(m-1)$ according to

$$\begin{aligned}\lambda_{k,m}\psi\binom{m\quad m-1}{r\qquad l}&=\psi\binom{m\quad m-1}{r\qquad l}(\lambda_{k,m}+\delta_{kr}),\\ \lambda_{k,m-1}\psi\binom{m\quad m-1}{r\qquad l}&=\psi\binom{m\quad m-1}{r\qquad l}(\lambda_{k,m-1}+\delta_{kl}).\end{aligned}$$

By our construction the shift components $\psi\binom{m\ m-1}{r\ l}$ are given by

$$\psi\begin{pmatrix} m & m-1 \\ r & l \end{pmatrix} = P\begin{pmatrix} m-1 & m \\ l & r \end{pmatrix}\psi(m)$$
$$= \psi(m)\bar{P}\begin{pmatrix} m & m-1 \\ r & l \end{pmatrix},$$

where $P\binom{m}{r}\binom{m-1}{l}$ may be interpreted as an $(m-1)\times m$ matrix of operators with entries

$$P\begin{pmatrix} m-1 & m \\ l & r \end{pmatrix}^i_j = \sum_{k=1}^{m-1} P\begin{pmatrix} m-1 \\ l \end{pmatrix}^i_k P\begin{pmatrix} m \\ r \end{pmatrix}^k_j,$$
$$i = 1,...,m-1, \quad j = 1,...,m.$$

Similarly, we define the operators $\bar{P}\binom{m}{r}\binom{m-1}{l}$.

More generally, an operator $a^l_{m+1}$ $(l < m+1)$ may be decomposed into a sum of shift components which simultaneously alter the representation labels of the subgroups $U(m)$, $U(m-1),...,U(l)$. We write this decomposition as

$$a^l_{m+1} = \sum_{i(\mathbf{k})} \psi\begin{pmatrix} m & m-1 & \cdots & l \\ i(m) & i(m-1) & \cdots & i(l) \end{pmatrix}^l, \tag{26}$$

where the summation symbol is shorthand notation for

$$\sum_{i(m)=1}^{m} \sum_{i(m-1)=1}^{m-1} \cdots \sum_{i(l)=1}^{l}.$$

Each shift component simultaneously alters the representation labels of the subgroups $U(m),...,U(l)$ according to

$$\lambda_{k,p}\psi\begin{pmatrix} m & m-1 & \cdots & l \\ i(m) & i(m-1) & \cdots & i(l) \end{pmatrix}$$
$$= \psi\begin{pmatrix} m & m-1 & \cdots & l \\ i(m) & i(m-1) & \cdots & i(l) \end{pmatrix}(\lambda_{k,p} + \delta_{k,i(p)}) \tag{27}$$

for $p = l,...,m$ and $k = 1,...,p$.

These shift components may be constructed by repeated application of the subgroup projectors as in the $a^{m-1}_{m+1}$ case. Let us denote the $l \times m$ matrix of operators with entries

$$\sum_{r=1}^{l} \cdots \sum_{q=1}^{m-2} \sum_{p=1}^{m-1} P\begin{pmatrix} l \\ i(l) \end{pmatrix}^i_r P\begin{pmatrix} l+1 \\ i(l+1) \end{pmatrix}^r_{\cdots} P\begin{pmatrix} m-1 \\ i(m-1) \end{pmatrix}^q_p$$
$$\times P\begin{pmatrix} m \\ i(m) \end{pmatrix}^p_j$$

simply by

$$P\begin{pmatrix} l & m-1 & m \\ i(l) & i(m-1) & i(m) \end{pmatrix}.$$

It is clear that these operators project out the simultaneous shift components of the generator $a^l_{m+1} = \psi(m)^l$ from the left:

$$\psi\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix} = P\begin{pmatrix} l & m \\ i(l) & i(m) \end{pmatrix}\psi(m). \tag{28}$$

Similarly, we define the projectors

$$\bar{P}\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix},$$

whose $(i,j)$ entry is given by

$$\sum_{p=1}^{m-1} \sum_{q=1}^{m-2} \cdots \sum_{r=1}^{l} \bar{P}\begin{pmatrix} m \\ i(m) \end{pmatrix}^p_i \bar{P}\begin{pmatrix} m-1 \\ i(m-1) \end{pmatrix}^q_p \cdots \bar{P}\begin{pmatrix} l \\ i(l) \end{pmatrix}^j_r$$

for $i = 1,...,m$ and $j = 1,...,l$. Clearly, these operators project out the simultaneous shift components of the generator $\psi(m)^l = a^l_{m+1}$ from the right:

$$\psi\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix} = \psi(m)\bar{P}\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix}. \tag{29}$$

In a similar way we define the operators

$$\bar{P}\begin{pmatrix} l & m-1 & m \\ i(l) & i(m-1) & i(m) \end{pmatrix}$$

and (30)

$$P\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix},$$

defined in the same way but with the order reversed.

By taking the Hermitian conjugate of Eqs. (26)–(29) we see that the generator $a^{m+1}_l$ $(l < m+1)$ may also be resolved into its simultaneous shift components according to

$$a^{m+1}_l = \sum_{i(\mathbf{k})} \psi^\dagger\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix}_l,$$

where each component

$$\psi^\dagger\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix}$$

may be constructed by aplying the projectors (30):

$$\psi^\dagger\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix}$$
$$= \bar{P}\begin{pmatrix} l & m-1 & m \\ i(l) & i(m-1) & i(m) \end{pmatrix}\psi^\dagger(m)$$
$$= \psi^\dagger(m)P\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix}.$$

We conclude this section by obtaining a generalization of Eqs. (23) for the multiple shift vectors

$$\psi\begin{pmatrix} m & m-1 & l \\ i(m) & i(m-1) & i(l) \end{pmatrix}.$$

We have

$$\psi^\dagger\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix}_l \psi\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix}^l$$
$$= \sum_{i,j=1}^{m} \bar{P}\begin{pmatrix} l & m \\ i(l) & i(m) \end{pmatrix}^i_l \psi^\dagger(m)_i \psi(m)^j \bar{P}\begin{pmatrix} m & l \\ i(m) & i(l) \end{pmatrix}^l_j$$
$$= \sum_{i,j=1}^{m-1} \bar{P}\begin{pmatrix} l & m-1 \\ i(l) & i(m-1) \end{pmatrix}^i_l \psi^\dagger\begin{pmatrix} m \\ i(m) \end{pmatrix}_i \psi\begin{pmatrix} m \\ i(m) \end{pmatrix}^j$$
$$\times \bar{P}\begin{pmatrix} m-1 & l \\ i(m-1) & i(l) \end{pmatrix}^l_j. \tag{31}$$

However, from Eqs. (23), we know that

$$\psi^\dagger\begin{pmatrix} m \\ i(m) \end{pmatrix}_i \psi\begin{pmatrix} m \\ i(m) \end{pmatrix}^j = M_{i(m),m}\bar{P}\begin{pmatrix} m \\ i(m) \end{pmatrix}^j_i$$

and it follows that Eq. (31) may be written

$$M_{i(m),m}\bar{P}\begin{pmatrix} l & m-1 \\ i(l) & i(m-1) \end{pmatrix}\bar{P}\begin{pmatrix} m \\ i(m) \end{pmatrix}\bar{P}\begin{pmatrix} m-1 & l \\ i(m-1) & i(l) \end{pmatrix}^l_l. \tag{32}$$

By repeated application of Eq. (20) this in turn may be written

$$\prod_{p=l+1}^{m} (\alpha_{i(p),p} - \alpha_{i(p-1),p-1} \quad -1)^{-1}(\alpha_{i(p),p} - \alpha_{i(p-1),p-1})^{-1}$$
$$\times \prod_{r=l}^{m} M_{i(r),r}\bar{C}_{i(r),r}. \tag{33}$$

Similarly we have

$$\psi\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l} \psi^{\dagger}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}_{l}$$
$$= \prod_{p=l+1}^{m} (\alpha_{i(p),p} - \alpha_{i(p-1),p-1} - 1)^{-1} \times (\alpha_{i(p),p} - \alpha_{i(p-1),p-1})^{-1} \prod_{r=l}^{m} \bar{M}_{i(r),r} C_{i(r),r}. \quad (34)$$

These are the required generalizations of Eqs. (25). They in fact determine the squares of the matrix elements of $a^{l}_{m+1}$ and $a^{m+1}_{l}$, respectively.

## 4. MATRIX ELEMENTS OF THE GROUP GENERATORS

Throughout this section we assume that we are working in a finite dimensional irreducible representation of U($n$) and we shall adopt the usual Gel'fand basis notation. Our aim is to evaluate the matrix elements of the generators $a^{l}_{m+1}$ and $a^{m+1}_{l}$ ($l \leqslant m$). The matrix of $a^{m+1}_{m+1}$ is of course diagonal with entries

$$\sum_{i=1}^{m+1} \lambda_{i,m+1} - \sum_{i=1}^{m} \lambda_{i,m}.$$

Suppressing the labels of U($m+2$), we may write an arbitrary Gel'fand pattern in the form

$$\left| \begin{matrix} \lambda_{i,m+1} \\ \lambda_{i,m} \\ \vdots \\ \lambda_{i,l-1} \\ (\nu) \end{matrix} \right\rangle,$$

where $(\nu)$ denotes a Gel'fand pattern for the subgroup U($l-2$). Let us fix this Gel'fand pattern and write it in the form $|\lambda_{j,k}\rangle$ for ease of notation. We begin by obtaining the matrix elements of the generators $a^{m}_{m+1}$ and $a^{m+1}_{m}$.

Resolving $a^{m}_{m+1}$ into its U($m$) shift components, we have

$$a^{m}_{m+1} |\lambda_{j,k}\rangle = \sum_{r=1}^{m} \psi\begin{pmatrix} m \\ r \end{pmatrix}^{m} |\lambda_{j,k}\rangle = \sum_{r=1}^{m} N^{m}_{r}[\lambda_{j,m+1}; \lambda_{j,m}; \lambda_{j,m-1}] \times |\lambda_{j,k} + \Delta_{r,m}\rangle,$$

where $|\lambda_{j,k} + \Delta_{r,m}\rangle$ is shorthand notation for the state obtained from $|\lambda_{j,k}\rangle$ by increasing the label $\lambda_{r,m}$ of the group U($m$) by one unit and leaving the remaining labels unchanged. The matrix elements $N^{m}_{r}$, in view of the Hermiticity property

$$\psi^{\dagger}\begin{pmatrix} m \\ r \end{pmatrix}_{m} = \left[\psi\begin{pmatrix} m \\ r \end{pmatrix}^{m}\right]^{\dagger}$$

and Eq. (25), are given by

$$N^{m}_{r}(\lambda_{j,m+1}; \lambda_{j,m}; \lambda_{j,m-1}) = \langle \lambda_{j,k} | M_{r,m} \bar{C}_{r,m} | \lambda_{j,k} \rangle^{1/2}. \quad (35)$$

(Strictly speaking, this matrix element is to be multiplied by a phase factor. However, it is customary to choose the phases of the matrix elements of $a^{m}_{m+1}$ to be real and positive. The question of phases shall be discussed more fully in the next section.) Substituting for $M_{r,m}$ and $\bar{C}_{r,m}$ using Eqs. (22) and (24) gives the result

$$N^{m}_{r} = \left( \frac{(-1)^{m} \prod_{p=1}^{m+1} (\lambda_{p,m+1} - \lambda_{r,m} + r - p) \prod_{l=1}^{m-1} (\lambda_{r,m} - \lambda_{l,m-1} + l - r + 1)}{\prod_{\substack{l=1 \\ \neq r}}^{m} (\lambda_{r,m} - \lambda_{l,m} + l - r)(\lambda_{r,m} - \lambda_{l,m} + l - r + 1)} \right)^{1/2}. \quad (36)$$

Similarly, the matrix elements of $a^{m+1}_{m}$ are

$$\bar{N}^{m}_{r}(\lambda_{j,m+1}; \lambda_{j,m}; \lambda_{j,m-1}) = \langle \lambda_{j,k} | \bar{M}_{r,m} C_{r,m} | \lambda_{j,k} \rangle^{1/2} = \left( \frac{(-1)^{m} \prod_{p=1}^{m+1} (\lambda_{p,m+1} - \lambda_{r,m} + r - p + 1) \prod_{l=1}^{m-1} (\lambda_{r,m} - \lambda_{l,m-1} + l - r)}{\prod_{\substack{l=1 \\ \neq r}}^{m} (\lambda_{r,m} - \lambda_{l,m} + l - r)(\lambda_{r,m} - \lambda_{l,m} + l - r - 1)} \right)^{1/2}. \quad (37)$$

The method for calculating the matrix elements of $a^{l}_{m+1}$ and $a^{m+1}_{l}$ is similar and, in view of Eqs. (33) and (34), no more difficult. Resolving $a^{l}_{m+1}$ ($l \leqslant m$) into its simultaneous shift components, we have

$$a^{l}_{m+1} |\lambda_{j,k}\rangle = \sum_{i(k)} \psi\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l} |\lambda_{j,k}\rangle = \sum_{i(k)} N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix} \times |\lambda_{j,k} + \Delta_{i(m),m} + \cdots + \Delta_{i(l),l}\rangle,$$

where $|\lambda_{j,k} + \Delta_{i(m),m} + \cdots + \Delta_{i(l),l}\rangle$ denotes the state obtained from $|\lambda_{j,k}\rangle$ by increasing the representation label $\lambda_{i(r),r}$ of the subgroup $U(r)$, $r = l,\ldots,m$, by one unit and leaving the other labels unchanged. In this case the matrix elements

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

are given by

$$\pm \langle \lambda_{j,k} | \psi^{\dagger}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}_{l} \psi\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l} |\lambda_{j,k}\rangle^{1/2},$$

which, by virtue of Eqs. (33) and (35), equals

$$\pm \prod_{r=l}^{m} N^{r}_{i(r)} \prod_{r=l+1}^{m} [(\lambda_{i(r),r} - \lambda_{i(r-1),r-1} + i(r-1) - i(r))^{-1} \times (\lambda_{i(r),r} - \lambda_{i(r-1),r-1} + i(r-1) - i(r) + 1)^{-1}]^{1/2}, \quad (38)$$

where $N^{r}_{i(r)}$ are the matrix elements of the generator $a^{r}_{r+1}$ which are given by Eq. (36). The undetermined phase ($\pm$) will be obtained in the next section.

Clearly,

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

corresponds to the matrix element

$$\left\langle \begin{matrix} \lambda_{j,m+1} \\ (\lambda') \end{matrix} \middle| a^{l}_{m+1} \middle| \begin{matrix} \lambda_{j,m+1} \\ (\lambda) \end{matrix} \right\rangle,$$

where $(\lambda') = (\lambda)$ except for $\lambda'_{i(r),r} = \lambda_{i(r),r} + 1$, $r = l,\ldots,m$.

Similarly, the matrix elements

$$\bar{N}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

of the generator $a^{m+1}_{l}$ $(l < m+1)$ are given by

$$\pm \left\langle \lambda_{j,k} \middle| \psi\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l} \psi^{\dagger}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}_{l} \middle| \lambda_{j,k} \right\rangle^{1/2},$$

which, in view of Eq. (34), equals

$$\pm \prod_{r=l}^{m} \bar{N}^{r}_{i(r)} \prod_{r=l+1}^{m} [(\lambda_{i(r),r} - \lambda_{i(r-1),r-1} + i(r-1) - i(r) + 1)^{-1} (\lambda_{i(r),r} - \lambda_{i(r-1),r-1} + i(r-1) - i(r))^{-1}]^{1/2},$$

where $\bar{N}^{r}_{i(r)}$ are the matrix elements of the generator $a^{r+1}_{r}$ which are given by Eq. (37).

## 5. CHOICE OF PHASES

In obtaining the matrix elements of the U($n$) generators there is a degree of freedom in that the phases of the generators $a^{m}_{m+1}$ may be chosen arbitrarily. Following Baird and Biedenharn,[3] we have chosen these phases to be positive [which agrees with the Condon–Shortley convention for SU(2)]. By Hermiticity it follows that the phases of the generators $a^{m+1}_{m}$ are also positive. The phases of the remaining generators are then dictated by the Lie algebra commutation relations. It follows from these considerations that the general matrix element

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

has phase[3]

$$S(i(m-1) - i(m))S(i(m-2) - i(m-1))\cdots S(i(l) - i(l+1)),$$

where $S(x)$ is the sign of $x$ and $S(0) = 1$.

It is interesting to note that the choice of phases may be obtained algebraically using the U($n$) characteristic identities as demonstrated in Baird and Biedenharn.[4]

## 6. ANALYSIS OF RESULTS

We have shown that the only nonvanishing matrix elements of the generator $a^{l}_{m+1}$ are of the form [suppressing the labels of the subgroup U($m+1$)]

$$\left\langle \begin{matrix} \lambda' \\ (\mu') \end{matrix} \middle| a^{l}_{m+1} \middle| \begin{matrix} \lambda \\ (\mu) \end{matrix} \right\rangle, \tag{39}$$

where $\lambda'$ is of the form $\lambda' = \lambda + \Delta_{i(m)}$, where $\Delta_{i(m)}$ is the U($m$) weight with 1 in position $i(m)$ and zero elsewhere. Also, since $a^{l}_{m+1}$ is a vector with respect to the subgroups U($l$),...,U($m-1$), we see that the only allowed patterns $(\mu')$ are of the form $(\mu') = (\mu)$ except $\mu'_{i(r),r} = \mu_{i(r),r} + 1$ for $r = l,\ldots,m-1$ and some $i(r)$ in the range $1,\ldots,r$. The matrix element in this case is

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

and is given by Eq. (38). On the other hand, using the Wigner–Eckart theorem, this matrix element may also be written

$$\langle \lambda + \Delta_{i(m)} \| \psi(m) \| \lambda \rangle \left\langle \begin{matrix} \lambda \\ (\mu) \end{matrix}; \begin{matrix} 1\dot{0} \\ l \end{matrix} \middle| \begin{matrix} \lambda + \Delta_{i(m)} \\ (\mu') \end{matrix} \right\rangle, \tag{40}$$

where the first term is the U($m$) reduced matrix element $(M_{i(m),m})^{1/2}$.

In the notation of Baird and Biedenharn[3] let us denote the U($l$) Wigner coefficients $(\bar{C}_{i(l),l})^{1/2}$ by $\binom{i(l):l}{l-1}$, the reduced matrix element $(M_{i(r),r})^{1/2}$ by $\binom{r+1}{i(r):r}$, and the corresponding "reduced Wigner coefficients" by $\binom{i(r):r}{i(r-1):r-1}$. Then the matrix element

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}$$

may be written in terms of reduced matrix elements, Wigner coefficients, and reduced Wigner coefficients according to[3]

$$N\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix} = \binom{m+1}{i(m):m} \prod_{r=l+1}^{m} \binom{i(r):r}{i(r-1):r-1} \binom{i(l):l}{l-1}.$$

It is interesting to note that by taking the trace of Eq. (20) we obtain the result

$$t_r\left(\bar{P}\begin{pmatrix} m & m+1 & m \\ r & k & r \end{pmatrix}\right) = \bar{C}_{k,m+1} M_{r,m} \bar{C}_{r,m} (\alpha_{k,m+1} - \alpha_{r,m} - 1)^{-1} \times (\alpha_{k,m+1} - \alpha_{r,m})^{-1}.$$

In terms of reduced Wigner coefficients this relation may be written in the form

$$t_r\left(\bar{P}\begin{pmatrix} m & m+1 & m \\ r & k & r \end{pmatrix}\right) = \binom{k:m+1}{r:m}^{2} t_r\left(\bar{P}\begin{pmatrix} m \\ r \end{pmatrix}\right),$$

which shows that the reduced Wigner coefficients are determined solely by the subgroup projectors.

Finally, from Eq. (32) we may write the matrix element (39) in the form

$$\left\langle \begin{matrix} \lambda \\ (\mu) \end{matrix} \middle| M_{i(m),m} \bar{P}\begin{pmatrix} l & \cdots & m \\ i(l) & \cdots & i(m) \end{pmatrix} \bar{P}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l}_{l} \middle| \begin{matrix} \lambda \\ (\mu) \end{matrix} \right\rangle^{1/2}.$$

Comparing this with the Wigner–Eckart factorization (40), we see that the general Wigner coefficient is given by

$$\left\langle \begin{matrix} \lambda \\ (\mu) \end{matrix} \middle| \bar{P}\begin{pmatrix} l & \cdots & m \\ i(l) & \cdots & i(m) \end{pmatrix} \bar{P}\begin{pmatrix} m & \cdots & l \\ i(m) & \cdots & i(l) \end{pmatrix}^{l}_{l} \middle| \begin{matrix} \lambda \\ (\mu) \end{matrix} \right\rangle = \left| \left\langle \begin{matrix} \lambda \\ (\mu) \end{matrix}; \begin{matrix} 1\dot{0} \\ l \end{matrix} \middle| \begin{matrix} \lambda + \Delta_{i(m)} \\ (\mu') \end{matrix} \right\rangle \right|^{2}. \tag{41}$$

This is clearly a generalization of Eq. (4) in Sec. 2.

## 7. CONCLUSION

Equation (41) shows that the general fundamental Wigner coefficients may be obtained solely from a knowledge of the subgroup projection operators. This form for the Wigner coefficients is useful and clearly may be generalized to arbitrary (multiplicity free) Wigner coefficients corresponding to the reduction of $V(\lambda) \otimes V(\mu)$, where $V(\lambda)$ is one

of the tensor representations. One simply applies the U($n$) projectors corresponding to the U($n$) tensor identity with reference representation $V(\lambda)$ (see Ref. 1 for further details) and the canonical subgroup tensor projectors with reference representation given by the decomposition of $V(\lambda)$ into irreducible representations of its subgroups. By this means we may give a general expression for the U($n$) Wigner operators of Biedenharn *et al.* as a polynomial in the group generators. This procedure is probably best described in the context of the pattern calculus and will be discussed more fully in a later publication.

Finally, we note that we have given an expression for the general matrix element (and the corresponding Wigner coefficients) as a polynomial in the group generators. This enables us to discuss "generalized matrix elements" without explicit reference to a basis state. It is therefore suggestive that this approach may be useful for obtaining generalized matrix elements for groups whose basis states are not known. In particular, it is hoped that useful information concerning the symplectic groups may be obtained by this method.


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# Reduction technique for matrix nonlinear evolution equations solvable by the spectral transform

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The main purpose of this paper is to describe a technique of reduction, whereby from the class of evolution equations for matrices of order $N$ solvable via the spectral transform associated to the (matrix) linear Schrödinger eigenvalue problem, one derives subclasses of nonlinear evolution equations involving less than $N^2$ fields. To illustrate the method, from the equations for matrices of order 2 two subclasses of equations for 2 fields (rather than 4) are obtained. The first class coincides, or rather includes, that solvable via the spectral transform associated to the generalized Zakharov–Shabat spectral problem; further reduction to nonlinear evolution equations for a single field reproduces a number of well-known equations, but also yields a novel one (highly nonlinear). The second class also yields highly nonlinear equations; some examples are given, including another novel evolution equation for a single field.

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## 1. INTRODUCTION

Recently we have introduced and discussed a class of matrix nonlinear evolution equations that can be solved via the spectral transform associated with the matrix Schrödinger spectral (or "scattering") problem.[1] These equations involve generally $N^2$ fields (here and below $N$ is the order of the matrices under consideration); but this number can be reduced by identifying equations (or rather classes of equations) that are satisfied by matrices having some special structure. For instance the requirement that a matrix of order $N$ be Hermitian halves the number of independent fields (from $N^2$ complex fields to $N^2$ real fields); the requirement that it be symmetrical reduces the number of independent fields to $\frac{1}{2}N(N+1)$; and so on. Such reductions are, however, rather trivial, and the corresponding restrictions on the class of evolution equations, that are required to guarantee compatibility with the time evolution, are easily established.[1] But other reductions are also possible, that decrease the number of independent fields by inducing nontrivial relations between different matrix elements that are compatible with the time evolution (for appropriately restricted classes of equations). The main purpose of the present paper is to introduce a technique to identify such reductions. The method is then illustrated by applying it to the case of matrices of order 2, thereby obtaining, from the general class of equations involving 4 independent fields, sublcasses of equations involving only two fields, or just a single one. One such class coincides with (or rather includes, since there is one added element of generality) that solvable via the spectral transform associated to the generalized Zakharov-Shabat spectral problem[2]; a result that has been obtained independently by Jaulent and Leon.[3]

For matrices of order 4, the simpler equation of the class solvable via the Schrödinger spectral transform has been analyzed by Bruschi, Levi, and Ragnisco.[4] This equation involves of course 16 fields; reduced versions involving respectively 10, 8, 6, 5, or 4 fields have also been obtained, by identifying the cases in which some of the 16 fields, if vanishing at the initial time, continue to vanish for all time.[4] Thus these reductions are rather simple; although the equations obtained in this manner are certainly far from trivial. All these reductions can be treated by the technique described in this paper, but this technique is actually richer. We plan to present the results obtained by its application to matrices of order 3 and 4 in separate papers.

The plan of this paper, and an outline of its content, can be evinced from the titles of the following sections and subsections. Here we merely report two novel, highly nonlinear evolution equations involving a single field, whose solvability is demonstrated below. The first reads

$$u_t = u_{xxx} - 6u_x\{u^2 - (u + u_{xx} - 2u^3)^2/[a^2 - 4(u^2 + u_x^2 - u^4)]\}; \tag{1.1}$$

$u \equiv u(x,t)$, $u(+\infty,t) = 0$, $u(-\infty,t) = 0$ if $a^2 \neq 1$,

$u(-\infty,t) =$ arbitrary constant if $a^2 = 1$.

The second reads

$$v_t = v_{xxx} - \tfrac{1}{8}v_x^3 + v_x[A\exp(v) + B\exp(-v) + C];$$

$v \equiv v(x,t)$, $v(+\infty,t) = 0$, $v(-\infty,t) = 0$

or

$$v(-\infty,t) = \ln(B/A). \tag{1.2}$$

## 2. PRELIMINARIES AND NOTATION

The class of matrix nonlinear evolution equations solvable via the spectral transform associated with the matrix Schrödinger spectral problem reads[1]

$$Q_t = \alpha_m(\underline{L})[\sigma_m, Q] + \beta_\mu(\underline{L})\underline{G}\sigma_\mu . \tag{2.1}$$

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Here and below $Q \equiv Q(x,t)$ is a matrix of order $N$ vanishing (sufficiently fast[1]) asymptotically,

$$Q(\pm\infty,t) = 0. \tag{2.2}$$

Latin subscripts run from 1 to $N^2-1$, Greek subscripts from 0 to $N^2-1$ and repeated subscripts are summed upon. The $N^2$ matrices $\sigma_\mu$ provide a basis for matrices of order $N$, with $\sigma_0 = \mathbf{1}$; the $2N^2-1$ functions $\alpha_m(z)$ and $\beta_\mu(z)$ are ratios of entire functions (in all interesting cases, they are in fact rational functions; in most interesting cases, they are just polynomials of low degree); except for these restrictions, these functions are arbitrary, and it is their choice that characterizes each particular evolution equation of the class (2.1). The possibility to solve the Cauchy problem for (2.1) via the spectral transform technique is maintained even if the functions $\alpha_m$ and $\beta_\mu$ depend explicitly on the time variable $t$; but we assume, for the sake of simplicity, that they are time independent. Then the evolution Eq. (2.1) is invariant under time translations; the (Cauchy) problem we shall always have in mind is the determination of $Q(x,t)$ for $t>0$ given by

$$Q(x,0) = \bar{Q}(x) \tag{2.3}$$

(of course with $\bar{Q}(\pm\infty) = 0$). Finally the integro-differential operators $\underline{L}$ and $\underline{G}$ are defined by the following formulas that detail their action on the generic matrix $F(x)$:

$$\underline{L}F(x) = F_{xx}(x) - 2\{Q(x,t),F(x)\} + \underline{G}\int_x^\infty dx'\,F(x'), \tag{2.4}$$

$$\underline{G}F(x) = \{Q_x(x,t),F(x)\} + \left[Q(x,t),\int_x^\infty dx'\,[Q(x',t),F(x')]\right]. \tag{2.5}$$

Here of course, as well as above and below, subscripted variables denote partial differentiation, and the square and curly brackets with a comma inside indicate as usual commutators and anticommutators:

$$[A,B] = AB - BA, \quad \{A,B\} = AB + BA. \tag{2.6}$$

The solvability via spectral transform of (2.1) hinges essentially on the fact that the corresponding evolution equation for the reflection coefficient $R(k,t)$ is linear[1]:

$$R_t(k,t) = [A(-4k^2),R(k,t)] + 2ik\{B(-4k^2),R(k,t)\}; \tag{2.7}$$

here and always below

$$A(z) \equiv \alpha_m(z)\sigma_m, \quad B(z) \equiv \beta_\mu(z)\sigma_\mu\,. \tag{2.8}$$

In fact, to solve completely the Cauchy problem via the spectral transform, the time evolution of the appropriate parameters corresponding to the discrete part of the spectrum (if any) must also be given[1]; but we assume for simplicity that these results can all be extracted by analytic continuation in $k$ of $R$ to the poles on the upper imaginary axis[1]; so that in the following we limit our analysis to the time evolution of $R$. This simplifies considerably our presentation; of course the results are then, strictly speaking, established only for Hermitian matrices $Q$ vanishing asymptotically faster than exponentially; but they clearly have a more general validity, as can be easily demonstrated by looking directly also at the time evolution of the part of the spectral transform associated to discrete eigenvalues.[1]

The basic tool of our treatment obtains from the Wronskian-type formulas[1]

$$2ik\,[F(-4k^2),R(k)] = \int_{-\infty}^{+\infty} dx\bar{\Psi}(x,k)\{f_m(\underline{L})[\sigma_m,Q(x)]\}\Psi(x,k), \tag{2.9a}$$

$$(2ik)^2\{H(-4k^2),R(k)\} = \int_{-\infty}^{+\infty} dx\bar{\Psi}(x,k)\{h_\mu(\underline{L})\underline{G}\sigma_\mu\}\Psi(x,k). \tag{2.9b}$$

Here and below, $f_m(z)$ and $h_\mu(z)$ are arbitrary entire functions (in fact, in all applications below, low-order polynomials);

$$F(z) \equiv f_m(z)\sigma_m, \quad H(z) \equiv h_\mu(z)\sigma_\mu\,; \tag{2.10}$$

$\bar{\Psi}$ and $\Psi$ are appropriate matrix solutions of the Schrödinger equation characterizing the spectral problem[1]; while the remaining symbols have already been defined. We have not indicated explicitly, in these equations, the time dependence (of $R$, $Q$, $\bar{\Psi}$, and $\Psi$); indeed these equations are merely a consequence of the spectral problem, having nothing to do with the time evolution. But they remain of course valid if $Q$, and therefore also $R$, $\bar{\Psi}$ and $\Psi$, depend on time (such dependence is indeed, from the spectral point of view, purely parametric).

## 3. REDUCTION TECHNIQUE

The task here is to identify matrices $Q$ having a special structure that is maintained as they evolve in time according to (2.1), or rather according to some appropriate subclass of (2.1). The essential requirement characterizing such a special structure is that it induce, at any given time, relations between the different matrix elements of $Q$, so as to reduce the number of these that can be assigned independently (as functions of $x$, for any given $t$ and in particular for $t=0$); *these relations need not be algebraic, but can in fact be integro-differential* (see below).

Since the time evolution (2.1) of $Q$ is complicated, while the corresponding time evolution (2.7) of $R$ is simple [indeed this simplicity constitutes the foundation of the spectral transform technique to solve (2.1)], it is clearly easier to find matrices $R$ that have a special structure compatible with the time evolution. On the other hand, since there is a one-to-one correspondence between $R$ and $Q$ (up to the discrete spectrum part of the spectral transform, that, as explained above, is ignored in this analysis), clearly to any reduction in the number of independent elements of $R$ (each being a function of $k$) there corresponds an analogous reduction in the number of independent elements of $Q$ (each being a function of $x$).

Thus the main question is to translate a special structure of $R$ into the corresponding special structure of $Q$; or rather, to identify those special structures of $R$ that make such a translation easy (namely, to identify those restrictions on $R$ such that the corresponding restrictions on $Q$ are easily ascertained). A convenient tool to achieve this goal was reported at the end of Sec. 2, for the results (2.9) imply that, if the matrix $Q(x,t)$ satisfies the (nonlinear integro-differential) equation

$$f_m(\underline{L})[\sigma_m,Q] + h_\mu(\underline{L})\underline{G}\sigma_\mu = 0, \tag{3.1}$$

the corresponding matrix $R(k,t)$ satisfies the linear equation

$$[F(-4k^2),R] + 2ik\{H(-4k^2),R\} = 0, \tag{3.2}$$

where the matrices $F$ and $H$ are of course defined by (2.10). Note that in these equations the $2N^2-1$ functions $f_m(z)$ and $h_\mu(z)$ are arbitrary (they must be entire; in all practical applications they will be low-order polynomials).

The matrix equation (3.2) yields of course, for given $F$ and $H$, $N^2$ homogeneous linear equations for the $N^2$ elements of $R$; thus, for a generic choice of $F$ and $H$, it is compatible only with the trivial solution $R=0$. But for appropriate choices of $F$ and $H$, the restriction (3.2) merely implies a reduction in the number of independent elements of $R$; and the corresponding relation for $Q$ is then explicitly given by (3.1). Note that this last equation is generally integro-differential and nonlinear [see (2.4) and (2.5)]; however, if the functions $f_m(z)$ and $h_\mu(z)$ are polynomials of very low order (zero, or perhaps one) (3.1) can be explicitly solved; namely the relations between the different matrix elements of $Q$ implied by (3.1) can be rewritten as explicit expressions of some elements in terms of the others (see below).

Of course this process of reduction can be applied more than once, namely it can be required that $R$ satisfy $n$ equations of type (3.2) (with $F(z)=F^{(j)}(z)$, $H(z)=H^{(j)}(z)$, $j=1,2,\ldots,n$), the corresponding $Q$ being then constrained by the $n$ corresponding equations of type (3.1).

Thus, this technique provides the possibility to translate appropriate types of constraint on $R(k)$ into the corresponding constraints on $Q(x)$, and vice versa. Let us emphasize that one is displaying here certain properties of the spectral transform, that have *a priori* nothing to do with the time evolution, and which may indeed also have applications just in the context of the spectral (or "scattering") problem. But of course if $Q$, and therefore $R$, evolve in time, the question of compatibility of any condition imposed on these matrices arises: if at the initial time $Q$ resp. $R$ satisfy a certain restriction of type (3.1) resp. (3.2), shall they satisfy it for all subsequent time? We identify below subclasses of the evolution Eq. (2.1) for which this is the case; clearly each evolution equation of these subclasses may be considered to describe the evolution of $M$ fields, with $M<N^2$ (the precise value of $M$ in each case depending on the specific case under consideration, see, for instance, the examples discussed below).

As we have already mentioned, rather than discussing the compatibility of a restriction of type (3.1) with the time evolution (2.1) of $Q$ it is convenient to consider the compatibility of the corresponding restriction of type (3.2) with the time evolution (2.7) of $R$; the correspondence between $R$ and $Q$ being then a guarantee that one kind of compatibility implies the other.

Let us thus define

$$Z(k,t) = [F(-4k^2),R(k,t)] + 2ik\{H(-4k^2),R(k,t)\}, \tag{3.3}$$

in order to ascertain when $Z(k,t)=0$ is compatible with (2.7). Differentiating with respect to $t$ and using (2.7) one easily obtains

$$Z_t(k,t) = [A(-4k^2),Z(k,t)] + 2ik\{B(-4k^2),Z(k,t)\} + C(k,t) \tag{3.4}$$

with

$$C(k,t) \equiv [R(k,t),([A(-4k^2),F(-4k^2)] - 4k^2[B(-4k^2),H(-4k^2)])] - 2ik\{R(k,t),([B(-4k^2),F(-4k^2)] + [A(-4k^2),H(-4k^2)])\}. \tag{3.5}$$

Thus $Z(k,0)=0$ implies $Z(k,t)=0$ for $t>0$ provided

$$C(k,t)=0; \tag{3.6}$$

this last equation is therefore the compatibility condition.

Note that $C$, as defined by (3.5), depends on the matrices $F$ and $H$, that characterize the restrictive condition (3.2), and on the matrices $A$ and $B$, that characterize the evolution equation (2.7); it depends moreover on $R$ itself, that is of course *a priori* unknown except for the requirement that it satisfy the restriction (3.2). Thus (3.6) is required to hold for any $R$ compatible with (3.2). Of course (3.6) is required to hold for all values of $k$.

There is always at least one evolution equation of the class (2.1) for which the compatibility condition holds, namely the "scalar" case corresponding to

$$\alpha_m(z)=\beta_m(z)=0, \tag{3.7a}$$

or equivalently

$$A=0, \quad B=\beta_0(-4k^2)\mathbb{1}. \tag{3.7b}$$

Examples in which the reduction process is compatible with a larger subclass of (2.1) than this are given below.

If the compatibility condition (3.6) is satisfied, a matrix $Q$, that has been reduced by the condition (3.1) to have only $M<N^2$ independent elements (each being a function of $x$, for given $t$), may be required to evolve in time according to (2.1). Then this matrix evolution equation, although corresponding formally to $N^2$ scalar equations, yields in fact only $M$ coupled evolution equations, the remaining $N^2-M$ being automatically satisfied. Thus one is finally left with a system of M coupled evolution equations for $M$ fields; these may be assigned (as functions of $x$, for $-\infty<x<\infty$) at any given time (and in particular at the initial time $t=0$), their values at all subsequent times being then determined by the requirement that they obey the system of evolution equations.

In conclusion, the process of reduction can be summarized as follows: (i) choose the matrices $F(z)$ and $H(z)$; (ii) ascertain the constraint they imply on $R$ through (3.2); (iii) ascertain the constraint implied on $A(z)$ and $B(z)$ by the requirement that (3.6) hold for any $R$ compatible with (3.2), as determined in step (ii) [of course with the same $F(z)$ and $H(z)$ in (3.6) as in (3.2)]. All these steps are algebraic, and they determine the class of reduced evolution equations. The corresponding structure for the matrix $Q$ is determined by (3.1); this last step need not be purely algebraic. This process of reduction may be performed more than once, with different (judicious!) choices of $F$ and $H$.

## 4. APPLICATION TO MATRICES OF ORDER 2

In this section the analysis is restricted to matrices of

order 2, in which case the natural choice for the basic matrices $\sigma_\mu$ identifies them with the standard Pauli matrices:

$$\sigma_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},$$
$$\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix};\qquad (4.1)$$
$$\{\sigma_m,\sigma_n\}=2\delta_{mn},\quad [\sigma_m,\sigma_n]=2i\epsilon_{mnl}\sigma_l\ .$$

Here of course $\delta_{mn}$ is the (symmetrical) Kronecker symbol ($\delta_{mn}=1$ if $m=n$, $\delta_{mn}=0$ if $m\neq n$) and $\epsilon_{mnl}$ is the (completely antisymmetrical) Ricci symbol ($\epsilon_{123}=1$). It will be convenient to represent also the matrices $Q(x,t)$ and $R(k,t)$ in this basis, writing

$$Q\equiv Q_\mu\sigma_\mu=Q_0+Q_m\sigma_m,\quad R\equiv R_\mu\sigma_\mu=R_0+R_m\sigma_m\ . \qquad (4.2)$$

Thus our task here is (i) to analyze the constraint condition (3.2) [for various possible choices of the matrices $F(z)$ and $H(z)$] and to investigate how it reduces the number of independent components of $R$; (ii) to identify, using the condition (3.6), the subclass of the nonlinear evolution equations (2.1) that are compatible with the constraint; (iii) to extract from the corresponding constraint (3.1) relations determining some of the elements of $Q$ in terms of the others, or equivalently some of the components $Q_\mu$ in terms of the remaining ones; (iv) to write explicitly the novel class of nonlinear evolution equations for the reduced number of fields, introducing at this stage if need be an appropriate notation (to make contact with known results) and discussing some specific examples.

We note first of all that, as can be easily shown, there is no choice of the matrices $F$ and $H$ in (3.2) that reduces the number of independent components of $R$ from 4 to 3. There exist instead several possibilities to reduce the independent components to 2; and then the reduction process can be applied once more (sometimes rather trivially, sometimes nontrivially; see below) to reduce to one field only. The more interesting instances are discussed in Sec. 4.1–4.4.

### 4.1 Simple example: The class of nonlinear evolution equations solvable via the generalized Zakharov–Shabat spectral problem as a subcase of the class of nonlinear evolution equations solvable via the matrix Schrödinger spectral problem

Set

$$F(z)=0,\quad H(z)=\sigma_3, \qquad (4.1.1)$$

in (3.2). There immediately follows

$$R(k,t)=R_1(k,t)\sigma_1+R_2(k,t)\sigma_2,\quad (R_0(k,t)=R_3(k,t)=0). \qquad (4.1.2)$$

It is also easy to obtain the corresponding relations for $Q(x,t)$ that obtain inserting (4.1.1) in (3.1):

$$Q(x,t)=Q_0(x,t)+Q_1(x,t)\sigma_1+Q_2(x,t)\sigma_2,\quad (Q_3(x,t)=0), \qquad (4.1.3)$$

$$Q_0(x,t)=\left[\int_x^\infty dx'\,Q_1(x',t)\right]^2+\left[\int_x^\infty dx'\,Q_2(x',t)\right]^2. \qquad (4.1.4)$$

To obtain the last equation, we have used the boundary condition $Q_0(+\infty,t)=0$; the condition $Q_0(-\infty,t)=0$ implies a constraint on $Q_1$ and $Q_2$ (see below).

We consider next the compatibility condition (3.6), and using (4.1.2) it is easily seen that it implies

$$A(z)=\alpha_3(z)\sigma_3,\quad (\alpha_1(z)=\alpha_2(z)=0), \qquad (4.1.5a)$$
$$B(z)=\beta_0(z),\quad (\beta_1(z)=\beta_2(z)=\beta_3(z)=0). \qquad (4.1.5b)$$

[Actually the compatibility condition does not constrain $\beta_3$, but the validity of (3.2) with (4.1.1) implies that the $\beta_3$ term does not contribute in the nonlinear evolution equation (2.1); thus by setting $\beta_3=0$ no generality is lost.]

Thus the subclass of nonlinear evolution equations for the two fields $Q_1$ and $Q_2$ reads

$$Q_t(x,t)=2\beta_0(\underline{L})Q_x(x,t)+\alpha_3(\underline{L})[\sigma_3,Q(x,t)], \qquad (4.1.6)$$

where of course $\underline{L}$ is defined by (2.4) and $Q$ is expressed in terms of $Q_1$ and $Q_2$ by (4.1.3) and (4.1.4). The corresponding equation for the reflection coefficient $R(k,t)$ reads of course

$$R_t(k,t)=4ik\beta_0(-4k^2)R(k,t)+\alpha_3(-4k^2)[\sigma_3,R(k,t)]. \qquad (4.1.7)$$

To show the complete correspondence of these equations to those solvable via the generalized Zakharov–Shabat spectral problem (Ref. 2) we introduce the matrix

$$V(x,t)=\begin{pmatrix}0&q(x,t)\\r(x,t)&0\end{pmatrix}=\sigma_1q_1(x,t)+i\sigma_2q_2(x,t), \qquad (4.1.8)$$

so that

$$q=q_1+q_2,\quad r=q_1-q_2;\quad q_1=\tfrac{1}{2}(q+r),\quad q_2=\tfrac{1}{2}(q-r), \qquad (4.1.9)$$

and we relate it to $Q(x,t)$ via the formula

$$Q=V_x+V^2=\begin{pmatrix}qr&q_x\\r_x&qr\end{pmatrix}, \qquad (4.1.10)$$

so that

$$\int_x^\infty dx'\,Q_1(x',t)=-q_1(x,t),$$
$$\int_x^\infty dx'\,Q_2(x',t)=-iq_2(x,t),$$
$$Q_1=q_{1x},\quad Q_2=iq_{2x}\ . \qquad (4.1.11)$$

This last formula provides some motivation for introducing the "matrix Miura transformation"[5] (4.1.10). The corresponding formula for $R$ reads

$$R(k,t)=\begin{pmatrix}0&\alpha^{(-)}(-k,t)\\\alpha^{(+)}(k,t)&0\end{pmatrix}. \qquad (4.1.12)$$

With these notations (4.1.6) and (4.1.7) become

$$\sigma_3v_t(x,t)+\gamma(\underline{L}_{ZS})v(x,t)=0, \qquad (4.1.13)$$
$$\alpha_t^{(\pm)}(k,t)\pm\gamma(k)\alpha^{(\pm)}(k,t)=0, \qquad (4.1.14)$$

with

$$v(x,t)\equiv\begin{pmatrix}r(x,t)\\q(x,t)\end{pmatrix} \qquad (4.1.15)$$
$$\gamma(k)=-4ik\beta_0(-4k^2)+2\alpha_3(-4k^2), \qquad (4.1.16)$$

the matrix integro-differential operator $\underline{L}_{ZS}$ being defined by the formula

$$L_{ZS}\begin{pmatrix} u^{(1)}(x) \\ u^{(2)}(x) \end{pmatrix} = \frac{1}{2i}\begin{pmatrix} u_x{}^{(1)}(x) \\ -u_x{}^{(2)}(x) \end{pmatrix} + i\begin{pmatrix} r(x,t) \\ q(x,t) \end{pmatrix} \times \int_x^\infty dx' \, [r(x',t)u^{(2)}(x') - q(x',t)u^{(1)}(x')], \quad (4.1.17a)$$

or equivalently

$$L_{ZS}u(x) = (2i)^{-1}\sigma_3 u_x(x) - v(x,t)\int_x^\infty dx' \, (v(x',t),\sigma_2 u(x')). \quad (4.1.17b)$$

The complete equivalence of these equations to those of Calogero and Degasperis[2] is apparent.

Actually the class of nonlinear evolution equations obtained here is more general than that of Calogero and Degasperis,[2] because there one had the condition that the two fields $q$ and $r$ vanish asymptotically ($x \to \pm\infty$) together with all their derivatives, while here one must require that $Q$ vanish asymptotically ($x \to \pm\infty$) with all its derivatives, namely [see (4.1.10)] all the derivatives of the two fields $q$ and $r$ are required to vanish asymptotically, but the two fields themselves need not both vanish as $x \to -\infty$ [that they should vanish as $x \to +\infty$ is implied by (4.1.11) and (4.1.9)]

$$q(x,t) \underset{x\to+\infty}{\to} 0, \quad r(x,t) \underset{x\to+\infty}{\to} 0, \quad q(x,t)r(x,t) \underset{x\to-\infty}{\to} 0. \quad (4.1.18)$$

To display an explicit example, we set

$$\alpha_3(z) = (2i)^{-1}(a+bz), \quad \beta_0(z) = \tfrac{1}{2}(c+dz). \quad (4.1.19)$$

Then the nonlinear evolution equations read

$$r_t = iar + ib\,[r_{xx} - 2(qr)r] + cr_x + d\,[r_{xxx} - 6(qr)r_x], \quad (4.1.20a)$$

$$q_t = -iaq - ib\,[q_{xx} - 2(qr)q] + cq_x + d\,[q_{xxx} - 6(qr)q_x], \quad (4.1.20b)$$

or equivalently [see (4.1.9)]

$$q_{1t} = -iaq_2 - ib\,[q_{2xx} - 2(q_1^2 - q_2^2)q_2] + cq_{1x} + d\,[q_{1xxx} - 6(q_1^2 - q_2^2)q_{1x}], \quad (4.1.21a)$$

$$q_{2t} = -iaq_1 - ib\,[q_{1xx} - 2(q_1^2 - q_2^2)q_1] + cq_{2x} + d\,[q_{2xxx} - 6(q_1^2 - q_2^2)q_{2x}]. \quad (4.1.21b)$$

A reduction of the class of nonlinear evolution equations solvable via the matrix Schrödinger spectral problem to the class solvable via the "generalized Zakharov–Shabat spectral problem" can be performed also in the case of matrices of order $N$, in close analogy to the treatment given here. We propose, however, to treat this problem in a separate paper, where we shall also provide a more detailed analysis of the connection between the two spectral problems [such an analysis may also serve to better motivate the transformations (4.1.10) and especially (4.1.12), that have been given here without much explanation of their origin].

### 4.2 Further reduction: Identification of a novel highly nonlinear class of solvable equations for a single field

In Sec. 4.1 we described the reduction of the class of nonlinear evolution equations solvable via the $2\times2$ matrix Schrödinger spectral problem to that solvable by the generalized Zakharov–Shabat problem Ref. 2. As is well-known, several classical nonlinear evolution equations are contained in this class, including in particular the nonlinear Schrödinger equation, the modified K dV equation and the sine-Gordon equation. These equations (in particular the last two, that are generally written for a single real field) can be obtained by applying once more the reduction technique; but these developments are too trivial and well-known to deserve reporting. In this section we consider instead a less trivial additional reduction of the class of evolution equations (4.1.6) [with (4.1.3) and (4.1.4)], namely that resulting from the choice, in (3.1) and (3.2), of

$$F(z) = \sigma_1 + i(c_0 + c_1 z)\sigma_2, \quad H(z) = 0, \quad (4.2.1)$$

where $c_0$ and $c_1$ are constant.

It is then immediately seen that

$$R(k,t) = R_1(k,t)[\sigma_1 + i(c_0 - 4k^2c_1)\sigma_2] = R_1(k,t)F(-4k^2). \quad (4.2.2)$$

The derivation of the corresponding formula for $Q$, resulting from the constraint (3.1) that now reads

$$[\sigma_1, Q] + i(c_0 + c_1 \underline{L})[\sigma_2, Q] = 0, \quad (4.2.3)$$

is less elementary; we outline the main steps in the Appendix. The final result is most conveniently written in terms of the fields $q_1$ and $q_2$ of Sec. 4.1 [see in particular (4.1.8–4.1.11)], and it reads

$$q_2 = [c_0 q_1 - c_1(2q_1^3 - q_{1xx})]/[1 - 4c_0c_1q_1^2 + 4c_1^2(q_1^4 - q_{1x}^2)]^{1/2}. \quad (4.2.4)$$

Next one considers the compatibility condition (3.6), and it is easily seen that it implies $\alpha_3 = 0$.

In conclusion, a class of nonlinear evolution equations for the single field

$$u(x,t) \equiv q_1(x,t), \quad (4.2.5)$$

solvable by the spectral transform technique obtains setting $\alpha_3 = 0$ in (4.1.6), letting $\beta_0(z)$ be an arbitrary entire function (or more generally, the ratio of two entire functions), and expressing the matrix $Q$ in terms of the single field $u$ as implied by (4.1.8)–(4.1.11), and (4.2.4–4.2.5). Equivalently but more simply, the same class of nonlinear evolution equations obtains from (4.1.13), with $\gamma(z)$ odd in $z$ and entire (or, more generally, the ratio of two entire functions), the fields $r$ and $q$ being given in terms of $u$ by (4.1.9), (4.2.4), and (4.2.5).

The asymptotic boundary conditions that must supplement this class of equations, so as to assure consistency, via (4.2.5), (4.1.11), (4.1.10), and (4.1.9), with the assumed asymptotic vanishing of $Q$ and its derivatives, require $u$ to vanish with its derivatives as $x \to +\infty$,

$$0 = u(+\infty,t) = u_x(+\infty,t) = u_{xx}(+\infty,t) = \cdots, \quad (4.2.6a)$$

and moreover that all the derivatives of $u$ vanish as $x \to -\infty$,

$$0 = u_x(-\infty,t) = u_{xx}(-\infty,t) = \cdots; \quad (4.2.6b)$$

but the value of $u$ itself as $x \to -\infty$ is required to vanish only

if $c_0^2 \neq 1$ (elementary algebra shows that, if $c_0^2 = 1$, any asymptotic value of $u$ is consistent with the requirement that the matrix $Q$ vanish asymptotically):

$$u(-\infty,t) = 0 \quad \text{if } c_0^2 \neq 1,$$

$$u(-\infty,t) = \text{arbitrary constant}, \quad \text{if } c_0^2 = 1. \tag{4.2.6c}$$

In fact it is easily seen that, provided $c_0^2 = 1$ and $c_1 \neq 0$, $u$ might even diverge as $x \to -\infty$ [but the derivatives of $u$ must vanish, see (4.2.6b)].

Of course another requirement on $u$ is that $q_2$, as given by (4.2.4) and (4.2.5), be finite for $-\infty < x < \infty$; a condition sufficient to guarantee this is the requirement that $u$ itself be regular and that the denominator on the right-hand side of (4.2.4) not vanish for real $x$. It is clearly sufficient that all these conditions hold at the initial time, since they are then automatically guaranteed to hold throughout the time evolution.

A simple example of nonlinear evolution equation of this class obtains inserting (4.2.4)–(4.2.5) in (4.1.21a) (of course with $a = b = 0$, as required by the consistency condition that forces $\alpha_3(z)$ to vanish; see above). It reads

$$u_t = cu_x + d\{u_{xxx} - 6u_x[u^2 - (c_0 u - 2c_1 u^3 + c_1 u_{xx})^2/ (1 - 4c_0 c_1 u^2 + 4c_1^2 u^4 - 4c_1^2 u_x^2)]\}. \tag{4.2.7}$$

The change of dependent and independent variables

$$u(x,t) = (c_0/c_1)^{1/2} u'(x',t'), \quad x = (c_0/c_1)^{1/2}(x + ct),$$
$$t' = d(c_0/c_1)^{3/2} t, \tag{4.2.8}$$

yields for $u'(x',t')$ the neater equation

$$u_t = u_{xxx} - 6u_x\{u^2 - (u - 2u^3 + u_{xx})^2/ [a^2 - 4(u^2 - u^4 + u_x^2)]\}, \tag{4.2.9}$$

that we have written omitting all primes (for notational convenience; and we persevere below), and setting $c_0 = 1/a$. The boundary conditions for this equation are

$$0 = u(+\infty,t) = u_x(+\infty,t) = u_{xx}(+\infty,t) = \cdots; \tag{4.2.10a}$$

$$0 = u_x(-\infty,t) = u_{xx}(-\infty,t) = \cdots; \tag{4.2.10b}$$

$$u(-\infty,t) = 0 \quad \text{if } a^2 \neq 1,$$

$$u(-\infty,t) = \text{arbitrary constant} \quad \text{if } a^2 = 1. \tag{4.2.10c}$$

Let us emphasize once more that the technique to solve this equation is through the equivalence of (4.2.7) to (2.1) with $\alpha_m = 0, \beta_m = 0, \beta_0(z) = \frac{1}{2}(c + dz)$ and $Q$ given in terms of $u$ by (4.1.8–4.1.11) and (4.2.4–4.2.5). This implies of course not only the possibility of solving the Cauchy problem[1] [given $u(x,0)$ one can clearly compute $Q(x,0)$; and given $Q(x,t)$ one can recover $u(x,t)$ with just one quadrature, as implied by (4.1.11)], but also to obtain all the results associated with the solvability of (2.1) by the spectral transform technique: An infinite number of conserved quantities, Bäcklund transformation, all the soliton phenomenology.[1] Here we merely report the single soliton solution of (4.2.9), that reads

$$u(x,t) = 2pa[(1 + 4p^2)^2 - a^2]^{-1/2}/\cosh\{2p[x - \xi(t)]\}, \tag{4.2.11}$$

with

$$\xi(t) = \xi_0 - 4p^2 t. \tag{4.2.12}$$

In writing this equation we assume that $p$ is a positive constant such that the square root on the right-hand side of (4.2.11) is real, or equivalently, such that the quantity $\nu$ defined setting

$$\coth\nu = (1 + 4p^2)/a, \tag{4.2.13}$$

is real. Note that the soliton of this equation moves with constant speed; this is in contrast with the generic behavior of the solitons associated with matrix nonlinear evolution equations,[1] but it agrees with the generic behavior of the solitons of the nonlinear evolution equations of the Zakharov–Shabat class (4.1.13),[2] of which after all (4.2.9) is merely a subcase (although one that would not have been easy to discover without the technique given above). We also report the spectral transform[1] of the matrix $Q$ corresponding to (4.2.11); it has of course $R = 0$, and a *two-fold degenerate* discrete eigenvalue $-p^2$, so that the matrix $C$ associated with it[1] has the structure

$$C = C_1 + C_2 \tag{4.2.14}$$

$$C_j = 2p \exp(2p\,\xi_j) P_j, \quad j = 1,2, \tag{4.2.15}$$

$$\xi_1 = \xi - (2p)^{-1} \ln\sinh\mu, \quad \xi_2 = \xi_1 - i\pi/(2p), \tag{4.2.16}$$

$$P_j = \tfrac{1}{2}(\mathbb{1} + \hat{n}_m^{(j)} \sigma_m), \quad j = 1,2, \tag{4.2.17}$$

$$\hat{n}_1^{(j)} = \cosh[\nu - (-)^j \mu], \quad \hat{n}_2^{(j)} = i\sinh[\nu - (-)^j \mu],$$
$$\hat{n}_3^{(j)} = 0, \quad j = 1,2. \tag{4.2.18}$$

Note that the constant $\mu$ is in fact not present in $C$,

$$C = 2p \exp(2p\xi)(\sigma_1 \sinh\nu + i\sigma_2 \cosh\nu), \tag{4.2.19}$$

and accordingly does not appear in (4.2.11). Let us emphasize that, for equations obtained by reduction, the fact that the solitons may correspond to degenerate discrete eigenvalues appears not to be exceptional.[4]

Let us finally discuss some limiting properties of the solutions $u(x,t;a)$ of Eq. (4.2.9).

Clearly $u(x,t;\infty)$ satisfies the mK dV equation

$$u_t = u_{xxx} - 6\eta u^2 u_x, \quad \eta = \pm 1 \tag{4.2.20}$$

(with $\eta = +1$); and indeed in this limit (4.2.11) yields the single-soliton solution of the mK dV equation (this solution is imaginary; indeed it is (4.2.20) with $\eta = -1$ that has real solitons).

Another limiting case obtains setting

$$u(\epsilon x, \epsilon^3 t; 2/\epsilon) = \int_x^\infty dx' \sin\left[2\int_{x'}^\infty dx''\, \bar{u}(x'',t)\right], \tag{4.2.21a}$$

$$\bar{u}(x,t) = \frac{1}{2}\frac{d}{dx}\arcsin\left[\frac{d}{dx} u(\epsilon x, \epsilon^3 t; 2/\epsilon)\right], \tag{4.2.21b}$$

with $\epsilon \to 0$. It is then easily seen that $\bar{u}(x,t)$ satisfies again the mK dV equation (4.2.20) (with $\eta = -1$).

A third limiting case obtains setting instead

$$u(\epsilon x, \epsilon^3 t; 1) = -\int_x^\infty dx' \exp\left[-2\int_{x'}^\infty dx''\, \tilde{u}(x'',t)\right], \tag{4.2.22a}$$

$$\tilde{u}(x,t) = \frac{1}{2}\frac{d}{dx}\ln\left[\frac{d}{dx} u(\epsilon x, \epsilon^3 t; 1)\right], \tag{4.2.22b}$$

again with $\epsilon \to 0$. It is easily seen that also $\tilde{u}(x,t)$ satisfies the mK dV equation (4.2.20) with $(\eta = +1)$.

It is remarkable that these three limiting procedures all yield solutions of the mK dV equation. It should however be noted that while the first two prescriptions produce solutions of mK dV that vanish asymptotically, the last one appears to yield solutions that diverge asymptotically; the way is thereby opened to the study of the Cauchy problem for the mK dV equation with diverging asymptotic behavior, that however does not appear to be anywhere as interesting and important as the analogous problem for the K dV equation.[6]

### 4.3. Another class of nonlinear evolution equations involving two fields

In this section we consider another reduction of the class of evolution equations (2.1) for matrices of order 2, that again decreases the number of independent fields from 4 to 2, but in a different fashion than in Sec. 4.1. It obtains setting in (3.2)

$$F(z) = -i(\gamma_0 + \gamma_1 z)\sigma_1, \quad H(z) = \gamma\sigma_3. \tag{4.3.1}$$

There immediately follows

$$R(k,t) = -[(\gamma_0 - 4k^2\gamma_1)/(2i\gamma k)]R_2(k,t) + R_1(k,t)\sigma_1 + R_2(k,t)\sigma_2, \quad (R_3(k,t) = 0), \tag{4.3.2a}$$

or equivalently

$$R(k,t) = R_0(k,t) + R_1(k,t)\sigma_1 - [2i\gamma k/(\gamma_0 - 4k^2\gamma_1)]R_0(k,t)\sigma_2, \quad (R_3(k,t) = 0). \tag{4.3.2b}$$

These two expressions display the fact that $R$ contains now only 2 independent components; while their equivalence is quite obvious, the first is to be preferred in the special case $\gamma_0 = \gamma_1 = 0$, the second in the special case $\gamma = 0$ (see below).

The corresponding expression for $Q$ obtains inserting (4.3.1) in (3.1). After some labor, that we consider sufficiently straightforward not to warrant any reporting, there obtains the result

$$Q(x,t) = Q_0(x,t) + Q_1(x,t)\sigma_1 + Q_2(x,t)\sigma_2, \quad (Q_3(x,t) = 0), \tag{4.3.3}$$

$$Q_0(x,t) = (\gamma + 2\gamma_1 W_2)^{-2}[\gamma_1(\gamma + 2\gamma_1 W_2)W_{2xx} - \gamma_1^2 W_{2x}^2 + W_2^2(\gamma + \gamma_1 W_2)^2 + \gamma_0 W_2(\gamma + \gamma_1 W_2) + \gamma^2 W_1^2 + 4\gamma_1^2 U^2 - 4\gamma_1\gamma U W_1], \tag{4.3.4}$$

$$W_j \equiv W_j(x,t) = \int_x^\infty dx'\, Q_j(x',t),$$

$$Q_j(x,t) = -W_{jx}(x,t), \quad j = 1,2, \tag{4.3.5}$$

$$U \equiv U(x,t) = -\int_x^\infty dx'\, Q_1(x',t)W_2(x',t), \tag{4.3.6a}$$

$$U(x,t) = -W_1(x,t)W_2(x,t) + \int_x^\infty dx'\, Q_2(x',t)W_1(x',t). \tag{4.3.6b}$$

Note the similarity of this definition of $W_j$ to the definition (4.1.11) of the fields $q_j$; the differences are caused by the need, in Sec. 4.1, to reproduce the notation of Calogero and Degasperis.[2]

We consider next the compatibility condition (3.6), and using (4.3.2) it is easily seen that it implies

$$\alpha_1(z) = i[(\gamma_0 + \gamma_1 z)/\gamma]\beta_3(z), \tag{4.3.7a}$$

$$\alpha_2(z) = \beta_2(z) = 0, \tag{4.3.7b}$$

$$\alpha_3(z) = i[\gamma z/(\gamma_0 + \gamma_1 z)]\beta_1(z), \tag{4.3.7c}$$

with $\beta_0(z), \beta_1(z)$, and $\beta_2(z)$ arbitrary entire functions, or rather ratios of entire functions. Note moreover that the constraint condition (3.2) with (4.3.1), together with (4.3.7a), implies that the $\alpha_1$ and $\beta_3$ terms in (2.1) cancel each other, so that one can set, without loss of generality,

$$\alpha_1(z) = \beta_3(z) = 0. \tag{4.3.7d}$$

In conclusion the class of nonlinear evolution equations that we have now obtained corresponds to (2.1) with the functions $\alpha_m(z)$ and $\beta_\mu(z)$ restricted by the conditions (4.3.7) and with the matrix $Q$ given by (4.3.3–4.3.6). This class, for any choice of the functions $\alpha_m$ and $\beta_\mu$ [compatible with (4.3.7)], yields two coupled evolution equations for the two fields $Q_1(x,t)$ and $Q_2(x,t)$, or equivalently for the fields $W_1(x,t)$ and $W_2(x,t)$ of (4.3.5) (indeed the evolution equations have generally a neater appearance when written in terms of the dependent variables $W_j$ rather than $Q_j$; see below). The boundary conditions to be required are clearly

$$0 = W_j(+\infty,t) = W_{jx}(+\infty,t) = W_{jxx}(+\infty,t) = \cdots, \quad j = 1,2, \tag{4.3.8a}$$

and

$$0 = W_{jx}(-\infty,t) = W_{jxx}(-\infty,t) = \cdots, \quad j = 1,2. \tag{4.3.8b}$$

As for the values of the fields $W_j$ as $x \to -\infty$, the relevant condition must be read from (4.3.4), corresponding to the requirement

$$Q_0(-\infty,t) = 0. \tag{4.3.8}$$

The first example we consider corresponds to the choice

$$\gamma_1 = 0, \quad \beta_0(z) = \tfrac{1}{2}(c + dz), \quad \beta_1(z) = -\tfrac{1}{2}b\gamma_0/\gamma. \tag{4.3.9}$$

Then one obtains for the two fields

$$u(x,t) \equiv W_1(x,t), \quad v(x,t) \equiv W_2(x,t) + \tfrac{1}{2}\gamma_0/\gamma \tag{4.3.10}$$

the evolution equations

$$u_t = -b[v_{xx} - 2v(u^2 + v^2 - C^2)] + cu_x + d[u_{xxx} - 6u_x(u^2 + v^2 - C^2)], \tag{4.3.11a}$$

$$v_t = b[u_{xx} - 2u(u^2 + v^2 - C^2)] + cv_x + d[v_{xxx} - 6v_x(u^2 + v^2 - C^2)], \tag{4.3.11b}$$

where we have introduce the constant

$$C = \tfrac{1}{2}\gamma_0/\gamma. \tag{4.3.12}$$

Assuming the constants $b, c, d$, and $C^2$, as well as the fields $u^2$ and $v^2$, to be real, one can introduce the complex field $\phi(x,t)$ setting

$$\phi(x,t) = u(x,t) + iv(x,t). \tag{4.3.13}$$

Then the two evolution equations (4.3.11) combine into the single equation

$$\phi_t = ib[\phi_{xx} - 2\eta(|\phi|^2 - |C|^2)\phi] + c\phi_x + d[\phi_{xxx} - 6\eta(|\phi|^2 - |C|^2)\phi_x], \quad \eta = \pm 1 \tag{4.3.14}$$

(for $\eta = +1$, $u$, $v$, and $C$ are real; for $\eta = -1$, they are imaginary). Moreover the boundary conditions for the field $\phi(x,t)$, besides requiring the asymptotic vanishing of all its derivatives, read

$$\phi(+\infty,t) = iC, \quad |\phi(-\infty,t)| = |C|. \tag{4.3.15}$$

Thus the field

$$\psi(x,t) = \exp(-iat + i\mu)\phi(x,t), \tag{4.3.16}$$

where $a$ and $\mu$ are real constants, satisfies the "generalized Hirota equation"[7]

$$\psi_t = -ia\psi + ib[\psi_{xx} - 2\eta(|\psi|^2 - |C|^2)\psi] + c\psi_x + d[\psi_{xxx} - 6\eta(|\psi|^2 - |C|^2)\psi_x], \tag{4.3.17}$$

with boundary conditions

$$|\psi(+\infty,t)| = |\psi(-\infty,t)| = |C|. \tag{4.3.18}$$

[Note that the last equation need not imply $\psi(+\infty,t) = \psi(-\infty,t)$.]

Of course subcases of this equation are the (generalized) versions of the nonlinear Schrödinger equation and of the mK dV equation, that obtain respectively for $a = c = d = 0$, $b = 1$, reading

$$i\psi_t = -\psi_{xx} + 2\eta(|\psi|^2 - |C|^2)\psi, \quad \eta = \pm 1, \quad |\psi(\pm\infty,t)| = |C|, \tag{4.3.19}$$

and for $a = b = c = 0$, $d = 1$, $\psi(x,t) = \psi^*(x,t) = u(x,t)$, reading

$$u_t = u_{xxx} - 6\eta(u^2 - |C|^2)u, \quad \eta = \pm 1, \quad u^2(\pm\infty,t) = |C|^2. \tag{4.3.20}$$

The second example we consider corresponds to the choice

$$\gamma_1 \neq 0, \quad \beta_0(z) = \tfrac{1}{2}(c + dz), \quad \beta_1(z) = 0. \tag{4.3.21}$$

One obtains then the two nonlinear evolution equations

$$W_{jt}(x,t) = cW_{jx}(x,t) + d[W_{jxxx}(x,t) - 6Q_0(x,t)W_{jx}(x,t)], \quad j = 1,2, \tag{4.3.22}$$

with $Q_0$ given in terms of $W_1$ and $W_2$ by (4.3.4)–(4.3.6). These equations are rather complicated; but they yield a simpler equation if a further reduction is performed. This is discussed in Sec. 4.4.

## 4.4 Further reduction: Novel solvable nonlinear evolution equation for a single field

The further reduction that we apply here is directly suggested by the structure of (4.3.22), that is clearly compatible with the position

$$W_2(x,t) \equiv u(x,t), \quad W_1(x,t) = \rho u(x,t), \tag{4.4.1}$$

$\rho$ being a constant. This implies [see (4.3.5)–(4.3.6)]

$$U(x,t) = -\tfrac{1}{2}\rho u^2(x,t) \tag{4.4.2}$$

and [see (4.3.4)]

$$Q_0(x,t) = (\gamma + 2\gamma_1 u)^{-2}\{\gamma_1(\gamma + 2\gamma_1 u)u_{xx} - \gamma_1^2 u_x^2 + u(\gamma + \gamma_1 u)[\gamma_0 + (1+\rho^2)(\gamma + \gamma_1 u)u]\}. \tag{4.4.3}$$

Thus one obtains now for the single field $u(x,t)$, or rather for the field

$$u'(x',t') = 2(\gamma_1/\gamma)u(x,t), \quad x' = \lambda x + \mu t, \quad t' = d\lambda^3 t, \tag{4.4.4}$$

the nonlinear evolution equation (hereafter all equations are written for the primed variables, but dropping all primes for notational convenience)

$$u_t = \frac{\partial}{\partial x}[u_{xx} - \tfrac{3}{2}u_x^2/(1+u) + \tfrac{1}{3}A(1+u)^3 - B/(1+u) + Cu], \tag{4.4.5}$$

where

$$A = -\tfrac{3}{8}(1+\rho^2)\gamma^2/(\gamma_1^2\lambda^2), \tag{4.4.6a}$$

$$B = A + \tfrac{3}{2}\gamma_0/(\gamma_1\lambda^2), \tag{4.4.6b}$$

$$C = -A - B + (c\lambda - \mu)/(d\lambda^3). \tag{4.4.6c}$$

Of course some of these constants can be eliminated or set to unity by appropriate choices of the constants $\lambda$ and $\mu$.

The boundary condition to be associated with (4.4.5) requires all derivatives of $u$ to vanish asymptotically, and moreover $u$ itself to vanish as $x \to +\infty$ (we are assuming $\lambda > 0$):

$$0 = u(+\infty,t) = u_x(+\infty,t) = u_{xx}(+\infty,t) = \cdots, \tag{4.4.7a}$$

$$0 = u_x(-\infty,t) = u_{xx}(-\infty,t) = \cdots. \tag{4.4.7b}$$

As for the value of $u$ as $x \to -\infty$, the following four possibilities are all compatible with the condition $Q_0(-\infty,t) = 0$:

$$u(-\infty,t) = -1 \pm 1, \quad u(-\infty,t) = -1 \pm (B/A)^{1/2}; \tag{4.4.7c}$$

of course the last one can be contemplated, for real $u$, only if the ratio $B/A$ is positive (this we assume below).

Another interesting version of the nonlinear evolution equation (4.4.5) obtains setting

$$u(x,t) = \exp[\tfrac{1}{2}v(x,t)] - 1, \tag{4.4.8}$$

since $v$ obeys then the nonlinear equation

$$v_t = v_{xxx} - \tfrac{1}{8}v_x^3 + v_x[A\exp(v) + B\exp(-v) + C], \tag{4.4.9}$$

while the boundary conditions read

$$0 = v(+\infty,t) = v_x(+\infty,t) = v_{xx}(+\infty,t) = \cdots, \tag{4.4.10a}$$

$$0 = v_x(-\infty,t) = v_{xx}(-\infty,t) = \cdots, \tag{4.4.10b}$$

$$v(-\infty,t) = 0 \quad \text{or} \quad v(-\infty,t) = \ln(B/A). \tag{4.4.10c}$$

Let us note that the expression of the (matrix) reflection coefficient corresponding to the matrix $Q$ of (4.3.3)–(4.3.5) and (4.4.1)–(4.4.3) reads

$$R(k,t) = R_0(k,t)[1 - 2ik\gamma(\gamma_0 - 4k^2\gamma_1)^{-1}(\rho\sigma_1 + \sigma_2)], \tag{4.4.11}$$

and evolves according to the simple equation

$$R_{0t}(k,t) = 2ik(c - 4k^2 d)R_0(k,t) \tag{4.4.12}$$

[here we are again using the unprimed $t$ variable; see (4.4.4)].

Finally let us note the limiting cases that can be obtained from (4.4.9) [or equivalently (4.4.5)], setting

$$v(x,t) = \epsilon\psi(x,t), \tag{4.4.13}$$

$$A = A_0 + \tfrac{1}{2}A_1\epsilon^{-1} + A_2\epsilon^{-2}, \tag{4.4.14a}$$

$$B = -\tfrac{1}{2}A_1\epsilon^{-1} + A_2\epsilon^{-2}, \tag{4.4.14b}$$

$$C = -2A_2\epsilon^{-2}, \tag{4.4.14c}$$

and considering the limit $\epsilon \to 0$. Then (4.4.9) becomes

$$\psi_t = \psi_{xxx} + \psi_x(A_0 + A_1\psi + A_2\psi^2) \tag{4.4.15}$$

with the boundary conditions

$$0 = \psi(\pm\infty,t) = \psi_x(\pm\infty,t) = \psi_{xx}(\pm\infty,t) = \cdots. \tag{4.4.16}$$

This equation is, however, already contained in the class considered in Sec. 4.3 [see (4.3.17)].

## 5. CONCLUDING REMARKS

The main purpose of this paper has been to present the method of reduction. Since the worth of any pie is apparent only in the eating, we have also applied it, but in the simplest context, namely to matrices of order 2. This has not only displayed the connection between the class of nonlinear evolution equations solvable by the spectral transform associated to the Zakharov–Shabat spectral problem[2] and those solvable by the matrix Schrödinger problem,[1,3] but has in fact provided some generalization of the Zakharov–Shabat class (by allowing a less restrictive asymptotic behavior of the solutions). Moreover novel classes of nonlinear evolution equations involving two fields, or a single field only, have been obtained; we have displayed some of these, that provide therefore novel additions to the stock of nonlinear partial differential equations of evolution type solvable by the spectral transform technique. All these equations possess of course all the properties characteristic of the "soliton" equations; and it is straightforward to display such properties using the formalism given in this paper and elsewhere.[1]

A number of additional applications are naturally suggested by the results of this paper; in particular we shall report separately the findings yielded by the application of this approach to matrices of order higher than two.


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## APPENDIX

In this Appendix we indicate how the nonlinear integro-differential equation (4.2.3) [with (4.1.8)–(4.1.11) and of course (2.4)–(2.5)] can be solved to yield (4.2.4).

Trivial algebra yields first of all

$$q_{2x} + ic_0q_{1x} + ic_1\Big[q_{1xxx} - 6q_{1x}q_1^2 + 4q_{1x}q_2^2 + 4q_{2x}q_1q_2 + 4q_{2x}\int_x^\infty dx'\, q_{2x}(x')q_1(x')\Big] = 0. \tag{A1}$$

It is then convenient to set

$$w(x) = \int_x^\infty dx' q_{1x}(x')q_2(x'), \tag{A2a}$$

$$q_2(x) = -w_x(x)/q_{1x}(x), \tag{A2b}$$

and to note that the left-hand side of (A1) is a perfect differential, so that integration from $x$ to $\infty$ yields

$$q_2 + ic_0q_1 + ic_1(q_{1xxx} - 2q_1^3 + 4q_2w) = 0. \tag{A3}$$

Multiply this equation by $q_{1x}$, and use (A2b) to eliminate $q_2$. One obtains again in this manner a perfect differential, whose integration from $x$ to $\infty$ yields the equation

$$2iw + c_0q_1^2 + c_1(q_{1x}^2 - q_1^4 + 4w^2) = 0. \tag{A4}$$

This is immediately solved for $w$ (to identify the correct solution out of the two possible ones note that $w$ must vanish when $q_{1x}$ and $q_1$ vanish, since this is what happens in the limit $x \to +\infty$), and subsequent insertion in (A2b) yields (4.2.4).


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[6] The typical diverging solution of the K dV equation behaves linearly in $x$ as $x$ diverges; removal of the divergent part by subtraction leaves for the nondivergent part an interesting equation, related to the so-called "cylindrical K dV equation" [see for instance, F. Calogero and A. Degasperis, Lett. Nuovo Cimento **23**, 150 (1978); L.A. Bordag and M.B. Matveev, Leipz. Prepr. (to be published); and the literature referred to in these papers.] The typical diverging solution of the mK dV equation behaves asymptotically proportionally to the square root of $x$; the equation one obtains after removal by substraction of the divergent part does not appear particularly interesting. This is connected with the fact that, while $q(x,t) = \frac{1}{6}(x/t)$ is an (asymptotically diverging) exact solution of the K dV equation $q_t - q_{xxx} + 6q_xq = 0$, no comparably simple solution of the mK dV equation exists; indeed the solution related to that written above via the Miura transformation (Ref. 5) involves Airy functions.

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# On one method of solving the Helmholtz equation. I

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A method is suggested to solve the Helmholtz equation in an arbitrary domain with general form boundary conditions. The method permits reducing this equation to that of Poisson and an infinite set of simultaneous linear algebraic equations. Convergence of the method is proved for any wave number. Thus, it becomes possible to solve the Helmholtz equation by using any known method developed to solve the Poisson equation. As an illustration, an effective algorithm is constructed to solve the two dimensional diffraction problem on the arbitrary periodic boundary for any wavelength by using the conformal mapping techniques. If the boundary contains irregular points, then the field in all approximations has in all these points singularities of the needed type.

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## INTRODUCTION

The Helmholtz equation describes a rather great number of physical processes, so the task of developing methods for its solution is important both for theory and applications. As explicit solutions of the Helmholtz equation are known only for a few domains of the simplest form, it is necessary to develop numerical algorithms for less specific cases. A lot of publications have been devoted to this problem. Application of general methods of numerical mathematics, such as variational and network methods, the moment methods, etc., enabled solution of many concrete problems. As the wave operator $-(\Delta + \mathbf{k}^2)$ is not positive definite, however, the amount of needed operations grows abruptly when the domain size increases or the domain form becomes more complicated; besides, no effective error estimates are known. Note also that these methods require a certain smoothness of the domain boundary. When applied to domains with irregular boundaries, the methods should be specially modified for each type of irregularity to capitalize on some particular features. This is especially bothersome when the boundary contains irregularities of different types, e.g., angle points with different angles. This all resulted in the construction for a number of special domains and boundary conditions of "hybrid" semianalytical methods which are highly effective in numerical calculations and take into account singularities in irregular boundary points in the natural way in the framework of the method.[1-4] The methods are effective only for domains with cylindrical or infinitely thin plane boundaries and they make substantial use of domain geometry. The situation in the field was pessimistically summed up by R. Mittra who wrote (Ref. 1, Chap. I): "As is the common feature of analytically oriented computer techniques, these methods cannot be applied to arbitrary configurations." Actually, the situation is not so hopeless because application of analytical transformations permits the construction of effective methods to solve many types of equations including the two dimensional Helmholtz one in the arbitrary configuration domain.[5,6]

In this work we present a general scheme for constructing an effective method to solve the Helmholtz equation in domains of arbitrary configuration and with general form boundary conditions. The method consists of reducing the Helmholtz equation $\Delta u + \mathbf{k}^2\mathbf{u} = f(x)$ ($\mathbf{k}$ is arbitrary) to the Poisson equation and a convergent infinite set of simultaneous linear algebraic equations. So it is possible to solve the Helmholtz equation in all cases when there exists an effective algorithm to solve the Poisson equation. As a specification of the scheme we consider the two dimensional problem of plane wave diffraction on an arbitrary periodic surface. Here the Poisson equation is solved explicitly by means of conformal mapping. This enables one to solve the diffraction problem with no assumptions as to boundary smoothness; besides, if the boundary has irregular points, then the field in all approximations has in these points singularities of the needed type. The solution obtained in this way is semianalytical for it is given by a series with numerically calculated coefficients that converges everywhere in the domain.

## 1. FORMULATION OF THE PROBLEM AND SOLUTION SCHEME

Consider the equation

$$\Delta\mathbf{u} + \mathbf{k}^2\mathbf{u} = f(\mathbf{x}), \quad \mathbf{x} = (\mathbf{x}_1,\ldots,\mathbf{x}_n), \tag{1.1}$$

in the domain $\Omega$ with the boundary $\Gamma$. A general form boundary condition

$$B[\mathbf{u}]|_\Gamma = \varphi(x), \tag{1.2}$$

providing that the unique solution exists, is given on $\Gamma$; if the domain $\Omega$ is infinite, then the operator $B$ also contains radiation (or equivalent) conditions on infinity. The formal scheme of the suggested method is as follows:

Rewrite Eq. (1.1) in the form

$$\Delta\mathbf{u} = f(x) - \mathbf{k}^2\mathbf{u}. \tag{1.3}$$

Partition the domain $\Omega$ into the sum of nonintersecting subdomains $\Omega_i$, $\Omega = \cup_{i=1}^{\infty}\Omega_i$. Let us take in each subdomain $\Omega_i$ a function system $\{\mathbf{u}_{in}(x)\}_{n=1}^{\infty}$ complete in a function class containing the solution. Generally speaking, the choice of $\Omega_i$ is arbitrary and made for convenient construction of the systems $\{\mathbf{u}_{in}(x)\}$ or for usage of *a priori* information on the solution. For example, if it is possible, one can choose $\Omega_i$ so that variables will separate; then corresponding partial solutions (modes) are taken as $\mathbf{u}_{in}(x)$. Let $l_{ij}$ be a

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system of linear functionals defined on functions continuous in $\Omega_i$. By definition this system is biorthogonal to $\{\mathbf{u}_{in}\}$: $l_{ij}(\mathbf{u}_{in}) = \delta_j^n$, where $\delta_j^n$ is the Kronecker symbol. Substituting the expansion of $\mathbf{u}(x)$ with respect to the functions $\mathbf{u}_{in}(x)$ in $\Omega_i$ to the right-hand side of Eq. (1.3):

$$\mathbf{u} = \sum_{n=1}^{\infty} A_{in}\mathbf{u}_{in}(x), \quad x \in \Omega_i, \tag{1.4}$$

we obtain

$$\Delta\mathbf{u} = f(x) - \mathbf{k}^2 \sum_{n=1}^{\infty} A_{in}\mathbf{u}_{in}(x), \quad x \in \Omega_i. \tag{1.5}$$

Denote $\tilde{u}_{in}(x) = \mathbf{u}_{in}(x)\psi_i$, where $\psi_i$ is a characteristic function of the subdomain $\Omega_i$, and let $R[g(x)]$ be a solution (or a generalized solution) of the Poisson equation with the right-hand side $g(x)$ and boundary conditions (1.2); if Eq. (1.2) includes radiation conditions, then while defining $R[g]$ they must be replaced by a condition of boundedness on infinity. Using this notation, Eq. (1.5) can be rewritten in the form

$$\mathbf{u} = R[f] - \mathbf{k}^2 \sum_{i=1}^{\mathscr{P}} \sum_{n=1}^{\infty} A_{in} R[\tilde{u}_{in}]. \tag{1.6}$$

Applying functionals $l_{ij}$ to both sides of Eq. (1.6) and taking into account Eq. (1.4), we obtain an infinite set of linear algebraic equations of the second kind to compute the coefficients

$$A_{ij} = l_{ij}(R[f]) - \mathbf{k}^2 \sum_{i=1}^{\mathscr{P}} \sum_{n=1}^{\infty} A_{in} l_{ij}(R[\tilde{u}_{in}]), \quad i = 1,\ldots,\mathscr{P}. \tag{1.7}$$

Equating to zero the determinant of Eq. (1.7), we obtain the characteristic equation that determines the Laplace operator spectrum for boundary conditions (1.2).

With some modifications this scheme can be applied to the Neumann problem which corresponds to the Poisson equation that has no solution for an arbitrary right-hand side.

The suggested scheme can be easily recognized as the somewhat generalized abstract method by Galerkin.[7,8] The generalization deals with the domain partitioning and introducing several systems of coordinate functions and corresponding functional systems. When $\mathscr{P} = 1$ we obtain the abstract Galerkin method with functionals biorthogonal to the coordinate functions. Such choice of functionals results in equations of the second kind for the sought coefficients.

Rigid formalization of this scheme and general theorems on convergence will be published elsewhere. In the present work we consider, as an illustration, the two dimensional problem of plane wave diffraction on a general configuration periodic surface.

By our method we shall be able to obtain a semianalytical solution of the problem that automatically accounts for the field singularities in irregular boundary points (if there are any). Such a solution is of interest by itself.

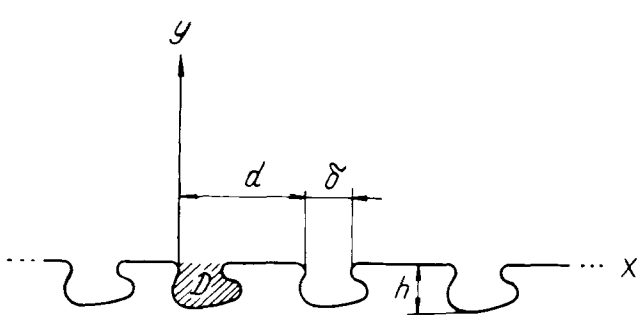


FIG. 1.

## 2. PLANE WAVE DIFFRACTION ON A PERIODIC BOUNDARY

Consider a two dimensional problem of plane wave diffraction on a periodic surface.

The domain $\Omega$ is a half-space with a periodic boundary $\Gamma$ with the period $\alpha$ (see Fig. 1).

That part of $\Omega$ that is bounded by one period of $\Gamma$ from below and by the segment $y = 0, 0 \leqslant x \leqslant \delta$, of the $OX$ axis from above will be called the main resonator $D$. All domains obtained by translating $D$ along the $OX$ axis by the integer number of periods will be also called resonators. Denote the boundary of $D$ by $\partial D$. The part of $\partial D$ which is coincident with $\Gamma$ will be called the actual boundary of $D$ and denoted by $\tilde{\partial} D$ while the segment $y = 0$, $0 \leqslant x \leqslant \delta$ will be called the resonator gap.

The plane wave $\mathbf{u}^{(0)} = A e^{i\beta x + \alpha y}$ meets $\Gamma$ with the incidence angle $\varphi$. Here $\beta = k \sin\varphi, \alpha = -ik\cos\varphi$, $k = 2\pi/\lambda = \omega/c$ is the wave number, $\omega$ is the frequency, and $c$ is the light velocity. The field $\mathbf{u}(x,y)$ to be found is the sum of $\mathbf{u}^{(0)}$ and the scattered field $\mathbf{u}_s$; $\mathbf{u}(x,y)$ will be determined from the Helmholtz equation (1.1) with $f(x) = 0$. As boundary conditions we take those of Neumann for

$$\left.\frac{\partial \mathbf{u}}{\partial n}\right|_{\Gamma} = 0 \tag{2.1}$$

(it is evident what changes should be made in all following considerations to treat the Dirichlet problem), those of Floquet for quasiperiodicity

$$\mathbf{u}(x + d, y) = e^{i\beta d}\mathbf{u}(x,y), \tag{2.2}$$

and the condition of radiation or limiting absorption. If $\Gamma$ contains sharp bends (angle points), then the Meixner conditions[9] must be added as well. By insignificant changes in the arguments of the papers,[10,11] one can demonstrate that the conditions suffice to determine the field sought for completely and uniquely.

According to conditions (2.2) and the radiation condition, the field at $y > 0$ can be given in the form

$$\mathbf{u} = \mathbf{u}^{(0)} + \sum_{n=-\infty}^{\infty} C_n e^{i\beta_n x - \alpha_n y}, \tag{2.3}$$

where

$$\beta_n = \beta + (2\pi n/d), \quad \alpha_n = (\beta_n^2 - k^2)^{1/2},$$

$$\alpha_0 \equiv \alpha, \quad \mathrm{Im}\,\alpha_n < 0; \quad \alpha_n > 0 \text{ if } \mathrm{Im}\,\alpha_n = 0.$$

Terms in Eq. (2.3) with $|\beta_n| < \mathbf{k}$ describe reflected propagating waves while terms with $|\beta_n| > \mathbf{k}$ describe surface waves. For the sake of simplicity we introduce the following notation:

$$e_n \equiv e^{i\beta_n x - \alpha_n y}, \quad e'_n \equiv e^{i\beta_n x' + \alpha_n y'},$$
$$e_+ \equiv e^{i\beta x + \alpha y}, \quad e'_+ \equiv e^{i\beta x' + \alpha y'}.$$

The field in the resonator $D$ will be given in the form similar to Eq. (1.4):

$$\mathbf{u} = \sum_{m=0}^{\infty} B_m \mathbf{u}_m(x,y), \tag{2.4}$$

where $\{\mathbf{u}_m(x,y)\}$ is a complete in $\mathscr{L}_2(D)$ orthonormal system of functions. The condition (2.2) permits one now to extend the field to all resonators.

Let us make certain changes in the general scheme to simplify further treatment, namely, instead of Eq. (1.5) we take the equation

$$\Delta U_M^{(N)} = -\mathbf{k}^2 \begin{cases} \mathbf{u}^{(0)} + \sum_{n=-N}^{N} \widetilde{C}_n e_n, & y > 0, \\ \sum_{m=0}^{M} \widetilde{B}_m \mathbf{u}_m(x,y), & (x,y) \in D. \end{cases} \tag{2.5}$$

The equation above is obtained from Eq. (1.5) by formal substitution of series in the right-hand side by their finite segments. Accordingly, instead of $\mathbf{u}, C_n$, and $B_m$ we introduce new variables $U_M^{(N)}, \widetilde{C}_n$, and $\widetilde{B}_m$, respectively. The right-hand side of Eq. (2.5) is, generally speaking, discontinuous, with a jump in the resonator gap. It is not difficult to see that the equation with the fixed coefficients $\widetilde{C}_n$, and $\widetilde{B}_m$ and boundary conditions discussed above has a unique solution continuous with the first derivatives in $\Omega$ (the solution is regarded as a generalized one[10] or classical everywhere but in the points $0 < x < \delta, y = 0$ where matching is made.) With $U_M^{(N)}$ found, we shall determine the coefficients $\widetilde{C}_n$, and $\widetilde{B}_m$ from Eq. (1.7) changed accordingly. $U_M^{(N)}$ will be constructed with the help of the quasistatic Green function.

## 3. CONSTRUCTION OF QUASISTATIC GREEN FUNCTION

The quasistatic Green function is defined as a Green function for the Laplace operator that satisfies the equation.

$$\Delta G = \delta(x - x', y - y'), \quad 0 < x < d, \ 0 < x' < d, \tag{3.1}$$

and the boundary conditions

$$\left.\frac{\partial G}{\partial n}\right|_{\Gamma} = 0,$$
$$G(x + d, y, x', y') = e^{i\beta d} G(x, y, x', y'); G(x, \infty, x', y') = 0. \tag{3.2}$$

[In general, the quasistatic Green function may be defined as a Green function for the Laplace operator with boundary conditions depending on the wave number. When $\varphi = 0$, i.e., when the incidence angle is right, the conditions (3.2) become independent of $\mathbf{k}$ and the problem (3.1) and (3.2) becomes a standard periodical static Neumann problem for which the Green function is known to be nonexistent. That can be seen from the formula (3.11). So the case of $\varphi = 0$ is a special one for the given method and must be regarded as a limit of the problem for slanting angles. More details will be given in part II of the present work.]

Let us construct the function $G$. To this end let us map conformally the domain $\Omega$ of the plane $\mathbf{z} = \mathbf{x} + i\mathbf{y}$ onto the half-plane $\eta > 0$ of the plane $\zeta = \xi + i\eta$ so that the point $\mathbf{z} = 0$ would be mapped into $\zeta = 0$, $\mathbf{z} = d$ into $\zeta = d$, and infinity into infinity.

This mapping will be further called canonical. Existence of a canonical mapping follows from the Riemann theorem.[11] It can easily be demonstrated that the mapping function $\zeta(\mathbf{z})$ has the form

$$\zeta(\mathbf{z}) = z + \varphi(\mathbf{z}), \tag{3.3}$$

where $\varphi(\mathbf{z})$ is a periodical function with the period $d$, $\varphi(\mathbf{z} + d) = \varphi(\mathbf{z})$, and the inverse mapping $\mathbf{z}(\zeta)$ has a similar form

$$\mathbf{z}(\zeta) = \zeta + \psi(\zeta), \quad \psi(\zeta + d) = \psi(\zeta). \tag{3.4}$$

Estimates in previous work[12] imply that

$$\varphi(\mathbf{z}) \to \text{const.}, \ y \to \infty; \ \psi(\zeta) \to \text{const.}, \ \eta \to \infty. \tag{3.5}$$

Direct calculation shows that Eq. (3.1) does not change in $\xi, \eta$ coordinates

$$\Delta_{\xi\eta} G = \delta(\xi - \xi', \eta - \eta'), \quad 0 < \xi < d, \ 0 < \xi' < d. \tag{3.1'}$$

($\zeta' = \xi' + i\eta'$ is the point corresponding to $\mathbf{z}' = x' + iy'$.)

General properties of conformal mappings, the condition $\zeta(\infty) = \infty$, and Eq. (3.3) imply that the conditions (3.2) are also invariant in the plane $\zeta$:

$$\left.\frac{\partial G}{\partial \eta}\right|_{\eta = 0} = 0, \quad G(\xi + d, \eta, \xi', \eta') = e^{i\beta d} G(\xi, \eta, \xi', \eta');$$
$$G(\xi, \infty, \xi', \eta') = 0. \tag{3.2'}$$

Hence, it is clear that $G$ can be sought as a series

$$G = \sum_{n=-\infty}^{\infty} e^{i\beta_n \xi} G_n(\eta, \xi', \eta'), \tag{3.6}$$

where

$$G_n = \frac{1}{d} \int_0^d e^{-i\beta_n \xi} G \, d\xi. \tag{3.7}$$

After some transformations we obtain $G_n$ from Eqs. (3.7), (3.1), and (3.2):

$$\frac{d^2 G_n}{d\eta^2} - \beta_n^2 G_n = \frac{1}{d} e^{-i\beta_n \xi'} \delta(\eta - \eta'), \tag{3.8}$$

$$\left.\frac{dG_n}{d\eta}\right|_{\eta = 0} = 0, \ G_n|_{\eta = \infty} = 0. \tag{3.9}$$

Hence,

$$G_n = -e^{-i\beta_n \xi'} \frac{e^{-|\beta_n||\eta - \eta'|} + e^{-|\beta_n||\eta + \eta'|}}{2|\beta_n| d}. \tag{3.10}$$

Substituting Eq. (3.10) into Eq. (3.7) we obtain $G$:

$$G = -\sum_{n=-\infty}^{\infty} e^{i\beta_n(\xi - \xi')} \times \frac{e^{-|\beta_n||\eta - \eta'|} + e^{-|\beta_n||\eta + \eta'|}}{2|\beta_n| d}. \tag{3.11}$$

From Eq. (3.11) characteristics of the function $G$ needed for further considerations can be derived:

$$\Delta_{x'y'} G = \delta(x - x', y - y'), \tag{3.12}$$

$$\left.\frac{\partial G}{\partial n'}\right|_{(x',y')\in\Gamma} = 0 \tag{3.13}$$

($\partial/\partial n'$ denotes differentiating with respect to the outward normal of $\Gamma$ by variables $x',y'$),

$$G(x,y,x'+d,y') = e^{-i\beta d}G(x,y,x',y'). \tag{3.14}$$

For the fixed $x,y$ and $y'\to\infty$ there exists the constant $C$ such that

$$|G(x,y,x',y')| < Ce^{-\beta y'}, \tag{3.15}$$

and for all $\mathbf{z}$, $\mathbf{z}'$ from $\Omega$ a representation

$$G = -\frac{1}{2\pi}\ln|\mathbf{z}-\mathbf{z}'| + g(\mathbf{z},\mathbf{z}'), \quad |g| < \infty \tag{3.16}$$

holds.

## 4. CONSTRUCTION OF $U_M^{(N)}$

Let us prove that the sought solution $U_M^{(N)}$ of Eq. (2.4) can be represented in the form

$$\begin{aligned} U_M^{(N)} &= -\mathbf{k}^2\Big\{\int_0^d dx'\int_0^\infty \Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)G\,dy' \\ &\quad + \iint\sum_{m=0}^{M}\widetilde{B}_m \mathbf{u}_m(x',y')G\,dx'dy'\Big\} \\ &\equiv Af^+(x,y) + \sum_{n=-N}^{N}\widetilde{C}_n f_n(x,y) + \sum_{m=0}^{M}\widetilde{B}_m g_m(x,y). \end{aligned} \tag{4.1}$$

Indeed, existence of improper integrals in Eqs. (4.1) is guaranteed by the estimates (3.15), and the fact that $U_M^{(N)}$ in the form (4.1) satisfies Eq. (2.4) follows from the construction method. Conditions (3.2) also imply that $U_M^{(N)}$ meets the quasiperiodicity condition and the Neumann condition on $\Gamma$. Equation (3.16) and well-known theorems on logarithmic potentials[13] imply that $U_M^{(N)}$ and $\partial U_M^{(N)}/\partial y$ are continuous on the resonator gap. One has only to check how $U_M^{(N)}$ behaves on infinity. To this end transform the first integral in Eq. (4.1) by means of the Green formula, taking into account the equality $-\mathbf{k}^2 e^{i\beta_n x'\pm\alpha_n y'} = \Delta(e^{i\beta_n x'\pm\alpha_n y'})$. We obtain

$$\begin{aligned} I &= -\mathbf{k}^2\int_0^d dx'\int_0^\infty G\Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)dy' \\ &= \int_0^d dx'\int_0^\infty G\Delta_{x'y'}\Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)dy' \\ &= \int_0^d dx'\int_0^\infty \Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)\Delta_{x'y'}G\,dy' \\ &\quad + \int_L\Big[G\frac{\partial}{\partial n'}\Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big) \\ &\quad - \Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)\frac{\partial G}{\partial n'}\Big]dl \equiv I_1 + I_2. \end{aligned}$$

Here $L$ is a contour made of rays $x'=0,y'\geqslant 0, x'=d,y'\geqslant 0$, and the segment $y'=0, 0\leqslant x'\leqslant d$.

Taking into account Eq. (3.12), we have

$$I_1 = Ae_+ + \sum_{n=-N}^{N}\widetilde{C}_n e_n .$$

Because of Eq. (3.14) the integrals along the rays $x'=0$ and $x'=d$ in $I_2$ cancel each other, so we are left with

$$\begin{aligned} I = I_1 + I_2 &= Ae_+ + \sum_{n=-N}^{N}\widetilde{C}_n e_n \\ &\quad - \int_0^d\Big[\Big(\alpha Ae'_+ - \sum_{n=-N}^{N}\widetilde{C}_n\alpha_n e'_n\Big)G \\ &\quad - \Big(Ae'_+ + \sum_{n=-N}^{N}\widetilde{C}_n e'_n\Big)\frac{\partial G}{\partial y'}\Big]_{y'=0}dx'. \end{aligned} \tag{4.2}$$

Making use of Eqs. (3.12), (3.4), and (3.5), it is not difficult to obtain for $G$ and $\partial G/\partial y'$ estimates similar to Eq. (3.15):

$$|G| < Ce^{-\beta y}, \quad \left|\frac{\partial G}{\partial y'}\right| < Ce^{-\beta y}, \tag{4.3}$$

which are valid when $y\to\infty$ for $x',y'$ in any fixed domain. Hence, it immediately follows that $I_2$ and functions $g_m(x,y)$ decrease as $e^{-\beta y}$ when $y\to\infty$. This remark together with Eq. (4.2) shows that $U_M^{(N)}$ satisfies necessary conditions on infinity, which completes the proof of the formula (4.1).

By using the quasiperiodicity condition this representation for $U_M^{(N)}$ is easily extended to the whole domain.

## 5. SIMULTANEOUS EQUATIONS TO DETERMINE COEFFICIENTS $\widetilde{C}_n$ and $\widetilde{B}_m$

To determine the unknown coefficients $\widetilde{C}_n$, and $\widetilde{B}_m$ in Eq. (4.1) we demand that for $y\geqslant 0$ the Fourier coefficients of $U_M^{(N)}$ with respect to the function system $\{e^{i\beta_n x}\}$ when $|n|\leqslant N$ should coincide with $\widetilde{C}_n e^{-\alpha_n y}$ while the coefficients with respect to the system $\{\mathbf{u}_m\}$ in the domain $D$ when $0\leqslant m\leqslant M$ should coincide with $\widetilde{B}_m$. This condition will be called the condition of coefficient coincidence. Applying it to Eq. (4.1), we obtain simultaneous linear algebraic equations to determine $\widetilde{C}_n$ and $\widetilde{B}_m$

$$\begin{aligned} &\frac{1}{d}\Big\{A\int_0^d f^+ e^{-i\beta_p x}dx + \sum_{n=-N}^{N}\widetilde{C}_n\int_0^d f_n \\ &\quad\times e^{-i\beta_p x}dx + \sum_{m=0}^{M}\widetilde{B}_m\int_0^d g_m e^{-i\beta_p x}dx\Big\} \\ &\quad = \widetilde{C}_p e^{-\alpha_p y} + \delta_0^p A e^{\alpha y}, \quad y\geqslant 0 (|p|\leqslant N); \end{aligned} \tag{5.1'}$$

$$\begin{aligned} &A\iint_D f^+\mathbf{u}_j dx\,dy + \sum_{n=-N}^{N}\widetilde{C}_n\iint_D f_n\mathbf{u}_j dx\,dy \\ &\quad + \sum_{m=0}^{M}\widetilde{B}_m\iint_D g_m\mathbf{u}_j dx\,dy \\ &\quad = \widetilde{B}_j \quad (0\leqslant j\leqslant M), \end{aligned} \tag{5.1''}$$

where $\delta_0^p$ is the Kronecker symbol.

The condition of coefficient coincidence is evidently an approximation of the exact equality (1.7) written for the concrete case considered. After formal passage to the limit with $N,M\to\infty$, Eqs. (5.1) turn to exact equations of Eq. (1.7) type. Foundation for the passage to the limit will be provided in the next section.

The right-hand side of Eq. (5.1') and their matrix elements depend on $y$. Let us show that the solution of Eqs. (5.1) is nevertheless independent of $y$. To this end transform the set of equations (5.1') so that it would be possible to exclude dependence on $y$.

Applying the Green formula to $f_n = \int_0^d dx'$

$\times \int_0^\infty G\Delta\,(e_n')dy'$, taking into account Eqs. (3.12)–(3.14), and the problem boundary conditions, we obtain

$$f_n(x,y) = e_n + \int_0^d \left(\alpha_n G + \frac{\partial G}{\partial y'}\right)\Big|_{y'=0} e^{i\beta_n x'}dx' \equiv e_n + \hat{f}_n(x,y), \tag{5.2}$$

where $\hat{f}_n$ is evidently a harmonic function (when $y>0$) that satisfies the Floquet condition (2.2) and the infinity condition $\hat{f}_n(x,\infty)=0$. Because of the Floquet condition $\hat{f}_n$ can be expanded into the Fourier series

$$\hat{f}_n = \sum_{s=-\infty}^{\infty} e^{i\beta_s x}\varphi_{ns}(y).$$

Substituting this series into the harmonic equation, we obtain the following for $\varphi_{ns}(y)$:

$$\varphi_{ns}'' - \beta_s^2\varphi_{ns} = 0.$$

From this equality and the condition $\hat{f}_n(x,\infty)=0$ we find

$$\varphi_{ns}(y) = \hat{f}_{ns}e^{-|\beta_s|y},$$

where $\hat{f}_{ns}$ are constant coefficients. Thus, $\hat{f}_n$ can be represented as

$$\hat{f}_n = \sum_{s=-\infty}^{\infty} \hat{f}_{ns}e^{i\beta_s x - |\beta_s|y}. \tag{5.3}$$

We get in a similar way

$$f^+(x,y) = e_+ + \sum_{s=-\infty}^{\infty} \hat{f}_s^+ e^{i\beta_s x - |\beta_s|y}, \quad y>0, \tag{5.4}$$

$$g_m(x,y) = \sum_{s=-\infty}^{\infty} \hat{g}_{ms}e^{i\beta_s x - |\beta_s|y}, \quad y>0. \tag{5.5}$$

Substituting Eqs. (5.2)–(5.5) into Eq. (5.1'), we get Eq. (5.1') in the form

$$A\hat{f}_p^+ + \sum_{n=-N}^{N} \tilde{C}_n\hat{f}_{np} + \sum_{m=0}^{M} \tilde{B}_m\hat{g}_{mp} = 0, \quad |p|\leqslant N. \tag{5.6}$$

Now we see that the sought values $\tilde{C}_n$ and $\tilde{B}_m$ are actually independent of $y$.

## 6. ANALYSIS OF EQS. (5.1)

To prove convergence we transform the set of equations (5.1) to the form without diagonal elements in the right-hand part and set $y$ to zero in Eq. (5.1'). We obtain

$$\tilde{C}_p = \sum_{\substack{n=-N\\(n\neq p)}}^{N} \tilde{C}_n \frac{f_{n\langle p\rangle}}{1-f_{p\langle p\rangle}} + \sum_{m=0}^{M} \tilde{B}_m \frac{g_{m\langle p\rangle}}{1-f_{p\langle p\rangle}} + A\frac{f_{\langle p\rangle}^+ - \delta_0^p}{1-f_{p\langle p\rangle}}, \tag{6.1'}$$

$$\tilde{B}_j = \sum_{\substack{m=0\\(m\neq j)}}^{M} \tilde{B}_m \frac{g_{mj}}{1-g_{jj}} + \sum_{n=-N}^{N} \tilde{C}_n \frac{f_{nj}}{1-g_{jj}} + A\frac{f_j^+}{1-g_{jj}}, \tag{6.1''}$$

where

$$f_{n\langle p\rangle} = \frac{1}{d}\int_0^d f_n(x,0)e^{-i\beta_p x}dx,$$

$$g_{m\langle p\rangle} = \frac{1}{d}\int_0^d g_m(x,0)e^{-i\beta_p x}dx,$$

$$f_{\langle p\rangle}^+ = \frac{1}{d}\int_0^d f^+(x,0)e^{-i\beta_p x}dx,$$

$$g_{mj} = \iint_D g_m \mathbf{u}_j dx\,dy,$$

$$f_{nj} = \iint_D f_n \mathbf{u}_j dx\,dy,$$

$$f_j^+ = \iint_D f^+\mathbf{u}_j dx\,dy.$$

[We shall demonstrate further that $f_{p\langle p\rangle}\to 0$ when $p\to\infty$ and $g_{jj}\to 0$ when $j\to\infty$. For a finite number of indices, however, $f_{p\langle p\rangle}$ and $g_{jj}$ may equal 1. In this case we leave Eqs. (5.1) in the original form.] Let us show that Eqs. (6.1) permit passage to the limit when $N,M\to\infty$, i.e., show that limits $C_n = \lim_{N,M\to\infty}\tilde{C}_n$ and $B_m = \lim_{N,M\to\infty}\tilde{B}_m$ exist and the sequences are summable quadratically, i.e., $\Sigma_{n=-\infty}^{\infty}|C_n|^2 < \infty$ and $\Sigma_{m=0}^{\infty}|B_m|^2<\infty$ and satisfy the infinite set of equations

$$C_p = \sum_{\substack{n=-\infty\\(n\neq p)}}^{\infty} C_n \frac{f_{n\langle p\rangle}}{1-f_{p\langle p\rangle}} + \sum_{m=0}^{\infty} B_m \frac{g_{m\langle p\rangle}}{1-f_{p\langle p\rangle}} + A\frac{f_{\langle p\rangle}^+ - \delta_0^p}{1-f_{p\langle p\rangle}}, \tag{6.2'}$$

$$B_j = \sum_{\substack{m=0\\(m\neq j)}}^{\infty} B_m \frac{g_{mj}}{1-g_{jj}} + \sum_{n=-\infty}^{\infty} C_n \frac{f_{nj}}{1-g_{jj}} + A\frac{f_j^+}{1-g_{jj}}, \tag{6.2''}$$

which is obtained from Eq. (6.1) by the formal passage to the limit. To prove that it will suffice to show that Eqs. (6.2) satisfy the Koch conditions[14] which reduce in this case to quadratic summability of coefficients and free terms.

Prove at first convergence of the series

$$S_1 = \sum_{n,p=-\infty}^{\infty} |f_{n\langle p\rangle}|^2, \quad S_2 = \sum_{m=0}^{\infty}\sum_{p=-\infty}^{\infty} |g_{m\langle p\rangle}|^2,$$

$$S_3 = \sum_{p=-\infty}^{\infty} |f_{\langle p\rangle}^+|^2, \quad S_4 = \sum_{mj=0}^{\infty} |g_{mj}|^2,$$

$$S_5 = \sum_{n=-\infty}^{\infty}\sum_{j=0}^{\infty} |f_{nj}|^2, \quad S_6 = \sum_{j=0}^{\infty} |f_j^+|^2.$$

It follows from the Parseval identity for Fourier series that

$$\sum_{p=-\infty}^{\infty} |f_{n\langle p\rangle}|^2 = \frac{1}{d}\int_0^d |f_n(x,0)|^2 dx,$$

$$\sum_{p=-\infty}^{\infty} |g_{m\langle p\rangle}|^2 = \frac{1}{d}\int_0^d |g_m(x,0)|^2 dx, \tag{6.3}$$

and that

$$S_3 = \frac{1}{d}\int_0^d |f^+(x,0)|^2 dx.$$

Thus, we proved convergence of $S_3$. When $\alpha_n > 0$, the value $I_n = (1/d)\int_0^d |f_n(x,0)|^2\,dx$ can be estimated as follows:

$$\frac{1}{d}\int_0^d |f_n(x,0)|^2\,dx$$
$$= \frac{k^4}{d}\int_0^d dx\left|\int_0^d dx'\int_0^\infty G(x,0,x',y')e'_n\,dy'\right|^2$$
$$< \frac{k^4}{d}\int_0^d dx\left\{\int_0^\infty e^{-\alpha_n y'}\,dy'\int_0^d |G(x,0,x',y')|\,dx'\right\}^2$$
$$< \frac{k^4 L^2}{\alpha_n^2}, \tag{6.3'}$$

where $L = \max\int_0^d |G(x,0,x',y')|\,dx'$. Using estimates (3.15) and (3.16), it is easy to see that $L < \infty$.

It evidently implies that the series $S_1$ converges and therefore the limit $f_{p\langle p\rangle} = 0$ exists.

To prove convergence of $S_2$ we use the second of identities (6.3). We obtain

$$S_{2,\nu} \equiv \frac{1}{d}\sum_{m=0}^{\nu}\int_0^d |g_m(x,0)|^2\,dx$$
$$= \frac{k^4}{d}\sum_{m=0}^{\nu}\int_0^d dx \times\left|\int\int_D \mathbf{u}_m(x',y')G(x,0,x',y')\,dx'\,dy'\right|^2$$
$$= \frac{k^4}{d}\int_0^d \sum_{m=0}^{\nu}\left|\int\int_D \mathbf{u}_m G(x,0,x',y')\,dx'\,dy'\right|^2 dx. \tag{6.4}$$

The Parseval identity for the function system $\{\mathbf{u}_m\}$ and the fact that $G\in\mathscr{L}_2(D)$ imply existence of the limit

$$\lim_{\nu\to\infty}\sum_{m=0}^{\nu}\left|\int\int_D \mathbf{u}_m G\,dx'\,dy'\right|^2 = \sum_{m=0}^{\infty}\left|\int\int_D \mathbf{u}_m G\,dx'dy'\right|^2$$
$$= \int\int_D |G|^2 dx'\,dy', \tag{6.5}$$

and it easily follows from here that

$$\lim_{\nu\to\infty} S_{2,\nu} = S_2$$
$$= \frac{k^4}{d}\int_0^d dx\int\int_D |G(x,0,x',y')|^2\,dx'dy' < \infty. \tag{6.6}$$

Convergence of the series $S_4, S_5, S_6$ is proved similarly, the sums for $S_4$ and $S_6$ being found explicitly:

$$S_4 = \int\int_D dx\,dy\int\int_D |G|^2 dx'\,dy',$$

$$S_6 = \int\int_D |f^+(x,y)|^2 dx\,dy.$$

Convergence of the series $S_4$ implies that $g_{jj}\to 0$ when $j\to\infty$. So denominators of matrix elements of Eqs. (6.2), i.e., $1 - f_{p\langle p\rangle}$ and $1 - g_{jj}$, tend to unity when $p\to\infty, j\to\infty$ and this together with the convergence of the series $S_1,\ldots,S_6$ guarantees that the Koch conditions are satisfied in Eqs. (6.2). Show at last that $U_M^{(N)}$ converges to the sought solution $\mathbf{u}$ when $M,N\to\infty$.

Note that as sequences of coefficients $\{C_n\}_{n=-\infty}^{+\infty}$ and $\{B_m\}_{m=0}^{\infty}$ are quadratically summable, the series

$$Ae_+ + \sum_{n=-\infty}^{\infty} C_n e_n, \quad y\geqslant 0;$$
$$\sum_{m=0}^{\infty} B_m u_m(x,y), \quad (x,y)\in D,$$

converge in $\mathscr{L}_2$ metric to a certain function $\sigma(x,y)\in\mathscr{L}_2$ and are defined as their sums in appropriate domains.

It was shown in Ref. 15 that solutions of finite sets of equations obtained by reducing infinite sets that satisfy the Koch conditions converge to the solution of the original set in $l_2$ metric. It means in our case that

$$\lim_{M,N\to\infty}\left[\sum_{n=-\infty}^{\infty}|\widetilde{C}_n - C_n|^2 + \sum_{m=0}^{\infty}|\widetilde{B}_m - B_m|^2\right] = 0, \tag{6.7}$$

where $\widetilde{C}_n = 0, |n| > N$ and $\widetilde{B}_m = 0, m > M$. Having written $U_M^{(N)}$ in the form

$$U_M^{(N)} = -k^2\left\{\int_0^d dx'\int_0^\infty\left(Ae'_+ + \sum_{n=-\infty}^{\infty} C_n e'_n\right)G\,dy'\right.$$
$$+\int\int_D\left[\sum_{m=0}^{\infty} B_m\mathbf{u}_m(x',y')\right]G\,dx'\,dy'$$
$$+\int_0^d dx'\int_0^\infty\sum_{n=-\infty}^{\infty}(\widetilde{C}_n - C_n)e'_n G\,dy'$$
$$\left.+\int\int_D\sum_{m=0}^{\infty}(\widetilde{B}_m - B_m)\mathbf{u}_m(x',y')G\,dx'\,dy'\right\}$$

and having used the estimate (6.7) and the Buniakovsky–Schwartz inequality, we show the existence of the limit

$$\lim_{M,N\to\infty} U_M^{(N)} \equiv v(x,y)$$
$$= -k^2\int_0^d dx'\int_0^\infty \sigma(x'y')G\,dy'$$
$$+\int\int_D \sigma(x',y')G\,dx'dy'. \tag{6.8}$$

Similarly, having passed to the limit in Eqs. (5.1) and taking into account Eqs. (6.8) and (4.1), we find

$$e^{-\alpha_n y}C_p + \delta_p^0 A\,e^{\alpha_n y} = \frac{1}{d}\int_0^d v(x,y)e^{-i\beta_r x}\,dx, \quad y\geqslant 0;$$

$$B_j = \int\int_D v(x,y)\mathbf{u}_j(x,y)\,dx.$$

From the Euler–Fourier formulas and completeness of function systems $\{e^{i\beta_r x}\}$ and $\{\mathbf{u}_j\}$ we conclude

$$\mathbf{v}(x,y)=\begin{cases} A\,e_* + \sum\limits_{p=-\infty}^{\infty} C_p e_p, & y\geqslant 0, \\ \sum\limits_{j=0}^{\infty} B_j \mathbf{u}_j(x,y), & (x,y)\in D, \end{cases} \tag{6.9}$$

i.e.,

$$\mathbf{v}(x,y)\equiv\sigma(x,y). \tag{6.10}$$

Substituting Eq. (6.10) into Eq. (6.8), we find that $v(x,y)$ satisfies the integral equation

$$\mathbf{v}(x,y) = -\mathbf{k}^2\int\int_{\Omega_0} \mathbf{v}(x',y')G\,dx'\,dy', \tag{6.11}$$

where $\Omega_0$ is the sum of the domains $(0<x<d, 0<y<\infty)$ and $D$. It is seen from Eq. (3.2) that $\mathbf{v}$ satisfies the quasiperiodicity condition and therefore is extended to all the domain $\Omega$. Using relations (3.12)–(3.16) and properties of potential-type integrals, it is easy to show that $\mathbf{v}(x,y)\in C^1(\Omega)$, the right side of Eq. (6.11), has generalized second derivatives and $\Delta\iint_{\Omega_0}\mathbf{v}G\,dx'\,dy' = \mathbf{v}(x,y)$ almost everywhere in $\Omega$; hence, $\Delta v = -\mathbf{k}^2\Delta\iint_{\Omega_0}\mathbf{v}G\,dx'\,dy' = -\mathbf{k}^2\mathbf{v}$, and $\mathbf{v}$ is a generalized solution of the Helmholtz equation.[10] The condition $\partial\mathbf{v}/\partial n|_\Gamma = 0$ follows from Eqs. (3.2) and (6.11); the validity of radiation conditions follows from Eq. (6.9). At last, from the theorem on uniqueness it follows that $\mathbf{v}(x,y) = \mathbf{u}(x,y)$, Q.E.D.

Passing to the limit $M,N\to\infty$ in Eq. (4.1), we find that the exact solution $u$ can be written as

$$\mathbf{u} = Af^*(x,y) + \sum_{n=-\infty}^{\infty} C_n f_n(x,y) + \sum_{m=0}^{\infty} B_m g_m(x,y). \tag{6.12}$$

It follows from the above estimates that the approximations $U_M^{(N)}$ uniformly converge to $\mathbf{u}$ in $\overline{\Omega}$. Note also that for all $M$ and $N$, $U_M^{(N)}$ has the needed singularities (satisfies the Meixner conditions exactly) in all boundary angle points. This follows from the method of constructing $U_M^{(N)}$ and can be immediately checked. It also follows from the given proof that determinants of equation sets (6.1) converge, when $M,N\to\infty$, to the determinant of the set (6.2). The latter determinant roots form the spectrum of the set eigenwaves and can be found as the limits for the roots of determinants in Eqs. (6.1) when $M,N\to\infty$.

## COMMENTS

(1) There are many publications where the Helmholtz equation is solved by means of conformal mapping (e.g., see Refs. 16–19). However, when conformal mapping is applied in a straightforward manner, it causes appearance of a variable refraction coefficient. It hinders further solution and permits one to receive only qualitative, asymptotic, or merely numerical results. Our method circumvents the difficulty as conformal mapping is used not directly for the Helmholtz equation but to the Poisson equation. That enabled receiving a semianalytical solution in the general case.

(2) In realizations of the described method for domains of complex configuration certain difficulties arise in constructing the conformal mapping $\zeta$ and in calculating integrals for matrix elements of Eqs. (5.1). The former difficulty is inherent in the problem considered because the Helmholtz equation transfers when $\mathbf{k}\to 0$ to the Laplace equation whose solution is equivalent to the construction of a conformal mapping. The latter difficulty is characteristic of all projection-type methods.[8] We regard the problem of constructing $\zeta$ as solved since numerical methods have been widely developed and many cases are known when the mapping can be found in the analytical form. As to matrix coefficients in Eq. (5.1), they can be simplified considerably, the order of integrals in them can be lowered, and some of the integrals can be even implicitly calculated. These equations as well as the development of the technique to solve Eqs. (5.1) will be treated in part II of the present work.

(3) In several cases our method permits one to obtain solutions in the analytical form.[6,20,21]

(4) It is evident that our method can be extended to more general operators whose dominant part can be effectively inverted. In the cases when the corresponding Green function is not quadratically summable (e.g., the Laplacian with $n>3$) the general scheme of the method must be somewhat changed, but we will not dwell on this question here.


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# A Bessel–Watson transform pair

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A Bessel–Watson type of transform pair is developed. Since this result differs from a previously published result, a comparison between these two results is also presented.

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## 1. INTRODUCTION

A new generalized transform pair is developed in Ref. 1. This transform pair is expected to be a generalization of the Fourier, Watson, and Kontorowich–Lebedev transforms which are frequently used in mathematical physics for solving boundary value problems. It appears, however, that the assumed properties, stated explicitly or implicitly and used in the proof for the development of the transform pair, are inconsistent. When these properties of the transform function, $E(\nu,\phi)$ are used in the integral representation of the solution, $E_z(\xi,\phi)$, it can be shown that $E_z(\xi,\phi)$ vanishes identically.

In this paper we first develop a Bessel–Watson type transform in Sec. 2 and then show in Sec. 3 why the previous result of Ref. 1 is inconsistent.

## 2. DEVELOPMENT OF THE TRANSFORM PAIR

A foundation on which many integral transform pairs in mathematical physics are based can be developed[2,3] from an appropriate spectral representation of Dirac's delta function in terms of a Green's function associated with a differential operator subject to appropriate boundary conditions. It may be emphasized that the Green's function is different for different transform pairs. The same technique can also be employed for the development of the transform pair presently being discussed in this paper. Let us consider the following differential equation defining a Green's function $G(\xi,\xi_0;\nu)$.

$$\frac{1}{\xi}\frac{d}{d\xi}\left(\xi\frac{d}{d\xi}G(\xi,\xi_0;\nu)\right)+\left(1-\frac{\nu^2}{\xi^2}\right)G(\xi,\xi_0;\nu) = -\frac{\delta(\xi-\xi_0)}{\xi}, \tag{2.1}$$

where $G(\xi_R,\xi_0;\nu)=0$ and $G(\xi,\xi_0;\nu)$ satisfies the radiation condition at $\xi=\infty$. The quantity $\nu^2$ is a complex parameter. Then the spectral representation of $\delta(\xi-\xi_0)$ can be shown[2,3] to have the form

$$\xi\delta(\xi-\xi_0) = -\frac{1}{2\pi i}\oint_C G(\xi,\xi_0;\nu)\,d\lambda, \quad \lambda=\nu^2, = -\frac{1}{\pi i}\int_C G(\xi,\xi_0;\nu)\,\nu\,d\nu, \tag{2.2}$$

where the contour $C$ encloses all the singularities of $G(\xi,\xi_0;\nu)$ in the complex $\nu$ plane in a clockwise sense (see Fig. 1). For the present problem defined by (2.1), the Green's function $G(\xi,\xi_0;\nu)$ is given by

$$G(\xi,\xi_0;\nu) = -(i\pi/4)\psi_\nu(\xi)H_\nu^{(2)}(\xi_0), \quad \xi_0<\xi = -(i\pi/4)\psi_\nu(\xi_0)H_\nu^{(2)}(\xi), \quad \xi_0<\xi. \tag{2.3}$$

The function $\psi_\nu(\xi)$ is defined by

$$\psi_\nu(\xi)=H_\nu^{(1)}(\xi)+R_\nu H_\nu^{(2)}(\xi), \tag{2.4a}$$

and

$$R_\nu = -H_\nu^{(1)}(\xi_R)/H_\nu^{(2)}(\xi_R), \tag{2.4b}$$

$\xi=Kr, \xi_R=KR$, $R$ is the radius of a cylinder, and $K$ = propagation constant. The quantities, $H_\nu^{(1)}(\xi)$ and $H_\nu^{(2)}(\xi)$ are Hankel functions of the first and second kind, respectively. Thus the desired spectral representation of the Dirac delta function is given by the following expression,

$$\xi\delta(\xi-\xi_0)=\frac{1}{4}\int_C \psi_\nu(\xi_<)H_\nu^{(2)}(\xi_>)\nu\,d\nu, \tag{2.5}$$

where $\xi_<$ is the smaller of $\xi$ and $\xi_0$. Similarly, $\xi_>$ is the larger of $\xi$ and $\xi_0$. Since the only singularities of $G(\xi,\xi_0;\nu)$ are the poles of $\psi_\nu(\xi_<)$ located at the zeros of $H_\nu^{(2)}(\xi_R)$, the

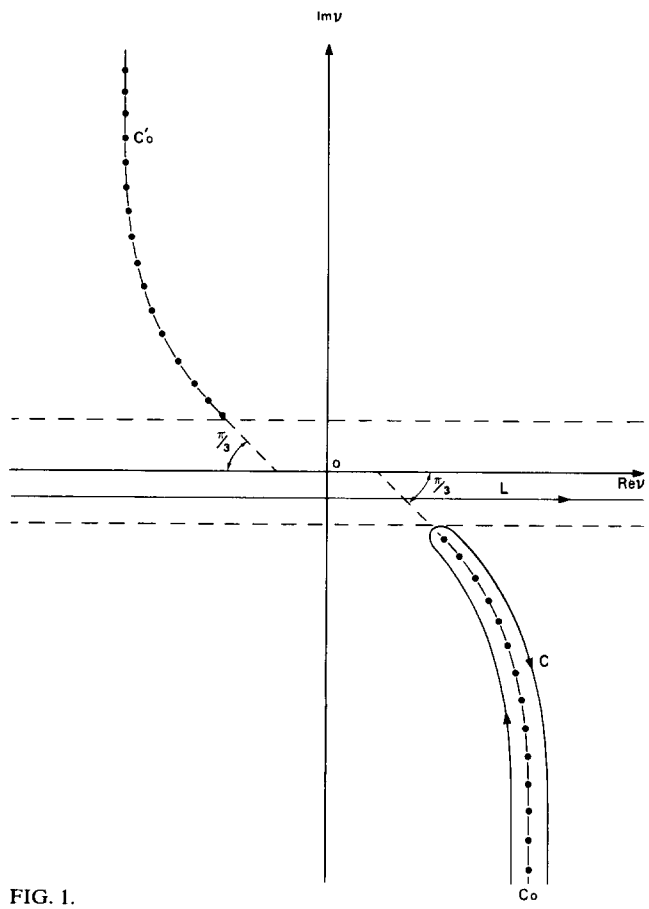


FIG. 1.

contour of integration $C$ in (2.5) encloses these zeros in the fourth quadrant of the $\nu$ plane (see Fig. 1). In view of (2.5) the desired integral transform pair may be expressed in the following manner:

$$E_z(\xi,\phi) = \int_C E(\nu,\phi)\psi_\nu(\xi)\,d\nu, \tag{2.6a}$$

and

$$\frac{E(\nu,\phi)}{\nu} = \frac{1}{4}\int_{\xi_R}^{\infty} E_z(\xi,\phi)\,H_\nu^{(2)}(\xi)\,\frac{d\xi}{\xi}, \tag{2.6b}$$

where $\phi$ is a parameter. In a boundary value problem $r$ and $\phi$ (with $\xi = Kr$) represent a polar coordinate system. We require that $E(\nu,\phi)$ decreases faster than $\nu H_\nu^{(2)}(\xi_>)$ in the lower half of the complex $\nu$ plane as $|\nu|$ approaches infinity, although $E(\nu,\phi)$ may have pole singularities in the neighborhood of, or along, the real axis. The necessity for such behavior of $E(\nu,\phi)$ at infinity will become clear later on. In order to prove the validity of (2.6a) and (2.6b) let us consider the following analysis,

$$\begin{aligned} E_z(\xi,\phi) &= \int_C E(\nu,\phi)\,\psi_\nu(\xi)\,d\nu \\ &= \int_C \psi_\nu(\xi)\,\frac{\nu\,d\nu}{4}\int_{\xi_R}^{\infty} E_z(\xi_0,\phi)\,H_\nu^{(2)}(\xi_0)\,\frac{d\xi_0}{\xi_0}. \end{aligned} \tag{2.7}$$

In view of (2.5) and its development, the spectral theory guarantees[2,3] that the interchange of the order of the integration in (2.7) is permissible. Then the right-hand side of (2.7) becomes $E_z(\xi,\phi)$ in view of (2.5). Thus the validity of the transform pair (2.6a) and (2.6b) is established.

Let us now investigate whether the contour $C$ can be shifted to anywhere in the lower half of the complex $\nu$ plane. In order to accomplish this it is first necessary to study the behavior of the respective integrands when $|\nu|$ approaches infinity in the lower half-plane. For this purpose let us first consider the integral in (2.5). From the asymptotic behavior[4,5] of the Bessel and Hankel functions for large order $\nu$ and with a fixed finite argument, it can be shown that

$$\nu\psi_\nu(\xi_<)\cdot H_\nu^{(2)}(\xi_>) \sim \frac{2i}{\pi}\left[\left(\frac{\xi_<}{\xi_>}\right)^\nu - \left(\frac{\xi_R^2}{\xi_<\xi_>}\right)^\nu\right] \tag{2.8}$$

in the region to the right side of the curve $C_0$ as $|\nu|$ approaches infinity in the fourth quadrant of the complex $\nu$ plane. The zeros of $H_\nu^{(2)}(\xi_R)$ are situated along the curves $C_0$ and $C_0'$ in the fourth and second quadrants, respectively. Initially the tangent to the curve $C_0$ makes[4-6] an angle of $-\pi/3$ with the real axis for a real value of $\xi_R$ and then becomes parallel to the imaginary axis as $|\nu|$ tends to infinity. In addition, one finds also that

$$\begin{aligned} &\nu\psi_\nu(\xi_<)\,H_\nu^{(2)}(\xi_>) \\ &\quad\sim \frac{-2i}{\pi}\left[\left(\frac{\xi_>}{\xi_<}\right)^\nu - \left(\frac{\xi_>\xi_<}{\xi_R^2}\right)^\nu\right] \end{aligned} \tag{2.9}$$

as $|\nu|$ approaches infinity in the third quadrant, as well as to the left of $C_0$ in the fourth quadrant of the complex $\nu$ plane. It may be noted that $C_0'$ can be obtained from $C_0$ by changing the sign of $\nu$. Let us also define a contour $L$ which is parallel to the real axis and lies between the real axis and the lowest order zero of $H_\nu^{(2)}(\xi_R)$ in the lower half of the $\nu$ plane. If $\xi_< \neq \xi_>$, the expression (2.8) vanishes as $|\nu|\to\infty$ and, therefore, the portion of $C$ running along the right side of $C_0$ can be deformed onto the portion of $L$ situated to the right side of the lowest order zero of $H_\nu^{(2)}(\xi_R)$. It may be noted that $\xi_R \leqslant \xi_< < \xi_>$. In view of the relation (2.9) the integrand (2.5) vanishes in the third quadrant; however, it diverges in the region of the fourth quadrant lying to the left of $C_0$ as $|\nu|$ approaches infinity. Therefore, the portion of the contour $C$ lying to the left of $C_0$ cannot be deformed onto the remaining portion of $L$.

Before considering the investigation of the deformability of the contour $C$ associated with the transform in (2.6a), let us first note that on $C_0$ where $H_\nu^{(2)}(\xi_R)$ vanishes, the quantity $|(2\nu/e\xi_R)^{\pm\nu}|$ approaches unity as $|\nu|\to\infty$ and the phase of $\nu$ is $-\pi/2+\epsilon_0$, $0<\epsilon_0\ll 1$. Then it can be shown that $\epsilon_0 \simeq \frac{1}{2}\pi/(\ln(2|\nu|/e\xi_R)) \ll 1$, where $\xi_R$ is a real positive finite number. The phase of $\nu$ in the region between $C_0$ and the negative imaginary axis is $-\pi/2+\epsilon$ ($\epsilon \leqslant \epsilon_0$), when $|\nu|$ approaches infinity. Therefore, in view of (2.9) one finds that

$$|\nu\psi_\nu(\xi_<)\,H_\nu^{(2)}(\xi_>)| \sim e^{|\nu|\epsilon\ln\tau}, \quad \tau>1, \tag{2.10}$$

in the region to the left of $C_0$ in the fourth quadrant as $|\nu|$ tends to infinity.

Let us now investigate whether $C$ in (2.6a) can be deformed onto $L$ if so, under what conditions. Since it is assumed that $E(\nu,\phi)$ decreases faster than $\nu H_\nu^{(2)}(\xi_>)$ in the lower half of the $\nu$ plane as $|\nu|$ approaches infinity, a comparison of the integrands of (2.5) and (2.6a) shows that the portion of the contour $C$ in (2.6a) lying to the right side of $C_0$ can be deformed onto a portion of $L$ in this case also, noting that this was possible for (2.5). The assumption that $E(\nu,\phi)$ decreases faster than $\nu H_\nu^{(2)}(\xi_>)$ at infinity in the $\nu$ plane is justified in many practical problems of interest. For instance, in a problem of scattering or diffraction of waves (acoustic or electromagnetic) by a cylinder, $E(\nu,\phi)$ contains a factor like $\exp(-i\nu\phi)$, where $\phi$ is the angular coordinate. If $\phi \neq 0$, then this expotential factor contributes to the rapid decay of the integrand in (2.6a) for $\mathrm{Im}\,\nu < 0$ as $|\nu|$ approaches infinity. For example, in many problems of interest one finds

$$E(\nu,\phi) \sim \nu H_\nu^{(2)}(\xi_>)\,e^{-i\nu\phi}, \tag{2.11a}$$

i.e.,

$$E(\nu,\phi)\,\psi_\nu(\xi) \sim G(\xi,\xi_0;\nu)\,e^{-i\nu\phi}, \tag{2.11b}$$

as $|\nu|\to\infty$.

By virtue of the property (2.9), it can easily be seen that the integrand $E(\nu,\phi)\,\psi_\nu(\xi)$ of (2.6a) vanishes in the third quadrant of the $\nu$ plane as $|\nu|$ approaches infinity. However, the relation (2.10) shows that in the fourth quadrant, between the negative imaginary axis and $C_0$, the integrand of (2.6a) behaves in the following manner as $|\nu|\to\infty$:

$$|E(\nu,\phi)\,\psi_\nu(\xi)| \sim e^{|\nu|(\epsilon\ln\tau-\phi)}, \tag{2.12}$$

where

$$\epsilon \leqslant \epsilon_0 \simeq \tfrac{1}{2}\pi/\ln(2|\nu|/e\xi_R) \ll 1.$$

Since $\tau>1$, the right-hand side of (2.12) vanishes if the following condition on $\phi$ and $\tau$ is satisfied

$$\epsilon\ln\tau < \phi,$$

$$\epsilon \ln\tau < \phi\,,$$
$$\text{or} \quad \tau < e^{\phi/\epsilon}\,, \tag{2.13}$$
$$\text{or} \quad \tau^{\pi/2\phi} < 2|\nu|/e\xi_R\,.$$

Note that the inequality (2.13) defines a relationship among the parameters, $\phi$, $\xi_<$, $\xi_>$, and $\xi_R$ for which (2.12) vanishes. Therefore, if condition (2.13) is satisfied, the contour $C$ in (2.6a) can be deformed onto $L$. It may be noted that since $\phi = 0$ in (2.5), condition (2.13) cannot be fulfilled and consequently the contour $C$ in (2.5) cannot be deformed onto the portion of $L$ lying to the left of the lowest order zero of $H_\nu^{(2)}(\xi_R)$.

It may be observed that expression (2.5) also gives the spectral representation of Dirac's delta function in terms of radial eigenfunctions. This can easily be seen by applying Cauchy's residue theorem in (2.5). In view of this observation, expression (2.6a) represents the radial eigenfunction expansion of the function of $E_z(\xi,\phi)$.

The transform pair (2.6a) and (2.6b) is suitable for a function $E_z(\xi,\phi)$ which satisfies a Dirichlet boundary condition at $\xi_R$. Similar transform pairs can also easily be obtained for functions which satisfy either a Neumann or mixed boundary condition at $\xi_R$. For all such problems, the starting point should be to construct an appropriate Green's function and then follow the steps similar to (2.2), (2.5)–(2.7). It may now be emphasized that in all such integral transforms, the initial contour of integration in the $\nu$ plane must enclose all the singularities (poles and branch cuts, if any) of the Green's function concerned, and then the asymptotic behavior of the integrand must be investigated before the initial contour can be deformed onto a new one.

## 3. COMPARISON OF THE PRESENT RESULT WITH A PREVIOUS ONE

The generalized transform pair developed in Ref. 1 is given by

$$E_z(\xi,\phi) = \int_L E(\nu,\phi)\cdot\psi_\nu(\xi)\,d\nu\,, \tag{3.1}$$

and

$$E(\nu,\phi) = \frac{1}{4}\int_{\xi_R}^{\infty} E_z(\xi,\phi)\,H_\nu^{(2)}(\xi)\,\nu\,\frac{d\xi}{\xi}\,, \tag{3.2}$$

where $r$, $\phi$, and $z$ represent a cylindrical coordinate system. The function $\psi_\nu(\xi)$ and $R_\nu$ are given by (2.4a) and (2.4b), respectively. The apparent discrepancy between these pairs of transforms (2.6a), (2.6b) and (3.1), (3.2) is in the choice of the contours $C$ and $L$, respectively. In addition, the method of approach in deriving (3.1) and (3.2) is entirely different from that used for (2.6a) and (2.6b). In the development of the pair (3.1) and (3.2), it is assumed implicitly that $E(\nu,\phi)$ is analytic in a horizontal strip bounded by two lines parallel to the real axis of the complex $\nu$ plane (one below and the other above). The integration path $L$ lies inside this strip. The boundary line lying in the lower half-plane is above the lowest order zero of $H_\nu^{(2)}(\xi_R)$ and the other boundary line is just a mirror image of this line with respect to the real axis. Since $\psi_\nu(\xi)$ is also analytic inside this strip, the path $L$ in (3.1) can be shifted onto the entire real axis of the $\nu$ plane. It is evident from the properties (3.3a) and (3.3b) that the integrand in (3.1) is an odd function $\nu$ and, therefore, the integral (3.1) vanishes identically.

$$H_{-\nu}^{(1,2)}(\xi) = \exp(\pm i\nu\pi)\cdot H_\nu^{(1,2)}(\xi)\,, \tag{3.3a}$$

and hence

$$E(-\nu,\phi) = -E(\nu,\phi)\exp(-i\pi\nu)\,, \tag{3.3b}$$

which follows from (3.3a) and (3.2).

It was shown earlier that the contour $C$ can be deformed onto $L$ provided the condition (2.13) is satisfied. Consequently, the following Dirac delta function representation as given in Ref. 1 is not valid.

$$\xi\delta(\xi-\xi_0) = \frac{1}{4}\int_L \psi_\nu(\xi)\,H_\nu^{(2)}(\xi_0)\,\nu\,d\nu\,. \tag{3.4}$$

It may now be observed that the representation s(2.6a) and (3.1) are equivalent provided the condition (2.13) is satisfied and the assumption of the analyticity of $E(\nu,\phi)$ is not imposed. However, when the contour $L$ is used, the transform pair (3.1) and (3.2) cannot be used for any arbitrary function, $E_z(\xi,\phi)$, which has a strong singularity like a delta function, $\delta(\xi-\xi_0)$. On the other hand, the transform pair (2.6a) and (2.6b) can represent a field as singular as $\delta(\xi-\xi_0)$.

The derivation of (3.1) and (3.2) presented in Ref. 1 is based on a method similar to that given by Kontorowich and Lebedev.[7] One of the main differences between these two transform pairs[1,7] is that the contour of integration $L$ is horizontal (below the real axis) in Ref. 1, whereas it is vertical for the Kontorowich–Lebedev transform.[7] It is very important to note that the transform function in Kontorowich–Lebedev transform is analytic inside a vertical strip including the imaginary axis of the $\nu$ plane. In the same way, in Ref. 1 the transform function $E(\nu,\phi)$ was implicitly treated as analytic inside a horizontal strip containing the real axis in the $\nu$ plane [see the development of Eqs. (2.6b)–(2.7b) of Ref. 1]. However, in many physical problems $E(\nu,\phi)$ may contain many pole singularities [see Eqs. (3.5)–(3.7) of Ref. 1] inside such a horizontal strip. This is the reason why the proof and the transform pair as given in Ref. 1 are invalid. Consequently, the derivation of the Kontorowich–Lebedev transform presented in Ref. 1, as a special case, is also invalid.


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# Nonorthogonal $R$-separable coordinates for four-dimensional complex Riemannian spaces

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We classify all $R$-separable coordinate systems for the equations $\Delta_4\Psi = \Sigma_{i,j=1}^4 g^{-1/2}\partial_j(g^{1/2}g^{ij}\partial_i\Psi) = 0$ and $\Sigma_{i,j=1}^4 g^{ij}\partial_i W\partial_j W = 0$ with special emphasis on nonorthogonal coordinates, and give a group theoretic interpretation of the results. For flat space we show that the two equations separate in exactly the same coordinate systems and present a detailed list of the possibilities. We demonstrate that every $R$-separable system for the Laplace equation $\Delta_4\Psi = 0$ on a conformally flat space corresponds to a separable system for the Helmholtz equations $\Delta_4\Phi = \lambda\Phi$ on one of the manifolds $E_4$, $S_1\times S_3$, $S_2\times S_2$, and $S_4$.

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## 1. INTRODUCTION

In this article we study the problem of $R$ separation of variables for the Laplace and Hamilton–Jacobi equations

$$\text{(a)}\Delta_4\Psi = \sum_{i,j=1}^4 g^{-1/2}\partial_i(g^{1/2}g^{ij}\partial_j\Psi) = 0\,,$$
$$\text{(b)}\sum_{i,j=1}^4 g^{ij}\partial_i W\partial_j W = 0\,. \tag{1.1}$$

ric, $g = \det(g_{ij}) \neq 0$, $\Sigma_{i,j=1}^4 g^{ij}g_{jk} = \delta_k^i$, $g_{ij} = g_{ji}$, and $\partial_j\Psi = \partial_{x^j}\Psi$. Some aspects of $R$ separation for these equations have been treated in an earlier paper.[1] In that paper we studied the *orthogonal* coordinate systems for which Eqs. (1.1) are $R$ separable. For conformally flat spaces it was shown that each $R$-separable orthogonal coordinate system for Eq. (1.1a) corresponds to coordinates which permit pure separation for the Helmholtz equation $\Delta_4\Phi = \lambda\Phi$ on one of the manifolds $E_4$ (flat space), $S_1\times S_3$, $S_2\times S_2$, or $S_4$, where $S_j$ is the $j$ dimensional sphere. In this paper we show that the same basic results hold for *nonorthogonal* coordinate systems. However, our methods here differ considerably from those of Ref. 1. It is easy to show that if a coordinate system $\{x^j\}$ (orthogonal or not) is $R$ separable for Eq. (1.1a) on a given Riemannian space, then it is also additively separable for Eq. (1.1b). For orthogonal coordinates on conformally flat spaces the condition that an additively separable system for Eq. (1.1b) also $R$ separates Eq. (1.1a) could be completely solved by employing the Robertson condition in the geometrical form due to Eisenhart.[2,3] However, the Robertson condition no longer holds in general for nonorthogonal coordinates[4] and in this paper we find it necessary to employ detailed facts concerning the structure of the conformal symmetry group of Eq. (1.1b) in order to obtain our results. Indeed the use of Lie theory appears to be absolutely essential in this regard.

The paper is arranged as follows: In Sec. 2 we classify the possible types of separable systems for the Hamilton–Jacobi equation (1.1b) and in Sec. 3 we give the corresponding (crude) classification of $R$-separable systems for the Laplace equation (1.1a). Then in Sec. 4 we study in detail the nonorthogonal separable systems for conformally flat spaces and obtain an explicit list. Finally, in Sec. 5 we use our detailed results to show that, even allowing nonorthogonal coordinates, the flat space equations (1.1a) and (1.1b) separate in exactly the same systems and that on a conformally flat space every $R$-separable system for Eq. (1.1a) corresponds to a separable system for the Helmholtz equation on one of the manifolds $E_4$, $S_1\times S_3$, $S_2\times S_2$, and $S_4$. Nonorthogonal coordinates arise only from $E_4$ and $S_4$. The extreme importance of these constant curvature manifolds for variable separation on conformally flat spaces is now clear.

The authors have already given an exhaustive study of nonorthogonal separation for the Helmholtz equations on $E_4$, $S_2$, and $S_3$.[4,5,7] The remaining case $S_4$ will be treated in a forthcoming paper. This paper will then conclude our analysis of variable separation for the Hamilton–Jacobi, Helmholtz, and Laplace equations on three and four dimensional Riemannian spaces.[6–9]

## 2. SEPARABLE SYSTEMS FOR THE HAMILTON–JACOBI EQUATION

We now discuss the classification of separable systems for Eq. (1.1b). Recall that separation of variables for this equation means $W = \Sigma_{i=1}^4 W^{(i)}(x^i)$. The existence of separable systems for Eq. (1.1b) is closely related to the symmetries of this equation. To define symmetry operators we employ a phase space formalism. The coordinates of this space are $(x^j, p_j)$, where $p_j = \partial_{x^j}W, j = 1,2,3,4$. The Poisson bracket of two functions $F$, $G$ on phase space is the function

$$\{F,G\}(x,p) = \sum_{j=1}^4 (\partial_{x^j}G\partial_{p_j}F - \partial_{x^j}F\partial_{p_j}G)\,. \tag{2.1}$$

A *first order symmetry* of Eq. (1.1b) is a function

$$\mathscr{L} = \sum_{i=1}^4 \xi^i(x)\,p_i \tag{2.2}$$

such that $\{\mathscr{L}, \Sigma_{i,j=1}^4 g^{ij}p_i p_j\} = \rho(x)\,(\Sigma_{i,j=1}^4 g^{ij}p_i p_j)$ for

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some analytic function $\rho$. The $\{\xi^i(x)\}$ are just the conformal Killing vector fields for the metric $\{g_{ij}\}$. The first order symmetries form a Lie algebra $\mathscr{H}$ under the Poisson bracket with $\dim\mathscr{H}\leqslant 15$ and the maximum dimension is achieved if and only if $g_{ij}$ is conformally flat, in which case $\mathscr{H}\cong O(6,C)$. A (*strictly*) *second order symmetry* is a function

$$\mathscr{L}' = \sum_{i,j=1}^{4} \eta^{ij}(x)\, p_i\, p_j, \quad \eta^{ij} = \eta^{ji}, \tag{2.3}$$

such that

$$\left\{\mathscr{L}', \sum_{i,j=1}^{4} g^{ij}\, p_i\, p_j\right\} = \mu(s,p)\left(\sum_{i,j=1}^{4} g^{ij}\, p_i\, p_j\right),$$

where $\mu(x,p)$ is a linear function of the $p_l$. The vector space of second order symmetries can be decomposed into orbits under the adjoint action of $\mathscr{H}$. We will show explicitly that every class of separable solutions $W$ of Eq. (1.1b) is characterized by a triplet of first or second order symmetries $\mathscr{L}_1$, $\mathscr{L}_2$, $\mathscr{L}_3$ which are in involution, i.e., $\{\mathscr{L}_i, \mathscr{L}_j\} = 0$ for $i \neq j$. The exact characterization is $\mathscr{L}_i = \lambda_i$ $(i = 1,2,3)$, where the $\lambda_i$ are the separation constants.

Our classification of separable systems is based on the number of ignorable and essential variables. A variable $x^i$ in a separable system is termed *ignorable* if $\mathscr{L} = p_i$ is a symmetry for Eq. (1.1b), where $p_i = \partial_{x^i} W$. Otherwise the variable $x^i$ is *essential*. If the separated ordinary differential equation in the essential variable $x^i$ is first degree, then $x^i$ is of *type* 1; if second degree, then $x^i$ is of *type* 2.

We consider a separable system for Eq. (1.1b) with two essential variables of type 2 $(x^1,x^2)$, one essential variable of type 1 $(x^3)$, and one ignorable variable $(x^4)$. (This is called a type $G$ equation.) With $W = \Sigma_{i,j=1}^{4} W^{(j)}(x^j)$, $W_j = \partial_j W$ we can write the separated ordinary differential equations in the form

$$\begin{aligned} &W_1^2 + f_1 W_4^2 + \lambda_1 a_1 + \lambda_2 b_1 \equiv \Phi_1 = 0, \\ &W_2^2 + f_2 W_4^2 + \lambda_1 a_2 + \lambda_2 b_2 \equiv \Phi_2 = 0, \\ &W_3 W_4 + \lambda_1 a_3 + \lambda_2 b_3 \equiv \Phi_3 = 0, \\ &W_4 = \lambda_3, \end{aligned} \tag{2.4}$$

where $f_j$, $a_j$, $b_j$ are function of $x^j$ and $\lambda_1, \lambda_2, \lambda_3$ are the separation constants. Making the trivial change of variable $x^j = X^j(\tilde{x}^j)$ if necessary, we can assume without loss of generality that $a_1 = b_2 = a_3 = 1$. To relate Eq. (1.1b) with Eqs. (2.4) we seek functions $\Theta_j(x^1,\ldots,x^4)$ such that

$$\sum_{j=1}^{3} \Theta_j \Phi_j \equiv \sum_{i,j}^{4} g^{ij} W_i W_j \tag{2.5}$$

identically in the separation constants, i.e., the coefficients of $\lambda_1, \lambda_2, \lambda_3$ should vanish in Eq. (2.5). As is easily verified, this condition determines the $\Theta_j$ up to an arbitrary multiple $Q(x^1,\ldots,x^4)$ and leads to the Hamilton–Jacobi equation

$$\begin{aligned} \text{(G)}\quad & Q\left[(a_2 b_3 - 1)(W_1^2 + f_1 W_4^2) + (b_1 - b_3)\right. \\ & \left.\times(W_2^2 + f_2 W_4^2) + (1 - a_2 b_1) W_3 W_4\right] = 0, \end{aligned} \tag{2.6}$$

with symmetry operators

$$\begin{aligned} \mathscr{L}_1 &= (a_2 b_1 - 1)^{-1}\,(p_1^2 + f_1 p_4^2 - b_1(p_2^2 + f_2 p_4^2)), \\ \mathscr{L}_2 &= (a_2 b_1 - 1)^{-1}\,(p_2^2 + f_2 p_4^2 - a_2(p_1^2 + f_1 p_4^2)), \\ \mathscr{L}_3 &= p_4. \end{aligned} \tag{2.7}$$

The most general metric tensor yielding separation of this type can be read off from Eq. (2.6) and the separation is characterized by $\mathscr{L}_j = \lambda_j, j = 1,2,3$.

In addition to the type $G$ separable equations above, the following Hamilton–Jacobi equations admit separation:

(A) Four ignorable variables:

$$\text{(A)}\quad Q\sum_{i=1}^{4} p_i^2 = 0, \mathscr{L}_i = p_i^2, \quad i = 1,2,3; \tag{2.8}$$

(B) Three ignorable variables:

$$\text{(B)}\quad Q\sum_{i,j=1}^{4} G^{ij}(x^4)\, p_i\, p_j = 0, \mathscr{L}_i = p_i, \quad i = 1,2,3; \tag{2.9}$$

(C) Two ignorable variables with two essential variables of type 2:

$$\begin{aligned} \text{(C)}\quad & Q\left[p_1^2 + p_2^2 + (e_1 + e_2) p_3^2 + 2(h_1 + h_2) p_3 p_4\right. \\ & \left. + (f_1 + f_2) p_4^2\right] = 0, \\ & \mathscr{L}_1 = p_3, \quad \mathscr{L}_2 = p_4, \\ & \mathscr{L}_3 = p_1^2 + e_1 p_3^2 + 2h_1 p_3 p_4 + f_1 p_4^2; \end{aligned} \tag{2.10}$$

(D) Two ignorable variables with one essential variable of each type: [It can be shown that (D2) is a special case of (D1).]

$$\begin{aligned} \text{(D1)}\quad & Q\left[p_1^2 + 2a_2 p_2 p_3 + 2b_2 p_2 p_4 + d_1 p_3^2\right. \\ & \left. + 2(f_1 + f_2) p_3 p_4 + e_1 p_4^2\right] = 0, \\ & \mathscr{L}_1 = p_3, \mathscr{L}_2 = p_4, \mathscr{L}_3 = 2a_2 p_2 p_3 + 2b_2 p_2 p_4 \\ & + 2f_2 p_3 p_4, \end{aligned} \tag{2.11}$$

$$\begin{aligned} \text{(D2)}\quad & Q\left[p_1^2 + 2p_2 p_4 + (d_1 + d_2) p_3^2\right. \\ & \left. + 2f_1 p_3 p_4 + e_1 p_4^2\right] = 0, \\ & \mathscr{L}_1 = p_3, \mathscr{L}_2 = p_4, \mathscr{L}_3 = 2p_2 p_4 + d_2 p_3^2; \end{aligned} \tag{2.12}$$

(E) Two ignorable variables with two essential variables of type 1:

$$\begin{aligned} \text{(E1)}\quad & Q(2a_1 p_1 p_3 + 2p_1 p_4 + 2a_2 p_2 p_3 + 2p_2 p_4 \\ & + (c_1 - c_2) p_3^2) = 0, \\ & \mathscr{L}_1 = p_3, \mathscr{L}_2 = p_4, \mathscr{L}_3 = 2a_2 p_2 p_3 + 2p_2 p_4 + c_2 p_3^2, \end{aligned} \tag{2.13}$$

$$\begin{aligned} \text{(E2)}\quad & Q(2p_1 p_4 + 2p_2 p_3 + 2b_2 p_2 p_4 \\ & + (d_1 + d_2) p_3^2) = 0, \quad b_2 \neq 0, \\ & \mathscr{L}_1 = p_3, \mathscr{L}_2 = p_4, \mathscr{L}_3 = 2p_2 p_3 + 2b_2 p_2 p_4 + c_2 p_3^2, \end{aligned} \tag{2.14}$$

$$\begin{aligned} \text{(E3)}\quad & Q(2p_1 p_4 + 2p_2 p_3 + c_1 p_3^2 + d_2 p_4^2) = 0, \\ & \mathscr{L}_1 = p_3, \mathscr{L}_2 = p_4, \mathscr{L}_3 = 2p_2 p_3 + d_2 p_4^2; \end{aligned} \tag{2.15}$$

(F) One ignorable variable with three essential variables of type 2:

$$\begin{aligned} \text{(F)}\quad & Q((q_2 - q_3) p_1^2 + (q_3 - q_1) + p_2^2 + (q_1 - q_2) p_3^2 \\ & + [r_1(q_2 - q_3) + r_2(q_3 - q_1) + r_3(q_1 - q_2)]\, p_4^2) \\ & = 0, \\ & \mathscr{L}_1 = p_4^2, \mathscr{L}_2 = \mathscr{Q}\left[(q_3^2 - q_2^2)\mathscr{P}_1^2\right. \\ & \left. + (q_1^2 - q_3^2)\mathscr{P}_2^2 + (q_2^2 - q_1^2)\mathscr{P}_3^2\right], \\ & \mathscr{L}_3 = \mathscr{Q}\left[q_2 q_3 (q_2 - q_3)\mathscr{P}_1^2 + q_1 q_3 (q_3 - q_1)\mathscr{P}_2^2\right. \\ & \left. + q_1 q_2 (q_1 - q_2)\mathscr{P}_3^2\right], \end{aligned} \tag{2.16}$$

where

$$\mathcal{Q} = [(q_1 - q_2)(q_1 - q_3)(q_2 - q_3)]^{-1}, \mathcal{P}_i^2 = p_i^2 + r_i p_4^2,$$

$i = 1,2,3;$

(H) No ignorable variables

$$\text{(H)} \quad Q\left(\sum_{j=1}^{4} M_{j,1}\, p_j^2\right) = 0, \qquad \mathcal{L}_i = \sum_{j=1}^{4} M_{j,i+1}\, p_j^2, \quad i = 1,2,3, \tag{2.17}$$

where $M_{jl}$ is the $(j,l)$ minor of a $4\times4$ Stäckel matrix $[\Phi_{km}(x^k)]$.

Just as noted in the case of three dimensions, there are no strictly $R$-separable solutions of the Hamilton–Jacobi equation which are not equivalent to one of the separable types listed above.[6] [An $R$-separable solution would have the form $W = W^0(x^1, x^2, x^3, x^4) + \Sigma_{j=1}^4 W^{(j)}(x^j)$.]

## 3. $R$-SEPARABLE SYSTEMS FOR THE LAPLACE EQUATION $\Delta_4\Psi = 0$

Here we classify the systems for which the Laplace equation (1.1a) admits $R$ separation of variables. Again the separable systems can be characterized by a triplet of commuting symmetry operators. Recall that

$$L = \sum_{j=1}^{4} \xi^j(x)\partial_{x^j} + \xi(x) \tag{3.1}$$

is a *first order symmetry operator* for Eq. (1.1a) if $[L, \Delta_4] = \rho(x)\Delta_4$ for some analytic function $\rho$. The set of all first order symmetries $L$ forms a Lie algebra $G$ under the commutator bracket $[A,B] = AB - BA$, called the *symmetry algebra* of Eq. (1.1a). The $\xi^j$ satisfy the Killing equations for a conformal Killing vector relative to the metric $g_{ij}$ and (factoring out the ideal generated by the trivial symmetry $L = 1$) $G$ is a subalgebra of the infinitesimal conformal group of the metric. When $g_{ij}$ corresponds to flat space then $\mathcal{G} \cong O(6,\mathbb{C})$, a 15-dimensional complex Lie algebra.

Similarly,

$$L' = \sum_{i,k=1}^{4} \eta^{jk}(x)\partial_{x^j x^k} + \sum_{l=1}^{4} \eta^l(x)\partial_{x^l} + \eta(x) \tag{3.2}$$

is a *second order symmetry operator* for $\Delta_4$ if $[L', \Delta_4] = K\Delta_4$, where $K$ is a first order differential operator of the form (3.1) (but $K$ is not necessarily a symmetry). If every $L'$ acting on the solution space of Eq. (1.1a) agrees with a linear combination of first and second order operators in the enveloping algebra of $\mathcal{G}$, then Eq. (1.1a) is said to be of *class* I; otherwise it is of *class* II.

We now proceed to classify all systems for which Eq. (1.1a) is $R$ separable, i.e., for which Eq. (1.1a) admits solutions of the form $\Psi = e^R \Pi_{i=1}^4 \Psi^{(i)}(x^i)$, where each $\Psi^{(i)}(x^i)$ satisfies an ordinary differential equation and $R$ is some specified function of the $x^j$. Substituting $\Psi = e^R\Phi$ into $\Delta_4\Psi = 0$ we obtain the equation

$$\sum_{i,j=1}^{4} b^{ij}\partial_{x^i x^j}\Phi + \sum_{i=1}^{4} b^i\partial_{x^i}\Phi + b_0\Phi = 0, \tag{3.3}$$

where

$$b^{ij} = g^{ij}, \quad b^i = \sum_{j=1}^{4} g^{ij}\partial_{x^j} \ln\,[g^{1/2}g^{ij}M^2],$$

$$b_0 = M^{-1}(\Delta_4 M), \quad M = e^R.$$

Clearly, an $R$-separable solution of Eq. (1.1a) corresponds to a purely separable solution of Eq. (3.3). In proceeding to classify $R$-separable systems we do not distinguish between purely separable and strictly $R$-separable systems for Eq. (1.1a) because the conditions for pure separation can be obtained from those for $R$ separation by setting $M = 1$.

The classification of $R$-separable types proceeds along the lines of the systems treated for the Hamilton–Jacobi equation. A variable $x^i$ in a separable system is *ignorable* if for some analytic function $\rho$, $L = \partial_{x^i} + \rho(x)$ is a symmetry operator for Eq. (1.1a); otherwise $x^i$ is *essential*. If the separated equation in the essential variable $x^i$ is first order, then $x^i$ is of *type* 1; if second order, then $x^i$ is of *type* 2. It is readily seen that for a given metric the separation of Eq. (1.1b) is necessary for the $R$ separation of Eq. (1.1a). Thus, the only possible systems permitting $R$ separation of Eq. (1.1a) are those listed in Sec. 2. However, there are additional conditions that must be satisfied by the multiplier $M$ in order for variables to $R$ separate.

To explain our method we treat one example, the analogy of the type $G$ equation for Sec. 2, in detail. Here there are two essential variables of type 2 $(x^1,x^2)$, one essential variable of type 1 $(x^3)$, and one ignorable variable $(x^4)$. With $\Psi = M\Pi_{j=1}^4 \Psi^{(j)}(x^j)$ we can write the separated ordinary differential equations as

$$\begin{aligned}
&\Psi_{11}^{(1)} + h_1\Psi_1^{(1)} + (f_1\lambda_3^2 + \lambda_1 a_1 + \lambda_2 b_1 + K_1)\Psi^{(1)} \\
&\quad \equiv \Phi_1\Psi^{(1)} = 0, \\
&\Psi_{22}^{(2)} + h_2\Psi_2^{(2)} + (f_2\lambda_3^2 + \lambda_1 a_2 + \lambda_2 b_2 + K_2)\Psi^{(2)} \\
&\quad \equiv \Phi_2\Psi^{(2)} = 0, \\
&\Psi_3^{(3)}\lambda_3 + (\lambda_1 a_3 + \lambda_2 b_3 + K_3)\Psi^{(3)} \equiv \Phi_3\Psi^{(3)} = 0, \\
&\Psi_4^{(4)} = \lambda_3\Psi^{(4)},
\end{aligned} \tag{3.4}$$

where $\Psi_{jj}^{(j)} = \partial_{jj}\Psi^{(j)}$. To relate Eqs. (3.3) with (3.4) one looks for functions $\Theta_j(x^1,\ldots,x^4)$ such that

$$\Phi\sum_{j=1}^{3}\Theta_j\Phi_j \equiv \sum_{i,j=1}^{4} b^{ij}\partial_{ij}\Phi + \sum_{i=1}^{4} b^i\partial_i\Phi + b_0\Phi = 0, \tag{3.5}$$

where $\Phi = \Pi_{j=1}^4 \Psi^{(j)}(x^j)$. Comparison of the coefficients of the second derivative terms and the $\lambda_i$ terms on both sides of Eq. (3.5) leads to the same solutions for $\Theta_j$ and $g^{ij}$ as found in Eq. (2.6). Comparison of the coefficients of the first derivative and constant terms yields the $R$-separation conditions

$$\begin{aligned}
&\frac{M^2}{Q} = \left[\prod_{i=1}^{3} A_i(x^i)\right] \\
&\qquad \times \exp(\alpha x^4)(1 - a_2b_1)[(a_2b_3 - 1)(b_1 - b_3)]^{1/2}, \\
&\Delta_4 M = MQ\,[K_1(a_2b_3 - 1) + K_2(b_1 - b_3) + K_3(1 - a_2b_1)], \\
&\alpha \in \mathbb{C}.
\end{aligned} \tag{3.6}$$

The symmetry operators $\mathcal{L}'_j$ for Eq. (3.5) such that $\mathcal{L}'_j\Phi = \lambda_j\Phi, j = 1,2,3$ can easily be obtained by solving for $\lambda_1, \lambda_2$, and $\lambda_3$ in Eqs. (3.4). The simplest of these is $\mathcal{L}'_3 = \partial_4$; the other two operators while straightforward to compute have rather lengthy expressions which we will not bother to

put down. Finally, the symmetry operators $\mathscr{L}_j$ for Eq. (1.1a) such that $\mathscr{L}_j\Psi = \lambda_j\Psi$ are given by $\mathscr{L}_j = M\mathscr{L}'_jM^{-1}$. The simplest of these is

$$\mathscr{L}_3 = \partial_4 - \frac{1}{2}\frac{Q_4}{Q} - \frac{1}{2}\alpha .$$

In the following we list the $R$-separable coordinates for Eq. (1.1a) in each of the cases (A)–(H), excluding (G) already listed. In each case we give the form of the metric $ds^2$ and the necessary and sufficient conditions to ensure $R$ separation. The Hamilton–Jacobi equations and the defining triplet of commuting symmetry operators can be obtained in a straightforward manner from these results:

(A) All variables ignorable:

$$ds^2 = Q\Big(\sum_{i=1}^{4}(dx^i)^2\Big),$$
$$M^2Q = \exp\Big(\sum_{i=1}^{4}\alpha_i x^i\Big), \Delta_4 M = \frac{M}{Q}\alpha_0, \quad \alpha_j\in\mathbb{C}; \tag{3.7}$$

(B) Three ignorable variables:

$$ds^2 = Q\Big(\sum_{i,j=1}^{4} g_{ij}(x^1)dx^i dx^j\Big),$$
$$M^2Q = f(x^1)\exp\Big(\sum_{i=1}^{4}\alpha_i x^i\Big), \tag{3.8}$$
$$\Delta_4 M = \frac{M}{Q}h(x^1), \quad \alpha_j\in\mathbb{C};$$

(C) Two ignorable variables and two essential variables of type 2:

$$ds^2 = Q\Big((dx^1)^2 + (dx^2)^2 + \frac{1}{(ef-h^2)} \times\{f(dx^3)^2 + e(dx^4)^2 - 2hdx^3dx^4\}\Big),$$
$$M^2Q = A_1(x^1)A_2(x^2)\exp(\alpha_3x^3+\alpha_4x^4)[ef-h^2]^{1/2}, \tag{3.9}$$
$$\Delta_4 M = \frac{M}{Q}(K_1+K_2),$$
$$e = e_1+e_2, h = h_1+h_2, f = f_1+f_2;$$

(D) Two ignorable variables with one essential variable of each type:

$$\text{(D1)}\quad ds^2 = Q\,[(dx^1)^2 + (2b_2f - e_1 - b_2^2d_1)^{-1}\{(e_1d_1 - f^2)(dx^2)^2 - (b_2dx^3 - dx^4)^2 + 2(b_2f-e_1)dx^2dx^3 + 2(f-b_2d_1)dx^2dx^4\}], f = f_1+f_2, \tag{3.10}$$
$$M^2Q = A_1(x^1)A_2(x^2)\exp(\alpha_3x^3+\alpha_4x^4) \times[2b_2f - e_1 - b_2^2d_1]^{1/2},$$
$$\Delta_4 M = \frac{M}{Q}(K_1+K_2),$$

$$\text{(D2)}\quad ds^2 = Q\Big[(dx^1)^2 + \frac{1}{d}\{(f_1^2 - e_1d)(dx^2)^2 + (dx^3)^2 - 2f_1dx^2dx^3 + 2d\,dx^2dx^4\}\Big],$$
$$M^2Q = A_1(x^1)A_2(x^2)\exp(\alpha_3x^3+\alpha_4x^4)(d)^{1/2}, \tag{3.11}$$
$$\Delta_4 M = \frac{M}{Q}(K_1+K_2), \quad d = d_1+d_2;$$

(E) Two ignorable variables with two essential variables of type 1: For systems of this type we supply some of the details of the $R$-separation conditions:

$$\text{(E1)}\quad ds^2 = Q\Big[-\Big(\frac{c_1-c_2}{a_1-a_2}\Big)(dx^1-dx^2)^2 + 2\,dx^3(dx^1-dx^2) + 2dx^4(a_1dx^2 - a_2dx^1)\Big]. \tag{3.12}$$

The (first derivative conditions for $R$ separation of $\Delta_4\Psi = 0$ are equivalent to

$$(\partial_1+\partial_2)\ln(M^2Q) = a_1+a_2,$$
$$(a_1\partial_1 + a_2\partial_2)\ln(M^2Q) = b_1+b_2, \tag{3.13}$$
$$\partial_j\ln(M^2Q) = \alpha_j\in\mathbb{C}, j = 3,4.$$

The solutions of these conditions fall into two classes:

Class (i): (a) $a_1 = \cosh x^1$, $a_2 = \cosh x^2$ or (b) $a_1 = e^{x^1}$, $a_2 = e^{x^2}$; (3.14)

then

$$M^2Q = \Big[\sinh\frac{1}{2}(x^1-x^2)\Big]^{\alpha}A_1(x^1)A_2(x^2) \times\exp(\alpha_3x^3+\alpha_4x^4), \tag{3.15}$$
$$\Delta_4 M = \frac{M}{Q}(K_1+K_2), \ \alpha, \ \alpha_j\in\mathbb{C};$$

Class (ii): $a_1$, $a_2$ are not of the form (3.14). (3.16)

The the $R$-separation conditions are of the form (3.15) wih $\alpha = 0$:

$$\text{(E2)}\quad ds^2 = Q\,[-(d_1+d_2)(b_2\,dx^1 - dx^2)^2 + 2dx^3(dx^2 - b_2\,dx^1) + 2dx^1\,dx^4]. \tag{3.17}$$

The (first derivative) conditions for $R$ separation of $\Delta_4\Psi = 0$ are equivalent to

$$(\partial_1 + b_2\partial_2)\ln(M^2Q) = a_1+a_2,$$
$$\partial_2\ln(M^2Q) = b_1+b_2, \partial_j\ln(M^2Q) = \alpha_j\in\mathbb{C}, \quad j = 3,4. \tag{3.18}$$

There are two solutions to these conditions:

Class (i): $b_2\neq x^2$, (3.19)

$$M^2Q = A_1(x^1)A_2(x^2)\exp(\alpha_3x^3+\alpha_4x^4),$$
$$\Delta_4 M = \frac{M}{Q}(K_1+K_2), \tag{3.20}$$

Class (ii): $b_2 = x^2$. (3.21)

Conditions (3.20) hold, except that now

$$M^2Q = A_1A_2\exp(x^2e^{-x^1} + \alpha_3x^3 + \alpha_4x^4), \tag{3.22}$$

$$\text{(E3)}\quad ds^2 = Q\,[-d_2(dx^1)^2 - c_1(dx^2)^2 + 2dx^1\,dx^4 + 2dx^2dx^3]. \tag{3.23}$$

The first derivative $R$-separation conditions are

$$\partial_1\ln(M^2Q) = a_1+a_2, \quad \partial_2\ln(M^2Q) = b_1+b_2,$$
$$\partial_j\ln(M^2Q) = \alpha_j, j = 3,4. \tag{3.24}$$

These conditions have the general solution

$$M^2Q = A_1A_2\exp(\epsilon x^1x^2 + \alpha_3x^3 + \alpha_4x^4), \quad \epsilon = 0,1,$$

$$\Delta_4 M = \frac{M}{Q}(K_1 + K_2)\,. \tag{3.25}$$

(F) One ignorable variable with three essential variables of type 2:

$$ds^2 = Q\left[\frac{(dx^1)^2}{q_2 - q_3} + \frac{(dx^2)^2}{q_3 - q_1} + \frac{(dx^3)^2}{q_1 - q_2} + \frac{(dx^4)^2}{[r_1(q_2 - q_3) + r_2(q_3 - q_1) + r_3(q_1 - q_2)]}\right],$$

$$M^2 Q = A_1 A_2 A_3 S \exp(\alpha_4 x^4),$$

$$S = [(q_2 - q_3)(q_3 - q_1)(q_1 - q_2)\{r_1(q_2 - q_3) + r_2(q_3 - q_1) + r_3(q_1 - q_2)\}]^{1/2}, \tag{3.26}$$

$$\Delta_4 M = \frac{M}{Q}[K_1(q_2 - q_3) + K_2(q_3 - q_1) + K_3(q_1 - q_2)];$$

(H) No ignorable variables:

$$ds^2 = Q\left(\sum_{i=1}^{4} \frac{S}{M_{i1}}\right), \quad S = \det\Phi \neq 0\,,$$

$$\Phi = (\Phi_{ij}(x^i)), \quad QM^2 = \frac{A_1 A_2 A_3 A_4}{S}\left[\prod_{j=1}^{4} M_{j1}\right]^{1/2},$$

$$\Delta_4 M = \frac{M}{Q}\left(\sum_{j=1}^{4} \frac{B_j M_{j1}}{S} + \alpha\right). \tag{3.27}$$

Here $M_{j1}$ is the $(j, 1)$ cofactor of the $4\times4$ Stäckel matrix $\Phi$.

## 4. CONFORMALLY FLAT NONORTHOGONAL *R*-SEPARABLE SYSTEMS

Here we specialize the results of Sec. 2 and 3 to flat space, limiting ourselves to nonorthogonal coordinates. (The orthogonal case has already been treated in Ref. 1.) In principle, the classification is straightforward: One need only compute the Riemann curvature tensor for each of the separable nonorthogonal metrics (A)–(G), require that it vanish identically, and classify all possibilities. In practice, however, the computations are hopelessly complicated. The problem becomes tractible only if detailed use is made of the conformal symmetry algebra O(6,C) of the flat space Laplace equation.

A basis for O(6,C) is given by

$$P_j = \partial_{z^j}, \quad j = 1,2,3,4\,,$$

$$I_{kl} = z^k\partial_{z^l} - z^l\partial_{z^k} = -I_{lk}, \quad 1 \leqslant k < l \leqslant 4\,,$$

$$D = -\left(1 + \sum_{i=1}^{4} z^i\partial_{z^i}\right), \tag{4.1}$$

$$K_j = 2z^j + (2(z^j)^2 - z\cdot z)\partial_{z^j} + 2z^j z^l\partial_{z^l} + 2z^j z^m\partial_{z^m} + 2z^j z^n\partial_{z^n}\,,$$

where $j,l,m,n = 1,2,3,4$ and no two are equal. Now every nonorthogonal $R$-separable system for the flat space Laplace equation

$$\sum_{j=1}^{4} \partial_{z^j}^2 \Psi = 0\,, \tag{4.2}$$

or any other Laplace equation, contains at least one ignorable variable $x^1$. Clearly there must exist an analytic function $\rho$ such that $\partial_{x^1} + \rho = L \in O(6,C)$. In general, a system with $m$ ignorable variables is associated with an $m$ dimensional Abelian subalgebra of O(6,C). Since we identify two systems if one can be obtained from the other by an action of the conformal symmetry group, to classify all possibilities for ignorable variables associated with Eq. (4.2) it is necessary and sufficient to determine all equivalence classes of Abelian O(6,C) subalgebras under the adjoint action of O(6,C).

We first list the classes of one dimensional subalgebras of O(6,C). To obtain most easily the results of Table I we have made use of the well known isomorphism $O(6,C) \cong sl(4,C)$ and the Jordan canonical forms for $4\times4$ matrices. We have also identified in this and the higher dimensional cases those subalgebras which can be mapped into one another under the outer automorphisms of spatial reflection and inversion. For each equivalence class we exhibit a representative element.

Suppose that $t$ is an ignorable variable belonging to the $R$-separable system $\{t, x^2, x^3, x^4\}$. Then we can assume the corresponding symmetry operator $L = \partial_t + \rho$ is identical with one of the five operators listed in Table I. From this relationship we can determine how the "standard" coordinates $z^1,\ldots z^4$ are associated to $t$ and the general form of the metric $ds^2$ in terms of $dt$. The ignorable variable $t$ is *orthogonal* if the corresponding metric can be written

$$ds^2 = Q\left[dt^2 + \sum_{i,j=2}^{4} g_{ij}(t,x^2,x^3,x^4)dx^i dx^j\right]. \tag{4.3}$$

Otherwise, $t$ is *nonorthogonal*. In Table II we list the metrics and coordinates corresponding to the operators in Table I.

It follows from Table II that the only operators associated with orthogonal ignorable variables are $I_{14}$, $I_{23}$, $D$, and $P_3$. Among nonorthogonal ignorable variables the only one for which the $(dt)^2$ term doesn't occur in the metric $ds^2$ is associated with the operator $P_3 + iP_4$. (Note that in each case $t$ is not unique; it can be replaced by $t' = t + f$ for arbitrary $f$. For nonorthogonal variables the assertion is that, no matter what the choice of $f$, the metric contains cross terms of the form $dt'\,da$.) This last possibility is of great interest, for it leads to "heat type" variables (slightly renormalized):

$$z^1 = a, z^2 = b, z^3 - iz^4 = 2t, z^3 + iz^4 = c\,. \tag{4.4}$$

If in these coordinates we assume a solution of Eq. (1.1a) of the form $\Psi = \Phi(a,b,c)e^{\beta t}$, the resulting equation becomes

$$(\partial_a^2 + \partial_b^2)\Phi = \beta\partial_c\Phi\,. \tag{4.5}$$

Note that here the ignorable variable $t$ is characterized by its nonorthogonality and the fact that there is no $(dt)^2$ term in the metric.

TABLE I. One-dimensional subalgebras of O(6,C).

1. $\alpha I_{14} + \beta I_{23} + \gamma D\,,\ \alpha,\beta,\gamma \in C$
2. $\alpha(-I_{14} + I_{23} - iD) + P_2 + iP_3 - I_{34} - iI_{24} + iI_{13} - I_{12},\ i = \sqrt{-1}$
3. $\alpha I_{14} + P_3$
4. $\alpha I_{21} + \beta(I_{34} - iD) + P_3 + iP_4$
5. $\frac{1}{2}(P_2 + iP_3) - iI_{24} - I_{34}$

TABLE II. Metrics and coordinates associated with ignorable variables.

1. $z^1 = a\,e^{-\gamma t}\cos(\alpha t + c)$, $z^2 = b\,e^{-\gamma t}\cos\beta t$
$z^3 = b\,e^{-\gamma t}\sin\beta t$, $z^4 = a\,e^{-\gamma t}\sin(\alpha t + c)$
$ds^2 = e^{-2\gamma t}[da^2 + db^2 - 2\gamma dt(ada + bdb)$
$+ \{\gamma^2(a^2 + b^2) + b^2\beta^2\}dt^2 + a^2(\alpha dt + dc)^2]$

Nonorthogonal unless two of $\alpha, \beta, \gamma$ are zero.

2. $z^1 - iz^4 = a\,e^{2i\alpha t}$, $z^1 + iz^4 = b + 2t^2$
$z^2 + iz^3 = (-2at + c)e^{2i\alpha t}$, $z^2 - iz^3 = 2t$
$ds^2 = e^{2i\alpha t}[da\,db + 2dt(dc + i\alpha a\,db) + 4(i\alpha c - a)dt^2]$.

Nonorthogonal.

3. $z^1 = a\cos\alpha t$, $z^2 = b$, $z^3 = t + c$, $z^4 = a\sin\alpha t$
$ds^2 = da^2 + \alpha^2 a^2 dt^2 + db^2 + (dt + dc)^2$

Nonorthogonal unless $\alpha = 0$.

4. $z^2 + iz^1 = a\,e^{i(\beta+\alpha)t}$, $z^2 - iz^1 = b\,e^{i(\beta-\alpha)t}$
$z^3 - iz^4 = 2t + c$, $z^3 + iz^4 = f\,e^{2i\beta t}$
$ds^2 = e^{2i\beta t}[da\,db + i(\beta + \alpha)a\,dt\,db + i(\beta - \alpha)b\,dt\,da + df\,dc$
$+ 2dt(df + i\beta f\,dc) + \{ab(\alpha^2 - \beta^2) + 4i\beta f\}dt^2]$

Nonorthogonal. No $dt^2$ term only if $\alpha = \beta = 0$.

5. $z^1 = a, z^2 + iz^3 = i\sqrt{2}(be^{\sqrt{2}t} - c\,e^{-\sqrt{2}t})$
$z^2 - iz^3 = t, z^4 = b\,e^{\sqrt{2}t} + c\,e^{-\sqrt{2}t}$.

Nonorthogonal.

A representative basis for each equivalence class of two-dimensional abelian subalgebras of O(6,C) is listed in Table III.

The corresponding results for three dimensional abelian subalgebras are listed in Table IV.

Finally, there is only one equivalence class of four dimensional abelian subalgebras of O(6,C). A representative has basis $P_1, P_2, P_3, P_4$.

The above results apply with only slight modification to the flat space Hamilton–Jacobi equation

$$\sum_{i=1}^{4} (\partial_{z^i} W)^2 = 0\,. \tag{4.6}$$

The symmetry algebra of this equation is again O(6,C) with basis

$$P_j = p_j, \quad j = 1,2,3,4,$$

$$I_{kl} = z^k p_l - z^l p_k = -I_{lk}\,, \quad 1 \leqslant k < l \leqslant 4\,, \tag{4.7}$$

$$D = -\sum_{i=1}^{4} z^i p_i,$$

$$K_j = (2(z^j)^2 - z\cdot z)\,p_j + 2z^j z^l p_l + 2z^j z^m p_m + 2z^j z^n p_n\,,$$

where $j,l,m,n = 1,2,3,4$ and no two are equal. To find all nonorthogonal metrics for Eq. (4.6) it is clearly sufficient to examine each of the general nonorthogonal separable metrics from the list (A)–(H) of Sec. 2 and determine which of these is conformally flat. All orthogonal separable metrics for Eq. (4.6) were already computed in Ref. 1, so here we omit the systems of type (A), (F), and (H). Note that every $R$-separable system for the Laplace equation (4.2) must correspond to one of these conformally flat metrics. We will show later that this correspondence is one to one.

The necessary and sufficient condition that a metric $ds^2 = Q(\Sigma g_{ij}dx^i dx^j) = Q\,d\hat{s}^2$ be conformally flat is that the conformal tensor $C_{ijkl}$ of the metric $d\hat{s}^2$ be identically zero.[10] Here,

$$C_{ijkl} = R_{ijkl} + \tfrac{1}{2}(g_{ik}R_{jl} - g_{il}R_{jk} + g_{jl}R_{ik} - g_{jk}R_{il}) + \tfrac{1}{6}R(g_{il}g_{jk} - g_{ik}g_{jl})\,, \tag{4.8}$$

where $R_{ijkl}$ is the Riemann curvature tensor, $R_{jl}$ is the Ricci tensor and $R$ is the scalar curvature. We will use this condition to determine the number of nonorthogonal conformally flat metrics of each type.

TABLE III. Two-dimensional abelian subalgebras of O(6,C).

1. $P_3 + iP_4 + \delta M_{23}, I_{34} - iD$
2. $P_3 + iP_4, P_1 + iP_2$
3. $P_3 + iP_4, I_{24} + iI_{32}$
4. $P_3 + iP_4, P_1 - iP_2 - iI_{14} + I_{31} + I_{24} + iI_{32}$
5. $P_3 + iP_4, P_1 - iP_2 - I_{34} + iD + I_{12}$
6. $P_3 + iP_4, P_3 - iP_4 - I_{24} - iI_{32} - iI_{14} + I_{31}$
7. $I_{41} + I_{23} - iD, P_2 + iP_3 - I_{34} - iI_{24} + iI_{13} - I_{12}$
8. $I_{43} + iI_{24} + I_{12} + iI_{13}, i(P_3 + K_3) + P_2 + K_2 + 2iI_{24} - 2I_{12}$
9. $I_{14} + P_3, I_{14} - iP_2$
10. $D, I_{24} + iI_{34}$
11. $P_3, P_2 + iP_3 + 2iI_{14}$
12. $iI_{24} + I_{43}, iI_{13} + I_{12}$
13. $iI_{24} + I_{43}, i(P_1 - K_1) - P_2 + K_2 + I_{43} - iI_{42} + I_{12} + iI_{13}$
14. $P_3 + I_{24} + iI_{12}, P_2 + I_{34} + iI_{13}$
15. $I_{23} - iD, P_2 + iP_3 + 2iI_{14}$
16. $I_{41} + I_{23} + \alpha(I_{23} - iD), I_{14} + iD + \beta(I_{23} - iD)$
17. $\alpha I_{14} + \beta(I_{23} - iD), P_2 + iP_3 + \delta(I_{23} - iD)$
18. $P_3 - iP_4 + \beta(D - iI_{34} - iI_{21}), D + P_2 + iP_1 - iI_{34} - iI_{21} - I_{14} + I_{32} + iI_{24} + iI_{31}$

TABLE IV. Three-dimensional abelian subalgebras of O(6,C).

1. $P_3 + iP_4, I_{43} + iD - I_{12}, P_1 - iP_2 - iI_{14} + I_{31} + I_{24} + iI_{32}$
2. $P_3 + iP_4, I_{43} + iD - I_{12}, iI_{24} - I_{32} + I_{14} + iI_{31}$
3. $P_3 + iP_4, I_{43} + iD - I_{12}, P_1 + iP_2$
4. $P_3 + iP_4, P_1 + I_{24} + iI_{32}, P_2 + I_{14} + iI_{31}$
5. $P_3 + iP_4, P_1 - iP_2 + iI_{14} - I_{31} + I_{24} + iI_{32}, P_1 + iP_2$
6. $P_3 + iP_4, P_1 - iP_2 + I_{14} + iI_{31} + iI_{24} - I_{32}, I_{14} + iI_{31} - iI_{24} + I_{32}$
7. $P_3 + iP_4, I_{24} + iI_{32}, I_{14} + iI_{31}$
8. $P_3 + iP_4, P_1, P_2 + iI_{24} - I_{32}$
9. $P_3 + iP_4, P_1 - iP_2, I_{14} + iI_{31} - iI_{24} + I_{32}$
10. $D, I_{14}, I_{23}$
11. $D, I_{23} + I_{41}, I_{42} + iI_{21} + iI_{43} - I_{31}$
12. $P_2, P_3, I_{41}$
13. $P_1, P_2, P_3$

(B) Three ignorable variables: For forms of type (B) the conformal flatness conditions prove too complicated to solve explicitly. Fortunately, group theory comes to our rescue: The possible separable systems of this type correspond to the three dimensional Abelian subalgebras listed in Table IV. Subalgebras 10, 12, 13 correspond to orthogonal coordinates. The subalgebra 4 does not give a separable system because the three Lie derivatives are functionally dependent. (In order to define a separable coordinate system the three Lie derivatives must be functionally independent.) The remaining subalgebras yield nonorthogonal coordinates all of heat type except 11 which, once a radial variable is separated, corresponds to the single nonorthogonal separable system for the Helmholtz equation on the complex sphere $S_3$.[7] [However, this system also arises in $E_4$ where the diagonalization of $D$ is accomplished by the diagonalization of the Casimir operator for the subalgebra O(4,C) generated by the $I_{jk}$.]

The coordinates and their relationship to the standard coordinates $z^j$ can be obtained from Tables I and II. For example, a suitable choice of coordinates for the operators of type 3 is

$$z^1 + iz^2 = e^{-2is}, \quad z^1 - iz^2 = t,$$
$$z^3 + iz^4 = w\,e^{-2is}, \quad z^3 - iz^4 = u, \tag{4.9}$$

where $\partial_s - i = I_{43} - I_{12} + iD$, $\partial_t = \frac{1}{2}(P_1 + iP_2)$, and $\partial_u = \frac{1}{2}(P_3 + iP_4)$. The corresponding differential form is

$$ds^2 = e^{-2is}[du\,dw - 2i\,ds(w\,du + dt)]. \tag{4.10}$$

We note that this metric also provides a separation of variables for the flat space Helmholtz equation $\Delta_4\Psi = E\Psi$. Indeed, if we set $x^1 = e^{-2is}, x^2 = t/2, x^3 = w/2, x^4 = u$ (these are equivalent coordinates), we obtain

$$ds^2 = 2\,dx^1\,dx^2 + 2\,dx^4(x^3\,dx^1 + x^1\,dx^3) \tag{4.11}$$

and the Helmholtz equation is

$$2\left[\partial_{12} + \frac{1}{x^1}(-x^3\partial_{23} + \partial_{34})\right]\Psi = E\Psi \tag{4.12}$$

with separation equations

$$\partial_2\Psi_2 = l_1\Psi_2, \quad \partial_4\Psi_4 = l_2\Psi_4,$$
$$(-2l_1x^3\partial_3 + 2l_2\partial_3)\Psi_3 = l_3\Psi_3, \tag{4.13}$$
$$(2l_1\partial_1 + 2l_3/x^1)\Psi_1 = E\Psi_1,$$

where $\Psi = \Pi_{j=1}^4 \Psi_j(x^j)$. The operators $\mathscr{L}_j$ which describe this separation are $\mathscr{L}_1 = \frac{1}{2}(P_1 + iP_2)$, $\mathscr{L}_2 = \frac{1}{2}(P_3 + iP_4)$, $\mathscr{L}_3 = \frac{1}{4}\{P_3 - iP_4, I_{13} + iI_{23} + iI_{14} - I_{24}\}$. The operators which characterize separation in this case are not all first order and would also suffice to describe the separation in the case of the Laplace equation $E = 0$. (The significance of two separate operator characterizations of the same coordinate system will be the topic of a separate paper.) Similar comments hold for subalgebras 1 and 2 on Table IV. Subalgebras 5 to 9 clearly directly define separation of the flat space Helmholtz equation. Thus, nonorthogonal coordinates of type (B) all correspond to coordinates that separate the Helmholtz equation on $E_4$.

(C) Two ignorable variables and two essential variables of type 2: It would be possible but extremely complicated to derive these metrics by directly requiring the metric (3.9) to be conformally flat. An easier method follows from the observation that for a conformally flat space the two Lie symmetries corresponding to the ignorable variables $x^3$, $x^4$ are taken from the list of commuting pairs of symmetries in Table III. For each pair of symmetries from this list there are constraints on the form $ds^2$ and the way in which the differentials $dx^3$ and $dx^4$ appear in it. For subalgebras 1–9 the corresponding metric is such that $e = 0$, i.e., the ignorable variable $x^4$ is nonorthogonal and there is no $(dx^4)^2$ term appearing in $ds^2$. Thus, to compute all coordinates corresponding to subalgebras 1–9 we can simply require that the metric

$$d\hat{s}^2 = (l_1 - l_2)[(dx^1)^2 + (dx^2)^2] + 2dx^3\,dx^4 + \left(\frac{m_1 - m_2}{l_1 - l_2}\right)(dx^3)^2 \tag{4.14}$$

be conformally flat.

Subalgebras 10–13 each contain an orthogonal ignorable variable so they do not correspond to type (C) metrics. Subalgebras 14–18 are somewhat more awkward to treat but in each case one can show that the metrics associated with these subalgebras are not of the form (3.9). Thus, none of these subalgebras correspond to type (C) coordinates.

Now suppose the conformally flat metric is of the form (4.14). The conditions of conformal flatness are

$$C_{1221} = \tfrac{1}{3}R_{1221} = 0, C_{1442} = R_{1442} = 0,$$
$$C_{1332} = R_{1332} + \tfrac{1}{3}\left(\frac{m_1 - m_2}{l_1 - l_2}\right)^2 R_{1442} = 0,$$
$$C_{1331} = \tfrac{1}{2}(R_{1331} - R_{2332}) + \frac{1}{(l_1 - l_2)^2} \times(\tfrac{1}{3} - \tfrac{1}{2}(m_1 - m_2))R_{1221} = 0, \tag{4.15}$$
$$C_{2332} = \tfrac{1}{2}(R_{2332} - R_{1331}) + \frac{1}{(l_1 - l_2)^2} \times(\tfrac{1}{3} - \tfrac{1}{2}(m_1 - m_2))R_{1221} = 0.$$

These conditions imply $R_{ijkl} = 0$ so the metrics $d\hat{s}^2$ are flat. We then obtain the following distinct solutions:

$$d\hat{s}^2 = (x^1 - x^2)\left[\frac{(dx^1)^2}{x^1} - \frac{(dx^2)^2}{x^2}\right] + 2\,dx^3dx^4 + (x^1 + x^2)(dx^4)^2, \tag{4.16}$$

$$d\hat{s}^2 = (x^1 - x^2)[(dx^1)^2 - (dx^2)^2] + 2\,dx^3dx^4 + (x^1 + x^2)(dx^4)^2, \tag{4.17}$$

$$d\hat{s}^2 = (dx^1)^2 + (dx^2)^2 + 2\,dx^3dx^4 + (ax^1 + bx^2)(dx^4)^2. \tag{4.18}$$

The remaining conformally flat metrics of this type are of the form

$$d\hat{s}^2 = d\sigma^2 + 2\,dx^3dx^4, \tag{4.19}$$

where $d\sigma^2$ is a separable metric in Euclidean two-space (see Ref. 11). Thus, all conformally flat metrics of type (C) correspond to coordinates that separate the flat space Helmholtz equation.

(D) Two ignorable variables and one essential variable of each type: We look for conformally flat metrics of type (D1) for which the Lie symmetries corresponding to the ignorable variables $x^3$, $x^4$ are taken from the list of commuting

pairs on Table III. Proceeding through the list we find that there can be no conformally flat metrics of this type, which are not already of type (D2).

For forms of type (D2) two of the conditions of conformal flatness are

$$C_{1331} = \tfrac{1}{3}R_{3113} = 0\,, C_{1223} = R_{1223} - \tfrac{1}{2}f_1 R_{1332} = 0\,. \tag{4.20}$$

These two conditions imply $d_1' = 0$ and $f_1 = 0$. The remaining conformal flatness condition is then $C_{1221} = \frac{1}{2} \times (R_{1221} - d_1 R_{3223}) = 0$, which is equivalent to $d_2'' - \frac{3}{5} \times (d_2')^2/d_2 - d_2 e_1'' = 0$. This equation can be solved to give the forms

$$d\hat{s}^2 = (dx^3)^2 + [1 + (x^2)^2](dx^1)^2 + 2\,dx^2dx^4 + \frac{1}{1 + (x^2)^2}(x^1dx^2)^2\,, \tag{4.21}$$

$$d\hat{s}^2 = (dx^3)^2 + x^2(dx^1)^2 + 2\,dx^2dx^4 + \frac{(x^1dx^2)^2}{x^2}\,, \tag{4.22}$$

$$d\hat{s}^2 = (x^2dx^1)^2 + ax^1\left(\frac{dx^2}{x^2}\right)^2 + (dx^3)^2 + 2\,dx^2dx^4\,. \tag{4.23}$$

(For these forms we have redefined $x^2$ and multiplied by a suitable function of $x^2$.) The forms (4.21)–(4.23) all define separation for the flat space Helmholtz equation.[8]

(E) Two ignorable variables and two essential variables of type 1: For metrics of type (E1) the conditions of conformal flatness imply that the metric $d\hat{s}^2$ is flat where $ds^2 = Qd\hat{s}^2$ is given by Eq. (3.12). Thus, from Ref. 8 we obtain the possibilities

$$d\hat{s}^2 = 2dx^3(dx^1 - dx^2) + 2\,dx^4\,[(x^1)^2dx^2 - (x^2)^2dx^1]\,, \tag{4.24}$$

$$d\hat{s}^2 = \left[A(x^1 + x^2) + \frac{B(x^1 + x^2) + C}{x^1 - x^2}\right](dx^1 - dx^2)^2 + 2dx^3(dx^1 - dx^2) + 2\,dx^4(x^1dx^2 - x^2dx^1)\,, \tag{4.25}$$

$$d\hat{s}^2 = \left[\frac{A}{x^1} + \frac{B}{(x^1)^2} + \frac{C}{x^2} + \frac{D}{(x^2)^2}\right]\frac{(x^2dx^1 - x^1dx^2)^2}{x^1 - x^2} + 2dx^3(x^2dx^1 - x^1dx^2) + 2\,dx^4(dx^2 - dx^1)\,. \tag{4.26}$$

For metrics of type (E2), (i) the conformal flatness conditions are

$$C_{1223} = \frac{1}{b_2}C_{2113} = \tfrac{1}{2}R_{1223} = 0\,,$$

$$C_{1221} = R_{1221} + (d_1 + d_2)(R_{2113} - b_2R_{1223}) = 0\,. \tag{4.27}$$

Solving these equations we obtain the conformally flat metric

$$d\hat{s}^2 = \left(\frac{B}{e^{2x^1}} + \frac{B}{e^{x^1}} + \frac{C}{(x^2)^2} + \frac{D}{x^2}\right)(x^2dx^1 - dx^2)^2 + 2dx^3(dx^2 - x^2dx^1) + 2dx^1dx^4\,. \tag{4.28}$$

This form is conformal to the type (E2), (i) metric of Ref. 8 which defines separation of the flat space Helmholtz equation. A similar computation shows that there are no type (E2), (ii) conformally flat metrics.

For metrics of type (E3) the relevant conformal flatness conditions are $C_{1221} = R_{1221} = 0$ and we obtain the metrics

$$d\hat{s}^2 = \left(\frac{x^2dx^1}{x^1}\right)^2 - (dx^2)^2 + 2\,dx^1dx^4 + 2(x^1)^2dx^2dx^3\,, \tag{4.29}$$

$$d\hat{s}^2 = (x^2dx^1)^2 - (x^1dx^2)^2 + 2\,dx^1dx^4 + 2\,dx^2dx^3\,, \tag{4.30}$$

$$d\hat{s}^2 = x^2\left(\frac{dx^1}{x^1}\right)^2 + x^1(dx^2)^2 + 2\,dx^1dx^4 + 2(x^1)^2dx^2dx^3\,, \tag{4.31}$$

$$d\hat{s}^2 = x^2(dx^1)^2 + x^1(dx^2)^2 + 2\,dx^1dx^4 + 2\,dx^2dx^3\,, \tag{4.32}$$

$$d\hat{s}^2 = x^2\left(\frac{dx^1}{x^1}\right)^2 + 2\,dx^1dx^4 + 2(x^1)^2dx^2dx^3\,. \tag{4.33}$$

As shown in Ref. 8 these metrics define variable separation for the flat space Helmholtz equation.

(G) One ignorable variable, two essential variables of type 2 and one of type 1: Comparing the type (G) metric with the metrics on Table II we see that the symmetry operator $P_3 + iP_4$ must correspond to the ignorable variable $x^4$. With this restriction only the nontrivial conformal flatness conditions are $C_{1331} = C_{2332} = 0$ and we obtain two groups of metrics:

$$\text{I:}d\hat{s}^2 = (dx^1)^2 + \frac{e^{2ix^1}}{(x^3 + a)}d\omega_k^2 - \frac{(dx^3)^2}{4(x^3 + a)^2}\,, \tag{4.34}$$

$$\text{II:}d\hat{s}^2 = (dx^1)^2 + d\omega_k^2 + Ax^1(dx^3)^2\,, \tag{4.35}$$

where

$$d\omega_1^2 = x^3(dx^2)^2 + 2\,dx^3dx^4 + \frac{(x^2dx^3)^2}{4x^3}\,,$$

$$d\omega_2^2 = (1 + (x^3)^2)(dx^2)^2 + 2\,dx^3dx^4 - \frac{(x^2dx^3)^2}{1 + (x^3)^2}\,,$$

$$d\omega_3^2 = (x^3dx^2)^2 + 2\,dx^3dx^4 - Bx^2\left(\frac{dx^3}{x^3}\right)^2\,, \tag{4.36}$$

$$d\omega_4^2 = (dx^2)^2 + 2\,dx^3dx^4 + Ax^2(dx^3)^2\,.$$

The metrics of type I determine separation for the Helmholtz equation on the four sphere $S_4$ and those of type II determine separation for the flat space Helmholtz equation.

This completes our classification of conformally flat nonorthogonal separable forms.

## 5. $R$-SEPARABLE COORDINATES FOR $\Delta_4\Psi = 0$

In our treatment of conformally flat metrics in Sec. 4 the original flat space metric was chosen in the form $ds^2 = Q(\Sigma g_{ij}dx^idx^j) = Q\,d\hat{s}^2$. In addition to the condition of conformal flatness for the metric $d\hat{s}^2$ the function $Q = e^{2\lambda}$ is determined by solving the equations

$$\lambda_{ij} = \tfrac{1}{2}(\tfrac{1}{6}g_{ij}R - R_{ij}) - \tfrac{1}{2}g_{ij}\left(\sum_{k,l=1}^{4} g^{kl}\lambda_{,k}\lambda_{,l}\right), \tag{5.1}$$

where $\lambda_{ij} = \lambda_{,ij} - \lambda_{,i}\lambda_{,j} = \partial_{x^i}\lambda$ and $\lambda_{,ij}$ is the second covariant derivative of $\lambda$ with respect to $g_{ij}$ (see Ref. 10).

As we have shown, the metrics $d\hat{s}^2$ correspond to only two manifolds: $E_4$ and $S_4$. The possible functions $Q$ relating flat space and these two manifolds are independent of coordinates and were already computed in Ref. 1. Furthermore, it was shown in that reference that always

$$\hat{\Delta}_4 Q^{1/2} + \frac{R}{6}Q^{1/2} = 0\,, \tag{5.2}$$

where $R$ is the (constant) scalar curvature, and $\hat{\Delta}_4$ is the Laplace–Beltrami operator on the manifold with metric $d\hat{s}^2$. When we studied orthogonal separation for $\Delta_4\Psi = 0$ in Ref.

1 we showed that we could always choose the multiplier $M = Q^{-1/2}$. Using this result as a guide we consider one of the nonorthogonal metrics $ds^2 = Qd\hat{s}^2$ listed in Sec. 4 and set $\Psi = Q^{-1/2}\Phi$. Substituting this expression into $\Delta_4\Psi = 0$ and making use of Eq. (5.2) we obtain

$$\hat{\Delta}_4\Phi + \frac{R}{6}\Phi = 0 \tag{5.3}$$

so that $\Phi$ satisfies a Helmholtz equation on the manifold corresponding to $d\hat{s}^2$. Since the Helmholtz equation separates in the coordinates $x^j$ corresponding to $d\hat{s}^2$, we can find separable solutions $\Phi = (\Pi_{j=1}^4 A_j(x^j)$ for Eq. (5.3) and $R$-separable solutions $\Psi = Q^{-1/2}\Pi_{j=1}^4 A_j(x^j)$ for the flat space Laplace equation. This proves that *all* nonorthogonal coordinate systems which separate Eq. (4.6) also $R$-separate Eq. (4.2). Combining these results with those of Ref. 1 we obtain the following:

*Theorem*: Let $\{x^j\}$ be a coordinate system (orthogonal or not) for which the equation

$$\sum_{l=1}^{4} (\partial_{z^l} W)^2 = 0 \tag{5.4}$$

is separable. Then

$$dx^2 = \sum_{l=1}^{4} (dz^l)^2 = Q\left(\sum_{i,j=1}^{4} g^{ij}dx^i dx^j\right) = Q\,d\hat{s}^2\,,$$

where $d\hat{s}^2$ is a metric on one of the spaces $\mathscr{M} = E_4$, $S_3 \times S_1$, $S_2 \times S_2$, $S_4$ and the coordinates $\{x^j\}$ are separable for the Helmholtz equation on $\mathscr{M}$. If $\{x^j\}$ is nonorthogonal, then we can assume that $\mathscr{M}$ is one of $E_4$ or $S_4$. The function $Q$ satisfies Eq. (5.3), where $R$ is the (constant) scalar curvature of $\mathscr{M}$. Furthermore, the Laplace equation

$$\sum_{j=1}^{4} \partial_{z^j}^2 \Psi = 0 \tag{5.5}$$

is $R$ separable in the coordinates $\{x^j\}$:

$$\Psi = Q^{-1/2} A_1(x^1)A_2(x^2)A_3(x^3)A_4(x^4)\,.$$

All separable systems for the Helmholtz equation on $\mathscr{M}$ yield $R$-separable systems for the flat space Laplace equation.

*Corollary*: Equations (5.4) and (5.5) separate in exactly the same coordinate systems (orthogonal or not).

*Corollary*: If $\{x^j\}$ is a separable coordinate system for the Laplace equation on a conformally flat space, then these coordinates permit separation of the Helmholtz equation on one of the manifolds $E_4$, $S_3 \times S_1$, $S_2 \times S_2$, or $S_4$.


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# Stability of constant-amplitude motions in slow-fluctuation approximation

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Oscillatory motions at constant amplitude admit of an especially simple description of their stability in phase space: orbital stability is equivalent to stability of the amplitudes alone, regardless of phase behavior, while Liapunov stability can subsequently be inferred from the phases alone. Stability arguments simplify further in slow-fluctuation approximation because of the availability of explicit quadratures for the amplitudes and phases depending ultimately on a single polynomial. Thus, all orbital stability information about near-resonant constant-amplitude motions in conservative, autonomous systems can be extracted solely from that one polynomial. Explicit analytic criteria for orbital stability are derived, and auxiliary methods for the construction of stability charts are developed. Liapunov stability is shown to be a rare exception, but Liapunov instability is encountered in distinctly varying degrees; a fairly wide class of motions in a fairly wide class of systems is shown to be Liapunov–unstable only in the third order of a certain approximation. Five examples are given at some length; they differ starkly in detail. Owing to their tractable stability properties the abundant constant-amplitude motions play in slow-fluctuation approximation the role of the often nonexistent, purely periodic solutions of the traditional theories.

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## I. INTRODUCTION

Autonomous, conservative, nonlinear oscillatory systems of many degrees of freedom (d.f.) with an internal near-resonance $\Sigma g_i \omega_i = \epsilon$ can be completely integrated in "slow-fluctuation" approximation, as we have described recently.[1] Referring to that paper[1] as SF and keeping its notation, we continue our study of the method.

We now turn to stability. Since this term appears even more protean in science than in politics, we hasten to explain that we follow Liapunov and Poincaré and define stability of motion in $2n$-dimensional phase space, not in the $n$-dimensional configuration space of the given d.f. This is often not done.[2] Among writers of practical texts known to us, Cunningham[3] and Leipholz[4] are distinguished for meticulous argument in phase space whenever it helps. Indeed, attempts at finding universal definitions of stability by the exercise of intuitive commonsense in configuration space have always ended with some disappointment. We quote Klein and Sommerfeld[5] as an outstanding example; the lucidity of these eminent authors commands admiration but does not point the way toward satisfactory, general concepts. Our method being extremely flexible and general, we naturally do not wish to be hampered by inadequate definitions of stability.

Let $\mathscr{C}$ be a system path in phase space and draw a (hyper) sphere of radius $\eta$ about each of its points. The envelope of this succession of spheres along $\mathscr{C}$ we call the "$\eta$-tube about $\mathscr{C}$". $\mathscr{C}$ is called "orbitally stable" iff for any preassigned $\eta$ there exists a $\rho$ with $0 < \rho \leqslant \eta$ such that any phase orbit $\mathscr{C}^*$ which passes somewhere within $\rho$ of $\mathscr{C}$ lies in its entirety within the $\eta$-tube about $\mathscr{C}$.

In the classic applications to celestial mechanics,[6] $\mathscr{C}$ is a closed curve corresponding to strictly periodic motion. This is not necessary. $\mathscr{C}$ can also represent a quasiperiodic motion for which $\mathscr{C}$ does "not quite" close while an $\eta$-tube may eventually penetrate itself. The stability definition still applies, at least in principle; in fact, it requires not periodicity but only boundedness of $\mathscr{C}$ (in the unbounded case it dissatifies inasmuch as even force-free uniform motion would be unstable). The quasi-periodic case is important to us because, as we were at pains to emphasize in SF, in near-resonant systems strictly periodic motions occur only under special circumstances. Thus our applications will be made to constant-amplitude (c-a) motions whose phase orbits normally do not close. In a sense, then, the abundant c-a motions take in slow-fluctuation theory the place of the elusive purely periodic solutions of the classical theories.

A motion will be orbitally unstable if for any $\eta$ there exists at least one orbit $\mathscr{C}^*$ which eventually leaves the $\eta$-tube, however small $\rho$ is chosen. Roughly speaking, in the unstable case certain arbitrarily small perturbations cause finite orbit changes. Still, possibly there are many $\mathscr{C}^*$ which remain safely within the $\eta$-tube even for a finite $\rho$. If so, one may speak of "conditional"[7] stability: roughly, perturbations of one type leave the orbit stable while the others change it materially. Phase space topologies of this kind are well known in the theory of differential equations; for instance, they play a prominent role in the study of generic properties of linear operators.[8] They are certainly not confined to recondite systems. With coupled oscillators they occur easily, as we show in Sec. III.C.

Sometimes orbital instability (whether conditional or absolute) results in monotonic amplitude growth, the disruptive event[9] called an "explosive instability" in plasma physics. Again, this is not infrequent, and we meet examples in Sec. V.

[a] This paper is based on a dissertation which will be submitted to Ohio University by M. F. A. in partial fulfillment of the requirements for the Ph.D. degree.

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It does not matter to the orbital stability of $\mathscr{C}$ how the distance between a phase point $P$ on $\mathscr{C}$ and the perturbed phase point $P^*$ on $\mathscr{C}^*$ evolves as the motion proceeds down the $\eta$-tube. At perturbation time $t_0$ the gap must have been less than $\rho$. Later it may grow indefinitely; usually it does, but sometimes not at all. $\mathscr{C}$ is called "Liapunov–stable" iff $\| P^*(t_0) - P(t_0)\| < \rho$ implies $\| P^*(t) - P(t)\| < \eta$ at all times $t > t_0$. (If $\rho$ can be chosen independently of $t_0$ the stability is furthermore called "uniform".) Liapunov–stable oscillators are perfect timepieces.[10] They are rare because nonlinear oscillators rarely have constant frequencies. However, if Liapunov *instability* is the rule, it can come in varying degrees, according to the actual rate of change of $\| P^*(t) - P(t)\|$. Since the subject may be of practical use, we discuss it in some detail in Sec. IV. We find, in particular, that there exist classes of c-a motions and systems for which Liapunov instability appears only in a higher approximation.

Stability arguments are fairly simple in slow-fluctuation approximation owing to the availability of explicit quadratures for amplitudes and phases. Central to our presentation is the simple fact, demonstrated in Sec. II, that orbital stability of c-a motions can be determined from the amplitudes alone, without regard to phases. Since in our approximation the amplitudes all arise from a single quadrature involving a polynomial, all orbital stability information about the various classes of c-a motions can be extracted merely from that one polynomial, as we show from several points of view in Sec. III. Liapunov stability of c-a motions can then be studied from the phase equations alone; see Sec. IV.

Throughout the paper our aim is not completeness. Rather, we want to show how the new slow-fluctuation method allows one to cut pathways of classification and understanding through the veritable jungle of detail rooted in the vast variety of nonlinear processes. Our list of examples in Sec. V is therefore purely illustrative, even sporadic, just a small hint of how much there is to be found.

Likewise, we again confine ourselves to systems with coupling Hamiltonians $H_1(q)$ dependent on coordinates alone, except for several asides. With momentum-dependent coupling, the separation of amplitudes and phases still holds good, and a single quadrature again furnishes all amplitudes. Using these facts, which were established in SF, stability arguments may be fashioned along the lines of the present paper in cases given explicitly.

We add a word of caution which could already have been said in SF but carries more weight in the context of stability arguments: an internal resonance occasionally is not quite what it purports to be. Consider a coupling $H_1(q) = \gamma q_1 q_2 q_3^2$ in three d.f. This is not at all unrealistic, cf. Sec. V.E, but if $m_1 = m_2$ and a resonance $\omega_1 = \omega_2$ is assumed it becomes tantamount to a degeneracy of the d.f. $q_1$ and $q_2$ which can be removed in standard fashion by a linear transformation, leading to a new Hamiltonian with a coupling of the type $\gamma_1 q_1^2 q_3^2 + \gamma_2 q_2^2 q_3^2$, and now there is no more resonance in the customary sense.[11] In order not to overburden our statements with exception clauses, we tacitly assume that such trompe–l'oeil degeneracies have been straightened out.

## II. GENERAL CONSIDERATIONS

The argument of this section is most conveniently couched in terms of amplitudes and phases. They are connected with the canonical variables by

$$q_i(t) = A_i \cos(\omega_i t + \beta_i),$$
$$p_i(t) = -m_i \omega_i A_i \sin(\omega_i t + \beta_i) \tag{2.1}$$

according to the transformations SF (2.1) and (2.2). It deserves mention that the simplicity and symmetry of these formulas is the result of a particular gauge. When a Lagrangian $L$ is replaced by an equivalent $L + dg/dt$, with some $g(q)$, then the generalized momenta $p_i = \partial L / \partial \dot{q}_i$ are replaced by $p_i + \partial g/\partial q_i$. The canonical transformation SF (2.1) implies that a choice of a particular $g$ has been made, a fact easily overlooked. The almost trivial simplicity of the following argument, too, results from this gauge; it would be lost under a homeomorphism $p_i \to p_i + \partial g/\partial q_i$ of the phase space which is still allowed in principle.

Consider a motion at constant amplitudes, say $A_i(t) = A_{i0}$. Its phase orbit $\mathscr{C}$ has projections onto the $p_i, q_i$ phase planes which are ellipses given by Eqs. (2.1) in terms of $t$ as parameter. $\mathscr{C}$ itself lies on the ($n$-dimensional) hypersurface defined by the intersection of the hypercylinders erected over the $n$ phase ellipses (2.1); it is not necessarily a closed curve.

One sees easily enough that orbital instability of $\mathscr{C}$ cannot be caused by the phases $\beta_i(t)$. Let us first assume that the amplitudes of $\mathscr{C}$ are stable in the following, obvious sense: for any preassigned $\eta'$ there exists a $\rho'$ with $0 < \rho' \leqslant \eta'$ such that on any perturbed phase orbit $\mathscr{C}^*$ which passes somewhere within $\rho'$ of $\mathscr{C}$,

$$|A_i^*(t) - A_{i0}| < \frac{\eta'}{\max(1, m_i \omega_i)}, \quad i = 1,\ldots,n \tag{2.2}$$

holds uniformly in $t$ for the perturbed amplitudes $A_i^*(t)$. Now preassign an $\eta > 0$, take $\eta' = \eta/\sqrt{n}$, note the pertaining $\rho' > 0$, draw an $\eta'$-tube about $\mathscr{C}$ and project it onto the $p_i$, $q_i$ phase planes, resulting in bands of width $2\eta'$ about the phase ellipses described above. Take any phase orbit $\mathscr{C}^*$ which comes somewhere within $\rho'$ of $\mathscr{C}$: because of the relations (2.2) and (2.1) its projections must lie within the elliptic $\eta'$-bands. However, it does not follow that $\mathscr{C}^*$ lies within the $\eta'$-tube about $\mathscr{C}$, because of possible foreshortening in the projection. The longest line segment which can have projections of length $\leqslant a$ onto all coordinate axes is the diagonal $d = a\sqrt{2n}$ of a hypercube of edges $a$ parallel to the axes; it will have equal projections $a\sqrt{2}$ onto the phase planes. Conversely, any point farther away from $\mathscr{C}$ than $\eta'\sqrt{n} = \eta$ will project outside the elliptical $\eta'$-band in at least one phase plane. At all events, $\mathscr{C}^*$ lies safely within the $\eta$-tube about $\mathscr{C}$, and hence the assumption (2.2) implies the orbital stability of $\mathscr{C}$.

Since the converse is obvious, we have the

*Theorem*: A motion at constant amplitudes is orbitally stable iff the neighboring amplitudes fulfill the conditions (2.2).

This holds regardless of the behavior of the perturbed phases $\beta_i^*(t)$; indeed, the projections of the perturbed phase

point may move within the elliptic $\eta'$-bands at any speeds. On the other hand, if in an orbitally stable case we subsequently look for Liapunov stability, we certainly need to prove no more than that $|\beta_i^*(t) - \beta_i(t)| < \eta'$ holds uniformly for all $i$.

This very convenient approach to stability of c-a motions results solely from the description in terms of amplitudes and phases, and depends in no way on the techniques used for solving the equations of motion. It becomes especially profitable in the slow-fluctuation approximation, for through the conservation laws SF (3.5) the $n$ conditions (2.2) are all fulfilled if the one for $A_1$ is fulfilled (or an equivalent one for $\bar{p}_1$). A study of solely the underlying polynomial $f(\bar{p}_1)$ thus yields all there is to know about orbital stability in any of the three classes of c-a motion, Case (I) and Case (II) with $r$ even or odd.

Motions at varying amplitudes present an altogether more difficult picture. Suppose for the sake of a quick orientation that we have found a phase path $\mathscr{C}$ in the neighborhood of which the amplitudes are stable in the sense of $|A_i^*(t) - A_i(t)| < \eta'$, analogous to condition (2.2). If the phases also remain stable, $\mathscr{C}$ is evidently Liapunov–stable, but if the phases are affected by the perturbations, $\mathscr{C}$ need not even be *orbitally* stable, for unless the phase changes $\beta_i^*(t) - \beta_i(t)$ are limited in just the right way, the perturbed phase point will gain distance not merely from the unperturbed phase *point* but from the unperturbed phase *curve* as well, since the amplitudes are now varying in time. Thus an orbital stability decision can no longer be based on a study of the amplitudes alone.

The general case also differs in its ergodic aspects. It suffices to consider a single phase plane.[12] The projection of $\mathscr{C}$ is no longer an ellipse, but a spiral which densely fills an annulus the edges of which are determined by the amplitude modulation range. The spiral will degenerate into a closed curve if and only if the modulation and oscillation periods are commensurate, a rare and exceptional case as emphasized in SF.[13] In general, then, a perturbed phase point $P^*(t)$ will continually lie arbitrarily close to points of $\mathscr{C}$ which the unperturbed point $P(t')$ reaches at certain other times. It may seem that in such a situation the usual concepts of stability lose meaning, but this is only a *Wiederkehreinwand* and we submit that it fails for the same reason as in statistical mechanics: the *Wiederkehr* times are fantastically long.[14] Commonsense suggests accordingly that stability be referred to a time scale. It is certainly legitimate to ask after what time interval $\tau(\eta,\rho)$ a perturbed $\mathscr{C}^*$ will leave the $\eta$-tube about $\mathscr{C}$. When in some sense this $\tau$ can be shown to have a uniform, positive lower bound $\tau_0$ as $\eta \to 0$, then $\mathscr{C}$ may be deemed "orbitally stable during $\tau_0$", and if $\tau_0$ is adequately long in relation to some given purpose, although in no way comparable to a Poincaré recurrence time, then the finding may be worth while.

Thus the general case represents an ample subject in its own right. We shall not pursue it here but it may well be mentioned because the surmise is a fair one that the reduction to quadratures inherent in our method can be exploited for general motions to yield useful results in practical cases where the existing, general theory of stability,[15] despite all the brilliant advances made in the last two or three decades, remains unmanageable.

## III. ORBITAL STABILITY

The developments of this section do not necessarily apply in full detail to the (possibly rare) exceptional cases defined in subsection A. Otherwise they are entirely general. They can also be adapted without substantial complications to the case of a momentum-dependent coupling.

### A. Some properties of the polynomial $f$

Recall the definition SF (3.9):

$$f(\bar{p}_1) = \overline{\overline{F}}^2 - \left[E - \sum_2^n \omega_i \alpha_i - \epsilon \bar{p}_1 - \overline{\overline{B}}\right]^2. \tag{3.1}$$

Polynomial $\overline{\overline{B}}(\bar{p}_1,\alpha)$ arises from the terms in the coupling $H_1(q)$ which contain only even powers of the coordinates, while $\overline{\overline{F}}(\bar{p}_1,\alpha)$ arises from the resonant terms after the substitutions SF (3.3) and (3.4), and has the general form

$$\overline{\overline{F}} = C(g_1\bar{p}_1)^{l_1/2}(g_2\bar{p}_1 + \alpha_2)^{l_2/2}\cdots$$
$$\cdots(g_n\bar{p}_1 + \alpha_n)^{l_n/2}\overline{\overline{Q}}(\bar{p}_1,\alpha), \tag{3.2}$$

as follows from the discussion in SF at the end of Sec. II. Here $C \neq 0$ is a system constant and the $l_i$ are integers $\geqslant 0$, with $l_1 \neq 0$ because of our numbering of the d.f., and with $\bar{p}_1 \geqslant 0$ because of the convention $g_1 > 0$ (see SF Sec. III); $\overline{\overline{Q}}$ is a polynomial which can be nonconstant only if there are several resonant terms in $H_1$.

From Eq. (3.2) it follows that $\overline{\overline{F}}(0,\alpha) = 0$ and therefore

$$f(0) \leqslant 0, \tag{3.3}$$

an inconspicuous but important fact.

Squaring Eq. (3.2) yields

$$\overline{\overline{F}}^2 = a_{l_1}\bar{p}_1^{\,l_1} + \cdots + a_j\bar{p}_1^{\,j}. \tag{3.4}$$

The highest nonvanishing coefficient $a_j$ sometimes depends only on system parameters, but if one or more d.f. with $g_i = 0$ are present, $a_j$ will also contain the amplitude constants $\alpha_i$ and then depends on initial conditions as well. The lower coefficients always contain the $\alpha_i$. Likewise, if

$$\overline{\overline{B}} = b_0 + b_1\bar{p}_1 + \cdots + b_m\bar{p}_1^{\,m}, \tag{3.5}$$

the highest coefficient $b_m$ may be independent of initial conditions but it does not have to be, and the lower ones normally are not, as is immediately clear from the origins of $\overline{\overline{B}}$ together with the transformation formulas SF (3.3).

From the definition (3.1), we now obtain

$$f(\bar{p}_1) = f_s\bar{p}_1^{\,s} + f_{s-1}\bar{p}_1^{\,s-1} + \cdots$$
$$+ \left[a_2 + 2b_2\left(E - \sum \omega_i\alpha_i - b_0\right) - (b_1 + \epsilon)^2\right]\bar{p}_1^{\,2}$$
$$+ \left[a_1 + 2(b_1 + \epsilon)\left(E - \sum \omega_i\alpha_i - b_0\right)\right]\bar{p}_1$$
$$- \left(E - \sum \omega_i\alpha_i - b_0\right)^2, \tag{3.6}$$

with the last coefficients written out in detail for later use. The highest nonvanishing coefficient $f_s$ may depend on system parameters only, but often enough it will depend on initial conditions as well. Consequently it may also go through zero for certain initial conditions. This is not obnoxious in itself, but if a zero occurs precisely for those initial conditions which also determine the c-a motion under consideration, various arguments will be in jeopardy. We have not found such cases, and possibly they are rare coincidences, but they are conceivable and must be treated on their own terms if and when they occur.

Thus we assume explicitly that $f_s$ has no zero within the range of values of $\alpha_2,\ldots,\alpha_n,E$ under consideration. As a consequence, the number of roots of $f(\bar{p}_1)$ will be invariant throughout this range. Furthermore, from the structure of the polynomial (3.6) it is clear that the roots will be continuous functions of $\alpha_2,\ldots,\alpha_n,E$ and that their product cannot change sign.

### B. Use of roots in special cases

The (nonnegative) roots of $f(\bar{p}_1)$ are the turning points of $\bar{p}_1(t)$, hence their behavior under perturbations determines the orbital stability of the motion. Unfortunately, simple formulas for the roots often do not exist. Some general stability criteria based on roots can nonetheless be obtained for restricted classes of c-a motions. We choose as example the fairly common Case (I) motions in which one single d.f. remains at rest [see SF Sec. V]. If the d.f. which does not move has $g_i = 0$, its amplitude is always constant [see SF Eq. (3.5)] and orbital stability depends on the other d.f.; thus we take it to be a resonant one with $g_i \neq 0$, and assume without loss of generality that it is $q_1$.

A glance at the exact equation of motion

$$\dot{p}_1 = -\frac{\partial H}{\partial q_1} = -m_1\omega_1^2 q_1 - \frac{\partial H_1}{\partial q_1}$$

shows that $q_1 \equiv 0$ is possible (nontrivially) only if $H_1$ contains no terms linear in $q_1$. Then in Eqs. (3.2) and (3.4) we must have $l_1 \geqslant 2$, and therefore $a_1 = 0$ in Eq. (3.6). Under these circumstances it is seen that $f(\bar{p}_1)$ cannot have a simple root at the origin, but will have a root of at least the second order there iff

$$E - \sum \omega_i \alpha_i - b_0 = 0. \tag{3.7}$$

Motion at $\bar{p}_1 \equiv 0$ requires such a higher-order root. Let us assume for brevity of exposition that it is exactly double, i.e. that the condition (3.7) holds together with

$$a_2 - (b_1 + \epsilon)^2 \neq 0, \tag{3.8}$$

and apply small perturbations to the motion. The condition (3.7) which had to be fulfilled to set up the c-a motion will now be violated and therefore the double root at the origin disappears. In its place there must still be two roots close by, because of continuity. The graph of $f(\bar{p}_1)$ now passes below the origin, because of the general condition (3.3); also, physical motion can only occur to the right and requires $f(\bar{p}_1) \geqslant 0$. It follows that at least one of the new roots must be (real and) positive.

Both roots may have moved towards the right. They may still coincide, or else they have separated and then $f(\bar{p}_1)$ must be positive in between. Thus the motion occurs at or between the displaced roots, and is orbitally stable because the displacement can be made arbitrarily small if the perturbations are taken small enough, satisfying the criterion (2.2).

The two roots may also have split with the origin between them. In this situation $\bar{p}_1$ must increase from the positive displaced root up to the next root, which will be at a finite distance from the origin, owing to condition (3.8), or may not even exist, in which case $\bar{p}_1$ must grow without bound. Inequality (2.2) can not be satisfied and the motion is orbitally unstable.

A formal stability criterion can be constructed from the sign of the product of the two displaced roots. Since all other roots are much larger, we can find the two small ones from the last three terms in the polynomial (3.6); their product has its sign opposite to the coefficient of $\bar{p}_1^2$ and therefore we find stability iff

$$a_2 - (b_1 + \epsilon)^2 < 0 \tag{3.9}$$

(which can in an explicit case be transformed back into a relation between the amplitudes).

### C. Use of derivatives in general

Multiple roots of $f(\bar{p}_1)$ as needed for c-a motion can occur in the four configurations sketched in Fig. 1. The order $\sigma$ of the root $R$ is even in Figs. 1a and 1b, odd (but not $\sigma = 1$) in Figs. 1c and 1d. Now apply small perturbations to $\alpha_2,\ldots,\alpha_n,E$; how will $\bar{p}_1(t)$ change in the four cases?

It is important to recognize at the outset that $\bar{p}_1$ is in general subject to restrictions resulting from the values of the

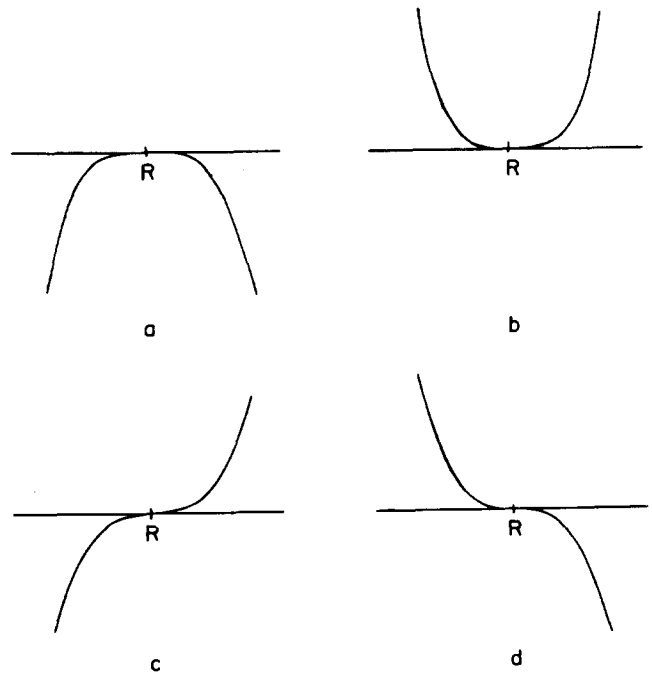


FIG. 1. The four possible configurations of multiple roots of the polynomial $f(\bar{p}_1)$.

constants $\alpha_2,...,\alpha_n$ regardless of the nature of the polynomial $f$. By virtue of the conservation laws SF (3.4), together with Eqs. SF (3.3) and the requirement $\bar{p}_i \geqslant 0$, an inequality

$$-g_i\bar{p}_1 \leqslant \alpha_i$$

must hold for every $i = 2,...,n$. For a near-resonant d.f. with $g_i = 0$ this is trivial. For a negative $g_i$, however, an upper bound to $\bar{p}_1$ is implied; an example of some interest occurs after Eq. (5.40) below. Likewise, a positive $g_i$ implies a lower bound $-\alpha_i \leqslant g_i\bar{p}_1$; there is the bound $0 \leqslant \bar{p}_1$ at all events, but it may be exceeded by one or more of the former. The closed interval from the largest lower bound (including zero) to the smallest upper bound we shall call the "domain of $\bar{p}_1$" resulting from the given $\alpha_2,...,\alpha_n$; it may be finite or right-infinite, and $\bar{p}_1$ can never lie outside at any time.

It can happen that the domain contracts into a single point. A simple example in three d.f. occurs after Eq. (5.60) below. In such a situation no amplitude variation is possible, and if we perturb $\alpha_2,..., \alpha_n$ a little, the perturbed domain will still be small. Hence any motion with a point domain is orbitally stable, irrespective of other considerations.

We may now turn to Fig. 1 under the assumption that the domain is a finite or right-infinite interval.

Consider Fig. 1a, the local maximum: regardless of where under small perturbations new zeros appear near $R$, the precondition $f(\bar{p}_1) \geqslant 0$ necessary for physical motion can only be met in the neighborhood of $R$, by continuity, and any c-a motion at $R$ is therefore orbitally stable.

Figure 1b, the local minimum: the opposite conclusion results, for extended regions with $f(\bar{p}_1) > 0$ always exist adjacent to $R$, so that certain perturbations will cause the amplitude to evolve away from $R$. Of course, the evolution can proceed only towards one side in case $R$ lies at an endpoint of the domain of $\bar{p}_1$. The instability can be conditional, though. For example, if $R$ is fourfold and splits into a quartet of distinct, real roots, then motion with a very small amplitude modulation, between the two inner roots, may occur after some perturbations.

Figure 1c: if $R$ lies at an inner point of the domain, instability follows as for Fig. 1b and is possibly conditional. However, if $R$ is a right domain endpoint, no finite evolution of $\bar{p}_1$ towards the right is allowed and orbital stability ensues.

Figure 1d: analogous to Fig. 1c. If $R$ is an inner point, there is instability, possibly conditional. If $R$ is a left domain endpoint, there is stability.

A summary of these results, expressed in terms of higher derivatives, is the

*Theorem*: With a point domain of $\bar{p}_1$, every motion has constant amplitudes and is orbitally stable. When the domain is an interval, a c-a motion $\bar{p}_1 = R$ at a root $R$ of multiplicity $\sigma \geqslant 2$ is orbitally stable iff
given $\sigma$ even:

$$(d^{\sigma}f/d\bar{p}_1^{\sigma})_{\text{at } R} < 0,$$

given $\sigma$ odd:

$$(d^{\sigma}f/d\bar{p}_1^{\sigma})_{\text{at } R} \gtrless 0 \quad \text{and} \quad R \begin{matrix}\text{upper}\\ \text{lower}\end{matrix} \text{endpoint.} \tag{3.10}$$

In the principal case $\sigma = 2$, a local minimum as in Fig. 1b could accordingly be stable if the domain is an isolated point. Actually, if $\sigma = 2$ it is just for a point domain that this configuration cannot occur in physical systems. For the proof, assume the contrary, apply small perturbations and note that in each of the alternative developments a contradiction follows. (a) If the real double root becomes complex, then $f(\bar{p}_1) > 0$ holds afterwards in some finite interval enclosing $R$ and the motion $\bar{p}_1(t)$ must become progressive, but this cannot happen because the domain of $\bar{p}_1$ can be held as small as we please. (b) If the root splits into two real ones, then $f(\bar{p}_1) < 0$ holds in between, the motion must be progressive from one of the roots outwards and the contradiction is the same. (c) If the double root never splits under any perturbation, c-a motion would always result. Now for any c-a motion in our nonlinear system, $R$ is determined by $\alpha_2,...,\alpha_n$ from one equation, either $\overline{F}(R,\alpha) = 0$ or SF (5.5), and $E$ then follows from another equation, either SF (5.2) or (5.6). However, $E$ is free for us to perturb independently of $\alpha_2,...,\alpha_n$, hence we may at will violate the latter equation, hence the amplitudes are not necessarily constant, hence the root cannot permanently stay double.

For a second-order root there is no further alternative similar to the above-mentioned splitting of a fourth-order root into a quartet with $f(\bar{p}_1)$ having a tiny bulge in the middle under which stable motion can continue. Odd-order roots, too, can develop such bulges and indeed these are necessary for continued stable motion in the vicinity of a point domain, or of a domain endpoint. Having thus characterized the special nature of the case $\sigma = 2$, we can state the simple

*Theorem*: C-a motion $\bar{p}_1 = R$ at a double root is orbitally stable iff

$$(d^2f/d\bar{p}_1^2)_{\text{at } R} < 0.$$

A simple example is the criterion (3.9); it effectively puts the second derivative of the polynomial (3.6) in a very practical form which could be attained because we had some explicit knowledge of the nature of the case. Such knowledge may not always be available, but it is still possible to develop more detailed, yet general, criteria if the distinction between Case (I) and Case (II) motions is introduced as in SF Sec. V. We do so in the remainder of this subsection, but confine ourselves to $\sigma = 2$, as the treatment of higher multiplicities will follow an analogous route. The required second derivative is obtained from the general formula (3.1)

$$\begin{aligned} f'' = d^2f/d\bar{p}_1^2 &= 2(\partial\overline{F}/\partial\bar{p}_1)^2 + 2\overline{F}\,\partial^2\overline{F}/\partial\bar{p}_1^2 \\ &\quad - 2(\epsilon + \partial\overline{B}/\partial\bar{p}_1)^2 \\ &\quad + 2\Big[E - \sum_2^n \omega_i\alpha_i - \epsilon\bar{p}_1 - \overline{B}\Big]\partial^2\overline{B}/\partial\bar{p}_1^2. \end{aligned} \tag{3.11}$$

Case (I) is defined by $\overline{F}(R,\alpha) \equiv 0$. Thus the second term on the right of Eq. (3.11) will vanish at $R$ except possibly if the second derivative of $\overline{F}$ is not bounded there. It could become unbounded, see Eq. (3.2), only if $l_i = 1$ or $l_i = 3$ for some $i$, together with $g_i\bar{p}_1 + \alpha_i = 0$ for $\bar{p}_1 = R$, which means in terms of amplitudes that $\bar{p}_i = 0$ and in fact, $\bar{p}_i \equiv 0$ because the motion is such that $\bar{p}_1 \equiv R$. But $q_i \equiv 0$ is possible (indepen-

dently of the other d.f.) only if $l_i \geqslant 2$, as we showed in Subsec. B for $i = 1$; hence we may discard the possibility $l_i = 1$. With $l_i = 3$, on the other hand, each term in the product $\bar{\bar{F}}(\partial^2\bar{\bar{F}}/\partial\bar{\bar{p}}_1^2)$ still contains $g_i\bar{p}_1 + \alpha_i$ to some positive power so that when this factor vanishes the product also does. Now from Eq. SF (5.2) it follows that the bracket in Eq. (3.11) vanishes at $R$, and hence we have the

*Theorem*: A case (I) c-a motion at a root $R$ of multiplicity $\sigma = 2$ is orbitally stable iff

$$|\partial\bar{\bar{F}}/\partial\bar{\bar{p}}_1|_{\text{at } R} < |\epsilon + \partial\bar{\bar{B}}/\partial\bar{\bar{p}}_1|_{\text{at } R}. \tag{3.12}$$

For the opposite sign there is instability, while equality can not arise for $\sigma = 2$.

Case (II) means $\sin\bar{\bar{q}}_1 \equiv 0$ and implies the relation SF (5.5):

$$\epsilon + \partial\bar{\bar{B}}/\partial\bar{\bar{p}}_1 = \pm\,\partial\bar{\bar{F}}/\partial\bar{\bar{p}}_1, \quad r\begin{matrix}\text{odd}\\ \text{even}\end{matrix}. \tag{3.13}$$

So now the first and third terms on the right of Eq. (3.11) cancel. In the bracket we set $\bar{\bar{p}}_1 = R$ and then substitute

$$E - \sum \omega_i\alpha_i - \epsilon R - \bar{\bar{B}}(R,\alpha) = \pm\,\bar{\bar{F}}(R,\alpha), \quad r\begin{matrix}\text{even}\\ \text{odd}\end{matrix}$$

from Eq. SF (5.6). Hence we have the

*Theorem*: A Case (II) c-a motion at a root $R$ of multiplicity $\sigma = 2$ is orbitally stable iff

$$\bar{\bar{F}}(R,\alpha)(\partial^2\bar{\bar{F}}/\partial\bar{\bar{p}}_1^2 \pm \partial^2\bar{\bar{B}}/\partial\bar{\bar{p}}_1^2)_{\text{at } R} < 0, \quad r\begin{matrix}\text{even}\\ \text{odd}\end{matrix}. \tag{3.14}$$

Again, equality is impossible for $\sigma = 2$, and $>$ means instability. In practice, the sign of $\bar{\bar{F}}$ is often constant, e.g., when $H_1(q)$ contains only one resonant term; then an obvious further simplification is possible.

The two formulas (3.12) and (3.14) are remarkably different: first derivatives in one, second derivatives in the other. Also, $\epsilon$ occurs explicitly in the former, while in the latter it remains concealed in the relation between the amplitudes $R,\alpha_2,..,\alpha_n$ of the c-a motion; cf. SF Eqs. (5.5) and (7.13) for detail.

### D. Existence surfaces and stability boundaries

We now introduce geometrical language[16] in order to interpret the analytical stability criteria of the preceding subsection. We represent every c-a motions as a point in an $n$-dimensional space having the amplitudes as rectangular cartesian coordinates. Actually, coordinates $\bar{p}_i$ will be more convenient than the $A_i$ themselves. In this $\bar{p}$-space all c-a motions of a particular class will be represented by a geometrical object which we call the "existence surface" of the class, for brevity; it will be a union of locally continuous sets of (generally) $n - 1$ dimensions, or bordered sheets of hypersurfaces, but we shall gloss over such details unless they matter to the purpose.

Case (I) motions are defined by $\bar{\bar{F}}(\bar{p}_1,\alpha) = 0$, a condition which by means of the substitutions SF (3.3) and (3.4) translates back from Eq. (3.2) into

$$\bar{F}(\bar{p}) = C\bar{p}_1^{\,l_1/2}\cdots\bar{p}_n^{\,l_n/2}\bar{Q}(\bar{p}) = 0. \tag{3.15}$$

Thus the Case (I) existence surface is not complicated. It consists mostly of planes $\bar{p}_i = 0$ (or rather, of hyperplane wedges, because of the physical restriction $\bar{p}_i \geqslant 0$ for all $i$) with $l_i \geqslant 2$ (for $l_i = 1$ a zero amplitude is usually ruled out as discussed in SF Sec. II); only the sheet $\bar{Q} = 0$ can become curved, but only if there are several resonant terms in $H_1(q)$, and of sufficiently high degree, too.

If we now apply the criterion (3.10) at each point, this existence surface will divide into subsets of different stability type which are disjoint but still locally continuous because $f(\bar{p}_1)$ as a polynomial has continuous derivatives. There is no need to deal with the points individually, of course; rather ask first, where does $f''$ vanish? In any connected region of the existence surface where the second derivative does not vanish, it must have the same sign throughout, by continuity; therefore it suffices to calculate this sign at one interior point in order to find the stability label for the entire region. All stable or unstable regions with $\sigma = 2$ can thus be recognized, and this disposes of a good deal of the stability problem.

The expression (3.11) for the second derivative can not be employed for the present purpose as it stands because it contains the energy constant $E$ which is not an independent one for c-a motions, see SF Sec. V, and must be eliminated, but this is precisely what we have done already to arrive at the criterion (3.12). In fact,

$$\pm\,(\partial\bar{\bar{F}}/\partial\bar{\bar{p}}_1)_{\text{at } R} = \epsilon + (\partial\bar{\bar{B}}/\partial\bar{\bar{p}}_1)_{\text{at } R} \tag{3.16}$$

is seen to be the condition to ensure that $f'' = 0$ for a Case (I) motion (at $\bar{\bar{p}}_1 \equiv R$ and with $\sigma > 2$).

Consider more generally the equation

$$\epsilon + \partial\bar{\bar{B}}/\partial\bar{\bar{p}}_1 = \pm\,\partial\bar{\bar{F}}/\partial\bar{\bar{p}}_1 \tag{3.17}$$

and translate it back into $\bar{p}$-space. The set of all points in $\bar{p}$-space satisfying Eq. (3.17) will be called, for brevity, the "2-stability boundary" of the Case (I) motion. It is in general a curved hypersurface, somewhat reminiscent of a hyperbolic paraboloid in three dimensions, as will be clear from a glance at Eq. (3.2), and it usually has two distinct sheets because of the $\pm$ sign. The points on the existence surface (3.15) which have $f'' = 0$ are now obtained by finding the intersection with the boundary (3.17). Note that the intersection may sometimes be only a contact.

Case (II) motions are defined by the condition (3.13) quoted above. This is seen to be identical with Eq. (3.17); only the $\pm$ sign needs to be interpreted as expressing the two possible values of $r$. Thus in $\bar{p}$-space the existence surface for Case (II) coincides with the 2-stability boundary for Case (I).

There is more such reciprocity. If on the Case (II) existence surface we again seek the points having $f'' = 0$, we must again eliminate $E$ from Eq. (3.11), but by the second route which led to the criterion (3.14), and recognize that

$$\bar{\bar{F}}(R,\alpha)(\partial^2\bar{\bar{F}}/\partial\bar{\bar{p}}_1^2 \pm \partial^2\bar{\bar{B}}/\partial\bar{\bar{p}}_1^2)_{\text{at } R} = 0, \quad r\begin{matrix}\text{even}\\ \text{odd}\end{matrix} \tag{3.18}$$

will make $f'' = 0$ for a Case (II) motion (at $\bar{\bar{p}}_1 \equiv R$ and with $\sigma > 2$). Obviously we can deal with this result much as with Eq. (3.16): we define a 2-stability boundary whose equation factorizes into $\bar{\bar{F}} = 0$ and the supplementary

$$\partial^2\bar{\bar{F}}/\partial\bar{\bar{p}}_1^2 \pm \partial^2\bar{\bar{B}}/\partial\bar{\bar{p}}_1^2 = 0, \quad r \begin{matrix}\text{even}\\ \text{odd}\end{matrix} \tag{3.19}$$

which happens to be the $\bar{\bar{p}}_1$-derivative of Eq. (3.17). The second factor could have singularities or become a constant (including zero), in which case we must not factor but consider the product (3.18) on its own merits; exceptions apart, however, the first factor $\bar{\bar{F}} = 0$ is merely the Case (I) existence condition (3.15).

It is this unexpected reciprocity which lends appeal to the geometrical approach. Roughly speaking, a study of only the two existence surfaces and their intersection, where the motions which are simultaneously Case (I) and (II) are found, will settle a major part of the stability question for *both* Cases (I) and (II). Of course, there are possible complications from Eq. (3.18); then the 3-stability boundaries still remain to be found in the intersection; and so forth. For reasons of space, we shall not attempt to do any of this in full generality, but refer instead to the specific examples in Sec. V. Here we only append one more discussion of a general nature.

The close connection between the stability problems for Cases (I) and (II) suggests exploitations of geometrical transformations. One example will suffice. Consider a system for which $\bar{\bar{F}}(\bar{p})$ is homogeneous while $\bar{\bar{B}}$ is zero, and apply a dilatation $\bar{p}_i \to \chi\,\bar{p}_i$ to $\bar{p}$-space. Since $\bar{\bar{F}}$ will simply multiply with some power of $\chi$, the existence surface (3.15) remains invariant. Now go from $\bar{p}$ to $\bar{\bar{p}}$. The pertinent transformation SF (3.3) is linear-homogeneous, hence $\bar{\bar{F}}$ will again be homogeneous, and its $\bar{\bar{p}}_1$-derivatives must also be homogeneous. Then in Eq. (3.19) the derivative will under the dilatation multiply with some power of $\chi$, and the supplementary 2-stability boundary is seen to be invariant. In Eq. (3.13) or (3.17) for the Case (II) existence surface the dilatation will also bring a power of $\chi$ to the derivative, but we cannot cancel it out, we can only put it as a denominator under the $\epsilon$. These last two arguments would obviously continue to hold if $\bar{\bar{B}}$ were not zero, but homogeneous and of the same degree as $\bar{\bar{F}}$, so that under dilatation $\bar{\bar{F}}$ and $\bar{\bar{B}}$ multiply with the *same* power of $\chi$, and their derivatives likewise. The result can be paraphrased thus: in a system with $\bar{\bar{F}}$ and $\bar{\bar{B}}$ homogeneous and of the same degree, or with $\bar{\bar{F}}$ homogeneous and $\bar{\bar{B}} \equiv 0$, a change of $\epsilon$ is tantamount to a dilatation of $\bar{p}$-space. This can be helpful in drawing stability diagrams. At the very least it follows that for $\epsilon = 0$ all $\sigma = 2$ stability regions are invariant under dilatation.

### E. Use of curvature boundaries in many cases

When the intersection of existence surfaces and 2-stability boundaries has been determined, the resultant 2-stability regions must still be labelled, using Eqs. (3.11) or (3.12) and (3.14), according as $f'' \gtrless 0$. In many cases the mechanical task of the calculation of the sign of $f''$ can be profitably linked to a more general, geometrical construction.

Suppose the polynomial $\bar{\bar{B}}(\bar{\bar{p}}_1, \alpha)$ is constant, or at most linear in $\bar{\bar{p}}_1$; then the fourth term on the right of formula (3.11) vanishes. In this case we call the set of all points in $\bar{p}$-space satisfying

$$(\partial\bar{\bar{F}}/\partial\bar{\bar{p}}_1)^2 + \bar{\bar{F}}\,\partial^2\bar{\bar{F}}/\partial\bar{\bar{p}}_1^2 - (\epsilon + \partial\bar{\bar{B}}/\partial\bar{\bar{p}}_1)^2 = 0 \tag{3.20}$$

the "curvature boundary" of $f(\bar{\bar{p}}_1)$. It will in general be a connected hypersurface of $n-1$ dimensions which divides $\bar{p}$-space into a "right" and a "left" part corresponding to $f'' \gtrless 0$. Calculation of the sign of $f''$ at a single point thus fixes the sign everywhere else, including the stability regions.

The benefit of this approach is that the curvature boundary often helps in the classification of the system motions which are possible in some more extended vicinity of a c-a motion under scrutiny. The projection of an arbitrary phase curve from $\bar{p},\bar{q}$-space into $\bar{p}$-subspace is in slow-fluctuation approximation a straight line segment given by the $n$ linear equations (see SF Sec. III)

$$\begin{aligned}\bar{\bar{p}}_1 &= g_1\bar{\bar{p}}_1,\\ \bar{\bar{p}}_i &= g_i\bar{\bar{p}}_1 + \alpha_i, \quad i = 2,\ldots,n\end{aligned} \tag{3.21}$$

in terms of the parameter $\bar{\bar{p}}_1$ (with $g_1 > 0$ but the other $g_i$ and the $\alpha_i$ possibly $\leqslant 0$). The turning points of the amplitude modulation, the segment end points, are determined by roots of $f(\bar{\bar{p}}_1) = 0$, which are often enough awkward to calculate. The equation $f''(\bar{\bar{p}}_1) = 0$ is of order 2 less and will usually be more manageable. For instance, a segment may cross the curvature boundary if and only if $f(\bar{\bar{p}}_1)$ has a point of inflection between the turning points; if now we find for some reason that this can not happen in a certain region, then we already know a good deal about the roots of $f(\bar{\bar{p}}_1)$ in the vicinity. Such perspectives can be developed *ad hoc*; we refer to a few hints in Sec. V.

If $\bar{\bar{B}}$ is of the second or higher order, then there is a separate $f'' = 0$ surface for every value of $E$. The family of these surfaces is linear in the parameter $E$; thus it does not have an envelope, but it follows from Eq. (3.11) that each member passes through the intersection of the surface (3.20) with the surface $\partial^2\bar{\bar{B}}/\partial\bar{\bar{p}}_1^2 = 0$. Evidently the structure of the family may be complicated. Useful geometrical arguments are still not ruled out for particular cases, but we have not perceived useful generalities worthy of elaboration.

## IV. LIAPUNOV STABILITY

We now seek c-a motions for which $|\beta_i^*(t) - \beta_i(t)| < \eta'$ holds (uniformly in $t$) in addition to the orbital stability condition (2.2) (under all perturbations which at time $t_0$ produce $\| P^*(t_0) - P(t_0)\| < \rho'$). A c-a motion is purely harmonic with constant periods, say $\omega_i + \dot{\beta}_{i0}$. The phase variations $\beta_i^*(t)$ of the perturbed motion will consist of constant parts close to the $\dot{\beta}_{i0}$, plus (small) parts having the same period $T^*$ as the amplitude modulations; see SF Sec. IV. Thus a phase variation change

$$\Delta\dot{\beta}_i = \dot{\beta}_i^*(t) - \dot{\beta}_{i0} \tag{4.1}$$

will in general consist of a small constant part plus a small part of period $T^*$.

Perfect, uniform Liapunov stability would result from $\Delta\dot{\beta}_i \equiv 0$. This would require that all motions in an entire $n$-dimensional neighborhood in $\bar{p}$-space have the same, constant period, including those off the c-a existence surface which are (faintly) amplitude modulated. Physically speaking, throughout this $n$-dimensional range of amplitude values the system would be required to exhibit an essentially

harmonic character with some faint, essentially harmonic coupling to account for faint, constant-frequency amplitude modulation. Such conditions are hard to conceive in a system with a polynomial coupling Hamiltonian.

The frequencies generally are not even constant inside the existence surfaces because the frequencies of c-a motions generally depend on the amplitudes. Only for Case (I) motions can they become constant, provided also $\bar{B} \equiv 0$. They are then identical with the normal frequencies $\omega_i$, and the system behaves as if it were exactly harmonic; see SF Sec. V. This class of motions (and systems) may have properties close to Liapunov stability.

Consider therefore a system with $\bar{B} = 0$. The Case (I) existence surface consists mostly of coordinate planes. Choose one of those, and without loss of generality call it $\bar{p}_1$. Thus the c-a motions to be considered have $\bar{p}_1 \equiv 0$ at a multiple root of $f(\bar{p}_1)$, which for brevity we assume to be exactly double; according to Eq. (3.6) this means that we must have both $E - \Sigma\omega_i\alpha_i = 0$ and

$$a_1 = 0, \tag{4.2}$$

a restriction on the system which happens to be included in the orbital stability problem discussed in Sec. III.B. From there we recall that after a perturbation $f(\bar{p}_1)$ has in the orbitally stable case two roots at, or close to the right of, the origin. To calculate them, we may exploit their smallness. Neglect $\bar{p}_1^{\,3}$ and higher powers in Eq. (3.6) so that

$$f^*(\bar{p}_1) = (a_2^* - \epsilon^2)\,\bar{p}_1^{\,2} + 2\epsilon\left(E^* - \sum \omega_i\alpha_i^*\right)\bar{p}_1 - \left(E^* - \sum \omega_i\alpha_i^*\right)^2, \tag{4.3}$$

where the star means "after perturbation". A short calculation shows that two real roots require $a_2^* \geqslant 0$ and the roots follow at once. The differential equation SF (3.10) can be integrated with the quadratic polynomial (4.3) and yields the elementary solution

$$\bar{p}_1(t) = \frac{E^* - \Sigma\omega_i\alpha_i^*}{\epsilon^2 - a_2^*} \times \{\epsilon + \sqrt{a_2^*}\,\sin[(\epsilon^2 - a_2^*)^{1/2}(t + \text{const})]\}, \tag{4.4}$$

where the argument of the sine is real on account of the orbital stability condition (3.9).

We now take the general equation SF (4.2) for the phase variations, set $\bar{B} \equiv 0$, recall that $\dot{\beta}_{i0} = 0$ for the given c-a motions, and write Eq. (4.1) as

$$\Delta\dot{\beta}_i = \frac{E^* - \Sigma\omega_i\alpha_i^* - \epsilon\bar{p}_1}{\bar{F}^*}\,\frac{\partial \bar{F}^*}{\partial\alpha_i^*}, \quad i = 2,\ldots,n. \tag{4.5}$$

Upon insertion of the explicit expression (4.4) into Eq. (4.5), $\Delta\dot{\beta}_i$ is seen to be in general a more or less complicated function of time, depending on the given $\bar{F}$. Hence there is in general no Liapunov stability; the best one could hope for is a kind of "stability over one modulation period" which would result if by happenstance the time average of $\Delta\dot{\beta}_i$ vanishes for all $i$ so that the perturbed phase point oscillates hence and forth about the unperturbed one.

However, it is also possible for $\bar{p}_1$ to be time-independent, namely if $a_2^* = 0$, according to Eq. (4.4); indeed the polynomial (4.3) becomes a perfect square for $a_2^* = 0$. Moreover, the constant value is

$$\bar{p}_1 = \left(E^* - \sum \omega_i\alpha_i^*\right)\Big/\epsilon, \tag{4.6}$$

provided $\epsilon \neq 0$, and if we substitute this into Eq. (4.5) the result is $\Delta\dot{\beta}_i \equiv 0$ for all $i = 2,\ldots,n$, regardless of $\bar{F}$; an analogous result follows for $i = 1$ from Eq. SF (4.3). This, then, is the way for constant frequencies to become possible in entire neighborhoods off the c-a existence surfaces: under perturbations the crucial multiple root of $f(\bar{p}_1)$ must not split but displace itself as one. A plausible result, perhaps, but it certainly was not obvious that systems of such nature are plentiful. In fact, the two conditions (4.2) and $a_2^* = 0$ are readily met by $l_1 \geqslant 3$ [see Eq. (3.4)]. The simplest example is a system in two d.f. with $H_1(q) = \gamma q_1^3 q_2$.

This argument rests upon the neglect of powers higher than the second in the polynomial (4.3). If in a system with coupling of type $q_1^3 q_2$ (or similar) it is permissible to neglect $q_1^3$, it will indeed behave in an essentially harmonic manner. Again a plausible result, but it no longer holds when the third power is admitted back into $f(\bar{p}_1)$: the double root will then split under perturbations, ever so slightly perhaps, but enough to bring *some* time dependence to $\bar{p}_1(t)$, and with it, to $\Delta\dot{\beta}_i$. Still we may call the motion "Liapunov unstable in the third order only".

Since the slow-fluctuation method is only an approximation one can hardly be disappointed at finding only approximate Liapunov stability. It astonishes one, on the other hand, to realize how frequently it arises, and as it may be relevant in many practical applications we believe that it is worth looking for routinely. Our arguments are easily modified to suit particular cases.

## V. EXAMPLES

The five examples in this section are partly culled from the literature, partly invented, partly tangible, and partly abstract. The selection was governed by a desire to present a handful of graphs and a handful of *ad hoc* methods which could fairly be called typical. In the same spirit we stopped short of developing every item down to its ultimate subdivisions, even though the results are mostly new.

All manipulative details are elementary and have been omitted. However, we indicate enough intermediate steps to enable the reader to follow the argument closely wherever it becomes convoluted. As a safeguard against ambiguities we have rigidly adhered to our elaborate, general notation.

### A. Coupling of pure $q_1^2 q_2$-type

We discuss first two d.f. coupled by

$$H_1(q) = \gamma q_1^2 q_2, \tag{5.1}$$

the simplest of all nonlinear systems of more than one d.f.[17] Only one resonance is possible:

$$2\omega_1 + g_2\omega_2 = \epsilon, \quad g_2 = \pm 1. \tag{5.2}$$

With $g_2 = -1$ the oscillator masses are positive and the

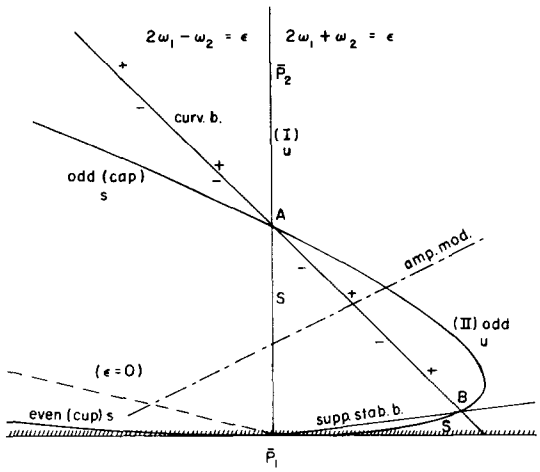


FIG. 2. Stability diagram for coupling $\gamma q_1^2 q_2$. (I) and (II) denote the existence lines for the Case (I) and (II) motions; *s* and *u* mean orbitally stable and unstable; even and odd refer to the parity of *r*; "curv. *b.*" is the boundary between regions of positive and negative curvature, marked + and −; the supplementary stability boundary for Case (II) is also indicated. The two important intersections are at $A\,(0, \frac{1}{2}\theta^2)$ and $B(\frac{4}{9}\theta^2, \frac{1}{18}\theta^2)$. The drawing assumes $\theta = \epsilon/\bar{\gamma} > 0$; for $\theta < 0$ interchange odd and even. At exact resonance the parabola contracts into the straight line marked $\epsilon = 0$. The dot-dash line is representative of motions at varying amplitude. For cup and cap, see Ref. 17.

Hamiltonian is positive-definite; this case represents a basic approximation in the theory of the elastic pendulum and many other, real systems.[17] With $g_2 = +1$ both $m_2$ and $\omega_2$ are negative; this case is familiar in celestial mechanics.[18] We treat both in the same formulation so as to bring their differences to the fore.

In either case, the equation of motion

$$\dot{p}_2 = -\partial H/\partial q_2 = -m_2\omega_2^2 q_2 - \gamma q_1^2$$

shows that $q_2 \equiv 0$ is not a solution unless also $q_1 \equiv 0$. The slow-fluctuation approximation (i.e. the passage from $\bar{H}$ to $\bar{S}$) becomes unreliable when the amplitude of $q_2$ tends towards zero, because it cannot reproduce the required fast phase variation; see SF Sec. VI. We accordingly crosshatch this sensitive strip on the stability graph, Fig. 2. For all other motions, as well as for the low-amplitude motions at times away from the minimum, the slow-fluctuation solutions are known to be extremely accurate, at least for values of $\gamma$ corresponding to an elastic pendulum.[17]

There is no polynomial $\bar{B}$, while $\bar{F}$ follows from the coupling (5.1) as

$$\bar{F}(\bar{p}_1, \alpha) = \bar{\gamma}\bar{p}_1[2(g_2\bar{p}_1 + \alpha_2)]^{1/2}, \tag{5.3}$$

where

$$\bar{\gamma} = \gamma(m_1^2\omega_1^2 m_2\omega_2)^{-1/2},$$
$$\bar{p}_1 = \tfrac{1}{2}\bar{p}_1, \quad \alpha_2 = \bar{p}_2 - \tfrac{1}{2}g_2\bar{p}_1. \tag{5.4}$$

The Case (I) existence line follows from Eq. (5.3) to be simply

$$\bar{p}_1 = 0. \tag{5.5}$$

($\bar{p}_2 = 0$ is equivalent to the $q_2 \equiv 0$ ruled out above). The Case (II) existence lines are found from Eq. (3.13) after transformation to $\bar{p}$ by means of Eqs. (5.4):

$$g_2\bar{p}_1 = -4\bar{p}_2 \mp \theta\sqrt{8\bar{p}_2},$$
$$\text{for } r \begin{matrix}\text{even}\\ \text{odd}\end{matrix} \text{ with } \theta = \epsilon/\bar{\gamma}. \tag{5.6}$$

With $g_2 = +1$ the equation can be satisfied for only one of the two signs, given the sign of $\theta$. On the other hand, at exact resonance $\epsilon = \theta = 0$ the parabola (5.6) degenerates into the straight line

$$g_2\bar{p}_1 + 4\bar{p}_2 = 0, \tag{5.7}$$

which can hold only for $g_2 = -1$, and then *r* may be either even or odd.

The supplementary stability boundary Eq. (3.19) becomes

$$g_2\bar{p}_1 - 8\bar{p}_2 = 0; \tag{5.8}$$

this can hold only for $g_2 = +1$. The curvature boundary Eq. (3.20) is found after some reduction to be the straight line

$$g_2\bar{p}_1 + \bar{p}_2 = \tfrac{1}{2}\theta^2 \tag{5.9}$$

for both values of $g_2$.

Equations (5.5)–(5.9) are best studied and applied by means of graphs. Note that they are all invariant under simultaneous change of sign of $g_2$ and $\bar{p}_1$. Hence we may in the first quadrant draw the curves for $g_2 = +1$, say, and continue them into the second to obtain a mirror image (or left-handed rendition) of the graph for $g_2 = -1$.

The equations contain $\epsilon$ and $\gamma$ only in the combination $\theta = \epsilon/\bar{\gamma}$. This is an obvious consequence of $\gamma$ being an overall factor in $H_1(q)$, and here as well as in other such cases reduces the number of needed graphs by one half. The given $H_1(q)$ has an additional property which entails a further symmetry: it contains one of the variables, here $q_2$, only in form of an odd power as an overall factor. Thus a change of sign of $\gamma$, or $\theta$, can be absorbed into this variable where it means a change of phase by an odd multiple of $\pi$; the sign of $\theta$ is therefore linked with the sign of *r*, again halving the number of graphs. Lastly, we conclude from Sec. III.D that a change of $\epsilon$ (or $\theta$) is equivalent to a dilatation; it follows, amongst other things, that the axis of the parabola (5.6) is always parallel to its limiting form (5.7).

We have drawn Fig. 2 for $\theta$ positive. The pertaining parity of *r* follows from Eq. (5.6). For negative $\theta$ merely interchange *r* odd and even (together with the descriptions "cup" and "cap" which are reminders of the appearance of these c-a motions in the type case, the elastic pendulum[17]).

The sign of $f''$ can be determined from Eq. (3.11) at a single point, say the origin. The stability labels follow as indicated. They are not affected by a change of sign of $\theta$.

Motions at varying amplitudes are represented by straight-line segments which according to Eqs. (3.21) and (5.4) all have the slope $g_2/g_1 = \pm\frac{1}{2}$, like the dot-dash line drawn.

The polynomial $f(\bar{p}_1)$ itself is finally calculated from Eqs. (3.1) and (5.3) as

$$f(\bar{p}_1) = 2g_2\bar{\gamma}^2\bar{p}_1^3 + (2\bar{\gamma}^2\alpha_2 - \epsilon^2)\bar{p}_1^2 + 2\epsilon(E - \omega_2\alpha_2)\bar{p}_1 - (E - \omega_2\alpha_2)^2. \tag{5.10}$$

Note the sign of its leading coefficient. It follows that of the

c-a motions with $\sigma = 3$, point A in Fig. 2 is unstable for $g_2 = +1$ but stable for $g_2 = -1$, while point B is always unstable; cf. Figs. 1c and 1d. It also follows that for $g_2 = +1$ unbounded motion is possible, since there is no upper bound on $\bar{\bar{p}}_1$. In fact, all unstable Case (I) and Case (II) motions are then in the neighborhood of unbounded motion.

It is a rewarding exercise to sketch quickly and qualitatively the appearance of the graph of $f(\bar{\bar{p}}_1)$ for the various regions and dividing lines of Fig. 2.

### B. Coupling of pure $q_1^2 q_2^2$-type

We now turn to the coupling

$$H_1(q) = \gamma q_1^2 q_2^2 \tag{5.11}$$

which seems not to have received much attention in the literature.[19] We present it here for contrast with the previous example. There is still only one resonance:

$$2\omega_1 + g_2\omega_2 = \epsilon, \quad g_2 = \pm 2, \tag{5.12}$$

but almost everything else has been altered by going from $q_2$ to $q_2^2$ in $H_1$.

First we calculate

$$\bar{\bar{B}}(\bar{\bar{p}}_1,\alpha) = 2\bar{\gamma}\bar{\bar{p}}_1(g_2\bar{\bar{p}}_1 + \alpha_2), \tag{5.13}$$

$$\bar{\bar{F}}(\bar{\bar{p}}_1,\alpha) = \bar{\gamma}\bar{\bar{p}}_1(g_2\bar{\bar{p}}_1 + \alpha_2), \tag{5.14}$$

where

$$\bar{\gamma} = \gamma/m_1\omega_1 m_2\omega_2,$$

$$\bar{\bar{p}}_1 = \tfrac{1}{2}\bar{p}_1, \quad \alpha_2 = \bar{p}_2 - \tfrac{1}{2}g_2\bar{p}_1. \tag{5.15}$$

From formula (5.14) we read off the Case (I) existence lines:

$$\bar{p}_1 = 0 \text{ and } \bar{p}_2 = 0. \tag{5.16}$$

The Case (II) existence lines are, from Eq. (3.13),

$$\tfrac{1}{2}g_2\bar{p}_1 + \bar{p}_2 + \tfrac{1}{3}\theta = 0, \quad r \text{ even},$$

$$\tfrac{1}{2}g_2\bar{p}_1 + \bar{p}_2 + \theta = 0, \quad r \text{ odd},$$

$$\text{where } \theta = \epsilon/\bar{\gamma}. \tag{5.17}$$

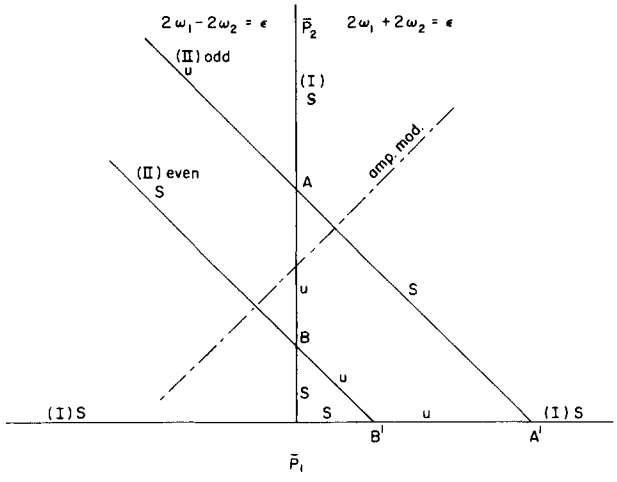


FIG. 3. Stability diagram for coupling $\gamma q_1^2 q_2^2$. Abbreviations as for Fig. 2, but here there is neither a curvature boundary nor a supplementary stability line. The intersections are $A\,(0, -\theta)$ and $B\,(0, -\frac{1}{3}\theta)$. The drawing assumes $\theta = \epsilon/\bar{\gamma} < 0$; for $\theta > 0$ the intercepts at $A$ and $B$ are below the $\bar{p}_1$-axis.

There is no supplementary stability boundary because the parenthesis in Eq. (3.18) reduces to a constant.

Equations (5.16) and (5.17) are again invariant under simultaneous sign change of $g_2$ and $\bar{p}_1$. Thus we again draw the two stability diagrams in one graph, Fig. 3, with $g_2 = +2$ on the right and the $g_2 = -2$ diagram being the mirror image of the left side. Since the polynomial (5.13) is quadratic there exists no energy-independent curvature boundary. The stability labels must therefore be ascertained one by one. At $\bar{p}_1 = 0$, the sign of $f''$ is quickly obtained from Eq. (3.11) or from the second-power coefficient in Eq. (5.18) below, but in the other cases we preferred to use Eqs. (3.12) and (3.14).

Fig. 3 is drawn for $\theta$ negative. For positive $\theta$, according to Eqs. (5.17) the two straight lines must shift downwards so as to make negative intercepts on the $\bar{p}_2$-axis; there are then no Case (II) motions possible for $g_2 = +2$. At exact resonance these lines coincide and pass through the origin; the stability of the Case (II) motions for $g_2 = -2$ then depends solely on the parity of $r$. Note also the alternation of the stability of the Case (I) motions, and in particular, how increasing the amplitude leads from instability back to stability (this still holds at positive $\theta$).

The dot-dash line again indicates the slope of the straight line segments (3.21) representing motion at varying amplitudes.

For reference we also quote the full polynomial

$$\begin{aligned} f(\bar{\bar{p}}_1) = &-12\bar{\gamma}^2\bar{\bar{p}}_1^4 - 2g_2\bar{\gamma}^2(2\theta + 3\alpha_2)\bar{\bar{p}}_1^3 \\ &- [3\bar{\gamma}^2\alpha_2^2 + 4\bar{\gamma}^2\theta\alpha_2 + \epsilon^2 - 4g_2\bar{\gamma}(E - \omega_2\alpha_2)]\bar{\bar{p}}_1^2 \\ &+ 2(\epsilon + 2\bar{\gamma}\alpha_2)(E - \omega_2\alpha_2)\bar{\bar{p}}_1 - (E - \omega_2\alpha_2)^2. \end{aligned} \tag{5.18}$$

Its leading coefficient is negative regardless of $g_2$, hence there can be no unbounded motion for $g_2 = +2$ despite the negative $m_2$ and the appearance of the dot-dash line!

### C. Coupling of $q_1^3 q_2$-type, with and without nonresonant addition

We now pass from $q_1^2$ in $H_1(q)$ to $q_1^3$. We also insert a second and nonresonant term; this could depend on the same two d.f. but for clarity we let it be introduced by a third d.f. Thus we take the coupling to be

$$H_1(q) = \gamma_1 q_1^2 q_2^2 + \gamma_2 q_1^3 q_3 \tag{5.19}$$

as in the detailed example of SF Sec. VII. There are several resonances possible, but all interesting features will become clear if we consider only

$$3\omega_1 - \omega_3 = \epsilon \tag{5.20}$$

as in SF. The results will be similar whether $m_2$, $\omega_2$ are positive or negative; only $\omega_1 \pm \omega_2$ must be significantly different from zero, otherwise there will be a second near-resonance due to the first term in $H_1$ (cf. SF, end of Sec. III).

First we take $\gamma_1 = 0$, i.e., $q_2$ remains decoupled from $q_1$, $q_3$. From SF Eq. (7.7) we read off

$$\bar{\bar{F}}(\bar{\bar{p}}_1,\alpha) = \tfrac{1}{2}\bar{\gamma}_2(3\bar{\bar{p}}_1)^{3/2}(-\bar{\bar{p}}_1 + \alpha_3)^{1/2}, \tag{5.21}$$

where

$$\bar{\gamma}_2 = \gamma_2 (m_1^3 \omega_1^3 m_3 \omega_3)^{-1/2},$$
$$\bar{p}_1 = \tfrac{1}{3}\bar{p}_1, \quad \alpha_3 = \bar{p}_3 + \tfrac{1}{3}\bar{p}_1. \tag{5.22}$$

The Case (I) existence line is

$$\bar{p}_1 = 0 \tag{5.23}$$

(with $\bar{p}_3 = 0$ ruled out because $q_3 \equiv 0$ is impossible unless also $q_1 \equiv 0$). The Case (II) existence line is found from SF Eq. (7.13) after some remodeling:

$$4\theta_2 (\bar{p}_3)^{1/2} \pm (\bar{p}_1)^{1/2} (9\bar{p}_3 - \bar{p}_1) = 0,$$
$$\text{for } r \begin{matrix} \text{even} \\ \text{odd} \end{matrix} \text{ with } \theta_2 = \epsilon/\bar{\gamma}_2. \tag{5.24}$$

This is not a conic section. Take $\theta_2$ positive, for the sake of discussion: with $r$ even, the parenthesis must be negative and hence we obtain a branch approaching the origin at low values of $\bar{p}_3$, while with $r$ odd the parenthesis is positive, so that $\bar{p}_3$ must sharply increase as $\bar{p}_1 \to 0$. At exact resonance the two branches degenerate into the straight lines

$$\bar{p}_1 = 0 \text{ and } 9\bar{p}_3 = \bar{p}_1. \tag{5.25}$$

The curvature boundary is best obtained from the polynomial SF (7.9); it is the hyperbola

$$\bar{p}_1^2 - 3\bar{p}_1\bar{p}_3 + \tfrac{4}{9}\theta_2^2 = 0, \tag{5.26}$$

which at exact resonance degenerates into

$$\bar{p}_1 = 0 \text{ and } 3\bar{p}_3 = \bar{p}_1. \tag{5.27}$$

The supplementary stability boundary is found from Eq. (3.19) after some algebra to be a degenerate conic section of which only the branch

$$\bar{p}_1 + (9 - 6\sqrt{3})\bar{p}_3 = 0 \tag{5.28}$$

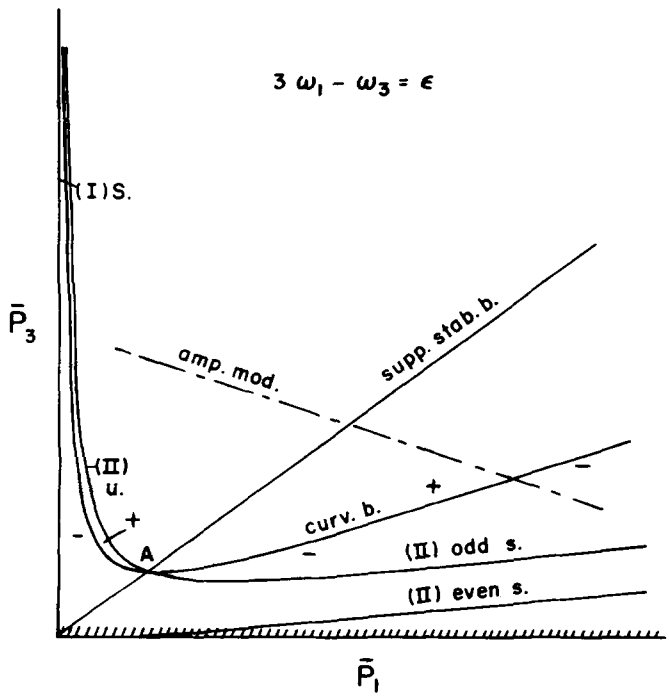


FIG. 4. Stability diagram for coupling $\gamma_2 q_1^3 q_3$ in the resonance $3\omega_1 - \omega_3 = \epsilon$. Abbreviations as for Fig. 2. The coordinates of point $A$ are both proportional to $|\theta_2|$. The drawing assumes $\theta_2 = \epsilon/\bar{\gamma}_2 > 0$; for $\theta_2 < 0$ interchange odd and even.

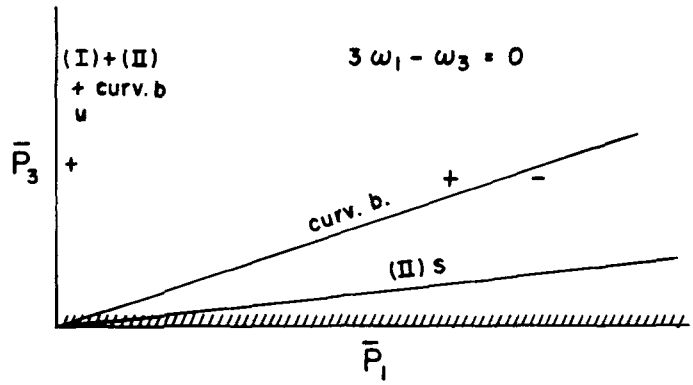


FIG. 5. The diagram of Fig. 4 degenerates into these straight lines at exact resonance $\epsilon = \theta_2 = 0$.

is admissible.

Existence lines, curvature, and stability boundaries are drawn in Fig. 4 for $\theta_2 > 0$. The dot-dash line indicates the slope of the straight-line segments (3.21) representing motion at varying amplitudes. For $\theta_2 < 0$, interchange $r$ even and odd.

We have drawn the case of exact resonance $\theta_2 = 0$ separately in Fig. 5 because it is starkly different. The upper part of the curvature boundary (in addition to the unstable part of the Case (II) existence line) has moved into the ordinate axis. Hence c-a motion at $\bar{p}_1 = 0$ now takes place at a *third*-order root of $f(\bar{p}_1)$. A glance at the formula SF (7.9) will show that the fourth root of $f(\bar{p}_1)$ is in this case $R_4 = \alpha_3$, and since $\alpha_3 > 0$ whereas $f(\bar{p}_1)$ eventually turns downwards it follows that the $\bar{p}_1 = 0$ motion is now orbitally *unstable* (cf. Fig. 1c) although for $\epsilon \neq 0$ it is *stable*. In fact, at $\epsilon \neq 0$ this motion is nearly Liapunov-stable as shown in Sec. IV! This abrupt, discontinuous change from a high degree of stability to orbital instability carries a lesson: system behavior at exact resonance is no unfailing guide to behavior off resonance, be the detuning ever so small. Right at the origin, of course, all four roots of $f(\bar{p}_1)$ coincide; the upper bound $\alpha_3$ also retreats into the origin and therefore the rest position of the system is orbitally stable, as one should expect.

A harbinger of this remarkable change of stability properties as $\epsilon \to 0$ is the close proximity in Fig. 4 of the curvature boundary to the two existence lines flanking it. Quite generally, such closeness foreshadows pronounced effects of *finite* perturbations on c-a motions. Figure 2 contains another example. The cap motion at small $\bar{p}_1$ is so close to the curvature boundary that a clumsy attempt at setting it up in an actual system may turn it into a motion in the vicinity of the *unstable* Case (I) motion nearby. Graphing $f(\bar{p}_1)$ roughly will help one to understand such $\bar{p}$-space topographies better.

Finally let $\gamma_1 \neq 0$; $q_2$ then moves at constant amplitude, although exchanging some energy with $q_1$ and $q_3$ via its phase (cf. SF Secs. III and IV). The offshoot is a $\bar{B}$-polynomial

$$\bar{B}(\bar{p}_1, \alpha) = 3\bar{\gamma}_1 \alpha_2 \bar{p}_1,$$

where

$$\bar{\gamma}_1 = \gamma_1/m_1\omega_1 m_2 \omega_2, \quad \alpha_2 = \bar{p}_2. \tag{5.29}$$

For the detailed derivation, see SF Eq. (7.2). This is quite

different from the quadratic polynomial (5.13); the reason is that in the present system $q_2$ does not resonate, hence $\bar{p}_2 = \text{const} = \alpha_2$ according to SF Eq. (7.5), while $\bar{p}_2$ is variable according to Eq. (5.15) if $\omega_1$ and $\omega_2$ resonate according to Eq. (5.12). In the slow-fluctuation Hamiltonian SF (3.6) this linear $\bar{B}$ adds to the term $\epsilon\bar{p}_1$. The effect is merely a replacement in all formulas of $\epsilon$ by $\epsilon + 3\bar{\gamma}_1\alpha_2$, i.e. a numerical change of $\epsilon$ which is equivalent to a dilatation of the stability diagram Fig. 4. The three-dimensional stability graph of the system of three d.f. can therefore be constructed simply by stacking cross sections similar to Fig. 4 from a bottom which is Fig. 5 and describes $\epsilon + 3\bar{\gamma}_1\alpha_2 = 0$.

If we had added a term $\gamma_1 q_1^2 q_3^2$ to $\gamma_2 q_1^3 q_3$ instead of $\gamma_1 q_1^2 q_2^2$, it would still not resonate; however, since $\bar{p}_3$ is not constant but varies according to Eq. (5.22), we then obtain a quadratic polynomial $\bar{B}$ after all and the stability diagram would differ markedly from Fig. 4.

### D. Three interacting waves

The coupling in three d.f.

$$H_1(q) = \gamma q_1 q_2 q_3 \tag{5.30}$$

has a diverse literature. In plasma physics, optics, and fluid dynamics it serves as a basic nonlinear approximation under the name of "the case of the three interacting waves." Some authors have attempted Hamiltonian formulations[20,21] without, however, exploiting them fully; other studies eschew the benefits of the Hamiltonian approach.[22] We consider only the Case (II) motions because their existence has generally been overlooked.[21]

The exact equations of motion are

$$\dot{p}_i = -m_i\omega_i^2 q_i - \gamma q_j q_k \quad \text{and cyclic}$$

Evidently $q_i \equiv 0$ is not possible unless also $q_j \equiv 0$ or $q_k \equiv 0$, and then the remaining $q$ varies harmonically. Each single d.f. is therefore a possible motion of Case (I) type, but this cannot be safely investigated in our approximation because of the fast phase changes accompanying amplitude zeros when the coupling contains only the first power, cf. SF Sec. VI.

Two different resonating systems are possible. One has

$$\omega_1 + \omega_2 + \omega_3 = \epsilon, \tag{5.31}$$

so that one or two frequencies must be negative, and correspondingly one or two masses negative. The three amplitudes vary in the same sense; explosive instability is possible.

The other system resonates at

$$\omega_1 - \omega_2 - \omega_3 = \epsilon \tag{5.32}$$

with all masses and frequencies positive. The amplitudes of $q_2$ and $q_3$ (the two "partial waves") vary in the same sense but in opposition to the amplitude of $q_1$ (the "sum wave"), according to

$$\bar{p}_2 + \bar{p}_1 = \alpha_2, \quad \bar{p}_3 + \bar{p}_1 = \alpha_3. \tag{5.33}$$

It follows that

$$\alpha_2 > 0, \quad \alpha_3 > 0 \tag{5.34}$$

($\alpha_2 = 0$ or $\alpha_3 = 0$ is possible only for the Case (I) type motions, which we cannot safely investigate anyway). Next we calculate

$$\bar{F} = \bar{\gamma}[\tfrac{1}{2}\bar{p}_1(\alpha_2 - \bar{p}_1)(\alpha_3 - \bar{p}_1)]^{1/2},$$
$$\bar{\gamma} = \gamma(m_1\omega_1 m_2\omega_2 m_3\omega_3)^{-1/2}, \quad \bar{p}_1 = \bar{p}_1. \tag{5.35}$$

Simple as this $\bar{F}$ appears to be, Eq. (3.13) leads to the Case (II) existence surface

$$3\bar{p}_1^2 - 2(\alpha_2 + \alpha_3)\bar{p}_1 + \alpha_2\alpha_3 = \mp\theta\,[8\bar{p}_1(\alpha_2 - \bar{p}_1)(\alpha_3 - \bar{p}_1)]^{1/2}$$
$$\text{for } r \begin{matrix}\text{even}\\ \text{odd}\end{matrix} \text{ with } \theta = \epsilon/\bar{\gamma}, \tag{5.36}$$

which is not easy to describe geometrically. We outline instead how to calculate it point by point.

First, at exact resonance $\theta = 0$, Eq. (5.36) is quadratic with roots

$$S_{1,2} = \tfrac{1}{3}(\alpha_2 + \alpha_3) \pm \tfrac{1}{3}(\alpha_2^2 - \alpha_2\alpha_3 + \alpha_3^2)^{1/2}. \tag{5.37}$$

Under the two numbering conventions $S_1 < S_2$ and $\alpha_2 \leqslant \alpha_3$, it is readily verified that

$$0 < S_1 < \alpha_2 \leqslant S_2 \leqslant \alpha_3. \tag{5.38}$$

From the conservation laws (5.33) it follows that for Case (II) motions always

$$\bar{p}_1 = \bar{p}_1 = \text{const} < \alpha_2 \tag{5.39}$$

($\bar{p}_1 \equiv \alpha_2$ implies $\bar{p}_2 \equiv 0$ which is only possible if also $\bar{p}_3 \equiv 0$, and we are back at a Case (I) type, also $\alpha_2 = \alpha_3$ follows). Thus $\bar{p}_1 \equiv S_2$ is not admissible, but $\bar{p}_1 \equiv S_1$ is and represents a unique amplitude of $q_1$ for any given pair of constants $0 < \alpha_2 \leqslant \alpha_3$; the amplitudes of $q_2$ and $q_3$ then follow from Eqs. (5.33).

When $\theta \neq 0$, Eq. (5.36) can be solved graphically through the intersections of the left- and right-hand sides, set separately equal to zero. The left always yields a parabola intercepting the $\bar{p}_1$-axis at $S_1$ and $S_2$; the right intercepts at 0, $\alpha_2$ and $\alpha_3$. Qualitative graphing in accordance with the magnitude relations (5.38) quickly shows that for any pair $0 < \alpha_2 < \alpha_3$ there are two distinct solutions of Eq. (5.36), called $R'$ and $R''$ in Fig. 6a, with $0 < R' < S_1 < R'' < \alpha_2$; one

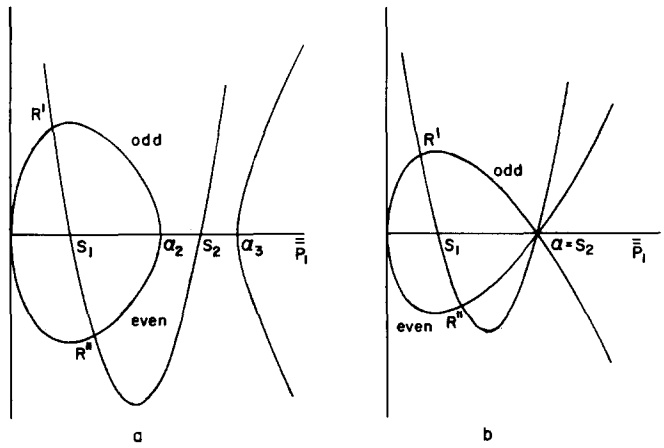


FIG. 6. Three interacting waves; coupling $\gamma q_1 q_2 q_3$ in the resonance $\omega_1 - \omega_2 - \omega_3 = \epsilon$. Graphical determination of the constant amplitudes of Case (II) motions if $\alpha_2 < \alpha_3$ and if $\alpha_2 = \alpha_3 = \alpha$, resp. For symbols, see text, Eq. (5.37) *et seq.*

occurs for $r$ odd, the other for $r$ even. In the degenerate case $\alpha_2 = \alpha_3$, $R''$ could slide up into $S_2$ or even beyond, (see Fig. 6b) and then Case (II) motion is possible only at $\bar{p}_1 = R'$.

The polynomial $f(\bar{p}_1)$ is of the third degree, and one easily sees from Eq. (5.35) that its highest coefficient is *positive*. Unbounded motion is nonetheless impossible. The product of the three roots is positive; they can easily be found with the aid of Eqs. (3.1) and (5.35) from

$$E - \omega_2\alpha_2 - \omega_3\alpha_3 - \epsilon\bar{p}_1 = \pm\bar{\gamma}[\tfrac{1}{2}\bar{p}_1(\alpha_2 - \bar{p}_1)(\alpha_3 - \bar{p}_1)]^{1/2}. \tag{5.40}$$

Solve graphically: the left side yields a straight line, the right a curve like the one in Fig. 6, except for a scale factor. If $\alpha_2 = \alpha_3$ there can be a double root at $\bar{p}_1 = \alpha_2$, but this is again the Case (I) type motion referred to above. Under all other circumstances the largest root of $f(\bar{p}_1)$ is seen to be necessarily real and *larger* than $\alpha_2$, which is an upper bound on $\bar{p}_1$ in any case. Thus there exist no initial conditions resulting in motion beyond the largest root in any case. By extension, physical motion can only take place between the two smallest roots. Case (II) motions therefore arise only from the configuration of Fig. 1a, and are always orbitally stable.

Regarding the system with the resonance (5.31), arguments can be fashioned along similar lines. However, $\alpha_2$ and $\alpha_3$ are now not necessarily positive, nor is there an upper bound on $\bar{p}_1$. Under these less favorable circumstances it no longer follows that a unique Case (II) motion exists for any pair $\alpha_2,\alpha_3$, nor can any quick conclusion be drawn about stability.

### E. An elastic double pendulum

Our last example is an idealized but not unrealistic system from technical mechanics, a double pendulum with the lower bob constrained to move in the vertical, the upper bob constrained to move in a vertical plane, and the inextensible threads replaced by linear springs. Mettler took it up in an important study;[23] he allowed the bob masses and spring constants to be different and investigated the 1:2 resonances between suspension and pendulum modes typical for any elastic pendulum.[17] On the other hand, we want to look for resonances involving all *three* d.f. For brevity of presentation, we take the masses and spring constants to be *equal*, see Fig. 7. Even so, the problem soon looks formidable because we have to develop the Hamiltonian to terms of order four, instead of three as Mettler did; however, physical and mathematical circumstances conspire to lead to a fairly simple, final result which we think interesting enough to describe.

Let the springs have lengths $l_1$ (upper) and $l_2$ (lower) under the static load of the two bobs, each of mass $m$; with equal unextended lengths $l_0$ we therefore have $k(l_1 - l_0) = 2mg$, $k(l_2 - l_0) = mg$

$$l_1/l_0 = 2l_2/l_0 - 1. \tag{5.41}$$

This determines the equilibrium position of Fig. 7 at $x = y_1 = y_2 = 0$. The exact expression for the potential energy is

$$V(x,y_1,y_2) = mg(y_1 + y_2)$$

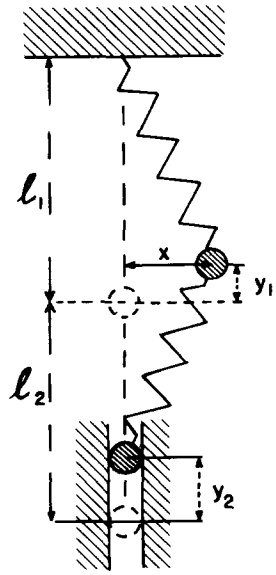


FIG. 7. The constrained elastic double pendulum with equal masses, equal unstretched lengths, and equal spring constants. The stretched lengths are $l_1$ and $l_2$ at rest; $y_1, y_2$ are measured positive upwards from rest.

$$+ \tfrac{1}{2}k\{[x^2 + (l_1 - y_1)^2]^{1/2} - l_0\}^2 + \tfrac{1}{2}k\{[x^2 + (l_2 - y_2 + y_1)^2]^{1/2} - l_0\}^2. \tag{5.42}$$

At small amplitudes,[24] binomial expansion and dropping of irrelevant constants leads in the fourth order to the Hamiltonian

$$\begin{aligned} H(x,y_1,y_2) = {} & \tfrac{1}{2}m(\dot{x}^2 + \dot{y}_1^2 + \dot{y}_2^2) \\ & + \tfrac{1}{2}d_1x^2 + ky_1^2 + \tfrac{1}{2}ky_2^2 - ky_1y_2 \\ & - \tfrac{1}{2}d_2x^2y_1 - \tfrac{1}{2}d_3x^2y_2 \\ & + \tfrac{1}{8}d_4x^4 - \tfrac{1}{2}d_4x^2y_1^2 \\ & - \tfrac{1}{2}\frac{d_3}{l_2}x^2y_2^2 + \frac{d_3}{l_2}x^2y_1y_2, \end{aligned} \tag{5.43}$$

where

$$d_1 = k\left(2 - \frac{l_0}{l_1} - \frac{l_0}{l_2}\right),$$
$$d_2 = k\left(\frac{l_0}{l_1^2} - \frac{l_0}{l_2^2}\right),$$
$$d_3 = k\frac{l_0}{l_2^2}, \quad d_4 = k\left(\frac{l_0}{l_1^3} + \frac{l_0}{l_2^3}\right). \tag{5.44}$$

If the upper bob where also constrained to move in the vertical, $x \equiv 0$, we would have a strictly harmonic system whose normal modes are therefore the proper coordinates to introduce for the following. The appropriate transformation is

$$x = q_1,$$
$$y_1 = -q_2\sin\phi + q_3\cos\phi,$$
$$y_2 = q_2\cos\phi + q_3\sin\phi, \tag{5.45}$$

and with $\tan 2\phi = -2$, or $\phi \approx 58.28°$, the Hamiltonian takes the desired form

$$H(q) = \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2) + \frac{m}{2}(\omega_1^2 q_1^2 + \omega_2^2 q_2^2 + \omega_3^2 q_3^2) + d_5 q_1^2 q_2 + d_6 q_1^2 q_3 + \gamma_1 q_1^4 + \gamma_2 q_1^2 q_2^2 + \gamma_3 q_1^2 q_3^2 + \gamma_4 q_1^2 q_2 q_3, \tag{5.46}$$

where

$$\omega_1^2 = d_1/m,$$

$$\omega_{2,3}^2 = \frac{k}{2m}(3 \pm \sqrt{5}), \text{ index}_3^2,$$

$$d_5 = \tfrac{1}{2}d_2 \sin\phi - \tfrac{1}{2}d_3 \cos\phi,$$

$$d_6 = -\tfrac{1}{2}d_2 \cos\phi - \tfrac{1}{2}d_3 \sin\phi,$$

$$\gamma_1 = d_4/8,$$

$$\gamma_2 = -\tfrac{1}{2}d_4 \sin^2\phi - \frac{d_3}{l_2}(\tfrac{1}{2}\cos^2\phi + \sin\phi\cos\phi),$$

$$\gamma_3 = -\tfrac{1}{2}d_4 \cos^2\phi - \frac{d_3}{l_2}(\tfrac{1}{2}\sin^2\phi - \sin\phi\cos\phi),$$

$$\gamma_4 = \tfrac{1}{2}d_4 \sin 2\phi + \frac{d_3}{l_2}(\cos 2\phi - \tfrac{1}{2}\sin 2\phi). \tag{5.47}$$

The normal modes $q_2$, $q_3$ are evidently antiphase and in-phase motions, respectively, with the former having much the higher frequency according to Eqs. (5.47).

The terms with coefficients $d_5$ and $d_6$ can have the resonances considered by Mettler.[23] Using Eqs. (5.41) and (5.47), it is easily calculated that

$$2\omega_1 - \omega_2 = 0 \text{ requires } l_2/l_0 = 1.337, \tag{5.48}$$

$$2\omega_1 - \omega_3 = 0 \text{ requires } l_2/l_0 = 1.034, \tag{5.49}$$

with $l_1/l_0$ determined by Eq. (5.41). For comparison, in the simple spring pendulum the resonant extension[25] is $l/l_0 = 1.333$. For completeness we also note that

$$\omega_1 - \omega_3 = 0 \text{ requires } l_2/l_0 = 1.161, \tag{5.50}$$

whereas $\omega_1 - \omega_2 = 0$ is physically impossible.

Now consider the last term in the Hamiltonian (5.46), the only one coupling all three d.f.; can it resonate at an extension safely different from those producing the other resonances? As above, we calculate that the obvious

$$2\omega_1 - \omega_2 + \omega_3 = 0 \text{ requires } l_2/l_0 = 1.097, \tag{5.51}$$

while the equally obvious

$$2\omega_1 - \omega_2 - \omega_3 = 0 \text{ requires } l_2/l_0 \approx 2.2,$$

which we discard at once as being physically too implausible. Since $\omega_1$ is not vastly different from $\omega_3$ for plausible extensions [see Eqs. (5.49) and (5.50)] the other combination frequencies in $q_1^2 q_2 q_3$ cannot resonate either. Thus we adopt

$$2\omega_1 - \omega_2 + \omega_3 = \epsilon, \quad |\epsilon| \ll \omega_1 \tag{5.52}$$

as the only realistic possibility. As the extension required at the exact resonance (5.51) is bracketed by the extensions in Eqs. (5.49) and (5.50), $\epsilon$ should remain fairly small—not an unreasonable restriction for a higher-order resonance.

For the near-resonance (5.52) we find in the usual way

$$\bar{\bar{B}} = 2(3\bar{\gamma}_1 - \bar{\gamma}_2 + \bar{\gamma}_3)\bar{p}_1^2 + 2(\bar{\gamma}_2\alpha_2 + \bar{\gamma}_3\alpha_3)\bar{p}_1, \tag{5.53}$$

$$\bar{\bar{F}} = \bar{\gamma}_4 \bar{p}_1[(\alpha_2 - \bar{p}_1)(\alpha_3 + \bar{p}_1)]^{1/2}, \tag{5.54}$$

where

$$\bar{\gamma}_1 = \gamma_1/m^2\omega_1^2, \quad \bar{\gamma}_2 = \gamma_2/m^2\omega_1\omega_2, \quad \bar{\gamma}_3 = \gamma_3/m^2\omega_1\omega_3,$$
$$\bar{\gamma}_4 = \gamma_4/m^2\omega_1\sqrt{\omega_2\omega_3}, \quad \bar{p}_1 = \tfrac{1}{2}\bar{p}_1,$$
$$\alpha_2 = \bar{p}_2 + \tfrac{1}{2}\bar{p}_1, \quad \alpha_3 = \bar{p}_3 - \tfrac{1}{2}\bar{p}_1. \tag{5.55}$$

Note that the two third-order terms in the Hamiltonian (5.46) (coefficients $d_{5,6}$) are *not* represented in the slow-fluctuation approximation because under the condition (5.52) they fluctuate much faster than the resonant term represented by the polynomial (5.54); on the other hand, the three nonresonant fourth-order terms (coefficients $\bar{\gamma}_{1,2,3}$) all contribute to the polynomial (5.53).

The equations of motion show that $q_1 \equiv 0$ is a possible solution, but $q_2 \equiv 0$ or $q_3 \equiv 0$ is not possible unless also $q_1 \equiv 0$. Hence the Case (I) existence surface is the plane

$$\bar{p}_1 = 0 \tag{5.56}$$

(i.e., the first quadrant of the $\bar{p}_2,\bar{p}_3$-plane with both axes included). The Case (II) existence surface is

$$\epsilon + (6\bar{\gamma}_1 - \bar{\gamma}_2 + \bar{\gamma}_3)\bar{p}_1 + 2\bar{\gamma}_2\bar{p}_2 + 2\bar{\gamma}_3\bar{p}_3 = \mp\bar{\gamma}_4[(\bar{p}_2\bar{p}_3)^{1/2} - \tfrac{1}{4}\bar{p}_1(\bar{p}_3/\bar{p}_2)^{1/2} + \tfrac{1}{4}\bar{p}_1(\bar{p}_2/\bar{p}_3)^{1/2}], \quad r \begin{matrix}\text{even}\\ \text{odd}\end{matrix}. \tag{5.57}$$

A study of the latter is beyond the scope of an illustrative example. Instead, we ask only the practically relevant question, is pure suspension motion stable?

The intersection of the existence surface (5.56) with its 2-stability boundary (5.57) is the conic

$$\epsilon + 2\bar{\gamma}_2\bar{p}_2 + 2\bar{\gamma}_3\bar{p}_3 = \mp\bar{\gamma}_4(\bar{p}_2\bar{p}_3)^{1/2}, \quad r \begin{matrix}\text{even}\\ \text{odd}\end{matrix}, \tag{5.58}$$

which can lie only in the first and/or third quadrant. Equations (5.47) quickly show that $\bar{\gamma}_2$, $\bar{\gamma}_3$, and $\bar{\gamma}_4$ are all negative, with $\bar{\gamma}_4$ being the smallest and $\bar{\gamma}_2$ the largest in amount (in fact, $\bar{\gamma}_2/\bar{\gamma}_4 \approx 7.5$ near resonance). It follows that the curve touches the coordinate axes at their intersections with the straight line

$$\epsilon + 2\bar{\gamma}_2\bar{p}_2 + 2\bar{\gamma}_3\bar{p}_3 = 0 \tag{5.59}$$

and lies rather narrowly along that line; hence it is an ellipse. For $\epsilon = 0$ it contracts into the origin (which is clearly stable in any case). For $\epsilon < 0$, it lies in the third quadrant; every suspension motion is then stable.

For $\epsilon > 0$, the ellipse lies in the first quadrant, and, since it does not enclose the origin, which is stable, its interior is orbitally unstable. We know of no intuitively simple reason why this instability should be there. The ellipse itself represents motion at a third-order root of $f(\bar{p}_1)$ at $\bar{p}_1 = 0$. In order to apply the criterion (3.10) to it, we calculate the coefficient of $\bar{p}_1^3$ in $f$ and find, using Eqs. (3.1), (5.53), and (5.54):

$$f_3 = \bar{\gamma}_4^2(\alpha_2 - \alpha_3) - 4(3\bar{\gamma}_1 - \bar{\gamma}_2 + \bar{\gamma}_3)(\epsilon + 2\bar{\gamma}_2\alpha_2 + 2\bar{\gamma}_3\alpha_3). \tag{5.60}$$

Since $\bar{\gamma}_4$ is fairly small, it is clear that $f_3 = 0$ happens to hold

approximately for all points of the straight line (5.59) which therefore represents approximately the 3-stability boundary. This line also divides the ellipse exactly into an $r$-even (left) and $r$-odd (right) half, see Fig. 8; calculation of the sign of $f_3$ in one half then shows that $r$ even (left) is stable, except perhaps near the points of contact where the argument is not safe.

This last detail is easily clarified. The domain of $\bar{p}_1$ has an upper bound determined by $\alpha_2$, hence it reduces to the isolated point $\bar{p}_1 = 0$ when $\alpha_2 = 0$. All points on the $\bar{p}_3$-axis, where $\bar{p}_2 = 0$, are therefore stable regardless of derivatives; in particular, the (upper) point of contact of the ellipse. Not so the (lower) point of contact with the $\bar{p}_2$-axis, where $\alpha_3 = 0$ which merely duplicates the lower bound at $\bar{p}_1 = 0$; the domain is then finite, and the contact must be unstable because $f_3 > 0$ there (see Fig. 1c). It now follows that the exact 3-stability boundary $f_3 = 0$ is slightly rotated clockwise against the line of contact (5.59).

For graphical display, we describe the system by the single parameter

$$\kappa = (l_1/l_2), \quad 1 < \kappa < 2, \tag{5.61}$$

with the range restriction inferred from Eq. (5.41). A convenient detuning measure is the dimensionless

$$\epsilon' = (\epsilon/\omega_1) = 2 - (\kappa + 1 - (2/\kappa))^{-1/2}; \tag{5.62}$$

thus at exact resonance we have $\kappa = 1.088$, and if $\epsilon'$ is increased from zero to 0.05, the concomitant increase of $\kappa$ is only $\frac{1}{2}\%$. Using also instead of $\bar{p}_2$ and $\bar{p}_3$ the dimensionless

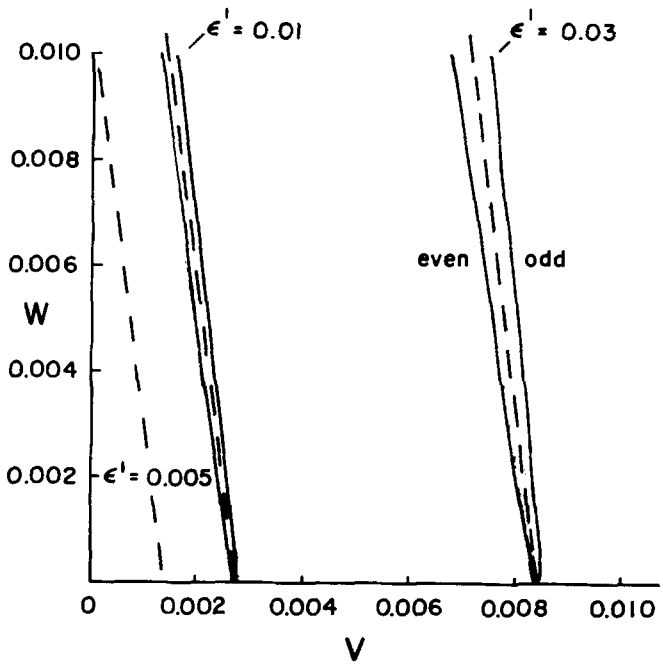


FIG. 8. Orbital stability of the suspension motions of the elastic pendulum; coupling $\gamma_4 q_1^2 q_2 q_3$ in the resonance $2\omega_1 - \omega_2 + \omega_3 = \epsilon$. Dimensionless amplitude squares $v,w$ as defined in Eq. (5.63); dimensionless detuning parameter $\epsilon' = \epsilon/\omega_1$. The insides of the ellipses are orbitally unstable. For $\epsilon' = 0.005$ the ellipse is too narrow to be printed; only the line joining its points of contact with the coordinate axes has been drawn as for the other ellipses. For $\epsilon' < 0$ there is no instability. The drawing has been cropped at the top because larger amplitudes would vitiate the approximation (5.43).

$$v = A_2^2/l_0^2, \quad w = A_3^2/l_0^2 \tag{5.63}$$

(with $A_{2,3}$ the amplitudes of the normal modes) the ellipse (5.58) becomes

$$\epsilon'(\kappa + 1 - 2\kappa^{-1})(2 - \kappa)^{-3} - (0.362\kappa^{-3} + 0.947)v - (0.138\kappa^{-3} + 0.053)w = \pm 0.224(1 - \kappa^{-3})\sqrt{vw}, \quad r \begin{matrix} \text{even} \\ \text{odd} \end{matrix}. \tag{5.64}$$

We plot this in Fig. 8 for two realistic values of $\epsilon'$. The difference between the exact 3-stability boundary points and the points of contact is too small to be visible on the graph.

Since $\bar{F}$ and $\bar{B}$ are in this example homogeneous and of the same degree, the two ellipses in Fig. 8 should be related by dilatation, but this is only approximately true because the $\bar{\gamma}$-coefficients in $\bar{F}$ and $\bar{B}$ themselves depend on $\epsilon$, i.e., one can not vary $\epsilon$ independently. As a result, the coefficients in the ellipse (5.64) depend slightly on $\epsilon$ via the parameter $\kappa$, and the two ellipses in Fig. 8 are slightly rotated against each other. However, the tilt is too small to be seen, and for most practical purposes the dilatation property still holds good.


[1] M. F. Augusteijn and E. Breitenberger, J. Math. Phys. (N.Y.) **21**, 462 (1980); Erratum **21**,2314 (1980).

[2] See also the historical essay by K. Magnus, Naturwiss. **46**, 590 (1959).

[3] W. J. Cunningham, *Introduction to Nonlinear Analysis* (McGraw-Hill, New York, 1958).

[4] H. Leipholz, *Stabilitätstheorie* (Teubner, Stuttgart, 1968): translated as *Stability Theory* (Academic, New York, 1970).

[5] F. Klein and A. Sommerfeld, *Über die Theorie des Kreisels*, 4 fasc. (Teubner, Leipzig 1897–1910; reprinted by Teubner, Stuttgart, 1965), pp. 342–54 and 947–9.

[6] For example, E. T. Whittaker, *A Treatise on the Analytical Dynamics of Particles and Rigid Bodies*, 4th ed. (Cambridge U.P., 1937), Chap. 15.

[7] The term is often used in this general sense; for example: E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill, New York, 1955), Sec. 13.4; M. Urabe, *Nonlinear Autonomous Oscillations* (Academic, New York, 1967), Sec. 6.1.

[8] For example, M. W. Hirsch and S. Smale, *Differential Equations, Dynamical Systems, and Linear Algebra* (Academic, New York, 1974), Chap. 7.

[9] Actually, every orbital instability has a certain disruptive air. The first well-understood case outside of celestial mechanics was probably the unbalanced rotor on an elastic support studied by A. Sommerfeld, Phys. Z. **3**, 266, 286 (1902). An earlier (1882) observation was the "hunting" of generators connected in parallel which initially bedevilled Edison's historic Pearl Street power station in Manhattan; cf. M. Josephson, *Edison* (McGraw-Hill, New York, 1959), pp. 262–3. However, hunting in a strict sense occurs only in nonconservative systems; e.g. J. J. Stoker, *Nonlinear Vibrations in Mechanical and Electrical Systems* (Interscience, New York, 1950), Sec. 4.5.

[10] Of course, real watches are not conservative systems; hence, although the balance wheel may have been Liapunov-stabilized by some device such as a Breguet overcoil, the operation depends foremost on the escape mechanism which establishes a limit cycle. See N. Minorski, *Nonlinear Oscillations* (Van Nostrand, Princeton, N.J., 1962), Secs. 3.11 and 28.5, and references given there.

[11] In fact, now $\bar{F} = 0$. Similar to Eq. (5.29) below, there is only a linear $\bar{B}$-polynomial, with the result that the $f$-polynomial becomes quadratic and touches the axis from below.

[12] Ergodic argument in full $p,q$-space is complicated by the existence of the amplitude conservation laws which effectively reduce the dimensionality of an $E$-surface from $2n - 1$ to $n$ (or $n - 1$ for c-a motions). Formulations become markedly more transparent in $\bar{p},\bar{q}$-space; for the reason see Eqs. (3.21).

[13] At this point we may also comment why we consistently call the barred variables "amplitudes and phases" but never "actions and angles": be-

cause crucial arguments repeatedly call for the use of amplitudes and phases in the precise, kinematical sense.

[14]General references: D. ter Haar, *Elements of Statistical Mechanics* (Holt, Rinehart and Winston, New York, 1954), Appendix I; M. Kac, Am. Math. Monthly, **54**, 369 (1947).

[15]General references: W. Hahn, *Stability of Motion* (Springer, Berlin, 1967); V. I. Arnold and A. Avez, *Ergodic Problems of Classical Mechanics* (Benjamin, New York, 1968); H. Leipholz, Ref. 4.

[16]General reference: D. M. Y. Sommerville, *Introduction to the Geometry of N Dimensions* (Constable, London, 1929; Dover reprint 1958).

[17]E. Breitenberger and R. D. Mueller, "The elastic pendulum: A nonlinear paradigm," submitted for publication to J. Math. Phys..

[18]For example, K. T. Alfriend, Celestial Mech. **3**, 247 (1971). He obtains both Case (I) and (II) motions, and investigates their stability.

[19]K. R. Subbaswamy and S. E. Trullinger, Phys. Rev. A **19**, 1340 (1979) met a related but more general Hamiltonian in a soliton problem.

[20]For example: J. Weiland and H. Wilhelmsson, *Coherent Non-Linear Interaction of Waves in Plasmas* (Pergamon, New York, 1977), Chaps. 7 and 9; also J. D. Meiss and K. M. Watson, *Topics in Non-linear Dynamics*, edited by S. Jorna (American Institute of Physics, New York, 1978), Vol. 46, pp. 296–323; J. D. Meiss, Phys. Rev. A **19**, 1780 (1979).

[21]F. Kh. Tsel'man, J. Appl. Math. Mech. (Pergamon translations from the Russian) **35**, 1038 (1971). With a Hamiltonian method formally similar to ours although conceptually quite different, cf. SF Footnote 19, he is led to a polynomial and to the recognition of the existence of Case (II) motions at exact resonance.

[22]For example: J. A. Armstrong, N. Bloembergen, J. Ducuing and P. S. Pershan, Phys. Rev. **127**, 1918 (1962); F. B. Bretherton, J. Fluid Mech. **20**, 457 (1964); K. M. Watson, B. J. West and B. I. Cohen, J. Fluid Mech. **77**, 185 (1976); C. H. McComas and F. B. Bretherton, J. Geophys. Res. **82**, 1397 (1977).

[23]E. Mettler, Ing. Arch. **28**, 213 (1959), especially pp. 219–22. In our terminology, this paper is a pioneer study of the orbital stability of Case (I) motions at exact resonance, using the Poincaré "method of generating solutions" (on which some comment is made in Ref. 17, Sec. IX).

[24]For the precise meaning of "small", see Ref. 17, Inequalities (2.6).

[25]Ref. 17, Eq. (2.5).

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# Independent variables in quantum mechanics

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It is conjectured that the particle states of quantum mechanics are represented by functions of independent variables. These functions obey a linear differential equation which has an invariance group homomorphic to the inhomogeneous Lorentz group, thus giving a linear, Lorentz-invariant theory. Simple one-particle examples of equations which lead to a discrete particle spectrum are given, using both space–time variable, $x_\mu$, and sets of spinlike variables (pairs of complex numbers). Some of the examples have internal symmetry. No examples of realistic "many-body" particle theories are given, but we can deduce general characteristics. The differential equation must be of second or higher order to give an interaction. Products of single-particle states will be solutions of the equation and will form a complete set for widely separated particles. But products of one-particle states are not solutions of the equation for strongly interacting particles, and this permits the creation of particles. The origin of antisymmetry in such a theory is not clear.

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## 1. INTRODUCTION

The problems to which the theory of quantum mechanics is applied can be ranked according to how much information is put in, *a priori* about the properties of the particles involved. The least fundamental ones, in which the mass, spin, and basic particle interactions are assumed known, would include the calculation of energy levels of the (Dirac) hydrogen atom and of electrons in crystals. At the other extreme, the most fundamental level, we have the "elementary particle" problem in which the goal is to derive the properties of the particles and their interactions from as few principles and/or equations as possible.

The less fundamental problems can be set up in two ways. One is the "first quantized" formulation in which the Hamiltonian is expressed in terms of functions of, and differential operators in, the "independent variables"—the position coordinates of the individual particles. The other is the "second quantized" formulation in which the Hamiltonian is expressed in terms of creation and annihilation operators for "particles". The first formulation is the primary one, from our point of view, while the second one is derived from the first and is used because it provides a compressed elegant notation which makes computations much easier.

The more fundamental problem is normally expressed only in the second quantized langauge of field theory. It is our purpose in this paper to explore the possibility that there is a first quantized formulation of the elementary particle problem which underlies quantum field theory.

There have been a number of first quantized theories of quantum mechanics proposed. Some of these deal only with single-particle equations[1] which may be second quantized to deal with many-particle systems. Others, like those of Bakamijian and Thomas,[2] can deal with many particles (or, at least variables) but either have difficulty with the separability of the interaction, or are only approximately relativistic.[3] None of these however is intended to be a theory underlying quantum field theory.

And, in fact, the many successes of QFT require that some justification be given for looking for such a theory. A partial justification can be given by observing that successful results are not always an indication that a theory is the "most fundamental" one, as the hydrogen atom attests. In addition: (1) There are those[4] who believe that the infinities encountered in $S$-matrix theory are an indication that a different formulation of the problem is needed. (2) According to the ideas of Weinberg[5] and Salam,[6] the vacuum state spontaneously breaks the internal symmetry of the original problem and thus contains a good deal of physical information. But there is no handle on $|0\rangle$ in field theory, i.e., no equation exists from which we can solve for its properties. Thus, if we believe these properties are subject to derivation, the Weinberg–Salam conjecture implies a deeper theory. (3) Even though QCD has made great strides in unifying the various forces of nature,[7] it is not clear that *all* the quantities we would like to calculate can be obtained from field theory. (4) Finally, the analogy between the less fundamental and more fundamental problems is suggestive. Suppose we are able to carry out our theory and that antisymmetrized spin $\frac{1}{2}$ particles emerged from it. Then, just as in the less fundamental problems, we would undoubtedly switch to field operators in order to do calculations efficiently. These creation operators would be labeled by space–time variables and spin indices, $\psi^*_\alpha(x_\mu)$, just as the usual creation operators are, because that is how particle states are (or can be) labeled. Thus, the operators of field theory are labeled *as if* they came from a deeper theory, which makes one suspect that that indeed might be the case. These reasons, we feel, are sufficient to justify the search for an underlying theory.

Such a theory must be able to take into account the three fundamental principles of the elementary particle problem—particleness, linear vector spaces, and Lorentz invariance. That is, there should be some mathematical principle which explains why we can describe nature in terms of particles, and the mathematical representative of these particles must be vectors in a linear vector space. The set of all vectors associated with a particle of mass $m$, spin $S$, are to

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form a basis for the $(m, S)$ irreducible representation of the inhomogeneous Lorentz group, ISL(2). In addition, a theory of elementary particles must be able to take into account the creation and annihilation of particles, and the antisymmetry of multifermion states.

The vectors assiciated with particle states in our formulation of quantum mechanics will be functions of a set, $U$ of independent variables. We must not confuse these functions with wavefunctions, nor labels with independent variables, so we explicitly make the distinction here. If $\Psi(p, \sigma{:}U)$ represents a particle with momentum $p$ and $z$-component of spin, $\sigma$, then a general state of the particle can be written as a linear combination, $\Sigma_\sigma \int \alpha^3\mathbf{p}\, \psi(\mathbf{p}, \sigma)\, \Psi(\mathbf{p}, \sigma{:}U)$; $\psi(\mathbf{p}, \sigma)$ is the *wave* function and the $\mathbf{p}$, $\sigma$, are the *labels*.

Neither these labels $\mathbf{p}$, $\sigma$ (or $\mathbf{x}$, $\sigma$, if we make a Fourier transform) nor the states themselves, tell us anything directly about the nature of the independent variables, so our first task is to examine possible choices. This is done in Sec. 2, where we start by examining the construction of basis vectors using sets of space–time variables, $x_\mu$ (used here as independent variables, not labels). Two sets of $x_\mu$ are found to be sufficient for the construction of basis functions for integer spin representations, but three sets are required for spin $\frac{1}{2}$ representations. The "intuitive" $x_\mu$ are not the only possible choice for independent variables, however. To illustrate this, we use a hybrid set in which the momentum part is a function of one set of $x_\mu$ while the spin part is a function of "spinlike" variables, which are pairs of complex variables. A relativistically invariant scalar product is given for these functions. The possibility of using only spinlike variables is tentatively explored by giving momentum operators constructed from first order differential operators in the spinlike variables.

The ability developed in Sec. 2 to construct basis functions for any positive mass does not give us a physical theory. What we need is some way to "pick out" the physical states. This is accomplished in our theory by assuming that (1) there exists an equation

$$\mathcal{O}\Psi = 0, \tag{1}$$

in which $\mathcal{O}$ is a *linear differential* operator in some set of independent variables, and $\Psi$ is a function of the independent variables; (2) there exists a continuous group of transformations, homomorphic to ISL(2), which leave $\mathcal{O}$ invariant; and (3) the mathematical entities representing physical states are to be solutions of the equation. This formulation assures us of a linear, Lorentz-invariant theory. We will call Eq. (1) the A equation, and its solutions will be called A functions.

Examples of A equations are given in Sec. 3. These have relatively few independent variables and can be considered as single-particle theories. The first example is the relativistic harmonic oscillator of Feynman et.al.,[8] in which two sets of $x_\mu$ are used as the independent variables. All representations $(m, S)$ of ISL(2) are allowed by the A equation for which $S$ is a whole integer and $m^2 = 2, 4, 6, \ldots$. There are also imaginary mass solutions which cause unitarity trouble in the many-body problem. The second example used one set of $x_\mu$ for the translational part of the basis functions, and two sets of spin variables for the spin part. The A equation is Klein–Gordon-like in the $x_\mu$ and harmonic-oscillatorlike in the spin variables. The masses allowed by the A equation are 2, 6, 10 ... for odd half integer spin, and 4, 8, 12, ... for whole integer spin. The third example uses one set of $x_\mu$ and four of spin variables, and is Dirac-like. There is an internal symmetry group isomorphic to SU(2) so that the representatives allowed by the A equation can be grouped into isospin multiplets.

The many-body problem will be much more difficult than the examples in Sec. 3, because there will be a very large number of independent variables, and so we do not consider specific examples here. Instead, in Sec. 4, we relate general particle properties to the form of the operator in, and solutions of, the A equation. We first find a large class of Lorentz-invariant operators. Then we consider physical states. There will presumably be a no-particle state, the vacuum state, represented by a function, $\Psi_0$. A single particle state will be represented by a function times $\Psi_0$, $f\Psi_0$, and multiparticle states by products of functions (i.e., $f_1 f_2 \Psi_0$ for two particles) when the represented particles are widely separated. The infinitesimal generators of the invariance group are first-order differential operators and therefore cause no interaction. But $\mathcal{O}$ itself can cause interactions, if it contains second-order differential operators, because a product is no longer, in general, an exact solution.

The "particleness" of the elementary particle problem is put in by saying the products of one-particle functions are complete when particles are widely separated and therefore not interacting. Or, perhaps better, products of one-particle functions are complete in the far distant past and future. When the interaction is nonzero, the one-particle functions are presumably *not* complete, because products are no longer solutions. This incompleteness during scattering allows for the possibility of creation and annihilation of particles.

The last general property we consider is that of antisymmetry. We speculate that it arises in an independent variable theory because of the need to exclude negative mass solutions of the A equation from arising during scattering.

Finally we note in Sec. 5 that a connection between the Lagrangian equations of quantum field theory and our A equation needs to be established in order to obtain guidelines for choosing a physically relevant $\mathcal{O}$, and to show that our theory leads to the same results as QFT.

## 2. INDEPENDENT VARIABLES AND BASIS FUNCTIONS

We will explore possible types of independent variables in this section, and show how to construct basis functions from them. The physical states yield no clues on the nature of the independent variables, so the procedure we follow is to lay down general criteria and then find independent variables satisfying them. A suitable set of independent variables is one from which we can construct basis funcitons for irreducible representations of ISL(2). In order to solve for the basis functions, we need ten infinitesimal generators which obey the commutation relations

$$[J_i, J_j] = i\epsilon_{ijk} J_k,$$

$$[J_i, K_j] = i\epsilon_{ijk} K_k,$$

$$
\begin{aligned}
&[J_i, J_j] = i\epsilon_{ijk}J_k,\\
&[J_i, K_j] = i\epsilon_{ijk}K_k,\\
&[K_i, K_j] = -i\epsilon_{ijk}J_k,\\
&[J_i, P_j] = i\epsilon_{ijk}P_k,\\
&[P_i, K_j] = -i\delta_{ij}P_o,\\
&[P_i, P_j] = 0,\\
&[P_0, J_i] = 0,\\
&[P_0, P_i] = 0,\\
&[P_0, K_i] = -iP_i,
\end{aligned}
\tag{2}
$$

of ISL(2). The construction of a basis for the $(m, S)$ representation $(m > 0)$ then proceeds by the method of the little group; $2S+1$ zero momentum functions $(\sigma = -S, \ldots, S)$ must be found which satisfy

$$P_o\psi_\sigma = m\psi_\sigma, \tag{3}$$

$$\mathbf{P}\psi_\sigma = 0, \tag{4}$$

and which serve as a basis for the spin $S$ representation of the "little group" SU(2).

We will examine the use of two different types of independent variables here—space–time variables and spinlike variables. There may be other suitable kinds, but it seems most efficient to exhaust the possibilities of these two before looking elsewhere.

The most obvious choice, based on our familiarity with "wave" functions of $x, y, z, t$ is a single set of space–time variables, with the associated infinitesimal generators

$$P_o = i\partial_t, \tag{5}$$

$$\mathbf{P} = -i\nabla, \tag{6}$$

$$\mathbf{J} = \mathbf{r}\times\mathbf{P}, \tag{7}$$

$$\mathbf{K} = \mathbf{r}P_0 + t\,\mathbf{P}. \tag{8}$$

This set of variables is not suitable, however, because $\mathbf{P}\psi = 0$ implies $\mathbf{J}\psi = \mathbf{r}\times\mathbf{P}\psi = 0$, and hence, only spin zero basis functions can be constructed. The reason for the failure is that there are no "internal" coordinates from which to construct the spin part of the functions. If we try two sets of $x_\mu$, then it is not difficult to construct representations for any integer spin—we could use $\exp[\mathrm{im}(t_1 + t_2)](r_1 - r_2)$, for example as the three zero momentum basis functions for a spin 1 representation of the little group. But we run into trouble again, because it is not possible to construct spin $\frac{1}{2}$ representations—which we will surely need for a theory which describes electrons, etc.—from two sets of space–time variables. If we go to three sets, however, then spin $\frac{1}{2}$ representations can be constructed, although somewhat awkwardly. Thus we could conceivably build our theory using only space–time variables.

On the other hand, there is no particular reason why the independent variables must be space–timelike; it is only the group structure and ability to construct basis functions that counts. To illustrate this, and at the same time, avoid the complications of spin $\frac{1}{2}$ space–time basis functions, we will show how to build basis functions from a combination of space-time and spinlike variables.

The spinlike complex variables, $u, v$, are associated with the group SL(2) which is the set of all homogeneous, linear transformations

$$
\begin{aligned}
&u' = a_{11}u + a_{12}v,\\
&v' = a_{21}u + a_{22}v,\\
&a_{11}a_{22} - a_{12}a_{21} = 1,
\end{aligned}
\tag{9}
$$

with the $a_{ij}$ complex. The infinitesimal generators of this group are

$$
\begin{aligned}
J_x &= \tfrac{1}{2}(u\partial_v + v\partial_u - \bar{u}\partial_{\bar{v}} - \bar{v}\partial_{\bar{u}}),\\
J_y &= \tfrac{1}{2}i(v\partial_u - u\partial_v + \bar{v}\partial_{\bar{u}} - \bar{u}\partial_{\bar{v}}),\\
J_z &= \tfrac{1}{2}(u\partial_u - v\partial_v - \bar{u}\partial_{\bar{u}} + v\partial_{\bar{v}}),
\end{aligned}
\tag{10}
$$

$$
\begin{aligned}
K_x &= \tfrac{1}{2}i(u\partial_v + v\partial_u + \bar{u}\partial_{\bar{v}} + \bar{v}\partial_{\bar{u}}),\\
K_y &= -\tfrac{1}{2}(v\partial_u - u\partial_v - v\partial_{\bar{u}} + \bar{u}\partial_{\bar{v}}),\\
K_z &= \tfrac{1}{2}i(u\partial_u - v\partial_v + \bar{u}\partial_{\bar{u}} - \bar{v}\partial_{\bar{v}}).
\end{aligned}
$$

Functions of $u, v, \bar{u}, \bar{v}$, can be used as basis functions for representations of SL(2). For example, a basis for the $(\frac{1}{2}, 0)$ representation is $u, v$; for the $(0, \frac{1}{2})$ representation, $\bar{u}, \bar{v}$; for the (1, 0) representation, $u^2, uv, v^2$; and for the $(\frac{1}{2}, \frac{1}{2})$ representation,

$$
\begin{aligned}
z_0 &= u\bar{u} + v\bar{v},\\
z_1 &= u\bar{v} + \bar{u}v,\\
z_2 &= i(\bar{u}v - u\bar{v}),\\
z_3 &= u\bar{u} - v\bar{v}.
\end{aligned}
\tag{11}
$$

We can now use a hybrid system of independent variables—one set of $(u, v)$ for the spin part of the wave function, and one set of $x_\mu$ for the translation part—for the construction of basis functions. The $P_\mu$ remain the same as in Eqs. (5) and (6) while the $\mathbf{J}, \mathbf{K}$ are the sum of a space–time part [Eqs. (7) and (8)], and a spin part [Eq. (10)]. Zero momentum basis functions for a spin $\frac{1}{2}$ mass $m$ representation can then be chosen as

$$
\begin{aligned}
\psi_{1/2} &= ue^{imt},\\
\psi_{-1/2} &= ve^{imt},
\end{aligned}
\tag{12}
$$

or as

$$
\begin{aligned}
\psi_{1/2} &= \bar{v}e^{imt},\\
\psi_{-1/2} &= \bar{u}e^{imt}.
\end{aligned}
\tag{13}
$$

Spin 1 basis functions are constructed similarly,

$$
\begin{aligned}
\psi_1 &= u^2e^{imt},\\
\psi_0 &= uve^{imt},\\
\psi_{-1} &= v^2e^{imt}.
\end{aligned}
\tag{14}
$$

A general requirement for a theory of quantum mechanics is that there must be a Lorentz-invariant scalar product defined for the vectors. In the case of the hybrid variables, the scalar product breaks into two parts, and we consider the spin part first. If we write $u = u_r + iu_i$, $v = v_r + iv_i$ ($u_r, u_i, v_r, v_i$ real), and if $f, g$ are two functions of $u, v, \bar{u}, \bar{v}$, then

$$\langle f, g\rangle_{\text{spin}} = \int\int\int\int_{-\infty}^{\infty} du_r\, du_i\, dv_r\, dv_i\, \bar{f}g = \int d^4u\, \bar{f}g \qquad (15)$$

satisfies all the requirements of a scalar product. Further, if we switch to new variables by means of Eq. (9), then the Jacobian of the transformation is $\det(A^* A)$; and since $\det(A) = 1$ for SL(2), the scalar product is Lorentz invariant.

This scalar product poses a problem for the basis functions of Eq. (12), because they have an undefined spin norm. This problem can be circumvented by mutliplying the basis functions by a function invariant under the little group, SU(2). Such an example appears in the next section and is

$$\psi_{1/2} = ue^{-(u\bar{u}+v\bar{v})}e^{imt},$$
$$\psi_{-1/2} = ve^{-(u\bar{u}+v\bar{v})}e^{imt}. \qquad (16)$$

These are still good spin $\frac{1}{2}$ represnetations of SU(2), and now have a well defined, finite spin form.

The space–time part of the scalar product may vary, depending on the problem at hand. But if the basis functions satisfy a Klein–Gordon equation, then we can use the usual one[9]

$$\langle fg\rangle = i\int_{-\infty}^{\infty} d^3x(\bar{f}_t g - g_t \bar{f}), \qquad (17)$$

or more generally

$$\langle fg\rangle = i\int_{\sigma} d\sigma^\mu(\bar{f}_\mu g - g_\mu \bar{f}), \qquad (18)$$

where $\sigma$ is any spacelike surface, and $f, g$ are positive energy solutions of the Klein–Gordon equation with the same mass. It is proved in Ref. 9 that this scalar product is Lorentz invariant and independent of $\sigma$.

We have thus been able, by using hybrid variables to construct basis functions from independent variables for any spin mass $> 0$. And we have constructed a Lorentz invariant scalar product under which the basis functions can be properly normalized.

We can also construct basis functions in the zero mass case. In order to demonstrate this, we will use the little group method again, this time for the energy–momentum vector $p_0 = p_3 = p, p_1 = p_2 = 0$. The equations to be satisfied by the single little group basis function, of spin $S$, are then

$$\begin{aligned}
(J_x - K_y)\psi &= \{-i(y\partial_z - z\partial_y + y\partial_t + t\partial_y) + v\partial_u - \bar{v}\partial_{\bar{u}}\}\\
&\quad\times\psi = 0,\\
(J_y + K_x)\psi &= \{-i(z\partial_x - x\partial_z - x\partial_t - t\partial_x) + iv\partial_u\\
&\quad + + i\bar{v}\partial_{\bar{u}}\}\psi = 0,\\
J_z\psi &= \{-i(x\partial_y - y\partial_x) + \tfrac{1}{2}(u\partial_u - v\partial_v - \bar{u}\partial_{\bar{u}} + v\partial_{\bar{v}})\}\psi\\
&= S\psi. \qquad (19)
\end{aligned}$$

These are solved by $\psi = v^{-2s} f(v\bar{v})\exp[i(pt - pz)]$ or $= \bar{v}^{2s} f(v\bar{v})\exp[i(pt - pz)]$, where $f$ is any function of $v$. Now, however, since $\psi$ does not depend on $u, \bar{u}$, the spin part of the scalar product gives infinity. We do not see how to escape this difficulty.

So far, we have used both space–time variables alone, and a hybrid system, to construct basis functions. Another possibility is to use sets of spinlike variables alone. The construction of normalizable basis functions looks quite difficult in this case, because of the large number of variables involved, so we will be satisfied here to take only the first step and find 10 infinitesimal generators for ISL(2). The **J**, **K** are simple enough—they are sums of operators like those of Eqs. (10). The $P_\mu$, which are not "natural" in the spin variables, must be Hermitian first-order differential operators which transform like 4-vectors. They are therefore of the form

$$P_\mu = \sum_{i=1}^{N}\sum_{j=1}^{N}(b_{ij}P_\mu^{\ ij} + \bar{b}_{ij}P_\mu^{ij+}), \qquad (20)$$

where there are $N$ sets of $(u, v)$,

$$\begin{aligned}
P_0^{ij} &= -v_i\partial_{\bar{u}_j} + u_j\partial_{\bar{v}_j},\\
P_1^{ij} &= -u_i\partial_{\bar{u}_j} + v_i\partial_{\bar{v}_j},\\
P_2^{ij} &= i(u_i\partial_{\bar{u}_j} + v_i\partial_{\bar{v}_j}),\\
P_3^{ij} &= v_i\partial_{\bar{u}_j} + u_i\partial_{\bar{v}_j},
\end{aligned} \qquad (21)$$

and the $b_{ij}$ are SL(2) invariants. If the $b_{ij}$ are constants, then the condition that $[P_\mu, P_\nu] = 0$ implies

$$\sum_{j=1}^{N} b_{ij}\bar{b}_{jk} = 0, \quad i, k = 1,\ldots,N. \qquad (22)$$

One solution to this set of equations is $b_{ij} = f_i g_j$ with $\Sigma\bar{g}_j f_j = 0$. This turns out to be an unsatisfactory solution because the resulting $P_\mu$ are not independent. That is, there exist four functions, $f_0, f_1, f_2, f_3$, of the $(u_i, v_i)$ such that $f_0P_0 + f_1P_1 + f_2P_2 + f_3P_3 = 0$. This condition implies there is no solution to the little group equations and hence these infintesimal generators would yield no massive representations of ISL(2). A better choice is to make a $P_\mu$ out of each pair of sets of $(u_i, v_i)$ and then add then together. If we have four sets of $(u, v)$, for example, we could construct

$$P_\mu = P_\mu^{21} + P_\mu^{43} + \text{h.a.} \qquad (23)$$

These $P_\mu$ then commute and form an independent set.

One consequence of the commutativity and independence of the $P_\mu$ is that there exist variables $x_\mu$ conjugate to them, i.e., they satisfy

$$[P_\mu, x_\nu] = i\,\delta_{\mu\nu}. \qquad (24)$$

The $x_\mu$ can be chosen to be

$$\begin{aligned}
x_0 &= \tfrac{1}{4}i\{\bar{u}_4u_1 + \bar{v}_4v_1 - (\bar{u}_2u_3 + \bar{v}_2v_3)\}/(u_4v_2 - v_4u_2) + \text{c.c.},\\
x_1 &= \tfrac{1}{4}i\{\bar{v}_4u_4 + \bar{u}_4v_1 - (\bar{v}_2u_3 + \bar{u}_2v_3)\}/(u_4v_2 - v_4u_2) + \text{c.c.},\\
x_2 &= \tfrac{1}{4}i\{\bar{u}_4v_1 - \bar{v}_4u_1 - (\bar{u}_2v_3 - \bar{v}_2u_3)\}/(u_4v_2 - v_4u_2) + \text{c.c.},\\
x_3 &= \tfrac{1}{4}i\{\bar{u}_4u_1 - \bar{v}_4v_1 - (\bar{u}_2u_3 - \bar{v}_2v_3)\}/(u_4v_2 - v_4u_2) + \text{c.c.},
\end{aligned} \qquad (25)$$

but they are not unique, because there are 16 real variables in the four sets of $(u, v)$, rather than just 4. With these $x_\mu$, we suspect that we could construct basis functions for irreducible representations of ISL(2) in a manner not too different from that used with one set of $x_\mu$, and one set of $(u, v)$. But it is not our purpose here to develop the spin-variable-only approach in detail. It has been pursued to the point of finding suitable $P_\mu$ simply to show the feasibility of a theory with not space–time variables. We will consider it not further at this

point and turn instead to a consideration of independent variable theories with $A$ equations.

## 3. SIMPLE $A$ EQUATIONS

As we indicated in the Introduction, the method we will use to formulate quantum mechanics for elementary particles is to construct an operator $\mathcal{O}$ from differential operators in the independent variables and then to require that the mathematical functions associated with physical states of particles satisfy the "$A$ equation", $\mathcal{O}\Psi = 0$. The theory is made Lorentz invariant by requiring that there exist ten infinitesimal generators (first-order differential operators) of ISL(2) which commute with $\mathcal{O}$,

$$[\mathcal{O}, \mathbf{J}] = [\mathcal{O}, \mathbf{K}] = [\mathcal{O}, P_\mu] = 0. \tag{26}$$

A complete physical theory will have many, perhaps an infinite number of, independent variables in order to be able to describe systems of many interacting particles. Such a theory will be extremely complicated, however, and so before considering it, we will give relatively simple illustrations of the method in which only a small number of independent variables are used.

Our first example is one already in the literature (although it is doubtful that the various authors viewed it as an example of the method of independent variables), namely, the relativistic harmonic oscillator proposed by Feynman, Kislinger, and Ravndal,[8] and pursued by Kim and Noz,[10] and Blaha,[11] among others. We will review the problem here, because it illustrates several points.

In the simplest version, two sets of space–time variables ${x_\mu}^1$ and ${x_\mu}^2$, are used, with an $A$ equation

$$\mathcal{O}\Psi(x^1, x^2) = \{\partial_\mu{}^1\partial_\mu{}^1 + \partial_\mu^2\partial_\mu^2 + V(x^1, x^2)\}\Psi(x^1, x^2) = 0. \tag{27}$$

The "potential", $V$, chosen for the harmonic oscillator problem is

$$V(x^1, x^2) = -\tfrac{1}{8}({x^1}_\mu - {x^2}_\mu)({x^1}_\mu - {x^2}_\mu). \tag{28}$$

If we switch to center of mass and internal coordinates,

$$\begin{aligned} X_\mu &= ({x_\mu}^1 + {x_\mu}^2)/2, \\ x_\mu &= ({x_\mu}^1 - {x_\mu}^2)/2, \end{aligned} \tag{29}$$

then the equation becomes

$$\{-P_\mu P_\mu + \partial_{x_\mu}\partial_{x_\mu} - x_\mu x_\mu\}\Psi(X, x) = 0, \tag{30}$$

where the momenta, $P_\mu$, are

$$\begin{aligned} P_0 &= i(\partial_0^1 + \partial_0^2), \\ \mathbf{P} &= i(\nabla^1 + \nabla^2). \end{aligned} \tag{31}$$

The above $P_\mu$, plus a $\mathbf{J}$, $\mathbf{K}$ which are sums of two sets of $\mathbf{J}$, $\mathbf{K}$, like those of Eqs. (7) and (8), give us a set of ten infinitesimal generators which obey the commutation relations ISL(2) and commute with $\mathcal{O}$, so the $A$ equation is Lorentz invariant.

Because of the Lorentz invariance, we expect to be able to catalog solutions of the equation by the representation of ISL(2) to which they belong. We will use the little group method in order to determine which irreducible representations $(m, S)$ are "allowed" by the equation. The zero momentum, $m > 0$, solutions must satisfy Eqs. (3) and (4), which implies they can be written as

$$\Psi(m, S; p = 0, \sigma: x_\mu, X_\mu) = e^{imX_0}f(m, S; p = 0, \sigma: x_\mu), \tag{32}$$

where the $2S + 1$ $f$'s form a basis for the spin $S$ representation of SU(2). If we put this form into the $A$ equation, then we obtain an eigenvalue equation for the allowed values of $m^2$,

$$(\partial^2_{x_0} - \partial^2_{x_1} - \partial^2_{x_2} - \partial^2_{x_3} - x_0{}^2 + x_1{}^2 + x_2{}^2 + x_3{}^2)f = m^2 f. \tag{33}$$

The solutions of Eq. (33) will be the product of four harmonic oscillator functions in the variables $x_0, x_1, x_2, x_3$,

$$f(n_0, n_1, n_2, n_3) = \prod_{\mu=0}^{3} \Psi_{n_\mu}(X_\mu), \tag{34}$$

with associated eigenvalues

$$m^2 = 2(n_1 + n_2 + n_3 - n_0) + 2. \tag{35}$$

The functions $\psi_n$ are harmonic oscillator functions, i.e., $\psi_0(x) = \exp(-x^2/2)$, $\psi_1(x) = x\exp(-x^2/2)$, etc.

The scalar product in this problem will consist of two parts: $\int \alpha^4 x$ on the internal variables, and a part like that of Eq. (17) for the external variables.

There seems to be some confusion in the literature about the form of the eigenfunctions. The tendency is to assume that the "ground state" $\Psi_0 = f(0, 0, 0, 0)$, must be SL(2) invariant, i.e., $\Psi_0 = \exp[(x_0{}^2 - x_1{}^2 - x_2{}^2 - x_3{}^2)/2]$. If this is assumed, then severe difficulties with the norm result, and much maneuvering[10] must be done to salvage the theory. But the ground state does *not*—when we are dealing with a one-body problem rather than the many-body problem—have to be SL(2) invariant in the little group method, only SU(2) invariant. Thus the ground state we have implicitly used above, $= \exp[-(x_0{}^2 + x_1{}^2 + x_2{}^2 + x_3{}^2)/2]$, is perfectly acceptable.

If $m^2 > 0$, the internal norm will be finite, because of the exponential $\Psi_0$, and states with different $n_\mu$ (and therefore different $m^2$) will be orthogonal. If $m^2 < 0$, however, then $m$ is pure imaginary and the center of mass norm gives infinity. Because of this difficulty, states with $m^2 < 0$ are excluded from consideration here. The negative $m^2$ states could not be dismissed as easily by Feynman et al.[8] because they were implicitly working on a many-body problem. There was no way to exclude the possibility that the scattering of an $m^2 > 0$ particle would produce an $m^2 < 0$ state, because all solutions of the $A$ equation, including those with $m^2 < 0$, might be part of the complete set of functions necessary to describe the outcome. Thus the negative $m^2$ states are worrisome in the many-body problem.

If $m^2 = 0$, i.e., $n_1 + n_2 + n_3 - n_0 = -1$, we must change the little group method, as mentioned in Sec. 2. It turns out that the $A$ equation has no $m^2 = 0$ solutions which also satisfy the little group equations, so no massless representations are allowed by (30).

Linear combinations of the $m^2 > 0$ solutions to Eq. (33) can be used to obtain solutions of definite spin as well as mass. For example, $f(0, 1, 0, 0)$, $f(0, 0, 1, 0)$, and $f(0, 0, 0, 1)$ form a spin 1 representation, with a mass squared of 4, and linear combinations of $f(0, n_1, n_2, n_3)$ with $n_1 + n_2 + n_3 = 2$ can be taken to obtain a spin 2 representation of $m^2 = 6$. A more complete treatment of the mass spectrum is given in

the references, so we will not pursue it here. We only remark that all representations have integer spin.

Our next example uses one set of $x_\mu$ and two sets of $(u, v)$ as the independent variables and will allow spin $\frac{1}{2}$ solutions. The $A$ equation for this example is chosen to be like the Klein–Gordon equation.

$$\mathcal{O}\Psi = (\partial_\mu \partial_\mu + m^2)\Psi = 0 \tag{36}$$

except that $m^2$ will be a differential operator in the spin variables rather than just a number. If we suppose that our $P_\mu$ are those of Eqs. (5) and (6) and the **J**, **K** are like those of Eq. (10) except that two sets of $(u, v)$ are used, then $\mathcal{O}$ commutes with them and will be Lorentz invariant provided $m^2$ is an SL(2)-invariant.

The number of candidates to be considered for $m^2$ can be cut down, and an additional quantum number introduced, if we assume that $\mathcal{O}$, and thus $m^2$, is to be invariant under a space inversion operation, $I_s$. The $I_s$ we choose is

$$I_s(x_0) = x_0 \quad I_s(x) = -x \tag{37}$$

$$I_s(u_1) = \bar{v}_2 \quad I_s(\bar{u}_1) = v_2 \quad I_s(u_2) = -\bar{v}_1 \quad I_s(\bar{u}_2) = -v_1,$$
$$I_s(v_1) = -\bar{u}_2 \quad I_s(\bar{v}_1) = -u_2 \quad I_s(v_2) = \bar{u}_1 \quad I_s(\bar{v}_2) = u_1, \tag{38}$$

and it takes $(P_0, \mathbf{P}, \mathbf{J}, \mathbf{K})$ into $(P_0, -\mathbf{P}, \mathbf{J}, -\mathbf{K})$, as it should.

We now choose an $m^2$ which is harmonic-oscillatorlike in the sense that it has second-order derivatives and quadratic terms in the $(u, v)$,

$$m^2 = (u_1 v_2 - v_1 u_2 + \bar{u}_1 \bar{v}_2 - \bar{v}_1 \bar{u}_2)/4 - (\partial_{u_1}\partial_{v_2} - \partial_{v_1}\partial_{u_2} + \partial_{\bar{u}_1}\partial_{\bar{v}_2} - \partial_{\bar{v}_1}\partial_{\bar{u}_2}). \tag{39}$$

It is not difficult to show that this operator is invariant under SL(2) and $I_s$.

Equation (36) can be solved by separation of variables. This is done by using linear combinations of variables which are eigenfunctions of $I_s$

$$\begin{aligned} u_+ &= (u_1 + \bar{v}_2)/\sqrt{2}, \\ v_+ &= (v_1 - \bar{u}_2)/\sqrt{2}, \\ u_- &= (u_1 - \bar{v}_2)/\sqrt{2}, \\ v_- &= (v_1 + \bar{u}_2)/\sqrt{2}. \end{aligned} \tag{40}$$

A bit of algebra shows that

$$\begin{aligned} m^2 &= -(\partial_{u_-}\partial_{\bar{u}_+} + \partial_{v_-}\partial_{\bar{v}_+} - u_+\bar{u}_+ - v_+\bar{v}_+) \\ &\quad + (\partial_{u_-}\partial_{\bar{u}_-} + \partial_{v_-}\partial_{\bar{v}_-} - v_-\bar{v}_- - u_-\bar{u}_-) \\ &= -\partial^2_{u_{-r}} + u^2_{+r} - \partial^2_{u_{-i}} + u^2_{+i} - \partial^2_{v_{-r}} \\ &\quad + v_{+r} - \partial^2_{v_{-i}} + v^2_{+i} \\ &\quad + \partial^2_{u_{+r}} - u^2_{-r} \\ &\quad + \partial^2_{u_{+i}} - u^2_{-i} + \partial^2_{v_{+r}} - v^2_{-r} + \partial^2_{v_{+i}} - v^2_{-i}, \end{aligned} \tag{41}$$

where $u_r$ indicates the real part of $u$, etc. Not surprisingly, $m^2$ splits up into eight harmonic oscillator operators.

To find the allowed values of $(m, S)$, we follow the same procedure as in the first example, where we considered only zero momentum basis functions and separated out the time dependence,

$$\Psi(m, S; p = 0, \sigma; x, U) = e^{imx_0} f(m, S; p = 0, \sigma; U). \tag{42}$$

The $A$ equation then becomes

$$m^2 f = m^2 f. \tag{43}$$

Its solutions will be products of eight harmonic-oscillator functions in the variables $u_{+r}, u_{+i}$, etc. If we relabel $(u_{+r}, u_{+i}, v_{+r}, v_{+i}, u_{-r}, u_{-i}, v_{-r}, v_{-i})$ by $(y_1, y_2, \ldots, y_8)$, then the eigenfunctions are $f(n_1, \ldots, n_8) = \Pi_{i=1}^8 \psi_{n_i}(y_i)$ with eigenvalues $m^2 = 2(n_1 + \ldots - n_8)$. We see that there are an infinite number of different eigenfunctions associated with each value of $m^2$. The trick is to organize them into states with definite spin and parity, and determine which $S$ and $P$ are allowed for a given mass. The method is tedious, but the results are fairly simple. A basis can be constructed for any whole integer representation of either parity if $m^2 \equiv 0 \bmod (4)$, and for any odd half-integer representation of either parity provided $m^2 \equiv 2 \bmod (4)$.

It is interesting to examine the structure of the basis functions for the $m = \sqrt{2}, S = \frac{1}{2}, P = 1$ representation. We note that $u_+, v_+$ form a basis for a spin $\frac{1}{2}$ representation of SU(2), with $J_z u_+ = \frac{1}{2}u_+, J_z v_+ = -\frac{1}{2}v_+$. And since $u_+ = y_1 + iy_2, v_+ = y_3 + iy_4$, we have

$$\Psi(\sqrt{2}, \tfrac{1}{2}, 1; p = 0, \sigma = \tfrac{1}{2}) = [\psi_1(y_1)\psi_0(y_2) + i\psi_0(y_1)\psi_1(y_2)] \prod_{i=3}^{8} \psi_0(y_i) e^{imt}, \tag{44}$$

$$\Psi(\sqrt{2}, \tfrac{1}{2}, 1; p = 0, \sigma = -\tfrac{1}{2}) = \psi_0(y_1)\psi_0(y_2)[\psi_1(y_3)\psi_0(y_4) + i\psi_0(y_3)\psi_0(y_4)] \times \prod_{i=5}^{8} \psi_0(y_i) e^{imt}.$$

Or, if we convert back to $u, v$ notation and let

$$\psi_0 = \prod_{i=1}^{8} \psi_0(y_i) = \exp[-(u_1\bar{u}_1 + v_1\bar{v}_1 + u_2\bar{u}_2 + v_2\bar{v}_2)/2], \tag{45}$$

then

$$\begin{aligned} \Psi(\sqrt{2}, \tfrac{1}{2}, 1; \quad p = 0, \quad \tfrac{1}{2}) &= (u_1 + \bar{v}_2)\Psi_0 e^{imt} \\ \Psi(\sqrt{2}, \tfrac{1}{2}, 1; \quad p = 0, \quad -\tfrac{1}{2}) &= (v_1 - \bar{u}_2)\Psi_0 e^{imt}. \end{aligned} \tag{46}$$

The $\mathbf{p} \neq 0$ basis functions will be Lorentz transforms of the above $p = 0$ basis functions. Hence the general form for an $m = \sqrt{2}\ S = \frac{1}{2}, P = 1$ function is

$$\Psi(\sqrt{2}, \tfrac{1}{2}, 1) = \int d^3p \ [f_1(\mathbf{p})u_1 + f_2(\mathbf{p})v_1 + f_3(\mathbf{p})\bar{u}_2 + f_4(\mathbf{p})\bar{v}_2] \times \exp[ip_\mu x_\mu - p_\mu(z^1_\mu + z^2_\mu)]; p_0 = \sqrt{2 + p^2}, \tag{47}$$

with $z_\mu$ defined as in Eq. (11). The $f_i(\mathbf{p})$ constitute the four components of the Dirac *wave* function in the momentum representation. Only two of the four can be specified independently, for each $\mathbf{p}$, corresponding to spin up and spin down. Thus there is a dependence among the $f$'s which can be expressed by the Dirac equation $(\gamma_\mu p_\mu - \sqrt{2})f(p) = 0$, where $f$ is a column vector with components $f_1(\mathbf{p}), f_2(\mathbf{p}), f_3(\mathbf{p}), f_4(\mathbf{p})$, and

$$\gamma_0=\begin{bmatrix}0&0&0&1\\0&0&-1&0\\0&-1&0&0\\1&0&0&0\end{bmatrix},\quad \gamma_1=\begin{bmatrix}0&0&-1&0\\0&0&0&1\\1&0&0&0\\0&-1&0&0\end{bmatrix}$$
$$\gamma_2=\begin{bmatrix}0&0&i&0\\0&0&0&i\\i&0&0&0\\0&i&0&0\end{bmatrix},\quad \gamma_3=\begin{bmatrix}0&0&0&1\\0&0&1&0\\0&-1&0&0\\-1&0&0&0\end{bmatrix}. \tag{48}$$

The scalar product for the solutions of Eq. (36) is like that for the hybrid functions of Sec. 2, except that $\int d^4u_1 \int d^4u_2$ replaces $\int d^4u$.

If $m^2>0$, the spin norm will be finite, because of the exponential $\Psi_0$, and states with different $n_i$ (and therefore different $m^2$) will be orthogonal. If $m^2<0$, however, the spin norm is still finite, but $m$ is pure imaginary and the space-time norm is infinite. Because of this difficulty, states with $m^2<0$ are excluded from consideration here. If $m^2=0$, then we must change the little group method as mentioned in Sec. 2. It turns out that there are $m^2=0$ solutions, but their spin norm is not well defined, so we must also exclude $m^2=0$ solutions as not being physical.

Our second example still had imaginary mass solutions because the eigenfunction equation was quadratic in $m$. Our third example, which uses one set of $x_\mu$ and four of $(u, v)$, avoids this problem by employing a Diraclike equation which is linear in the eigenvalue $m$. The $A$ equation is

$$\mathcal{O}\Psi=(iD_\mu\partial_\mu-m)\Psi=0, \tag{49}$$

where

$$m=(u_1v_3-v_1u_3-u_2v_4-v_2u_4)/4+\text{c.c.}\\ -(\partial_{u_1}\partial_{v_3}-\partial_{v_1}\partial_{u_3}+\partial_{u_2}\partial_{v_4}-\partial_{v_2}\partial_{u_4})+\text{h.a.}, \tag{50}$$

and the differential operators

$$\begin{aligned}D_0&=u_1\partial_{\bar v_3}-v_1\partial\bar u_3+u_2\partial_{\bar v_4}-v_2\partial_{\bar u_4}+\text{h.a.},\\ D_1&=-u_1\partial_{\bar u_3}+v_1\partial_{\bar v_3}-u_2\partial_{\bar u_4}+\text{h.a.},\\ D_2&=+i(u_1\partial_{\bar u_3}+v_1\partial_{\bar v_3}+u_2\partial_{\bar u_4}+v_2\partial_{\bar v_4})+\text{h.a.},\\ D_3&=u_1\partial_{\bar v_3}+v_1\partial_{\bar u_3}+u_2\partial_{\bar v_4}+v_2\partial_{\bar u_4}+\text{h.a.}\end{aligned} \tag{51}$$

have replaced the Dirac matrices $\gamma_\mu$.

To find the allowed values of $(m, S)$, we again look only at the zero momentum solutions and write $\Psi=\exp(-imx_0)f$ to obtain the eigenfunction equation

$$mD_0f=mf, \tag{52}$$

for $m, f$. The operators $D_0$ and $m$ commute, so we can diagonalize them separately. The diagonalization procedure for $m$ is quite similar to that followed in example 2; we define two sets of $\pm$ variables

$$\begin{aligned}u_1^+&=(u_1+\bar v_3)/\sqrt2, & u_1^-&=(u_1-\bar v_3)/\sqrt2,\\ v_1^+&=(v_1-\bar u_3)/\sqrt2, & v_1^-&=(v_1+\bar u_3)/\sqrt2,\\ u_2^+&=(u_2+\bar v_4)/\sqrt2, & u_2^-&=(u_2-\bar v_4)/\sqrt2,\\ v_2^+&=(v_2-\bar u_4)/\sqrt2, & v_2^-&=(v_2+\bar u_4)/\sqrt2,\end{aligned} \tag{53}$$

which are eigenfunctions of the space inversion operator $I_s$, i.e.,

$$I_s(u^\pm{}_n)=\pm u^\pm{}_n, I_s(v^\pm{}_n)=\pm v^\pm{}_n. \tag{54}$$

We then find that

$$m=-\sum_{i=1}^{8}(\partial^2{}_{y_i}-y_i{}^2)+\sum_{i=9}^{16}(\partial^2{}_{y_i}-y_i{}^2), \tag{55}$$

where

$$(y_i,\ldots,y_{16})=(u^+{}_{1r}, u^+{}_{1i}, v^+{}_{1r}, v^+{}_{1i}, u^+{}_{2r}, u^+{}_{2i}, v^+{}_{2r}, v^+{}_{2i}, u^-{}_{1r},\ldots).$$

The eigenfunctions are $f(n_1,\ldots,n_{16})=\Pi\psi_{n_i}(y_i)$ with eigenvalues

$$m=2(n_1+\cdots+n_8-n_9\cdots n_{16}).$$

If we re-express $D_0$ in terms of the $\pm$ variables, we get

$$\begin{aligned}D_0=&u_1^+\partial_{u_1^+}+v_1^+\partial_{v_1^+}-u_1^-\partial_{u_1}-v_1^-\partial_{v_1}\\ &+u_2^+\partial_{u_2^+}+v_2^+\partial_{v_2^+}-u_2^-\partial_{u_2}-v_2^-\partial_{v_2^-}+\text{h.a.}\end{aligned} \tag{56}$$

This operator acting on the ground state, $\Psi_0=f(0,\text{---}0,)$ gives zero, so $D_0$ essentially acts only on the spin part $(f/\Psi_0)$ of the basis functions.

It is interesting to observe that the $\mathcal{O}$ of this example has an "internal" symmetry group, isomorphic to SU(2), which rotates sets of $(u, v)$ into each other according to

$$\begin{bmatrix}(u_1',v_1')\\(u_2',v_2')\\(u_3',v_3')\\(u_4',v_4')\end{bmatrix}=\begin{bmatrix}a_{11}&a_{12}&0&0\\a_{21}&a_{22}&0&0\\0&0&\bar a_{11}&\bar a_{12}\\0&0&\bar a_{21}&\bar a_{22}\end{bmatrix}\begin{bmatrix}(u_1,v_1)\\(u_2,v_2)\\(u_3,v_3)\\(u_4,v_4)\end{bmatrix}, \tag{57}$$

(that is, $u_1'=a_{11}u_1+a_{12}u_2$, $v_1'=a_{11}v_1+a_{12}v_2$, etc.), where the matrix is unitary with a determinant of one. The ISL(2) and $I_s$-invariant infinitesimal generators of the internal symmetry group are

$$\begin{aligned}2I_x=&u_1\partial_{u_2}+u_2\partial_{u_1}-u_3\partial_{u_4}-u_4\partial_{u_3}\\ &+v_1\partial_{v_2}+v_2\partial_{v_1}-v_3\partial_{v_4}-v_4\partial_{v_3}+\text{h.a.},\\ 2I_y=&i(u_2\partial_{u_1}-u_1\partial_{u_2}+u_4\partial_{u_3}-u_3\partial_{u_4}\\ &+v_2\partial_{v_1}-v_1\partial_{v_2}+v_4\partial_{v_3}-v_3\partial_{v_4})+\text{h.a.},\\ 2I_z=&u_1\partial_{u_1}-u_2\partial_{u_2}-u_3\partial_{u_3}+u_4\partial_{u_4}\\ &+v_1\partial_{v_1}-v_2\partial_{v_2}-v_3\partial_{v_3}+v_4\partial_{v_4}+\text{h.a.},\\ =&u_1^+\partial_{u_1^+}-u_2^+\partial_{u_2^+}+v_1^+\partial_{v_1^+}-v_2^+\partial_{v_2^+}\\ &+u_1^-\partial_{u_1}-u_2^-\partial_{u_2}+v_1^-\partial_{v_1}-v_2^-\partial_{v_2}.\end{aligned} \tag{58}$$

We will denote $2I_z$ as the "charge" operator and can then label the representations by mass, isospin, charge, and parity. As an example, there will be 8 representations with $|m|=2$, $|Q|=1, I=\frac12$. They can be grouped into four pairs, with each pair being an isospin doublet. The basis functions $(f/\Psi_0)$ and their associated mass, charge, and parity are $(u_1^+, v_1^+: 2, 1, 1)$, $(u_2^+, v_2^+: 2, -1, 1)$, $(u_1^-, v_1^-: 2, 1, -1)$, $(u_2^-, v_2^-: 2, -1, -1)$; $(\bar u_1^+, \bar v_1^+: -2, -1, 1)$; $(\bar u_2^+, \bar v_2^+: -2, 1, 1)$; $(\bar u_1^-, \bar v_1^-: -2, -1, -1)$, $(\bar u_2^-, \bar v_2^-: -2, 1, -1)$.

We are not certain which representations should be considered the antiparticles of the first two. In the conventional Dirac equation, the antiparticle has a negative energy.

But in reality, the physical antiparticle has a positive energy. So we would favor the fourth and third, as being the antiparticles of the first and second, resp. But the question probably does not have a clear-cut answer except in the context of a many-body problem.

This example is "flawed" as an illustration of an internal symmetry because the $\mathcal{O}$ separates, i.e., $\mathcal{O} = \mathcal{O}_{13} + \mathcal{O}_{24}$. One way to correct this is to introduce a term in the mass operator, $m$, proportional to the $I_x$ of Eq. (58). This would couple the 13 and 24 variables and break the SU(2) symmetry. The eigenfunctions of $\mathcal{O}$ would then be those linear combinations of eigenfunctions of $I_z$ which are eigenfunctions of $I_x$, and the mass would depend on the eigenvalue, i.e., there would be a mass splitting for the doublets.

It is possible to use six sets of $(u, v)$ instead of four and obtain an $\mathcal{O}$ with an internal symmetry isomorphic to SU(3). We could then add terms to $\mathcal{O}$ which break the symmetry in such a way that the physical spectrum can be imitated fairly well. But more representations of SU(3) occur in the solution space than occur physically; states of all triality[12] occur, rather than the physical triality of zero. In addition, the similarity of this spectrum to the physical one seems to be due solely to the group structure. Hence, we do not believe these results are significant.

And in retrospect, we do not really expect physically significant results at the single-particle (i.e., few independent variables) level, because, although the mass spectrum is a kinematic quantity, it is evidentally tied to the many-body problem. We are therefore led to discuss this much more complicated problem in the next section.

## 4. THE MANY-BODY PROBLEM

We now turn from the relatively simple, but unphysical, single-particle theories of Sec. 3 to the more realistic many-body problem. The $A$ equation will be extremely difficult to solve in detail in this problem, because of the large number of independent variables—at least one set for every fermion in the universe. Because of this, we will not examine the content of a particular equation here. We will instead only "rough out" the problem by looking for those general properties of the $A$ equation and its solutions which correspond to the physical properties of particles.

A very general property of nature is its Lorentz-invariant character. We can build this into our theory by requiring that the mathematical representative of a physical state satisfy the $A$ equation, $\mathcal{O}\Psi = 0$, where $\mathcal{O}$ is a linear differential operator with an invariance group of transformations of the independent variables, homorphic to ISL(2). The first step, then, is the construction of classes of Lorentz-invariant $\mathcal{O}$'s from which we will eventually, by the use of more powerful heuristic techniques than we have now, choose the "physically correct" operator.

A related problem is the construction of the infinitesimal generators of the invariance group. In some methods of setting up quantum mechanics, it is this construction which is all important, because the Hamiltonian is responsible for the interaction. But the fact that the group is a transformation group implies that the infinitesimal generators are first-order differential operators, which in turn implies that the infinitesimal generators are not directly responsible for the interaction in our theory. It is caused instead, as we shall see, by a suitable $\mathcal{O}$. Because of this, our procedure will be to choose the infinitesimal generators and therefore the invariance group to be as simple as possible. It is then a relatively easy job to construct classes of $\mathcal{O}$'s which commute with the infinitesimal generators, thus obtaining relativistically invariant theories.

We consider first the case where the independent variables are space–timelike. In this case, the infintesimal generators will simply be chosen as sums of operators like those of Eqs. (5)–(8), e.g., $P_0 = i\Sigma\partial_{x_0}$, where we have assumed a finite number, $N$, of variables. Then a class of "Klein–Gordon-like" operators which commute with these ten infinitesimal generators, and are therefore Lorentz invariant, is

$$\mathcal{O} = \sum_{m=1}^{n} \partial_\mu{}^{(m)}\partial_\mu{}^{(m)} + V, \tag{59}$$

with the "potential" $V$ being a function of the $(x_\mu{}^{(m)} - x_\mu{}^{(n)})$ $(x_\mu{}^{(m)} - x_\mu{}^{(n)})$. On the other hand, if the variables are spinlike, the **J**, **K** will be sums of the spinlike **J**, **K** of Eq. (10), and the $P_\mu$ will be

$$P_\mu = \sum_{m=1}^{n} p_\mu{}^{(m)}, \tag{60}$$

with the $p_\mu{}^{(m)}$ being operators like those of Eq. (21). An example of Dirac-like ISL(2)-invariant operators in this case is

$$= \sum d_\mu{}^{(m)} p_\mu{}^{(m)} + V, \tag{61}$$

where the $d_\mu{}^{(m)}$ are Hermitian operators, analogous to the $D_\mu$ of Eq. (51), which must commute with $p_\nu{}^{(n)}$, $x_\nu{}^{(n)}$ for all $n, \nu$. The potential could be constructed, as before, from functions of $(x_\mu{}^{(m)} - x_\mu{}^{(n)})$ $(x_\mu{}^{(m)} - x_\mu{}^{(n)})$, but could also include ISL(2)-invariant functions of the spin variables. We note that the operator of Eq. (61) is also suitable when a hybrid system of variables is used.

Since we are now able to construct a large class of $A$ equations which are Lorentz invariant, we can begin an analysis of how other physical properties of particles bear on the form of the $A$ equation and its solutions. A second general property is that physical states are catalogued according to the number and kind of particles present (if the interactions are not too strong). The lowest state will be one with no particles present. This ground or vacuum state $\Psi_0$ will be a function which satisfied the $A$ equation, and which is an ISL(2) invariant. According to the ideas of Weinberg[5] and Salam[6] $\Psi_0$ is not simply a "background" but contains a good deal of physical information. That is, they argue that the original problem (the $A$ equation in our case, the Lagrangian in theirs) is invariant under the internal symmetries, with the broken symmetry arising from spontaneous symmetry breaking—a "crystallizing"—in the vacuum state, (in analogy to an asymmetric Ising model vacuum state arising from a symmetric Hamiltonian). Thus, our theory holds out the possibility of being able to show why the symmetry is broken as it is, because we have an equation for the vacuum state.

The next states of physical interest are the one-particle states. In many-body problems such as phonons in crystals, and $^4$He, functions representing "particles" are the product of the ground state and an "excitation function; we will assume the same thing here. That is, the function representing a single particle of mass $m$, spin $S$, momentum $p$, and $z$-component of spin $\sigma$ is

$$\Psi(m, p, s, \sigma) = f(m, p, s, \sigma)\Psi_0. \tag{62}$$

where the $f$'s form a basis for the $(m, s)$ irreducible representation of ISL(2).

There are two interesting points about the equation for $f$ obtained by putting this $\Psi$ into the $A$ equation. One is that the potential $V$ never enters. If we write $\Psi_0 = \exp(\Phi_0)$, then Eqs. (60) and (61) become the equations

$$\sum(p_\mu{}^{(m)}p_\mu{}^{(m)}f + 2p_\mu{}^{(m)}fp_\mu{}^{(m)}\Phi_0) = 0, \tag{63}$$

$$\sum(d_\mu{}^{(m)}p_\mu{}^{(m)}f + d_\mu{}^{(m)}fp_\mu{}^{(m)}\Phi_0 + p_\mu{}^{(m)}fd_\mu{}^{(m)}\Phi_0) = 0, \tag{64}$$

resp., for $f$. Thus even though the vacuum problem may prove to be too difficult, we can still calculate with the theory by choosing $\Psi_0$ as a real normalizable, ISL(2)-invariant function and starting the problem from there.

The other point is that the $A$ equation can be made into an eigenvalue equation for the mass, or the mass squared. In order to see this, we write

$$f(m, 0, s, \sigma) = e^{-imX_0}f_{\text{int}}(m, 0, s, \sigma), \tag{65}$$

where

$$[p_\mu{}^{(m)}, X_0] = \delta_{\mu_0}/N \tag{66}$$

for the zero momentum basis functions of an $(m, S)$ representation of ISL(2). The "internal" functions must be translationally invariant,

$$P_\mu f_{\text{int}} = 0, \tag{67}$$

and satisfy

$$m^2 f_{\text{int}} + \sum(p_\mu{}^{(m)}p_\mu{}^{(m)}f_{\text{int}} + 2p_\mu{}^{(m)}f_{\text{int}}p_\mu{}^{(m)}\Phi_0) = 0, \tag{68}$$

or

$$m(\mathscr{D}_0 f_{\text{int}} + f_{\text{int}}\mathscr{D}_0\Phi_0) + \sum(d_\mu{}^{(m)}f_{\text{int}}p_\mu{}^{(m)}\Phi_0 + p_\mu{}^{(m)}f_{\text{int}}d_\mu{}^{(m)}\Phi_0) = 0,$$

$$\mathscr{D}_0 = \sum d_0{}^{(m)} \tag{69}$$

obtained from Eq. (63) or (64), resp., by the use of Eq. (65).

The $m^2$ of Eq. (68) and the $m$ of Eq. (69) must be real since all operators involved are Hermitian, but until we solve a particular equation, we do not know whether they will be positive or negative. We would like to avoid those $\mathscr{O}$, $\Psi_0$ which give negative $m^2$ solutions to Eq. (68), if that is the form we choose for the $A$ equation, because of the unitarity problem alluded to in Sec. 3. There will most surely be negative mass solutions to Eq. (68), and, we suspect from the examples of Sec. 3, there is a good chance of having negative mass solutions to Eq. (69). These negative mass solutions are unphysical, because such particles are never observed, and must somehow be eliminated from the theory. There are two possibilities. One is to use Eq. (69) and search for a $V$ (or a $\Psi_0$) which gives no negative mass solutions. The other is to construct the many-particle solutions so that, even though negative mass solutions exist and are part of a complete set, they are not "activated" in a scattering process between positive mass solutions. Without further detailed investigation, there is no way of knowing which, if either, of these remedies will work.

We now consider those solutions of the $A$ equation which correspond to several particles, ignoring symmetrization properties for the time being. Our initial expectation is that a many-particle state is mathematically represented by something like a product, e.g., the solution of the $A$ equation that corresponds to one particle with momentum $p_1$, and another with momentum $p_2$ is

$$\Psi = f_{p_1}f_{p_2}\Psi_0. \tag{70}$$

Now if $\mathscr{O}$ contained derivatives no higher than the first, then the $\Psi$ of Eq. (70) would be an exact solution of the $A$ equation provided $\Psi_0, f_{p_1}\Psi_0$, and $f_{p_2}\Psi_0$ are. But such a theory would be one without interactions, because, since the time evolution operator is a first-order differential operator,

$$\exp(iP_0X_0)f_{p_1}f_{p_2}\Psi_0 = \exp[i(p_{10} + p_{20})x_0]f_{p_1}f_{p_2}\Psi_0, \tag{71}$$

which says mathematically that there is no energy of interaction—each particle evolves in time as if the others were not there. A similar analysis would show that $\mathscr{O}$ must not be a separable operator. The implications of this argument are that $\mathscr{O}$ must not be separable, and it must contain differential operators of at least second order. Conversely, we see that if $\mathscr{O}$ does have second-order derivative terms, then the cross terms—in our examples, these would be $p_\mu{}^{(m)}f_{p_1}p_\mu{}^{(m)}f_{p_2}$ or $d_\mu{}^{(m)}f_{p_1}p_\mu{}^{(m)}f_{p_2}$—imply that the product is, in general, no longer an exact solution.

Suppose, on the other hand, that we use "localized" states, $f_x = \int d^3p\, g(p)e^{ip\cdot x}f_p$, with the precise form of $g(p)$ depending on spin and the properties one wants for $f_x$. Then for *any* reasonable theory of quantum mechanics, we expect the "interactions" between localized particles to go to zero as their separation goes to infinity. In our theory, this would imply that the cross terms go to zero. But then, the product of "distant" particle functions,

$$\Psi = f_{x_1}f_{x_2}\Psi_0, \tag{72}$$

is a solution of the $A$ equation.

We can illuminate these ideas, and expand on them somewhat if we consider a scattering process. Suppose we start out with two widely separated electrons at a large negative time, say $-t_0$. Then the solution corresponding to the electrons will be a product like Eq. (72). As time progresses and the electrons get closer, the interaction cross terms will no longer be negligible, and so the solution will not be as simple as a product. If the interaction is weak, we would expect that the solution at time $t$ might be something like

$$\Psi_{\text{out}}(t) = \exp[i(t + t_0)P_0]\Psi(-t_0) = \int d^3x_1 \int d^3x_2\, \psi(x_1, x_2, t)f_{x_1}f_{x_2}\Psi_0, \tag{73}$$

i.e., a sum of products, with $\psi$ being the conventional wavefunction of quantum mechanics. But the above would not be exactly correct; there will be an "extra" part to the solution, outside the vector space spanned by products of one-particle solutions, corresponding roughly to particles (photons, virtual pairs, etc.) "off the mass shell." After the scattering is finished, and the constituents have widely separated from each other, we again expect the results to be describable as a sum of products of one particle states, even if there are photons and/or particle–antiparticle pairs present, i.e.,

$$\begin{aligned}\Psi(t)_{\text{out}} = &\int d^3x_1\, d^3x_2\, \psi_1(x_1, x_2, t) f^e_{x_1} f^e_{x_2} \Psi_0 \\ &+ \int d^3x_1\, d^3x_2\, d^3x_3\, \psi_2(x_1, x_2 x_3, t) f^e_{x_1} f^e_{x_2} f^{\text{ph}}_{x_3} \Psi_0 \\ &+ \int d^3x_1\, d^3x_2\, d^3x_3\, d^3x_4 \Psi(x_1, x_2, x_3, x_4, t) \\ &\times f^e_{x_1} f^e_{x_2} f^e_{x_3} f^{\bar{e}}_{x_4} \Psi_0 \\ &+ \cdots, \end{aligned} \tag{74}$$

where $f^e, f^{\bar{e}}, f^{\text{ph}}$ identify functions corresponding to single electrons, positrons, and photons, resp. So in this scheme, products of one-particle states are complete for systems of widely separated particles, but are not complete when the particles are interacting significantly. The incompleteness provides for the possibility of creation and annihilation of particles, while the "asymptotic completeness" is the mathematical principle corresponding to our description of nature in terms of particles.

Thus we have a theory which, in principle, is Lorentz–invariant, is capable of describing nature in terms of particles, and which can account for the creation and annihilation of particles in a manner which does not seem overly contrived. The last principle, however, that of symmetrization—and antisymmetry in particular—is not a "natural" one in an independent variable theory. In fact, part of the motivation for using field theory is that antisymmetry is considered to be a "basic" principle which can be put in only by the use of antisymmetric operators as the building blocks of an elementary particle theory.

On the other hand, there is no reason why antisymmetrization should be impossible to include in an independent variable theory. One possible reason for its occurring might be that only antisymmetric solutions of the $A$ equation are *stable*. That is, suppose our $A$ equation has both positive and negative mass solutions for fermions, but only positive mass solutions (or else positive and negative solutions, but the negative solutions are never brought into play in a scattering process) for bosons. Then one could imagine that if fermion states were not antisymmetrized, the scattering of two positive mass fermions would produce a cascade of positive and negative mass pairs. The only way to obtain stable many-particle states would be to antisymmetrize, thereby excluding the scattering to negative mass states.

The actual form for symmetric and antisymmetric solutions cannot be known until we solve a particular problem. But we can give examples, in order to have some idea of what sort of solutions to try. The symmetric case is very simple; we can just use a product like that of Eq. (70), provided the two $f$'s are functions of the same variables [not $f_p(u_1) f_p(u_2)$, for example]. The constructions are so simple, in fact, that one hardly feels compelled to "explain" why symmetric solutions occur.

The antisymmetric case requires a more complicated construction. Let us suppose that, as in the $^4$He example, a one-particle fermion state is of the form

$$\Psi_{p,s} = \left[\sum g_{p,s}(u_i)\right] \Psi_0, \tag{75}$$

where the $u_i$ represent different sets of independent variables. (Actually, the $g$'s will depend on more than one set of variables, as in the Feynman wavefunctions that take backflow into account,[13] but the main dependence is on $u_i$.) Then a function antisymmetric in the two sets of labels $(p_1, s_1)$ and $(p_2, s_2)$ is

$$\Psi_{p_1,s_1,p_2,s_2} = \sum\sum [g_{p_1,s_1}(u_i) g_{p_2,s_2}(u_j) - g_{p_1,s_1}(u_j) g_{p_2,s_2}(u_i)] \Psi_0. \tag{76}$$

In a way, the function of Eq. (76) is interesting for what is left out; nothing is said about the symmetry properties of $\Psi_0$. The reason is that the only thing we know about particle states is that they are antisymmetric in the *labels*, i.e., $|x_2, x_1\rangle = -|x_1, x_2\rangle$. We know nothing at all about symmetry properties with respect to the *independent variables*. In particular, we do not know whether $\Psi_0$ must be antisymmetrized in the independent variables in order to "exclude" negative mass states. We suspect that the picture of every negative mass state being occupied in $\Psi_0$ is naive, because there are a continuous infinity of states and that makes for an extremely messy theory.

In summary, we see that the idea of spin $\frac{1}{2}$ solutions of the $A$ equation being antisymmetric in the labels can, in principle, be fit into the independent variable approach. But it does not fit in naturally. We must await more detailed work on a specific example in order to see how, or whether, antisymmetry occurs.

## 5. SUMMARY AND CONCLUSIONS

We have proposed a theory of quantum mechanics in which physical states are mathematically represented by functions which are solutions of a Lorentz-invariant differential equation in some set of independent variables. In Sec. 2, we explored different types of variables and concluded that either space–timelike or spinlike variables were suitable. We then used these variables in Sec. 3 to give examples of different types of simple one-particle $A$ equations with discrete mass spectra.

Consideration of the many-body problem in Sec. 4 was initiated by showing how to construct large classes of Lorentz-invariant differential equations in either type of variable. Then we made several assumptions, based partly on analogy with many-body problems, about the form of solutions of the $A$ equation, in order to be able to explain particleness, interactions, and creation and annihilation. (1) We assume there exists an ISL(2)-invariant vacuum state. (2) We assume there exists one-particle solutions of the form $f\Psi_0$ where $f$ is a function which has a definite mass and spin. (3) We assume multiparticle states are "something like" products, i.e., $\Psi = f_1 f_2 \Psi_0$. Second-order differential operators

in the $A$ equation will then cause an interaction. (4) We assume that if the $f$'s corresponding to localized particles, then the "interaction" goes to zero as the separation goes to infinity. Thus if the single particle functions, $f\Psi_0$, are complete for one-particle states, the widely separated functions will be complete for widely separated many-particle states. (5) These states will presumably not be complete for interacting particles, however, and this appears to allow for the creation and annihilation of particles. (6) Finally, we assume that antisymmetry in the labels of the solutions is made necessary by the need to exclude negative mass solutions from the theory.

It is obvious from the number of assumptions we have made that what we have here is not a physical theory, but only the suggestion for the form of a theory. Thus, although the theory has the possibility of satisfying all requirements, we cannot properly judge it until we choose a specific $A$ equation and see if our assumptions about the form of the solutions are valid. It is particularly crucial to investigate whether and how antisymmetry arises, since that concept seems "forced" here.

One last remark. Since the Lagrangian equations of motion of quantum field theory yield so much correct information, we would expect those equations, perhaps in some approximation, to follow from our theory. This essentially means there must be a connection between our $A$ equation and the Lagrangian equations. Some inkling of such a connection can be seen if we assume the general form of a solution to the $A$ equation is like that of Eq. (74), only the functions for the various particles, in particular the phonon and electron–positron pair, are not necessarily the functions for physical particles, but rather may be "off the mass shell." This idea will not be pursued further here, but its development is crucial both for choosing a physically relevant $A$ equation, and for examining the physical content of the $A$ equation.


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# Representation and properties of para-Bose oscillator operators. II. Coherent states and the minimum uncertainty states

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The energy, position, and momentum eigenstates of a para-Bose oscillator system were considered in paper I. Here we consider the Bargmann or the analytic function description of the para-Bose system. This brings in, in a natural way, the coherent states $|z;\alpha\rangle$ defined as the eigenstates of the annihilation operator $\hat{a}$. The transformation functions relating this description to the energy, position, and momentum eigenstates are explicitly obtained. Possible resolution of the identity operator using coherent states is examined. A particular resolution contains two integrals, one containing the diagonal basis $|z;\alpha\rangle\langle z;\alpha|$ and the other containing the pseudodiagonal basis $|z;\alpha\rangle\langle -z;\alpha|$. We briefly consider the normal and antinormal ordering of the operators and their diagonal and discrete diagonal coherent state approximations. The problem of constructing states with a minimum value of the product of the position and momentum uncertainties and the possible $\alpha$ dependence of this minimum value is considered.

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## 1. INTRODUCTION

In paper[1] I of this work we have given a detailed study of the energy, position, and momentum eigenstates of a para-Bose oscillator system characterized by the commutation relation

$$[\tfrac{1}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger),\hat{a}] = -\hat{a} \tag{1.1}$$

and by a parameter $\alpha$ denoting the minimum eigenvalue of the Hamiltonian $\frac{1}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)$ ($\alpha = \frac{1}{2}$ being the normal Bose case). We had in particular considered the relationship between the matrix and the wave mechanical descriptions of the para-Bose operators. In the present paper we consider the Bargmann (or the entire function space) description, operator ordering, and construction of states with minimum value of the product of uncertainties in position–momentum variables and related matters. We begin in Sec. 2 by constructing the Bargmann representation using a suitably defined Hilbert space of entire analytic functions for the SL(2,$R$) Lie algebra relevant to us, and then for the para-Bose system. This brings in, in a natural way, the coherent states, i.e., the eigenstates of the para-Bose annihilation operator. The transformations relating this description to the energy, coordinate, and momentum descriptions will be explicitly obtained. Possible resolution of the identity operator using coherent states is examined. As is well known, in the normal Bose case a diagonal resolution of the identity operator does exist, viz.,

$$\hat{1} = \frac{1}{\pi}\int |z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|d^2z\,. \tag{1.2}$$

However, it turns out that for other values of $\alpha$, no such diagonal resolution exists. This is because a certain moment problem has no solution in the general case. An alternative resolution of the identity valid for all $\alpha$ will be developed and its uniqueness discussed. This resolution contains two integrals: one consisting of the diagonal basis $|z;\alpha\rangle\langle z;\alpha|$ and the other consisting of the pseudodiagonal basis $|z;\alpha\rangle\langle -z;\alpha|$. This second integral is of course absent in the normal Bose case $\alpha = \frac{1}{2}$. In Sec. 3, we discuss the possibilities of various operator descriptions such as the normal ordered, the antinormal ordered, and the diagonal and the discrete diagonal coherent state approximations. In Sec. 4, we consider the problem of constructing states with the minimum product of the uncertainties in position and momentum variables, and their $\alpha$ dependence. Section 5 comprises concluding remarks and some general questions.

## 2. BARGMANN REPRESENTATION OF PARA-BOSE OPERATORS

Para-Bose operators $\hat{a},\hat{a}^\dagger$, and $\hat{H} = \frac{1}{2}(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)$ leave the representation space $\mathscr{D}_\alpha$ invariant. This space is spanned by the eigenstates $|n;\alpha\rangle, n = 0,1,\cdots$ of $\hat{H}$ with the corresponding eigenvalues $n + \alpha$. The parameter $\alpha$ denotes the minimum eigenvalue of $\hat{H}$. Using the representation of the operator $\hat{\mathbf{a}}$ in space $\mathscr{D}_\alpha$, one can construct its eigenstate $|z;\alpha\rangle$ with eigenvalue $z$, where $z$ is any complex number.[2] We call such a state the para-Bose coherent state in analogy with the normal Bose case. Instead of following this procedure for obtaining these states, we show that they appear in a natural way in the Bargmann description of $\mathscr{D}_\alpha$. We begin in Sec. 2A with the Bargmann[3] type description of the representation $D_\beta$ of the SL(2,$R$) Lie algebra, using a Hilbert space of entire functions. This involves working with the eigenfunctions of $J_-$. This is used in Sec. 2B to construct a similar description of the para-Bose representation $\mathscr{D}_\alpha$. We are then directly led to the coherent states $|z;\alpha\rangle$. One of the outcomes of this procedure is a particular resolution of the identity in terms of the coherent states. The possibility of having a diagonal expression for the identity operator is examined in Sec. 2C.

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### A. Bargmann description of SL(2,R) representation $D_\beta$

In Sec. 2 of part I, we introduced the para-Bose operators and the relations satisfied by them. The para-Bose operator algebra is determined in terms of the Hamiltonian (I2.2):

$$\hat{H} = \tfrac{1}{2}(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \tag{2.1}$$

and the commutation relation [Eq. (I2.1)]

$$[\hat{a},\hat{H}] = \hat{a}\,. \tag{2.2}$$

We have seen that the operators $\hat{J}_0$, $\hat{J}_1$, and $\hat{J}_2$ defined as

$$\hat{J}_0 = \tfrac{1}{2}\hat{H},\quad \hat{J}_1 = \tfrac{1}{4}(\hat{a}^2 + \hat{a}^{\dagger 2}),\quad \hat{J}_2 = (i/4)(\hat{a}^2 - \hat{a}^{\dagger 2})\,, \tag{2.3}$$

obey commutation relations which correspond to the SL(2,$R$) Lie algebra [Eq. (I2.8)]. The eigenvectors of $\hat{J}_0$, viz., $|n;\beta\rangle$, form a complete orthonormal basis:

$$\hat{J}_0|n;\beta\rangle = (n+\beta)|n;\beta\rangle\,, \tag{2.4}$$

$$\langle n';\beta\,|n;\beta\rangle = \delta_{n',n}\,. \tag{2.5}$$

We ask for a realization of the representation $D_\beta$ of the SL(2,$R$) Lie algebra in which the vector $|n;\beta\rangle$ is realized as the $n$th power of a complex variable $\omega$ and $\hat{J}_+ \equiv \hat{J}_1 + i\hat{J}_2$ is realized as a simple multiplication by $\omega$:

$$|n;\beta\rangle \to \mu_n\omega^n\,, \tag{2.6}$$

$$J_+ \to \omega\,. \tag{2.7}$$

A set of constants $\mu_n$ are introduced since $\hat{J}_+$ has definite nontrivial matrix elements. Equation (I2.13) leads to a recursion relation for $\mu_n$:

$$\mu_{n+1} = [(n+1)(n+2\beta)\,]^{-1/2}\mu_n\,. \tag{2.8}$$

With the choice $\mu_0 = 1$, we are led to a solution

$$\mu_n = \left[\frac{\Gamma(2\beta)}{n!\Gamma(n+2\beta)}\right]^{1/2}. \tag{2.9}$$

Equation (2.4) implies that $\hat{J}_0$ is realized according to

$$\hat{J}_0 \to \beta + \omega\frac{d}{d\omega}\,. \tag{2.10}$$

The form of $\hat{J}_- = \hat{J}_1 - i\hat{J}_2$ in this realization is obtained using Eqs. (I2.13) and (2.9):

$$\hat{J}_- \to \omega\frac{d^2}{d\omega^2} + 2\beta\,\frac{d}{d\omega}\,. \tag{2.11}$$

A general vector $|g\rangle$ in $D_\beta$ now determines the function $g(\omega)$ as follows:

$$|g\rangle = \sum_{n=0}^{\infty} g_n|n;\beta\rangle$$

$$\to g(\omega) = \sum_{n=0}^{\infty} g_n\mu_n\omega^n\,. \tag{2.12}$$

If $|g\rangle$ has a finite norm, i.e., if $\{g_n\}$ is $l_2$, the behavior of $\mu_n$ for large $n$ ensures that $g(\omega)$ is an entire analytic function of $\omega$. Thus, $D_\beta$ has been realized in a Hilbert space of entire functions. The inner product in this realization can be exhibited in the form

$$\langle g'|g\rangle = \sum_{n=0}^{\infty} g_n'^* g_n = \int d^2\omega\, K(\omega;\beta)g'^*(\omega)g(\omega)\,. \tag{2.13}$$

Here

$$d^2\omega \equiv du\,dv\quad(\omega = u + iv)\,, \tag{2.14}$$

and the integration extends over the entire complex $\omega$ plane. Taking $|g\rangle$ to be the vector $|n;\beta\rangle$ and using Eq. (2.7) along with the orthonormality of $|n;\beta\rangle$, we find that $K$ is a function of $|\omega|$ only and that it obeys the relation

$$\int_0^\infty d\,|\omega|K(|\omega|;\beta)|\omega|^{2n+1} = (2\pi\mu_n^2)^{-1} = n!\Gamma(n+2\beta)\,[2\pi\Gamma(2\beta)]^{-1}\,. \tag{2.15}$$

In writing the last line (2.15), we have substituted for $\mu_n$ from Eq. (2.9). A solution for $K(|\omega|;\beta)$ exists in terms of the Bessel function $K_\nu(x)$ [see Ref. 4, p. 684, formula (6.561. 16)].

$$K(|\omega|;\beta) = 2(\pi\Gamma(2\beta))^{-1}|\omega|^{2\beta-1}K_{2\beta-1}(2|\omega|)\,. \tag{2.16}$$

We show in Appendix A that this is a unique positive solution.

Let us now view $g(\omega)$ as the inner product of the ket $|g\rangle$ with a ket $|\omega^*;\beta\rangle$ labeled by $\omega^*$:

$$g(\omega) = N_\beta(|\omega|)\langle\omega^*;\beta\,|g\rangle\,, \tag{2.17}$$

where $N_\beta(|\omega|)$ is some real positive function of $|\omega|$ to be adjusted later for proper normalization [cf. Eq. (2.20) below]. The action of $\hat{J}_+$ given in Eq. (2.7) implies that the bras (kets) are the eigenstates of $\hat{J}_+(\hat{J}_-)$

$$\langle\omega^*;\beta\,|\hat{J}_+ = \omega\langle\omega^*;\beta\,|,\quad \hat{J}_-|\omega;\beta\rangle = \omega|\omega;\beta\rangle\,. \tag{2.18}$$

Taking $|g\rangle$ to be $|n;\beta\rangle$ and using Eqs. (2.12) and (2.17) we find that

$$\langle\omega^*;\beta\,|n;\beta\rangle = \mu_n\omega^n[N_\beta(|\omega|)]^{-1}\,,$$

which implies, on taking the Hermitian adjoint of this equation and substituting for $\mu_n$ from Eq. (2.9), that (cf. Barut and Girardello, Ref. 3).

$$|\omega;\beta\rangle = [N_\beta(|\omega|)]^{-1}\sum_{n=0}^{\infty}\left[\frac{\Gamma(2\beta)}{n!\Gamma(n+2\beta)}\right]^{1/2}\omega^n|n;\beta\rangle\,. \tag{2.19}$$

The ket $|\omega;\beta\rangle$ is obviously a finite norm vector, and in fact we may choose $N_\beta(|\omega|)$ such that $|\omega;\beta\rangle$ is normalized. Using the orthonormality of $|n;\beta\rangle$ we find from Eq. (2.19) that

$$\langle\omega;\beta\,|\omega;\beta\rangle = [N_\beta(|\omega|)]^{-2}\sum_{n=0}^{\infty}\frac{\Gamma(2\beta)|\omega|^{2n}}{n!\Gamma(n+2\beta)} = [N_\beta(|\omega|)]^{-2}\Gamma(2\beta)|\omega|^{1-2\beta}I_{2\beta-1}(2|\omega|)\,,$$

where $I_\nu(x)$ is the modified Bessel function. Hence, we take

$$N_\beta(|\omega|) = \{\Gamma(2\beta)|\omega|^{1-2\beta}I_{2\beta-1}(2|\omega|)\}^{1/2}\,. \tag{2.20}$$

It may however be noted that the eigenvectors of $\hat{J}_-$ are not orthogonal. We find that

$$\langle|\omega';\beta\,|\omega;\beta\rangle = \{N_\beta(|\omega'|)N_\beta(|\omega|)\}^{-1}\Gamma(2\beta)(\omega'^*\omega)^{1/2-\beta}\times I_{2\beta-1}(2(\omega'^*\omega)^{1/2})\,. \tag{2.21}$$

The use of Eqs. (2.16), (2.17), and (2.20) in the inner product expression (2.13) leads to the resolution of the identity operator in the space of the representations $D_\beta$:

$$\hat{1}_\beta = \frac{2}{\pi}\int d^2\omega\, I_{2\beta-1}(2|\omega|)K_{2\beta-1}(2|\omega|)|\omega;\beta\rangle\langle\omega;\beta\,|\,. \tag{2.22}$$

The subscript $\beta$ on $\hat{1}$ indicates the space wherein this resolution holds. It is shown in Appendix A that a resolution of the identity in the form

$$\hat{1}_\beta = \int F(\omega)|\omega;\beta\rangle\langle\omega;\beta|d^2\omega \tag{2.23}$$

is unique as long as we restrict $F(\omega)$ to be a positive definite function.

### B. Bargmann description of $\mathscr{D}_\alpha$

There are two ways in which a similar description of the para-Bose representation $\mathscr{D}_\alpha$ can be constructed. One is to use the representation just constructed for $D_\beta$ and use the fact that $\mathscr{D}_\alpha$ is the direct sum of $D_\beta$ and $D_{\beta+1/2}$ [cf. Eq. (I2.16)]. Alternatively, we may start afresh and require that $\hat{a}^\dagger$ be realized as multiplication by a complex number $z$ while $|n;\alpha\rangle$ is realized essentially as the $n$th power of $z$. We follow here the first method.

$\mathscr{D}_\alpha$ is realized in a space which is the direct sum of two spaces carrying $D_\beta$ and $D_{\beta+1/2}$ :

$$\mathscr{D}_\alpha = D_\beta \oplus D_{\beta+1/2}\ , \quad \alpha = 2\beta.$$

In each of the constituent spaces we can set up the eigenvectors of $J_-$. Equation (I2.19) shows that $\hat{a}$ acts on these states as follows:

$$\hat{a}|\omega;\beta\rangle = [N_{\beta+1/2}(|\omega|)/N_\beta(|\omega|)](2/\alpha)^{1/2}\omega|\omega;\beta+\tfrac{1}{2}\rangle\ , \tag{2.24a}$$

$$\hat{a}|\omega;\beta+\tfrac{1}{2}\rangle = [N_\beta(|\omega|)/N_{\beta+1/2}(|\omega|)](2\alpha)^{1/2}|\omega;\beta\rangle\ . \tag{2.24b}$$

The state $|\omega;\beta\rangle$ is orthogonal to the state $|\omega';\beta+\frac{1}{2}\rangle$:

$$\langle\omega;\beta|\omega';\beta+\tfrac{1}{2}\rangle = 0\ . \tag{2.25}$$

An eigenstate $|z,\alpha\rangle$ of $\hat{a}$ with an arbitrary complex number $z$ as the eigenvalue

$$\hat{a}|z;\alpha\rangle = z|z;\alpha\rangle \tag{2.26}$$

can now be constructed as a linear superposition of $|\omega;\beta\rangle$ and $|\omega;\beta+\frac{1}{2}\rangle$. We find that the $|z;\alpha\rangle$ satisfying Eq. (2.26) is given by

$$|z;\alpha\rangle = \mathscr{N}_\alpha(|z|)[N_\beta(\tfrac{1}{2}|z|^2)|\tfrac{1}{2}z^2;\beta\rangle + N_{\beta+\frac{1}{2}}(\tfrac{1}{2}|z|^2)(z/\sqrt{2\alpha})|\tfrac{1}{2}z^2;\beta+\tfrac{1}{2}\rangle]\ . \tag{2.27}$$

The overall real positive factor $\mathscr{N}_\alpha(|z|)$ is to be so chosen that $|z;\alpha\rangle$ is properly normalized:

$$\langle z;\alpha|z;\alpha\rangle = 1\ . \tag{2.28}$$

We therefore write

$$\mathscr{N}_\alpha(|z|) = \left[\{N_\beta(\tfrac{1}{2}|z|^2)\}^2 + \{N_{\beta+1/2}(\tfrac{1}{2}|z|^2)\}^2\frac{|z|^2}{2\alpha}\right]^{-1/2} \tag{2.29}$$

and from Eq. (2.20) we find that

$$\mathscr{N}_\alpha(|z|) = [2^{\alpha-1}\Gamma(\alpha)\mathscr{F}_\alpha(|z|^2)]^{-1/2}\ , \tag{2.30}$$

where $\mathscr{F}_\alpha(z)$ is the function introduced in paper I [Eq. (I3.16)], viz.,

$$\mathscr{F}_\alpha(z) = z^{1-\alpha}(I_{\alpha-1}(z) + I_\alpha(z))\ . \tag{2.31}$$

On substituting from Eq. (2.19) into (2.27) we find that

$$|z;\alpha\rangle = \mathscr{N}_\alpha(|z|)\sum_{n=0}^{\infty}\left\{\frac{\Gamma(2\beta)}{n!\Gamma(n+2\beta)}\right\}^{1/2}(\tfrac{1}{2}z^2)^n \times[|n;\beta\rangle + (z/2^{1/2})(n+2\beta)^{-1/2}|n;\beta+\tfrac{1}{2}\rangle]\ . \tag{2.32}$$

Recalling from paper I [Eq. (I(2.17)] that

$$|l;\beta\rangle = |2l;\alpha\rangle \text{ and } |l;\beta+\tfrac{1}{2}\rangle = |2l+1;\alpha\rangle\ , \tag{2.33}$$

we obtain the following expansion for the coherent state $|z;\alpha\rangle$ in terms of the eigenstates $|n;\alpha\rangle$ of the Hamiltonian $\hat{H}$ (cf. Ref. 2):

$$\begin{aligned}|z;\alpha\rangle &= \mathscr{N}_\alpha(|z|)\sum_{n=0}^{\infty}\left[\frac{\Gamma(\alpha)}{n!\Gamma(n+\alpha)}\right]^{1/2}\{(z/2^{1/2})^{2n}|2n;\alpha\rangle \\ &\quad + (z/2^{1/2})^{2n+1}(n+\alpha)^{-1/2}|2n+1;\alpha\rangle\} \\ &= \{2^{\alpha-1}\mathscr{F}_\alpha(|z|^2)\}^{-1/2} \\ &\quad \times\sum_{n=0}^{\infty}\left\{\left[\frac{n}{2}\right]!\Gamma\left(\left[\frac{n+1}{2}\right]+\alpha\right)\right\}^{-1/2} \\ &\quad \times(z/2^{1/2})^n|n;\alpha\rangle\ .\end{aligned} \tag{2.34}$$

Here $[K]$ stands for the integral part of $K$ i.e., the largest integer smaller than or equal to $K$.

Equation (2.34) gives the coherent states of the para-Bose representation $\mathscr{D}_\alpha$. Several important properties readily follow from here. These states are not mutually orthogonal. The inner product of $|z;\alpha\rangle$ with $|z';\alpha\rangle$ is given by

$$\langle z';\alpha|z;\alpha\rangle = \mathscr{F}_\alpha(z'^*z)/\{\mathscr{F}_\alpha(|z|^2)\mathscr{F}_\alpha(|z'|^2)\}^{1/2}\ . \tag{2.35}$$

It is interesting to note that the entire function $\mathscr{F}(x)$ also appears in the momentum eigenfunction $\langle x;\alpha|k;\alpha\rangle$ Eq. (IB.15)].

Finally, we derive the coordinate and momentum representations of the coherent state. From Eqs. (2.34) and (I3.10) we find that

$$\begin{aligned}\langle x;\alpha|z;\alpha\rangle &= \exp(-\tfrac{1}{2}x^2)|x|^{\alpha-1/2}\{2^{\alpha-1}\mathscr{F}_\alpha(|z|^2)\}^{-1/2} \\ &\quad \times\sum_{n=0}^{\infty}(-1)^n\frac{z^{2n}}{2^n\Gamma(n+\alpha)} \\ &\quad \times\left[L_n^{\alpha-1}(x^2) + \frac{zx}{2^{1/2}}(n+\alpha)\right]L_n^\alpha(x^2)\ ,\end{aligned} \tag{2.36}$$

where $L_n^\alpha$ is the associated Laguerre polynomial. On making use of the generating function relation [Ref. 4, p. 1038 formula (8.975.3)]

$$(xz)^{-(1/2)\alpha}e^zJ_\alpha(2(xz)^{1/2}) = \sum_{n=0}^{\infty}\{\Gamma(n+\alpha+1)\}^{-1}L_n^\alpha(x)z^n\ , \tag{2.37}$$

and on simplification, we may rewrite Eq. (2.36) as

$$\begin{aligned}\langle x;\alpha|z;\alpha\rangle &= 2^{(\alpha-1)/2}|x|^{\alpha-(1/2)}\exp[-\tfrac{1}{2}(x^2+z^2)] \\ &\quad \times\{\mathscr{F}_\alpha(|z|^2)\}^{-1/2}\mathscr{F}_\alpha(\sqrt{2}xz)\ .\end{aligned} \tag{2.38}$$

Again, from Eqs. (2.34), (2.37), and (I3.13) we obtain on simplification

$$\begin{aligned}\langle k;\alpha|z;\alpha\rangle &= 2|k|^{\alpha-(1/2)}\exp[-\tfrac{1}{2}(k^2+z^2)] \\ &\quad \times\{\mathscr{F}_\alpha(|z|^2)\}^{-1/2}\mathscr{F}_\alpha(\sqrt{2}ikz).\end{aligned} \tag{2.39}$$

To set up the representation $\mathscr{D}_\alpha$ in a Hilbert space of entire functions, we must associate with every vector $|f\rangle$ an entire function $f(z)$. This is achieved using coherent states in the following manner:

$$|f\rangle \to f(z) = [2^{\alpha-1}\Gamma(\alpha)\mathscr{F}_\alpha(|z|^2)]^{1/2}\langle z^*;\alpha|f\rangle\ . \tag{2.40}$$

In particular, from Eq. (2.34) we find that the vector $|n;\alpha\rangle$ is realized as

$$|n;\alpha\rangle = \{\Gamma(\alpha)\}^{1/2}\left\{\left[\frac{n}{2}\right]!\Gamma\left(\left[\frac{n+1}{2}\right]+\alpha\right)\right\}^{-1/2} \times (z/\sqrt{2})^n . \tag{2.41}$$

Further, since the coherent states are the eigenstates of $\hat{a}$, or equivalently

$$\langle z^*;\alpha|\hat{a}^\dagger = z\langle z^*;\alpha| , \tag{2.42}$$

it is evident that $\hat{a}^\dagger$ is realized as multiplication by $z$. In fact, this requirement along with the relations [Eqs. (I2.20 c,d)]

$$\hat{a}^\dagger|2n;\alpha\rangle = (2n+2\alpha)^{1/2}|2n+1;\alpha\rangle , \tag{2.43a}$$

$$\hat{a}^\dagger|2n+1;\alpha\rangle = (2n+2)^{1/2}|2n+2;\alpha\rangle , \tag{2.43b}$$

would lead us directly to the numerical factors present in Eq. (2.41). On the other hand, the action of $\hat{a}$ is different on even and odd entire functions of $z$. From Eqs. (2.41) and (I2.20 a,b), viz.,

$$\hat{a}|2n;\alpha\rangle = (2n)^{1/2}|2n-1;\alpha\rangle , \tag{2.44a}$$

$$\hat{a}|2n+1;\alpha\rangle = (2n+2\alpha)^{1/2}|2n;\alpha\rangle , \tag{2.44b}$$

we find that the action of $\hat{a}$ on an even entire function is $df(z)/dz$ whereas its action on an odd entire function is $[d/dz)+(2\alpha-1)/z]f(z)$. Hence, if we write $f(z)$ as a sum of an even part and an odd part

$$f(z) = f_+(z) + f_-(z) , \tag{2.45}$$

then $\hat{a}$ is realized by

$$\hat{a} \to \frac{d}{dz} + \frac{(\alpha-1/2)}{z}(1-\hat{P}) , \tag{2.46}$$

where $\hat{P}$ is the parity operator

$$\hat{P}f(z) = f(-z) . \tag{2.47}$$

Alternatively, if we express $f(z)$ as a column vector

$$\begin{pmatrix} f_+(z) \\ f_-(z) \end{pmatrix} , \tag{2.48}$$

then $\hat{a}^\dagger$ and $\hat{a}$ are realized by matrix operators

$$\hat{a}^\dagger \to \begin{pmatrix} 0 & z \\ z & 0 \end{pmatrix}, \quad \hat{a} \to \begin{pmatrix} 0 & \frac{d}{dz}+\frac{2\alpha-1}{z} \\ \frac{d}{dz} & 0 \end{pmatrix} \tag{2.49}$$

In the space $\mathscr{D}_\alpha$, a vector $|f\rangle$ is determined by the $l_2$ sequence $\{f_n\}$:

$$|f\rangle = \sum_{n=0}^{\infty} f_n|n;\alpha\rangle . \tag{2.50}$$

Now since $\mathscr{D}_\alpha$ is the direct sum of $D_\beta$ and $D_{\beta+(1/2)}$, $\beta = \alpha/2$, the even members $\{f_{2l}\}$ define a vector lying in the subspace carrying the representation $D_\beta$, while the odd members $\{f_{2l+1}\}$ determine a vector lying in the complimentary space $D_{\beta+(1/2)}$. Each of these in turn gives an entire function of $\omega$ via Eq. (2.12) and a similar one with $\beta+\frac{1}{2}$ in place of $\beta$. Thus, we have

$$|f\rangle = \sum_{l=0}^{\infty} f_{2l}|l;\beta\rangle \oplus \sum_{l=0}^{\infty} f_{2l+1}|l;\beta+\tfrac{1}{2}\rangle \to f_1(\omega), f_2(\omega) , \tag{2.51}$$

$$f_1(\omega) = [\Gamma(\alpha)]^{1/2}\sum_{l=0}^{\infty} f_{2l}[n!\Gamma(n+\alpha)]^{-1/2}\omega^l , \tag{2.52}$$

$$f_2(\omega) = [\Gamma(\alpha+1)]^{1/2}\sum_{l=0}^{\infty} f_{2l+1}[n!\Gamma(n+\alpha+1)]^{-1/2}\omega^l . \tag{2.53}$$

From Eq. (2.27) and the relations (2.17) and (2.40) we readily find that the pair of entire functions of $f_1$ and $f_2$ are related to the single entire function $f(z)$ by the equation

$$f(z) = f_1(\tfrac{1}{2}z^2) + [z/(2\alpha)^{1/2}]f_2(\tfrac{1}{2}z^2) . \tag{2.54}$$

Thus, $f_1$ and $f_2$ determine the even and the odd parts, respectively, of $f$:

$$f_+(z) = f_1(\tfrac{1}{2}z^2) , \tag{2.55a}$$

$$f_-(z) = (z/(2\alpha)^{1/2})f_2(\tfrac{1}{2}z^2) . \tag{2.55b}$$

We can now develop an expression for the inner product in the Hilbert space of entire functions of $z$ carrying the para-Bose representation $\mathscr{D}_\alpha$. We begin with

$$\langle f'|f\rangle = \int d^2\omega [K(\omega;\beta)f_1'(\omega)^* f_1(\omega) + K(\omega;\beta+\tfrac{1}{2})f_2'(\omega)^* f_2(\omega)] , \tag{2.56}$$

obtained using Eq. (2.13) within $D_\beta$ and a similar equation with $D_{\beta+(1/2)}$. $K(\omega;\beta)$ is given by Eq. (2.16). We now make the change of variable

$$\omega = z^2/2, \quad d^2\omega = |z|^2 d^2z , \tag{2.57}$$

and also allow for the fact that $\omega$ covers the complex plane twice while $z$ covers it once. Using Eqs. (2.16) and (2.55), we then get:

$$\begin{aligned}\langle f'|f\rangle &= \left(\frac{2^{1-\alpha}}{\pi\Gamma(\alpha)}\right)\int d^2z|z|^{2\alpha}[K_{\alpha-1}(|z|^2)f'_+(z)^* f_+(z) \\ &\quad + K_\alpha(|z|^2)f'_-(z)^* f_-(z)] \\ &= \frac{1}{2\alpha\pi\Gamma(\alpha)}\int d^2z|z|^{2\alpha}[(K_{\alpha-1}(|z|^2)+K_\alpha(|z|^2)) \\ &\quad \times f'(z)^* f(z) + (K_{\alpha-1}(|z|^2)-K_\alpha(|z|^2)) \\ &\quad \times f'(z)^* f(-z)] .\end{aligned} \tag{2.58}$$

Substituting for $f(z)$ and $f'(z)$ from Eq. (2.40) and observing that $|f\rangle$ and $|f'\rangle$ are arbitrary, we obtain the following resolution of the identity operator in $\mathscr{D}_\alpha$:

$$\begin{aligned}\hat{1}_\alpha &= \frac{1}{2\pi}\int d^2z|z|^{2\alpha}\mathscr{F}_\alpha(|z|^2)[\{K_{\alpha-1}(|z|^2+K_\alpha(|z|^2)\} \\ &\quad \times|z;\alpha\rangle\langle z;\alpha|] + \{K_{\alpha-1}(|z|^2)-K_\alpha(|z|^2)\} \\ &\quad \times|z;\alpha\rangle\langle -z;\alpha| .\end{aligned} \tag{2.59}$$

The appearance of the "nondiagonal" terms may be unexpected, but this formula has the virtue of being valid for all $\alpha$ and that the functions appearing in the integrand are all well behaved. For $\alpha = \frac{1}{2}$, we observe that $K_{1/2}(x) = K_{-1/2}(x)$ and Eq. (2.59) reduces to the diagonal resolution of the identity operator

$$\hat{1}_{1/2} = \frac{1}{\pi}\int |z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|d^2z . \tag{2.60}$$

It is interesting to note as shown in Appendix A that a resolution of the identity in the form

$$\hat{1}_\alpha = \int F_1(z)|z;\alpha\rangle\langle z;\alpha||d^2z + \int F_2(z)|z;\alpha\rangle\langle -z;\alpha|d^2z \tag{2.61}$$

is also unique as long as we require that $F \pm F_2$ are positive definite functions.

It may further be observed that the nondiagonal nature of the representation (2.59) disappears if we rewrite it in terms of the eigenstates of $\hat{J}_- = \frac{1}{2}\hat{a}^2$, viz., $|\omega;\beta\rangle, |\omega,\beta + \frac{1}{2}\rangle$. Essentially, this appears in Eq. (2.56). Viewed differently, we may define

$$|z_\pm,\alpha\rangle = \frac{1}{\sqrt{2}}\{|z;\alpha\rangle \pm |-z;\alpha\rangle\} \tag{2.62}$$

and rewrite Eq. (2.59) in the form

$$\hat{1}_\alpha = \frac{1}{2\pi}\int d^2z|z|^{2\alpha}\mathcal{F}_\alpha(|z|^2)\{K_{\alpha-1}(|z|^2)|z_+;\alpha\rangle\langle z_+;\alpha| + K_\alpha(|z|^2)|z_-;\alpha\rangle\langle z_-;\alpha|\}, \tag{2.63}$$

which is essentially a "diagonal" representation. The states $|z_\pm;\alpha\rangle$ are orthogonal to each other, but are not properly normalized. They are in fact proportional to $|\omega;\beta\rangle$ and $|\omega;\beta + \frac{1}{2}\rangle$, respectively.

One may observe that the operator $\hat{R}_1$ introduced in Eq. (I2.22) has the effect of changing $|z;\alpha\rangle$ to $|-z;\alpha\rangle$:

$$\hat{R}_1|z;\alpha\rangle = |-z;\alpha\rangle, \tag{2.64}$$

so that

$$\hat{R}_1|z_\pm;\alpha\rangle = \pm|z_\pm;\alpha\rangle. \tag{2.65}$$

### C. Diagonal coherent state representation of the identity operator in $\mathcal{D}_\alpha$

We now consider the question whether a diagonal resolution of the identity in terms of the coherent states exists in $\mathcal{D}_\alpha$:

$$\hat{1}_\alpha = \int d^2z\,\chi(z;\alpha)|z;\alpha\rangle\langle z;\alpha|. \tag{2.66}$$

On taking the matrix elements of Eq. (2.66) between the number states $|m;\alpha\rangle$ and $|n;\alpha\rangle$, it is readily seen from the orthogonality of these states that $\chi(z;\alpha)$, if it exists, depends on $z$ through $|z|$ only and does not depend on the phase of $z$. We write

$$\rho = \tfrac{1}{2}|z|^2 \tag{2.67}$$

and take $\chi$ to be a function of $\rho$. We also write

$$\mathcal{K}(\rho;\alpha) = 2^{2-\alpha}\pi\{\Gamma(\alpha)\mathcal{F}_\alpha(2\rho)\}^{-1}\chi(\rho;\alpha). \tag{2.68}$$

For $m = n$, we then obtain using Eq. (2.34) the following moments of $\mathcal{K}$:

$$\int_0^\infty \rho^n\mathcal{K}(\rho;\alpha)d\rho = \{\Gamma(\alpha)\}^{-1}\left[\frac{n}{2}\right]!\Gamma\left(\left[\frac{n+1}{2}\right]+\alpha\right),$$
$$= \{\Gamma(\alpha)\}^{-1}l!\Gamma(l+\alpha), \quad n = 2l,$$
$$= \{\Gamma(\alpha)\}^{-1}l!\Gamma(l+1+\alpha), \quad n = 2l+1. \tag{2.69}$$

If Eq. (2.69) has a solution, then Eq. (2.66) is established. It follows from the results of Appendix A [uniqueness of representation (2.59)] that Eq. (2.69) has no solution if $\mathcal{K}(\rho;\alpha)$ was restricted to a positive definite function except for the case $\alpha = \frac{1}{2}$, (when $\mathcal{K} = 2e^{-2\rho}$). Hence, in Eq. (2.69), we have to give up the positivity of $\mathcal{K}$.

Introducing a new variable $\sigma$, we may convert the moment conditions (2.69) into the equation

$$\int_0^\infty \mathcal{K}(\rho;\alpha)e^{i\rho\sigma}d\rho = \{\Gamma(\alpha)\}^{-1}\sum_{l=0}^{\infty}\left\{\frac{l!\Gamma(l+\alpha)}{(2l)!}(i\sigma)^{2l} + \frac{l!\Gamma(l+1+\alpha)}{(2l+1)!}(i\sigma)^{2l+1}\right\}, \tag{2.70}$$

valid within the radius of convergence of the power series on the right hand side, i.e., $|\sigma| < 2$. We rewrite Eq. (2.70) using the hypergeometric function

$$F(a,b;c;u) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{l=0}^{\infty}\frac{\Gamma(a+l)\Gamma(b+l)}{l!\Gamma(c+l)}u^l \tag{2.71}$$

in the form

$$\int_0^\infty \mathcal{K}(\rho;\alpha)e^{i\rho\sigma}\,d\rho = h(\sigma;\alpha), \tag{2.72}$$

where

$$h(\sigma;\alpha) = F(\alpha,1;\tfrac{1}{2};-\tfrac{1}{4}\sigma^2) + i\alpha\sigma F(\alpha+1,1;\tfrac{3}{2};-\tfrac{1}{4}\sigma^2). \tag{2.73}$$

We can now state a precise condition that will determine, for each $\alpha$, whether $\mathcal{K}$ exists. Equation (2.72) allows us to analytically continue the right hand side of Eq. (2.70) outside the circle $|\sigma| = 2$. Since the integral on the left hand side of Eq. (2.72) runs from 0 to $\infty$, a solution to our problem exists if and only if the right-hand side of Eq. (2.73) is free of singularities in the upper half of the complex $\sigma$ plane. In general, the hypergeometric function (2.71) has a branch point at $u = 1$, with a cut conventionally drawn along the real axis from $u = 1$ to $u = \infty$, and in the cut plane it has no singularities. Thus, the function on the right hand side of Eq. (2.73) in general has a branch point on the positive imaginary axis at $\sigma = 2i$, with a cut from $\sigma = 2i$ to $\sigma = i\infty$. (The branc point at $\sigma = -2i$ is not relevant to us here.) Let us first calculate the discontinuity across the cut.

We must evaluate the limits of $h(\sigma,\alpha)$ as $\sigma$ approaches a point on the positive imaginary axis beyond $2i$ from the right and from the left half-planes. For this we must use standard continuation formulas to deal with the hypergeometric function outside the circle of convergence of its power series definition. For the moment, assume $\alpha \neq 1,2,3,\cdots$. Then the relevant formulas are [Ref. 4, p. 1043, formula (9.132.2)]

$$F(\alpha,1;\tfrac{1}{2};u) = [\pi^{1/2}\Gamma(1-\alpha)/\Gamma(\tfrac{1}{2}-\alpha)](-u)^{-\alpha}F(\alpha,\alpha+\tfrac{1}{2};\alpha;1/u) + [2u(1+\alpha)]^{-1}F(1,\tfrac{3}{2};2-\alpha;1/u),$$
$$F(\alpha+1,1;\tfrac{3}{2};u) = \tfrac{1}{2}\pi^{1/2}[\Gamma(-\alpha)/\Gamma(\tfrac{1}{2}-\alpha)](-u)^{-\alpha-1}F(\alpha+1,\alpha+\tfrac{1}{2};\alpha+1;1/u)$$
$$-\tfrac{1}{2}(u\alpha)^{-1}F(1,\tfrac{1}{2};1-\alpha;1/u), \quad |\arg(-u)| < \pi. \tag{2.74}$$

We can now calculate the jump of $h$ across its cut. With $y$ a real number greater than 2, we find that

$$h(iy-\epsilon;\alpha) - h(iy+\epsilon;\alpha) = [\pi^{1/2}\Gamma(1-\alpha)/\Gamma(\tfrac{1}{2}-\alpha)](e^{i\pi\alpha} - e^{-i\pi\alpha})(y^2/4)^{-\alpha}F(\alpha,\alpha+\tfrac{1}{2};\alpha;4/y^2)$$
$$-\alpha y[\pi^{1/2}\Gamma(-\alpha)/\{2\Gamma(\tfrac{1}{2}-\alpha)\}](e^{i\pi(\alpha+1)} - e^{-i\pi(\alpha+1)})(y^2/4)^{-\alpha-1}F(\alpha+1,\alpha+\tfrac{1}{2};\alpha+1;4/y^2)$$

$$= [2i\pi^{3/2}/\{\Gamma(\alpha)\Gamma(\tfrac{1}{2}-\alpha)\}](\tfrac{1}{4}y^2)^{-\alpha}(1-2/y)F(\alpha,\alpha+\tfrac{1}{2};\alpha;4/y^2)\,. \tag{2.75}$$

It turns out that this final result is valid even if $\alpha = 1,2,3,\cdots$, though to obtain it in these cases one must use formulas other than Eq. (2.74) to perform the analytic continuation. So Eq. (2.75) is valid for all $\alpha > 0$ (and, of course, $y > 2$). It follows that for all values of $\alpha$ other than $\frac{1}{2},\frac{3}{2},\frac{5}{2},\cdots$, $h(\sigma;\alpha)$ certainly has a branch point at $\sigma = 2i$, with a nonzero discontinuity across the cut, so no solution exists for the moment problem (2.69). Thus, in the para-Bose representation $\mathscr{D}_\alpha$ with $\alpha \neq \frac{1}{2},\frac{3}{2},\frac{5}{2},\cdots$, there is no diagonal coherent state resolution of the identity.

If $\alpha = m + \frac{1}{2}$ with $m = 0,1,2,\cdots$, the expression (2.75) vanishes, so $h(\sigma;m+\frac{1}{2})$ has no branch point in the upper half $\sigma$ plane. We must now check whether it has a pole at $\sigma = 2i$. As mentioned earlier, it definitely has no singularities anywhere else in the upper half $\sigma$ plane. It turns out that we are able to express $h$ in quite elementary form for the set of values of $\alpha$ being considered. One has, in fact, the results

$$F(m+\tfrac{1}{2},1;\tfrac{1}{2};u) = -\tfrac{1}{2}[\Gamma(m+1)/\{\Gamma(m+\tfrac{1}{2})(1-u)^{m+1}\}]\sum_{n=0}^{m}\frac{\Gamma(n-\frac{1}{2})(1-u)^n}{n!},$$

$$F(m+\tfrac{3}{2},1;\tfrac{1}{2};u) = \frac{\Gamma(m+1)}{2\Gamma(m+3/2)(1-u)^{m+1}}\sum_{n=0}^{m}\frac{\Gamma(n+\frac{1}{2})(1-u)^n}{n!}, m = 0,1,2,\cdots. \tag{2.76}$$

[See, for example, Ref. 5, p. 110, formula (14)]. This leads to the following explicit expression for $h$:

$$h(\sigma;m+\tfrac{1}{2}) = -\tfrac{1}{2}[m!/\Gamma(m+\tfrac{1}{2})](1+\tfrac{1}{4}\sigma^2)^{-m-1}\sum_{n=0}^{m}\Gamma(n-\tfrac{1}{2})[1+i(\tfrac{1}{2}-n)\sigma](1+\tfrac{1}{4}\sigma^2)^n/n!, \quad m = 0,1,2,\cdots. \tag{2.77}$$

For the normal Bose case $m = 0$, the potential pole at $\sigma = 2i$ due to the factor standing ahead of the sum is killed by the sum (actually just one term) and

$$h(\sigma;\tfrac{1}{2}) = (1-\tfrac{1}{2}i\sigma)^{-1}, \tag{2.78}$$

so the moment problem has a solution and we get $\mathscr{K}$ inverting the Fourier transform in (2.72):

$$\mathscr{K}(\rho;\tfrac{1}{2}) = \frac{1}{2\pi}\int_{-\infty}^{\infty}d\sigma\exp(-i\rho\sigma)h(\sigma;\tfrac{1}{2}) = \begin{cases}2e^{-2\rho}, & \rho > 0,\\ 0, & \rho < 0.\end{cases} \tag{2.79}$$

This, when used in Eq. (2.68), leads to the known diagonal resolution of the identity for the normal Bose case:

$$\hat{1}_{1/2} = \frac{1}{\pi}\int d^2z|z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|\,. \tag{2.80}$$

However, for $\alpha = \frac{3}{2},\frac{5}{2},\cdots$, i.e., $m = 1,2,\cdots, h(\sigma;\alpha)$ always has a pole, of order $m$, at $\sigma = 2i$. Thus, except for the very special case $\alpha = \frac{1}{2}$, $h(\sigma;\alpha)$ always has a singularity at $\sigma = 2i$ in the upper half-plane, this being either a branch point ($\alpha \neq \frac{3}{2},\frac{5}{2},\cdots$) or a pole ($\alpha = \frac{3}{2},\frac{5}{2},\cdots$). We conclude that the moment problem (2.69) has no solution if $\alpha \neq \frac{1}{2}$.

A quick way to reach this conclusion avoiding an analysis of singularities in the complex $\sigma$ plane is to note that the Fourier inverse transform of $h(\sigma;\alpha)$ is explicitly calculable [Ref. 4, p. 853 formulas (7.531.1), (7.531.2)]:

$$\mathscr{K}'(\rho;\alpha) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty}\exp(-i\rho\sigma)h(\sigma;\alpha)d\sigma$$
$$= 2|\rho|^{\alpha}[\Gamma(\alpha)]^{-1}\{K_{\alpha-1}(2|\rho|)+\epsilon(\rho)K_{\alpha}(2|\rho|)\}, \quad -\infty < \rho < \infty\,. \tag{2.81}$$

Thus, if Eq. (2.69) or (2.72) has a solution, it must be given by Eq. (2.81), which should automatically vanish for $\rho < 0$. This happens only when $\alpha = \frac{1}{2}$.

*Hence, we find that a diagonal coherent state resolution* (2.66) *of the identity operator does not exist, even if we allow* $\mathscr{K}$ *to be a distribution (as usually defined) in any para-Bose representation* $\mathscr{D}_\alpha$ *except* $\mathscr{D}_{1/2}$.

## 3. PARA-BOSE OPERATOR DESCRIPTION

We now consider some aspects of the description operators acting on a space carrying the para-Bose representations $\mathscr{D}_\alpha$. We first recall the situation in the familiar $\alpha = \frac{1}{2}$ case and then consider the problem of generalizing those results.

In the $\mathscr{D}_{1/2}$ space we can write the coherent state $|z;\frac{1}{2}\rangle$ in the form

$$|z;\tfrac{1}{2}\rangle = e^{z\hat{a}^\dagger - z^*\hat{a}}|0;\tfrac{1}{2}\rangle$$
$$= e^{-(1/2)|z|^2}e^{z\hat{a}^\dagger}|0;\tfrac{1}{2}\rangle\,. \tag{3.1}$$

A fairly large and important class of operators can be described by the Weyl representation

$$\hat{A} = \int d^2z\,F(z)e^{z\hat{a}^\dagger - z^*\hat{a}}, \tag{3.2}$$

which is analogous to a Fourier representation with a $c$-number weight function $F(z)$. We also have the diagonal coherent state representation valid for a certain class of operators

$$\hat{A} = \int \phi(z)|z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|d^2z\,. \tag{3.3}$$

There is close relationship between a particular ordered form of $\hat{A}$ and the various representations of $\hat{A}$ such as $F(z)$ or $\phi(z)$.[6] From the commutation relations of $\hat{a}$ and $\hat{a}^\dagger$ one obtains the operator relations

$$\begin{aligned} e^{z\hat{a}^\dagger + z'\hat{a}} &= e^{z\hat{a}^\dagger}e^{z'\hat{a}}e^{zz'/2} \\ &= e^{z'\hat{a}}e^{z\hat{a}^\dagger}e^{-zz'/2}\,, \end{aligned} \tag{3.4}$$

with $z,z'$ any two complex numbers. Such relations when used in Eq. (3.2) allow us to express $\hat{A}$ in normal ordered form with dependences on $\hat{a}^\dagger$ standing to the left of the dependences on $\hat{a}$, or in the antinormal ordered form with the dependences on $\hat{a}$ to the left of the dependences on $\hat{a}^\dagger$. Putting $z' = -z^*$ in Eq. (3.4) we find that the normal (antinormal) ordered description involves better (worse) behaved weight function relative to that of Weyl representation. Thus, for example, we obtain the following normal and antinormal ordered forms of $\hat{A}$ from Eq. (3.2):

$$\hat{A} = \int F(z)e^{-(1/2)|z|^2}e^{z\hat{a}^\dagger}e^{-z^*\hat{a}}d^2z\,, \tag{3.5}$$

$$= \int F(z)e^{(1/2)|z|^2}e^{-z^*\hat{a}}e^{z\hat{a}^\dagger}d^2z\,. \tag{3.6}$$

Using the resolution of the identity (2.60), one can immediately obtain the diagonal coherent state representation $\hat{A}$ from its antinormal ordered form

$$\begin{aligned} \hat{A} &= \frac{1}{\pi}\int F(z')e^{(1/2)|z'|^2}e^{-z'^*\hat{a}}|z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|e^{z'\hat{a}^\dagger}d^2z\,d^2z' \\ &= \int d^2z\int d^2z'F(z')\exp\{\tfrac{1}{2}|z'|^2 - z'^*z + z'z^*\}|z;\tfrac{1}{2}\rangle\langle z;\tfrac{1}{2}|\,. \end{aligned} \tag{3.7}$$

Thus, we find

$$\phi(z) = \frac{1}{\pi}\int d^2z'F(z')e^{(1/2)|z'|^2}\exp(z^*z' - zz'^*)\,. \tag{3.8}$$

Similarly, the normal ordered form of $\hat{A}$ is related to the diagonal matrix elements of $\hat{A}$ in the coherent state:

$$\langle z|\hat{A}|z\rangle = \int d^2z'F(z')e^{-(1/2)|z'|^2}\exp(z^*z' - zz'^*)\,. \tag{3.9}$$

It is unfortunately not easy to obtain generalizations of these results in the para-Bose representation $\mathscr{D}_\alpha$ for $\alpha \neq \frac{1}{2}$. For example, we have seen in Sec. 2 that even the identity operator does not have a diagonal coherent state representation for $\alpha \neq \frac{1}{2}$. Most of the statements we can make about operator descriptions in $\mathscr{D}_\alpha$ rest on general arguments and not on any explicit calculations.

From Eqs. (I2.20) and (2.34) we obtain the following generalizations of Eq. (3.1):

$$|z;\alpha\rangle = \mathscr{N}_\alpha(|z|)\Gamma(\alpha)2^{\alpha-1}\mathscr{F}_\alpha(z\hat{a}^\dagger)|0;\alpha\rangle\,, \tag{3.10}$$

where $\mathscr{N}_\alpha$ and $\mathscr{F}_\alpha$ are given by Eqs. (2.30) and (2.31), respectively.

We now consider whether we can express an operator in normal or antinormal ordered forms for general $\alpha$. An operator $\hat{A}$ is clearly determined by the values of its coherent state matrix elements

$$\langle z';\alpha|\hat{A}|z;\alpha\rangle \tag{3.11}$$

in the sense that if this matrix element vanishes for all $z$ and $z'$, then $\hat{A}$ must vanish. Now that bra and ket vectors involved above depend on $z$ and $z'$ such that the function

$$\langle z';\alpha|\hat{A}|z;\alpha\rangle/\langle z';\alpha|z;\alpha\rangle \tag{3.12}$$

is analytic in $z'^*$ and $z$. This is evident from the relation (2.34). We may thus define an analytic function $f(z'^*,z)$, which does not depend on $z'$ and $z^*$, as

$$f(z'^*,z) = \langle z';\alpha|\hat{A}|z;\alpha\rangle/\langle z';\alpha|z;\alpha\rangle\,. \tag{3.13}$$

If in $f$ we set $\hat{a}^\dagger$ in place of $z'^*$ and $\hat{a}$ in place of $z$, and always keep the former to the left of latter, we obtain an operator $:f(\hat{a}^\dagger|\hat{a}):$ in a normal ordered form all of whose coherent state matrix elements coincide with those of $\hat{A}$. The two operators must then be equal

$$\hat{A} = :f(\hat{a}^\dagger|\hat{a}):\,. \tag{3.14}$$

We have used a bar rather than a coma to separate the arguments of $f$ to stress the normal ordered nature of this operator. Thus, in principle, every operator is expressible as some normal ordered function of $\hat{a}^\dagger$ and $\hat{a}$. It is perhaps important to stress that this argument rests on the properties of coherent states and not on a recipe for moving $\hat{a}^\dagger$ and $\hat{a}$ past each other.[7]

One can show that any normal ordered operator can be rewritten as the sum of two parts in the form

$$:f(\hat{a}^\dagger|\hat{a}): = \text{“}g(\hat{a}|\hat{a}^\dagger)\text{”} + \hat{R}_1\text{”}h(\hat{a}|\hat{a}^\dagger)\text{,”} \tag{3.15}$$

where $\hat{R}_1$ is defined from the relation

$$[\hat{a},\hat{a}^\dagger] = 1 + (2\alpha - 1)\hat{R}_1\,, \tag{3.16}$$

and $g$ and $h$ are both antinormal normal ordered and uniquely determined by $f$. One reaches this conclusion by working with simple monomials and obtaining results such as

$$\hat{a}^\dagger\hat{a}^{2l} = \hat{a}^{2l}\hat{a}^\dagger - 2l\hat{a}^{2l-1}\,, \tag{3.17a}$$

$$\hat{a}^\dagger\hat{a}^{2l+1} = \hat{a}^{2l+1}\hat{a}^\dagger - (2l+1)\hat{a}^{2l} - (2\alpha-1)\hat{R}_1\hat{a}^{2l}\,, \tag{3.17b}$$

$$\hat{a}^{\dagger 2l}\hat{a} = \hat{a}\hat{a}^{\dagger 2l} - 2l\hat{a}^{\dagger 2l-1}\,, \tag{3.17c}$$

$$\hat{a}^{\dagger 2l+1}\hat{a} = \hat{a}\hat{a}^{\dagger 2l+1} - (2l+1)\hat{a}^{\dagger 2l} - (2\alpha-1)\hat{R}_1\hat{a}^{\dagger 2l}\,. \tag{3.17d}$$

These relations can be established by induction. Using these relations, one may verify that the general expression

$$\hat{a}^{+m}\hat{a}^n$$

can be systematically transformed to finally assume the form of the right-hand side of Eq. (3.15). Unfortunately, no simple analytical expression can be worked out for general $m$ and $n$; if it were, one could try generalizing Eq. (3.4) for $\alpha \neq \frac{1}{2}$ (but with $\hat{R}_1$ present in the expressions). Thus, we see that any operator has, in addition to the normal ordered form (3.14), the possibility of being expressed in the form (3.15), which way be called a quasi-antinormal ordered form. This result of course neither confirms nor denies the possibility of achieving a true antinormal ordered form, which is possible if $\hat{R}_1$ itself is expressible in antinormal form.

Using the structure (3.15) and inserting the resolution of identity (2.59) in between $\hat{a}$ and $\hat{a}^\dagger$ and also using the obvious result

$$\hat{R}_1|z;\alpha\rangle = |-z;\alpha\rangle\,, \tag{3.18}$$

we readily see that every operator $\hat{A}$ posseses, in principle, a representation

$$\hat{A} = :f(\hat{a}^\dagger|\hat{a}): = \int \phi_1(z,z^*)|z;\alpha\rangle\langle z;\alpha|d^2z + \int \phi_2(z,z^*)|z;\alpha\rangle\langle -z;\alpha|d^2z\,. \tag{3.19}$$

Here

$$\phi_1(z,z^*) = F_1(|z|^2)g(z,z^*) + F_2(|z|^2)h(-z,z^*)\,, \tag{3.20a}$$

$$\phi_2(z,z^*) = F_2(|z|^2)g(z,-z^*) + F_1(|z|^2)h(-z,-z^*)\,, \tag{3.20b}$$

and

$$F_1(x) = \frac{1}{2\pi}x^\alpha \mathscr{F}_\alpha(x)\{K_{\alpha-1}(x) + K_\alpha(x)\}\,, \tag{3.21a}$$

$$F_2(x) = \frac{1}{2\pi}x^\alpha \mathscr{F}_\alpha(x)\{K_{\alpha-1}(x) - K_\alpha(x)\}\,. \tag{3.21b}$$

Thus, we find that if we are given $g$ and $h$ we obtain $\phi_1$ and $\phi_2$. Conversely, knowing a representation of the type (3.19), i.e., $\phi_1$ and $\phi_2$, we may determine $g$ and $h$. For this, we regard $\phi_1$, $\phi_2$, $g$, and $h$ as functions of two independent complex variables. We rewrite Eq. (3.20b) by replacing $z^*$ with $-z^*$:

$$\phi_2(z,-z^*) = F_2(-|z|^2)\,g(z,z^*) + F_1(-|z|^2)h(-z,z^*)\,. \tag{3.22}$$

We then obtain, from Eqs. (3.20a) and (3.22) the following expressions for $g$ and $h$:

$$g(z,z^*) = \frac{F_1(-|z|^2)\phi_1(z,z^*) - F_2(|z|^2)\phi_2(z,-z^*)}{F_1(|z|^2)F_1(-|z|^2) - F_2(|z|^2)F_2(-|z|^2)}\,, \tag{3.23}$$

$$h(-z,z^*) = \frac{F_2(-|z|^2)\phi_1(z,z^*) - F_1(|z|^2)\phi_2(z,-z^*)}{F_2(|z|^2)F_2(-|z|^2) - F_1(|z|^2)F_1(-|z|^2)}\,. \tag{3.24}$$

Lastly, we discuss the existence of diagonal and discrete diagonal coherent state approximations (not representations) to operators. For definiteness let us restrict ourselves to the family of Hilbert–Schmidt (H–S) operators $\hat{A}$ for which

$$\mathrm{Tr}(\hat{A}^\dagger\hat{A}) < \infty\,. \tag{3.25}$$

The expression

$$(A,B) = \mathrm{Tr}(\hat{A}^\dagger\hat{B}) \tag{3.26}$$

serves as an inner product among such operators, making them elements of a Hilbert space. Condition (3.25) can be expressed in the basis $|n;\alpha\rangle$ as

$$\sum_m\sum_n |\langle m;\alpha|\hat{A}|n;\alpha\rangle|^2 < \infty\,, \tag{3.27}$$

so that these matrix elements of $\hat{A}$ are surely bounded, and in fact go to zero for large values of $m$ and $n$. Using the argument used in Ref. 8, it now follows that the diagonal coherent matrix elements of $\hat{A}$ are separately analytic, in fact entire, in the real and imaginary parts of $z$, the eigenvalue of $\hat{a}$. Thus, using Eq. (2.34),

$$\begin{aligned}\langle z;\alpha|\hat{A}|z;\alpha\rangle = \mathscr{N}_\alpha^2\Gamma(\alpha)\sum_{l,m=0}^{\infty} 2^{-m-l} &\times[m!l!\Gamma(\alpha+m)\Gamma(\alpha+l)]^{-1/2}\\ &\times\Big\{(x-iy)^{2m}(x+iy)^{2l}A_{2m,2l}\\ &+\frac{(x-iy)^{2m}(x+iy)^{2l+1}}{(2\alpha+2l)^{1/2}}A_{2m,2l+1}\\ &+\frac{(x-iy)^{2m+1}(x+iy)^{2l}}{(2\alpha+2m)^{1/2}}A_{2m+1,2l}\\ &+\frac{(x-iy)^{2m+1}(x+iy)^{2l+1}}{2[(\alpha+m)(\alpha+l)]^{1/2}}A_{2m+1;2l+1}\Big\}\end{aligned} \tag{3.28}$$

is the boundary value, for real $x$ and $y$, of an entire analytic function in two complex variable $\xi$ and $\eta$, say, defined by the replacement $x\to\xi$ and $y\to\eta$ on the right hand side of Eq. (3.28). This allows us to assert that an (H–S) operator $\hat{A}$ is fully determined by its diagonal coherent state matrix elements since by the principle of uniqueness of analytic continuation

$$\langle z;\alpha|\hat{A}|z;\alpha\rangle = 0 \text{ for all } z \Rightarrow \hat{A} = 0\,. \tag{3.29}$$

Using the inner product notation (3.26) we could state this result as

$$(|z;\alpha\rangle\langle z;\alpha|,\hat{A}) = 0, \quad \text{all } z \Rightarrow \hat{A} = 0\,. \tag{3.30}$$

However, this has the interpretation that in the Hilbert space of all H–S operators, "linear combinations" of the (continuous) family of elements $|z;\alpha\rangle\langle z;\alpha|$ form a dense set, so that any operator $\hat{A}$ can be approximated arbitrarily closely by such linear combinations. We can therefore assert that the diagonal coherent state approximation to a given operator $\hat{A}$:

$$\hat{A} \sim \int d^2z\varphi(z)|z;\alpha\rangle\langle z;\alpha| \tag{3.31}$$

can be found to arbitrary accurary.

Actually, it is possible to replace Eq. (3.29) by a much more economical one. It is well known that an entire function vanishes identically if it vanishes on a suitably chosen infinite sequence of points in the complex plane. For example, a sequence with a finite limit point has this property. In general, a set of points in the complex plane with the property that the only entire function (out of the class of entire functions under discussion) that vanishes on this set is the zero function is called a characteristic set. For entire functions in two variables, characteristic sets are defined in the product of the complex plane by itself. We can now replace Eq. (3.29) by the following one: choose two characteristic sets $\{x_j\}$, $\{y_k\}$ in the complex plane, both restricted to the real axis. Define the set of points $z_{jk}$ by

$$z_{jk} = x_j + iy_k\,. \tag{3.32}$$

Then

$$\langle z_{jk};\alpha|\hat{A}|z_{jk};\alpha\rangle = 0, \text{ all } j \text{ and } k \Rightarrow \hat{A} = 0\,. \tag{3.33}$$

Alternatively,

$$(|z_{jk};\alpha\rangle\langle z_{jk};\alpha|,\hat{A}) = 0, \quad \text{all } j \text{ and } k \Rightarrow \hat{A} = 0\,. \tag{3.34}$$

Thus, such a denumerable sequence of coherent state projection operators already yields via its linear combinations a dense set in the Hilbert space of H–S operators, leading to the existence of discrete diagonal coherent state approximations to a given $\hat{A}$:

$$\hat{A} \sim \sum_{j,k} \varphi_{ik} |z_{jk};\alpha\rangle\langle z_{jk};\alpha| \tag{3.35}$$

to any desired accuracy.

## 4. POSITION–MOMENTUM UNCERTAINTY PRODUCT

In this section we consider the problem of constructing states with a minimum value of the product of the uncertainties in position and momentum variables. It is well known that if

$$[\hat{A},\hat{B}] = i\hat{C}, \tag{4.1}$$

where $\hat{A}$, $\hat{B}$, and $\hat{C}$ are Hermitian operators, then one has the inequality

$$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geqslant \tfrac{1}{4}|\langle\hat{C}\rangle|^2, \tag{4.2}$$

where

$$\langle(\Delta\hat{A})^2\rangle = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2, \tag{4.3}$$

and the sharp brackets denote the quantum expectation values in the given state. Relation (4.2) reduces to an equality if and only if the given state is an eigenstate of $(\hat{A} + i\lambda\hat{B})$, where $\lambda$ is some real number. Let us now identify $\hat{A}$ and $\hat{B}$ as the position and momentum variables respectively of the para-Bose system

$$\hat{A} = \hat{q} = \frac{\hat{a} + \hat{a}^\dagger}{\sqrt{2}}, \quad \hat{B} = \hat{p} = \frac{\hat{a} - \hat{a}^\dagger}{(\sqrt{2})i}, \tag{4.4}$$

so that

$$[\hat{A},\hat{B}] = i[\hat{a},\hat{a}^\dagger] = i\{1 + (2\alpha - 1)\hat{R}_1\}, \tag{4.5}$$

where [cf. Eq. (I2.22)]

$$\hat{R}_1|n;\alpha\rangle = (-1)^n|n;\alpha\rangle. \tag{4.6}$$

We then find that

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant \tfrac{1}{4}\langle[\hat{a},\hat{a}^\dagger]\rangle^2. \tag{4.7}$$

We may readily verify that relation (4.7) is an equality for the para-Bose coherent states (being the eigenstates of the operator $\hat{q} + i\hat{p}$). However, since $[\hat{a},\hat{a}^\dagger]$ is in general not a $c$-number, the right-hand side of (4.7) itself depends on the given state. Hence, the para-Bose coherent states do not minimize the product of the uncertainties in $\hat{q}$ and $\hat{p}$ in the absolute sense, except for the ordinary Bose case where $\alpha = \frac{1}{2}$. Relation (4.7) gives the minimum value of the product of the uncertainties only in a restricted sense. Consider all those states for which $\frac{1}{4}\langle[\hat{a},\hat{a}^\dagger]\rangle^2$ is a given definite number. The uncertainty product in any of these states is greater than or equal to this number. There is no guarantee that such states would include any coherent state.

In order to determine the minimum value of the uncertainty product, we consider the cases $\alpha < \frac{1}{2}$, $\alpha = \frac{1}{2}$, and $\alpha > \frac{1}{2}$ separately.

*Case* 1: $\alpha < \frac{1}{2}$. The commutator $[\hat{a},\hat{a}^\dagger]$ can be expressed in the form [cf. Eq. (4.5)]

$$[\hat{a},\hat{a}^\dagger] = 2\alpha\hat{P}_e + 2(1-\alpha)\hat{P}_o, \tag{4.8}$$

where $\hat{P}_e$ and $\hat{P}_o$ are the projection operators on the even and odd number states respectively:

$$\hat{P}_e = \sum_{n=0}^{\infty} |2n;\alpha\rangle\langle 2n;\alpha|, \tag{4.9a}$$

$$\hat{P}_o = \sum_{n=0}^{\infty} |2n+1;\alpha\rangle\langle 2n+1;\alpha|. \tag{4.9b}$$

Since $\hat{P}_e + \hat{P}_o = \hat{1}$, we readily find from Eq. (4.8) that

$$2(1-\alpha) - 2(1-2\alpha)\,\hat{P}_e = [\hat{a},\hat{a}^\dagger] = 2\alpha + 2(1-2\alpha)\,\hat{P}_o. \tag{4.10}$$

Further, $\alpha < \frac{1}{2}$ and both $\hat{P}_e$ and $\hat{P}_o$ are positive definite operators; we have

$$2(1-\alpha) \geqslant \langle[\hat{a},\hat{a}^\dagger]\rangle \geqslant 2\alpha. \tag{4.11}$$

From the equalities (4.7) and (4.11) we the obtain

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant \alpha^2, \tag{4.12}$$

giving us a lower bound to the product of the uncertainties in $\hat{q}$ and $\hat{p}$. In order to search for the states for which this lower bound is actually reached, we observe that for such states we must have [cf. relations (4.7), (4.11), and (4.12)]

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle = \tfrac{1}{4}\langle[\hat{a},\hat{a}^\dagger]\rangle^2 \tag{4.13}$$

and

$$\langle[\hat{a},\hat{a}^\dagger]\rangle = 2\alpha \tag{4.14}$$

separately. For Eq. (4.13) to hold, the given state must be an eigenstate of $\hat{q} + i\lambda\hat{p}$ for some real $\lambda$ (in fact $\lambda \geqslant 0$, since there are no eigenstates of $\hat{q} + i\lambda\hat{p}$ for $\lambda < 0$). Also, from Eqs. (4.10) and (4.14) we find that such a state could contain only the even number states and hence

$$\langle\hat{q} + i\lambda\hat{p}\rangle = 0, \tag{4.15}$$

which follows from the fact that $\hat{q}$ and $\hat{p}$ have nonzero matrix elements between the neighboring number states only [cf. Eq. (I2.20)].

We thus conclude that for $\alpha < \frac{1}{2}$, the minimum value of the product of the uncertainties $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$ is $\alpha^2$, and that this is achieved for the states which are the eigenstates of $\hat{q} + i\lambda\hat{p}$ with eigenvalue zero. One may readily see that this state is given by

$$|\psi\rangle = \left\{\sum_{n=0}^{\infty} \frac{\Gamma(\alpha+n)}{n!}\left(\frac{\lambda-1}{\lambda+1}\right)^{2n}\right\}^{-1/2} \times \sum_{n=0}^{\infty}\left\{\left(\frac{\Gamma(\alpha+n)}{n!}\right)^{1/2}\left(\frac{\lambda-1}{\lambda+1}\right)^n|2n;\alpha\rangle\right\}, \tag{4.16}$$

which in fact contains only the even number states.

For such a state, we find that[9]

$$\langle(\Delta\hat{q})^2\rangle = \lambda\alpha, \tag{4.17a}$$

$$\langle(\Delta\hat{p})^2\rangle = \alpha/\lambda. \tag{4.17b}$$

We also have, therefore,

$$\langle(\Delta\hat{q})^2\rangle + \langle(\Delta\hat{p})^2\rangle \geqslant 2\alpha, \tag{4.18}$$

with equality holding only if $\lambda = 1$, i.e., for the ground state $|0;\alpha\rangle$.

It is interesting to note that the minimum uncertainty state (4.16) may also be written directly as

$$|\psi\rangle = \exp\{\tfrac{1}{4}\log\lambda\,(\hat{a}^{\dagger 2} - \hat{a}^2)\}|0;\alpha\rangle, \tag{4.19}$$

which follows from the fact that

$$e^{(1/4)\log\lambda\,(\hat{a}^{\dagger 2} - \hat{a}^2)}\hat{a}e^{-(1/4)\log\lambda\,(\hat{a}^{\dagger 2} - \hat{a}^2)} = \hat{q} + i\lambda\hat{p}, \quad \lambda > 0, \tag{4.20}$$

and that $|0;\alpha\rangle$ is an eigenstate of $\hat{a}$ with eigenvalue 0.

*Case* 2: $\alpha = \frac{1}{2}$. This is the familiar case of the ordinary Bose oscillator. In this case the commutator $[\hat{a},\hat{a}^\dagger]$ is a $c$-number, and the situation is very simple and in fact well known. The minimum uncertainty product $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$ is now $\frac{1}{4}$ and this is achieved for the eigenstates of the operator $\hat{q} + i\lambda\hat{p}$, $\lambda > 0$. Again, here also, we find that $\langle(\Delta\hat{q})^2\rangle + \langle(\Delta\hat{p})^2\rangle \geqslant 1$ and the minimum value 1 is reached for the coherent states, i.e., the eigenstates of $\hat{q} + i\hat{p}$.

*Case* 3: $\alpha > \frac{1}{2}$. Consider first the case when $\frac{1}{2} \leqslant \alpha \leqslant 1$. From Eq. (4.10), we find in this case that

$$\langle[\hat{a},\hat{a}^\dagger]\rangle \geqslant 2(1-\alpha)$$

and hence

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant (1-\alpha)^2 . \tag{4.21}$$

It may readily be seen that equality in (4.21) can never hold. For if it does, the given state must be an eigenstate of $\hat{q} + i\lambda\hat{p}$ and in addition we must have

$$\langle[\hat{a},\hat{a}^\dagger]\rangle = 2(1-\alpha) .$$

Equation (4.10) then shows that the minimum uncertainty state should contain only the odd number states and such a state can never be an eigenstate of $\hat{q} + i\lambda\hat{p}$ for any real positive $\lambda$.

For the case when $\alpha \geqslant 1$, we can have states for which $\langle[\hat{a},\hat{a}^\dagger]\rangle = 0$; however, such a state can never be an eigenstate of $\hat{q} + i\lambda\hat{p}$ so that the product of the uncertainties in $\hat{q}$ and $\hat{p}$ can never be made to vanish.

It is believed that when $\alpha > \frac{1}{2}$, the lower bound of $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$ is $\frac{1}{4}$, the same as in the ordinary Bose case. This conjecture is based on the following observations:

(1) The coherent states are the eigenstates of $\hat{q} + i\lambda\hat{p}$ with $\lambda = 1$. For such states we have

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle = \tfrac{1}{4}|\langle z;\alpha|[\hat{a},\hat{a}^\dagger]|z;\alpha\rangle|^2 . \tag{4.22}$$

Further, we find from Eqs. (4.5), (2.64), and (2.35) that[2]

$$\langle z;\alpha|[\hat{a},\hat{a}^\dagger]|z;\alpha\rangle = 1 + (2\alpha-1)\frac{I_{\alpha-1}(|z|^2) - I_\alpha(|z|^2)}{I_{\alpha-1}(|z|^2) + I_\alpha(|z|^2)} , \tag{4.23}$$

where $I_\alpha$ is the modified Bessel functions. Hence, for coherent states we obtain

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle = \tfrac{1}{4}\left\{1 + (2\alpha-1) \times \frac{I_{\alpha-1}(|z|^2) - I_\alpha(|z|^2)}{I_{\alpha-1}(|z|^2) + I_\alpha(|z|^2)}\right\}^2 . \tag{4.24}$$

We show in Appendix B that

$$I_{\alpha-1}(|z|^2) > I_\alpha(|z|^2), \quad \alpha \geqslant \tfrac{1}{2} , \tag{4.25}$$

so that from Eq. (4.24) we find for $\alpha \geqslant \frac{1}{2}$ the inequality

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle > \tfrac{1}{4} . \tag{4.26}$$

It may be observed that there is no coherent state for which the uncertainty product actually takes the value $\frac{1}{4}$. However, by letting $z$ be very large we may approach this value as close as we like.

(2) Consider any stationary state represented by a density operator $\hat{\rho}$. This implies that $\hat{\rho}$ commutes with the Hamiltonian, i.e., $\hat{\rho}$ is diagonal in the number representation

$$\hat{\rho} = \sum_{n=0}^{\infty} \rho_n |n;\alpha\rangle\langle n;\alpha| . \tag{4.27}$$

For such a state we find that $\langle\hat{q}\rangle = \langle\hat{p}\rangle = 0$ and

$$\langle q^2\rangle = \langle\hat{p}^2\rangle = \sum_{n=0}^{\infty} \rho_n(n+\alpha) \geqslant \alpha, \tag{4.28}$$

with equality holding only for the ground state ($\rho_n = \delta_{n,0}$). Hence

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant \alpha^2. \tag{4.29}$$

(3) From Eq. (4.10) we find that

$$\langle[\hat{a},\hat{a}^\dagger]\rangle = 2(1-\alpha) + 2(2\alpha-1)\langle\hat{P}_e\rangle . \tag{4.30}$$

Thus, if $\langle\hat{P}_e\rangle \geqslant \frac{1}{2}$ (and $\alpha \geqslant \frac{1}{2}$),

$$\langle[\hat{a},\hat{a}^\dagger]\rangle \geqslant 1 . \tag{4.31}$$

Hence, for all those states for which $\langle\hat{P}_e\rangle \geqslant \frac{1}{2}$ we find

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant \tfrac{1}{4} . \tag{4.32}$$

Also, if $\langle\hat{P}_e\rangle \leqslant [\alpha - (3/2)]/(2\alpha-1)$, we have

$$\langle[\hat{a},\hat{a}^\dagger]\rangle \leqslant -1 ,$$

and again we find that

$$\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle \geqslant \tfrac{1}{4}. \tag{4.33}$$

Of course, it is not necessary that the lower bound is actually obtained in these cases. Thus, we find that the product of the uncertainties cannot be less than $\frac{1}{4}$ if either $\langle\hat{P}_e\rangle \geqslant \frac{1}{2}$ or $\langle\hat{P}_e\rangle \leqslant [\alpha - (3/2)]/(2\alpha-1)$. For $\alpha$ very large, it includes almost the whole range.

In Table I below, we summarize the results of this section.

It is interesting to observe that the ground state $|0;\alpha\rangle$ is actually an extremum state for the uncertainty product $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$ for all $\alpha$ in the sense that it satisfies

$$\delta\{\langle\psi|(\hat{q} - \langle\hat{q}\rangle)^2|\psi\rangle\langle\psi|(\hat{p} - \langle\hat{p}\rangle)^2|\psi\rangle\} = 0 , \tag{4.34}$$

subject to the condition $\langle\psi/\psi\rangle = 1$. For $\alpha < \frac{1}{2}$, the ground state $|0;\alpha\rangle$ is the minimum uncertainty product state as discussed earlier. For $\alpha > \frac{1}{2}$ it turns out that $|0;\alpha\rangle$ is actually the maximum uncertainty product state. However, this maximum is only a local maximum, i.e., if we look into neighborhood of the ground state, we get $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$, a maximum for the ground state. The inequality (4.29) is not a contradiction, since any stationary state other than the ground state is not in the neighborhood of it. It appears that the general solution of Eq. (4.34) for $|\psi\rangle$ is the eigenstate of $\hat{q} + i\lambda\hat{p}$ with eigenvalue 0 [except for the normal Bose case $\alpha = \frac{1}{2}$, for which the general solution of Eq. (4.34) is any eigenstate of $\hat{q} + i\lambda\hat{p}$].

## 5. CONCLUDING REMARKS

We have considered energy, position, and momentum eigenstates and the Bargmann description of the para-Bose system with one degree of freedom. Using the coherent states, a resolution of the identity operator containing the diagonal and pseudodiagonal term has been obtained. Normal and antinormal ordering of para-Bose operators has been discussed. We also discussed the minimum value of the product of the uncertainties in position and momentum var-

TABLE I. Lower bound of the uncertainty product $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$.

| $\alpha$ | Restriction on the state | Lower bound of $\langle(\Delta\hat{q})^2\rangle\langle(\Delta\hat{p})^2\rangle$ | Remarks |
|---|---|---|---|
| $\alpha<\frac{1}{2}$ | All states | $\alpha^2$ | Lower bound is obtained for the eigenstate of $\hat{q}+i\lambda\hat{p}$, with eigenvalue 0 ($\lambda\geqslant 0$). |
| $\alpha=\frac{1}{2}$ | All states | $\frac{1}{4}$ | Lower bound is obtained for any eigenstate of $\hat{q}+i\lambda\hat{p}$. |
| $\alpha>\frac{1}{2}$ | Coherent states | $>\frac{1}{4}$ | By taking $z$ large, we can approach the value $\frac{1}{4}$ as close as we like. |
| | $\langle\hat{P}_e\rangle\geqslant\frac{1}{2}$ <br> $\langle\hat{P}_e\rangle\leqslant\frac{\alpha-3/2}{2\alpha-1}$ | $>\frac{1}{4}$ | |
| All $\alpha$ | Stationary states $[\hat{\rho},\hat{H}]=0$ | $\alpha^2$ | Lower bound is obtained for the ground state $\lvert 0;\alpha\rangle$. |

iables. We have tried to generalize the several known results for the normal Bose case ($\alpha=\frac{1}{2}$) to the para-Bose case (general $\alpha$). We have found significantly different results in the general case.

It is obvious that the coherent states form an overcomplete set. For the case $\alpha=\frac{1}{2}$, it has been shown[10] that the existence of a diagonal coherent state representation is analogous to the existence of an expansion of a given state in terms of coherent states with imaginary eigenvalues, i.e., in terms of the states of the form $|ix\rangle$, with $x$ real. This is demonstrated by introducing "super operators" whose action on the space consisting of ordinary operators is suitably defined. It will be of interest to see if such a formalism could be generalized for the para-Bose system. It is necessary, for this purpose, to consider first a para-Bose system with more than one degree of freedom. Unfortunately, the algebra for systems with more than one degree of freedom becomes much complicated[11] especially because even the operators belonging to different modes need not commute. One may then naturally ask for the minimum value of the uncertainty product $\langle(\Delta\hat{q}_1)^2\rangle\langle(\Delta\hat{p}_2)^2\rangle$ for the position and momentum variables in different modes. It will also be of interest to study the Weyl representation for para-Bose systems with one or more degrees of freedom.

## APPENDIX A: A MOMENT PROBLEM

In this Appendix we consider the moment problem

$$\int_0^\infty dx\, K(x,\alpha)x^{2n+1}=n!\Gamma(\alpha+n)/(2\pi\Gamma(\alpha)), \tag{A1}$$

and show that if we restrict $K(x,\alpha)$ to be positive, it has a unique solution. We further show that this leads to unique resolutions of the identity operator in the spaces of the representations $D_\beta$ [Eq. (2.23)] and $\mathscr{D}_\alpha$ [Eq. (2.61)] as long as the corresponding weight functions $F(\omega)$ or $F_1(z)\pm F_2(z)$ are restricted to be positive definite.

We set

$$x^2=t, \tag{A2}$$

$$\pi\Gamma(\alpha)K(x,\alpha)=\phi(t), \tag{A3}$$

and write Eq. (A1) in the form

$$\int_0^\infty \phi(t)t^n dt=n!\Gamma(\alpha+n). \tag{A4}$$

A solution of Eq. (A4) is given by

$$\phi(t)=2t^{(\alpha-1)/2}K_{\alpha-1}(2t^{1/2}), \tag{A5}$$

where $K_{\alpha-1}$ is the modified Bessel function of the second kind.[12]

Shohat and Tamarkin give a sufficient condition under which the moment problem

$$\int_0^\infty \varphi(t)t^n dt=\mu_n \tag{A6}$$

is determined [i.e., $\varphi(t)$ is unique as long as $\varphi(t)$ is restricted to be positive]. This condition is (Ref. 13, theorem 1.11, p. 20) that the series

$$\sum_{n=1}^{\infty}\mu_n^{-1/(2n)} \tag{A7}$$

is divergent. In the present case the moment problem (A4) is determined, i.e., has a unique positive definite solution (A5), if the series

$$\sum_{n=1}^{\infty}[n!\Gamma(\alpha+n)]^{-1/(2n)} \tag{A8}$$

is divergent. It is readily seen that the $n$th term of this series for large $n$ behaves as $n^{-1}$ and hence the series is in fact divergent. This establishes the required result.

Consider the resolution (2.23) of the identity operator in the space of the representation $D_\beta$:

$$\hat{1}_\beta=\int F(\omega)|\omega;\beta\rangle\langle\omega;\beta|d^2\omega. \tag{A9}$$

One may readily show using Eq. (2.19) and comparing Eq. (A9) with the relation

$$\sum_{n=0}^{\infty} |n;\beta\rangle\langle n;\beta| = \hat{1}_{\beta}). \tag{A10}$$

That $F(\omega)$ must be a function of $|\omega|$ only and that it must satisfy the moment condition

$$\int_0^{\infty} \beta\,[F(|\omega|)\{I_{2\beta-1}(2|\omega|)\}^{-1}|\omega|^{2\beta-1}]|\omega|^{2n+1}\,d|\omega| = \frac{n!\Gamma(\alpha+n)}{2\pi}. \tag{A11}$$

Since $I_{2\beta-1} > 0$ for $\beta > 0$, we conclude that as long as $F(\omega)$ is positive, it is given by

$$F(|\omega|) = \frac{2}{\pi} I_{2\beta-1}(2|\omega|)K_{2\beta-1}(2|\omega|). \tag{A12}$$

Finally, we consider the resolution of the identity operator in the space of the representation $\mathscr{D}_{\alpha}$:

$$\hat{1}_{\alpha} = \int \{F_1(z)|z\rangle\langle z| + F_2(z)|z\rangle\langle -z|\}d^2z. \tag{A13}$$

Again using Eq. (2.34) and comparing Eq. (A13) with the relation

$$\hat{1}_{\alpha} = \sum_{n=0}^{\infty} |n;\alpha\rangle\langle n;\alpha|, \tag{A14}$$

one may readily show that both $F_1 \pm F_2$ must be functions of $|z|^2$ only. This implies $F_1$ and $F_2$ must also separately be functions of $|z|^2$ only. Further, one finds that

$$\int_0^{\infty} \{F_1(|z|^2) + F_2(|z|^2)\}\{\mathscr{F}_{\alpha}(|z|^2)\}^{-1}|z|^{4n+1}d|z| = \pi^{-1}2^{2n+\alpha-2}n!\Gamma(n+\alpha) \tag{A15}$$

and

$$\int_0^{\infty} \{F_1(|z|^2) - F_2(|z|^2)\}\{\mathscr{F}_{\alpha}(|z|^2)\}^{-1}|z|^{4n+3}d|z| = \pi^{-1}2^{2n+\alpha-1}n!\Gamma(n+\alpha+1). \tag{A16}$$

Setting $|z|^2 = 2x$, Eqs. (A15) and (A16) may be written in the form

$$\int_0^{\infty} \{F_1(2x) + F_2(2x)\}\{x\mathscr{F}_{\alpha}(2x)\}^{-1}x^{2n+1}dx = \pi^{-1}2^{\alpha-2}n!\Gamma(n+\alpha), \tag{A17}$$

$$\int_0^{\infty} \{F_1(2x) - F_2(2x)\}\{\mathscr{F}_{\alpha}(2x)\}^{-1}x^{2n+1}dx = \pi^{-1}2^{\alpha-2}n!\Gamma(n+\alpha+1). \tag{A18}$$

Since $\mathscr{F}_{\alpha}(2x)$ is always positive for $\alpha > 0$, we conclude that as long as $F_1 \pm F_2$ are positive they are uniquely determined. The resolution of the identity operator (2.59) is unique under this restriction.

## APPENDIX B: PROOF OF THE INEQUALITY $I_{\alpha-1}(z) > I_{\alpha}(z)$

In this Appendix we show that for $\alpha \geqslant \frac{1}{2}$ and $z \geqslant 0$, we have the inequality

$$I_{\alpha-1}(z) > I_{\alpha}(z), \tag{B1}$$

where $I_{\alpha}(z)$ is the modified Bessel function

$$I_{\alpha}(z) = \left(\frac{z}{2}\right)^{\alpha} \sum_{n=0}^{\infty} \frac{(z/2)^{2n}}{n!\Gamma(n+\alpha+1)}. \tag{B2}$$

Define a function $f(z,\alpha)$ as

$$f(z,\alpha) = I_{\alpha-1}(z) - I_{\alpha}(z). \tag{B3}$$

From Eqs. (B2) and (B3) we find that

$$f(z,\alpha) = \sum_{n=0}^{\infty} \frac{(z/2)^{2n+\alpha-1}}{n!\Gamma(n+\alpha+1)}[n+\alpha-z/2]. \tag{B4}$$

Each term on the right-hand side of Eq. (B4) is positive for $\alpha > z/2$. Hence, it follows that

$$f(z,\alpha) > 0, \quad \text{for } 0 \leqslant z \leqslant 2\alpha. \tag{B5}$$

Further, for large values of $z$, we know the asymptotic nature of $I_{\alpha}(z)$:

$$I_{\alpha}(z) \sim (2\pi z)^{-1/2}e^{z}\left[1 - \frac{1}{2z}(\alpha^2 - \tfrac{1}{4})\right] \tag{B6}$$

so that

$$f(z,\alpha) \sim (8\pi z^3)^{-1/2}e^{z}(2\alpha - 1). \tag{B7}$$

Hence, it also follows that for some large and positive number $M$, and $2\alpha > 1$,

$$f(z,\alpha) > 0, \quad z > M. \tag{B8}$$

Further, we also know that $f(z,\alpha)$ is an analytic function of $z$ for $z > 0$. Hence, from Eqs. (B5) and (B8), it follows that if $f(z,\alpha)$ was negative for some $z$, such that $z\alpha < z < M$, then it must have a minimum at some point where its value is negative. Thus, $f(z,\alpha)$ can be negative for $2\alpha < z < M$ only if for some $z = z_0$, we have the following three conditions satisfied:

$$f(z_0,\alpha) < 0, \frac{d}{dz}f(z_0,\alpha) = 0, \text{ and } \frac{d^2}{dz^2}f(z_0,\alpha) > 0. \tag{B9}$$

Now $I_{\alpha}(z)$ satisfies the differential equation[12]

$$\left[z^2\frac{d^2}{dz^2} + z\frac{d}{dz} - (z^2+\alpha^2)\right]I_{\alpha}(z) = 0,$$

from which it follows that for all $z$,

$$z^2\frac{d^2}{dz^2}f(z,\alpha) + z\frac{d}{dz}f(z,\alpha) - (z^2+\alpha^2)f(z,\alpha) + (2\alpha-1)I_{\alpha-1}(z) = 0. \tag{B10}$$

Since[14] $I_{\alpha-1}(z) > 0$ for $z > 0$ and $\alpha > \frac{1}{2}$, Eq. (B10) at $z = z_0$ is obviously in contradiction with Eq. (B9). Hence, $f(z,\alpha)$ cannot take any negative value. This established the inequality (4.25) of the text, viz.,

$$I_{\alpha-1}(z) > I_{\alpha}(z), \quad z \geqslant 0, \alpha \geqslant \tfrac{1}{2}. \tag{B11}$$


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# Ermakov systems, velocity dependent potentials, and nonlinear superposition

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We derive new Ermakov systems with velocity-dependent potentials. The extended Ermakov system presented contains all known one-dimensional cases and many new systems. These Ermakov systems lead to a nonlinear superposition law for the solutions.

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## I. INTRODUCTION

In earlier work[1] we have applied Noether's theorem to the Lagrangian

$$L = \tfrac{1}{2}(\dot\rho^2 - \omega^2(t)\rho^2) + \sum_i G_i(t)F_i(\rho), \tag{1.1}$$

where $G_i$ and $F_i$ are initially arbitrary functions of their arguments. The following results are obtained by applying Noether's theorem to this Lagrangian:

$$G_i = G_{0i}x^{2m_i-2}, \tag{1.2}$$

$$F_i = F_{0i}\rho^{-2m_i}, \tag{1.3}$$

where $G_{0i}$, $F_{0i}$, and $m_i$ are arbitrary constants. Here $x$ is an auxiliary function, associated with the time part of the Noether symmetry transformation, and satisfying the equation

$$\ddot x + \omega^2(t)x = \kappa/x^3, \tag{1.4}$$

where $\kappa$ is an arbitrary constant. The equation of motion for $\rho$ takes the form

$$\ddot\rho + \omega^2(t)\rho = \sum_i c_i x/\rho^{2m_i-1}/(x\rho^2), \tag{1.5}$$

and the Noether invariant the form

$$I = \tfrac{1}{2}\left[(x\dot\rho - \rho\dot x)^2 + \kappa\left(\frac{\rho}{x}\right)^2 + \sum_i \frac{c_i}{m_i}\left(\frac{x}{\rho}\right)^{2m_i}\right], \tag{1.6}$$

where $c_i = -2m_iG_{0i}F_{0i}$. The invariant $I$ is constant if $\rho$ is any solution to (1.5) and $x$ is any solution to (1.4). For the details of the calculation we refer to Ref. 1. The idea for that calculation arose from the work of Lutzky[2] who obtained the above results for $c_i = 0$. These calculations represent an interesting application of Noether's theorem. For arbitrary $G_i$ and $F_i$ the Lagrangian (1.1) does not allow a Noether symmetry transformation. Noether's theorem applied to this Lagrangian forces $G_i$ and $F_i$ to have the above forms so that the Lagrangian will allow a Noether symmetry.

Previous to arriving at the above results we had introduced[3] more general Ermakov systems containing the above Ermakov systems as special cases. The equation of motion for these more general Ermakov systems has the form

$$\ddot\rho + \omega^2(t)\rho = f(x/\rho)/(\rho^2 x), \tag{1.7}$$

where $f$ is an arbitrary function. The auxiliary equation and invariant have the form

$$\ddot x + \omega^2(t)x = g(\rho/x)/(x^2\rho), \tag{1.8}$$

$$I = \tfrac{1}{2}(x\dot\rho - \rho\dot x)^2 + \int^{x/\rho} f(\eta)\,d\eta + \int^{\rho/x} g(\eta)\,d\eta, \tag{1.9}$$

where $g$ is also an arbitrary function. $I$ is constant if $\rho$ satisfies (1.7) and $x$ satisfies (1.8). We refer to (1.7) and (1.8) as an Ermakov pair of equations and to (1.9) as the Ermakov invariant associated with this pair. It is clear that the Ermakov system (1.5), (1.4), and (1.6) is a special case of the more general Ermakov system (1.7), (1.8), and (1.9).

An important property of Ermakov type systems such as (1.7), (1.8), and (1.9) is that they imply a general nonlinear superposition law relating the solutions to the Ermakov pair of equations. The nonlinear superposition law can be derived by using the new dependent variable $r = \rho/x$ and independent variable $d\tau = dt/x^2$. In terms of these quantities the invariant $I$ has the form

$$I = \tfrac{1}{2}r'^2 + v(r), \tag{1.10}$$

where the prime implies differentiation with respect to $\tau$ and $v(r)$ is defined by

$$v(r) = \int^r g(\eta)\,d\eta + \int^{1/r} f(\eta)\,d\eta. \tag{1.11}$$

For obvious reasons we refer to $I$ as the energy and $v(r)$ the potential energy of the Ermakov system. The energy integral (1.10) can be integrated to obtain

$$\tau + c = \frac{1}{\sqrt 2}\int \frac{dr}{(I - v(r))^{1/2}}, \tag{1.12}$$

where $c$ is an arbitrary constant of integration. Equation (1.12) is the key equation for the existence of a nonlinear superposition law for the Ermakov pair. Suppose we choose a particular solution to (1.8), say, $x$, then the general solution to the $\rho$ equation (1.7) can be written

$$\rho = xr\left(\int dt/x^2 + c, I\right), \tag{1.13}$$

where $r$ is obtained by solving (1.12). Equation (1.13) is the general solution to (1.7), the integration constants being $I$ and $c$. Thus, the nonlinear superposition law (1.13) gives the general solution to (1.7) in terms of a particular solution to (1.8). Examples of the use of this nonlinear superposition law can be found in Refs. 4 and 5 and an example of a more general nonlinear superposition law of the same general type is in Ref. 6. For the present purposes it is sufficient to note that the implicit nonlinear superposition law (1.13) can become explicit, that is, constructive for certain choices of $f$

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and $g$. It, therefore, represents a practical method of constructing solutions of the $\rho$ equation in terms of solutions to the $x$ equation. Also such nonlinear superposition laws have utility in numerical analysis, where the accurate determination of particular solutions yields the general solution through the nonlinear superposition law.[7]

The purpose of the present paper is to derive more general Ermakov systems involving velocity-dependent potentials and forces. We shall employ Noether's theorem to obtain new Ermakov systems and then generalize these systems in the same way that the more general Ermakov system (1.7), (1.8), and (1.9) can be obtained by generalizing the Noether theorem results (1.4), (1.5), and (1.6). In Sec. II we start from the Lagrangian

$$L = \tfrac{1}{2}(\dot\rho^2 - \omega^2(t)\rho^2) + P(\rho,\dot\rho,t), \tag{1.14}$$

containing a velocity-dependent potential and give the Noether theorem results for this Lagrangian. In Sec. III we generalize these results to more general Ermakov systems. In Sec. IV we discuss various examples of these more general Ermakov systems. Finally in Sec. V we shall give our conclusions along with suggestions for further work.

The inclusion of linear friction in Ermakov systems can be obtained by a change in the independent variable as explained in Ref. 4, hence, without loss of generality we can consider only the friction-free equations.

## II. NOETHER'S THEOREM INVARIANTS

The Lagrangian under investigation is the time-dependent harmonic oscillator with the velocity-dependent potential

$$L = \tfrac{1}{2}(\dot\rho^2 - \omega^2(t)\rho^2) + P(\rho,\dot\rho,t). \tag{2.1}$$

We use the formulation of Noether's theorem as given by Lutzky.[2] A symmetry transformation for a system is described by the group operator

$$X = \xi(\rho,t)(\partial/\partial t) + \eta(\rho,t)(\partial/\partial\rho). \tag{2.2}$$

If $X$ is a symmetry transformation then the following combination of terms must be a total time derivative of a function $f(\rho,t)$, i.e.,

$$\xi\frac{\partial L}{\partial t} + \eta\frac{\partial L}{\partial\rho} + (\dot\eta - \dot\rho\dot\xi)\frac{\partial L}{\partial\dot\rho} + \dot\xi L = \dot f. \tag{2.3}$$

If (2.3) is satisfied then the Noether invariant is

$$I = (\xi\dot\rho - \eta)\frac{\partial L}{\partial\dot\rho} - \xi L + f. \tag{2.4}$$

The details of the calculation involve solving Eq. (2.3), which is an identity in $\rho,\dot\rho$, for $\eta, f, \xi$, and $P$. Since the details of this type of calculation have been given in Ref. 1 and 2 we only give the results for the Lagrangian (2.1). In the following calculation we assume that $P$ is as general as possible subject to the requirement that Noether's theorem produces explicit invariants.

The terms proportional to $\dot\rho^3$ in (2.3) imply $\xi$ depends only on $t$. The $\dot\rho^2$ terms give $\eta$ as

$$\eta = \tfrac{1}{2}\dot\xi\rho + \psi(t), \tag{2.5}$$

where $\psi(t)$ is an arbitrary function of time.

The $\dot\rho$ terms then yield $f$

$$f = \tfrac{1}{2}\ddot\xi\rho^2 + \dot\psi\rho + \chi(t), \tag{2.6}$$

where $\chi$ is an arbitrary function of time. Here we have assumed $P(\rho,\dot\rho,t)$ is general enough so that the terms in (2.3) involving $P$ are not proportional to $\dot\rho, \dot\rho^2$, and $\dot\rho^3$. If this is not the case then the above results will be modified in a way that depends on the explicit form of $P$. The $\rho^2$ terms in (2.3) now yield the equation

$$\dddot\xi + 4\omega^2\dot\xi + 4\omega\dot\omega\xi = 0 \tag{2.7}$$

which can be integrated to the form

$$\ddot x + \omega^2(t)x = \kappa/x^3, \quad \xi = x^2, \tag{2.8}$$

where $\kappa$ is an arbitrary integration constant. The $\rho$ terms of (2.3) yield

$$\dot\psi + \omega^2(t)\psi = 0. \tag{2.9}$$

In obtaining these last two results (2.8) and (2.9) we have assumed that the terms involving $P$ in (2.3) do not contain terms proportional to $\rho$ and $\rho^2$. Next from (2.3) we obtain $\dot\chi = 0$ which implies that we may choose $\chi = 0$. Finally then (2.3) takes the form

$$\xi P_t + (\tfrac{1}{2}\dot\xi\rho + \psi)P_\rho + (\tfrac{1}{2}\ddot\xi\rho - \tfrac{1}{2}\dot\xi\dot\rho + \dot\psi)P_{\dot\rho} + \dot\xi P = 0. \tag{2.10}$$

From this point it is not possible to progress further in the solution without some restrictions on the form of the potential $P$, that is, the Lagrangian cannot allow a Noether symmetry for arbitrary $P$. This same type of result occured in Ref. 8, where the potential initially having the form $F(\rho,t)$ is forced by Noether's theorem to have the form $G(t)F(k(t)\rho)$, where the functions $G(t)$, $k(t)$ follow from Noether's theorem. For the present case Noether's theorem implies $P$ has the form

$$P = G(t)F(q(t)\rho, k(t)\rho + h(t)\dot\rho), \tag{2.11}$$

where $G, q, k$, and $h$ are to be determined. In the following we denote the derivative of $F$ with respect to its first argument as $F_1$ and the derivative with respect to its second argument as $F_2$. We now deduce the explicit forms for $G, q, k$, and $h$ from Noether's theorem. Using the form (2.11), Eq. (2.10) takes the form

$$\begin{aligned}&\xi(\dot GF + GF_1\dot q\rho + GF_2(\dot k\rho + \dot h\dot\rho) + (\tfrac{1}{2}\dot\xi\rho + \psi)\\ &\times(GF_1q + GF_2k) + (\tfrac{1}{2}\ddot\xi\rho - \tfrac{1}{2}\dot\xi\dot\rho + \dot\psi)GF_2h + \dot\xi GF = 0.\end{aligned} \tag{2.12}$$

Next the coefficients of $F, F_1, F_2, \rho F_1, \rho F_2$, and $\dot\rho F_2$ must separately vanish in order for $F$ to remain arbitrary. The $\dot\rho F_2$ terms yield

$$\xi\dot h - \tfrac{1}{2}\dot\xi h = 0 \tag{2.13a}$$

or

$$h = c_1x, \tag{2.13b}$$

where $\xi = x^2$ and $c_1$ is an arbitrary integration constant. The $\rho F_2$ terms yield

$$\xi\dot k + \tfrac{1}{2}\dot\xi k + \tfrac{1}{2}\ddot\xi h = 0, \tag{2.14a}$$

which integrates, after using (2.13b) to

$$k = c_2/x - c_1\dot x, \tag{2.14b}$$

where $c_2$ is another integration constant. The $\rho F_1$ terms yield

$$\xi\dot{q} + \tfrac{1}{2}\dot{\xi}q = 0, \tag{2.15a}$$

or

$$q = c_3/x, \tag{2.15b}$$

where $c_3$ is another integration constant. The $F_1$ terms yield

$$\psi = 0, \tag{2.16}$$

and the $F$ terms

$$G = 1/x^2. \tag{2.17}$$

Summarizing the results of the calculation we have obtained the function $P$ as

$$P = F(c_3\rho/x, c_2\rho/x + c_1(x\dot{\rho} - \rho\dot{x}))/x^2, \tag{2.18}$$

where $F$ is an arbitrary function of its arguments and the constants $c_1$, $c_2$, and $c_3$ are arbitrary constants. Since the function $F$ is an arbitrary function of its arguments we lose no generality in taking $c_3 = 1, c_2 = 0, c_1 = 1$ in which case $P$ has the form

$$P = F(\rho/x,\ x\dot{\rho} - \rho\dot{x})/x^2, \tag{2.19}$$

where $F$ is still an arbitrary function. The Lagrangian takes the form

$$L = \tfrac{1}{2}(\dot{\rho}^2 - \omega^2(t)\rho^2) + F(\rho/x,\ x\dot{\rho} - \rho\dot{x})/x^2. \tag{2.20}$$

For convenience in writing the formulas let

$$r = \rho/x, \tag{2.21}$$

$$W = x\dot{\rho} - \rho\dot{x}. \tag{2.22}$$

The utility of using these variables has been emphasized by Lutzky.[9] Here $r$ is the ratio variable that was introduced in our earlier discussion of nonlinear superposition and $W$ is defined the same as the Wronskian for linear equations. It is important to note, however, that $W$ is not constant in general. We note the following important relation between these two new variables:

$$x^2\frac{dr}{dt} = W, \tag{2.23}$$

and if we introduce the new independent variable $d\tau = dt/x^2$, we obtain

$$r' = \frac{dr}{dt} = W, \tag{2.24}$$

which was used in our earlier discussion of nonlinear superposition.

In terms of these new variables the results of this section can be summarized as follows: The velocity-dependent Lagrangian which allows a Noether symmetry has the form

$$L = \tfrac{1}{2}(\dot{\rho}^2 - \omega^2(t)\rho^2) + F(r,W)/x^2, \tag{2.25}$$

the equation of motion associated with this Lagrangian is

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{x^3}\frac{\partial F}{\partial r} + \frac{W}{x^3}\frac{\partial^2 F}{\partial W \partial r} + \frac{\dot{W}}{x}\frac{\partial^2 F}{\partial W^2} = 0, \tag{2.26}$$

where $x$ satisfies the auxiliary equation

$$\ddot{x} + \omega^2(t)x = \kappa/x^3 \tag{2.27}$$

and the Noether invariant is

$$I = \frac{1}{2}W^2 + \frac{1}{2}\kappa r^2 - F + W\frac{\partial F}{\partial W}. \tag{2.28}$$

Note that in the equation of motion (2.26) the term $\dot{W}$ contains $\ddot{\rho}$ and $\ddot{x}$ since

$$\dot{W} = x\ddot{\rho} - \rho\ddot{x}. \tag{2.29}$$

We could use this result to make the $\ddot{\rho}$ dependence explicit, however, we prefer to do this after we have derived the generalized Ermakov system in the next section.

In the special case $\partial F/\partial W = 0$ these results reduce to the Ermakov system

$$\ddot{\rho} + \omega^2(t)\rho = \frac{1}{x^3}\frac{\partial F}{\partial r} = \frac{1}{\rho^2 x}f\left(\frac{\rho}{x}\right), \tag{2.30}$$

$$\ddot{x} + \omega^2(t)x = \kappa/x^3 \tag{2.31}$$

which we have previously derived from Noether's theorem.[8]

As a final point in this section, we return to the idea of a nonlinear superposition law between the $\rho$ and $x$ equations (2.26) and (2.27). Using the new independent variable $d\tau = dt/x^2$ and (2.24) we obtain

$$I = \frac{1}{2}r'^2 + \frac{1}{2}\kappa r^2 - F(r,r') + r'\frac{\partial F}{\partial r'}, \tag{2.32}$$

which still leads to the nonlinear superposition law

$$\rho = xr\left(\int dt/x^2 + c, I\right), \tag{2.33}$$

if we can solve (2.32) for $r'$, integrate and then solve for $r = r(\int dt/x^2 + c, I)$. Even if this cannot be done explicitly it might still be useful for numerical solutions of the $\rho$ equation.[7] The fact that the nonlinear superposition law (2.33) can become explicit has been mentioned earlier and is discussed in Refs. 4, 5, and 6.

## III. ERMAKOV GENERALIZATIONS

In this section we discuss the equation of motion (2.26) derived in the last section

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{x^3}\frac{\partial F}{\partial r} + \frac{W}{x^3}\frac{\partial^2 F}{\partial r \partial W} + \frac{\dot{W}}{x}\frac{\partial^2 F}{\partial W^2} = 0, \tag{3.1}$$

where $x$ satisfies the auxiliary equation

$$\ddot{x} + \omega^2(t)x = \kappa/x^3. \tag{3.2}$$

Now in the Ermakov derivation of the invariant for (3.1) and (3.2) we eliminate $\omega^2(t)$ between these equations, multiply by $W$ and notice that the resulting equation implies that the quantity

$$I = \tfrac{1}{2}W^2 + \tfrac{1}{2}\kappa r^2 - F(r,W) + W\frac{\partial F}{\partial W} \tag{3.3}$$

is constant. After performing this latter calculation we are in a position to generalize these results by generalizing the auxiliary equation from (3.2) to

$$\ddot{x} + \omega^2(t)x - \frac{1}{\rho^3}\frac{\partial G}{\partial \bar{r}} + \frac{W}{\rho^3}\frac{\partial^2 G}{\partial \bar{r}\partial W} - \frac{\dot{W}}{\rho}\frac{\partial^2 G}{\partial W^2} = 0, \tag{3.4}$$

where $G = G(\bar{r}, W)$ is an arbitrary function and

$\tilde{r} = x/\rho = r^{-1}$. Elimination of $\omega^2(t)$ and multiplication by $W$ leads to the Ermakov invariant

$$I = \frac{1}{2}W^2 - F + W\frac{\partial F}{\partial W} - G + W\frac{\partial G}{\partial W} \tag{3.5}$$

for the pair (3.1) and (3.4). Equations (3.1), (3.4), and (3.5) represent an extended Ermakov system of a fairly general form.

As another genralization of the form of the extended Ermakov pair (3.1) and (3.4) we may replace the first terms in these equations by $m(W)\ddot{\rho}$ and $m(W)\ddot{x}$, where $m$ is an arbitrary function. The Ermakov invariant then takes the form of (3.5) except that the first term is replaced by

$$\int^{W} \eta m(\eta)\, d\eta. \tag{3.6}$$

The Ermakov invariant (3.5) corresponds to the choice $m = 1$. It is not yet clear whether or not this type of term can be introduced using Noether's theorem applied to a different Lagrangian than employed in this paper. The addition of the term $m(W)$ to the Ermakov system is also discussed in Ref. 6.

Through the change in independent variable $dt/x^2$ the invariant (3.5) is converted into a function of $r$, $r'$ and therefore we have the same implicit nonlinear superposition law connecting (3.1) and (3.4) as discussed in the previous section. This is still true if we add the function $m$ just discussed.

## IV. EXAMPLES

The extended Ermakov system (3.1), (3.4), and (3.5) contains all previous Ermakov systems as special cases and many new Ermakov systems. It is the first example of an Ermakov system with velocity-dependent forces except for the special case discussed in Ref. 6.

As a first example suppose neither $F$ or $G$ depend on $W$:

$$\frac{\partial F}{\partial W} = 0, \quad \frac{\partial G}{\partial W} = 0. \tag{4.1}$$

The Ermakov pair (3.1) and (3.4) then become

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{x^3}\frac{dF}{dr} = 0, \tag{4.2}$$

$$\ddot{x} + \omega^2(t)x - \frac{1}{\rho^3}\frac{dG}{d\tilde{r}} = 0, \tag{4.3}$$

which is just our original Ermakov system[3] if we define $f$ and $g$ as

$$\frac{1}{\rho^2}f(x/\rho) = \frac{1}{x^2}\frac{dF}{dr}, \tag{4.4}$$

$$\frac{1}{x^2}g(\rho/x) = \frac{1}{\rho^2}\frac{dG}{d\tilde{r}}. \tag{4.5}$$

As pointed out previously the Ermakov pair (3.1) and (3.4) contain $\ddot{\rho}$ and $\ddot{x}$ in the $\dot{W}$ terms. When this dependence is made explicit, the equations take on a different and sometimes startling form. For instance, if we assume that $F$ and $G$ depend only on $W$ then the Ermakov pair (3.1) and (3.4) become

$$\ddot{\rho} + \omega^2(t)\rho + \frac{\dot{W}}{x}\frac{d^2F}{dW^2} = 0, \tag{4.6}$$

$$\ddot{x} + \omega^2(t)x - \frac{\dot{W}}{\rho}\frac{d^2G}{dW^2} = 0. \tag{4.7}$$

Using (2.29) and solving the resulting equations for $\ddot{\rho}$ and $\ddot{x}$ one finds

$$\ddot{\rho} + \omega^2(t)\rho = 0, \tag{4.8}$$

$$\ddot{x} + \omega^2(t)x = 0, \tag{4.9}$$

that is, the Ermakov pair for (4.6) and (4.7) are equivalent to two uncoupled time-dependent harmonic oscillators. For this case $W = \text{const}$ and the $F$ and $G$ terms in the Ermakov invariant (3.5) are superfluous.

As another example we consider the partially coupled system

$$F = -r - W^2/2 + 1/(6W^2), \tag{4.10}$$

$$G = 0. \tag{4.11}$$

The Ermakov pair take the form

$$\ddot{\rho} + \omega^2(t)\rho + x^5\dot{r}^4 = 0, \tag{4.12}$$

$$\ddot{x} + \omega^2(t)x = 0, \tag{4.13}$$

and the Ermakov invariant is

$$I = r - 1/(2W^2). \tag{4.14}$$

If we use the new independent variable $d\tau = dt/x^2$ then (4.14) can be written

$$I = r - 1/(2r'^2). \tag{4.15}$$

Solving (4.15) for $r'$ and integrating we easily derive the nonlinear superposition law between (4.12) and (4.13)

$$\rho = x_1 I + 3^{2/3}(x_2 x_1^{\,1/2}/W_0 + c x_1^{\,3/2})^{2/3}/2, \tag{4.16}$$

where $x_1$ and $x_2$ are solutions to the linear auxiliary equation (4.13) with Wronskian $W_0$ and $\rho$ is the general solution to (4.12), $I$ and $c$ being the arbitrary integration constants. This same example was discussed in Ref. 6, where it arose by introducing the function $m(W)$ in the original Ermakov system (1.7), (1.8), and (1.9).

We shall let these examples serve to illustrate the extended Ermakov system (3.1), (3.4), and (3.5).

## V. CONCLUSIONS

In this paper we have started from the Lagrangian for the time-dependent harmonic oscillator with a velocity-dependent potential

$$L = \tfrac{1}{2}(\dot{\rho}^2 - \omega^2(t)\rho^2) + P(\rho\dot{\rho},t). \tag{5.1}$$

Applying Noether's theorem to this Lagrangian we determine the form of the function $P$ so that $L$ admits a Noether symmetry. The result we are led to is that $P$ has the form

$$P = F(\rho/x, x\dot{\rho} - \rho\dot{x})/x^2 = F(r,W)/x^2. \tag{5.2}$$

The resulting equations of motion and invariants, have a simpler form in terms of the variables $r$ and $W$, as emphasized by Lutzky.[9] The Ermakov equations of motion and invariant are

$$\ddot{\rho} + \omega^2(t)\rho - \frac{1}{x^3}\frac{\partial F}{\partial r} + \frac{W}{x^3}\frac{\partial^2 F}{\partial r \partial W} + \frac{\dot{W}}{x}\frac{\partial^2 F}{\partial W^2} = 0, \tag{5.3}$$

$$\ddot{x} + \omega^2(t)x = \kappa/x^3, \tag{5.4}$$

and

$$I = \frac{1}{2}W^2 + \frac{1}{2}\kappa r^2 - F + W\frac{\partial F}{\partial W}. \tag{5.5}$$

In this Noether's theorem approach to Ermakov systems the auxiliary equation (5.4) is uncoupled from the $\rho$ equation. This will always be true for Lagrangians of the type under investigation since Noether's theorem leads to

$$\frac{\partial \xi}{\partial \rho} = 0 = \frac{\partial x}{\partial \rho} = 0. \tag{5.6}$$

In Sec. III we found that the Ermakov type derivation of the invariant by elimination of $\omega^2$ between the pair leads to an immediate "symmetric" generalization of auxiliary equation from (5.4) to

$$\ddot{x} + \omega^2(t)x - \frac{1}{\rho^3}\frac{\partial G}{\partial \bar{r}} + \frac{W}{\rho^3}\frac{\partial^2 G}{\partial \bar{r}\partial W} - \frac{\dot{W}}{\rho}\frac{\partial^2 G}{\partial W^2} = 0. \tag{5.7}$$

The Ermakov invariant now becomes

$$I = \frac{1}{2}W^2 - (F+G) + W\frac{\partial}{\partial W}(F+G). \tag{5.8}$$

This extended Ermakov system (5.3), (5.7), and (5.8) contains all previous Ermakov systems as special cases and many new Ermakov systems. It is the first example of an Ermakov system with velocity-dependent forces except for the special case discussed in Ref. 6.

Apart from their intrinsic interest, Ermakov systems deserve study for two main reasons. The first is that the have proven useful in solving time-dependent quantum problems. As an example we mention Ref. 10 and the references contained therein. Here one finds the eigenfunctions of the quantum mechanical operator associated with Ermakov invariants used to construct the wave functions of the Schrödinger equation in exact closed form. Also one finds the Feynman propagator expressed in terms of the eigenfunctions of the Ermakov invariant. One key reason that Ermakov invariants are useful in describing quantum systems is that one of the pair of variables $\rho$, $x$ becomes a $q$-number while the other remains a $c$-number. The Ermakov invariant thus becomes an exact quantum mechanical invariant. Special cases of the Ermakov invariants discussed in this paper could prove useful in quantum treatment of physical systems. The second practical application of Ermakov systems is the existence of a nonlinear superposition law relating the solutions of the Ermakov pair. A key point in the nonlinear superposition law is the form the Ermakov invariant takes in terms of $r$ and $r'$. We are left, in principle, with only one integral to perform before the superposition law becomes explicit. We have presented a simple example of the use of the nonlinear superposition law for the extended Ermakov system in Sec. IV.

Although it may be "beyond our fondest dreams"[11] to hope for a nonlinear superposition law of universal validity, Ermakov systems represent an important subset of nonlinear equations for which one always has a nonlinear superposition law. In cases where this law becomes explicit it is of practical value and furnishes the general solution. As a final point we mention that nonlinear superposition laws obtain for Ermakov systems associated with systems of several degrees of freedom.[12,13]


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# Random walks and quantum currents in networks [a)]

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The free electron network model of a metal is reformulated in terms of restricted random walks; this allows direct calculation of the propagator. The reformulation gives more freedom in the choice of boundary conditions and is suitable for the investigation of topologically disordered networks.

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## INTRODUCTION

The quantum network model has had a long history (at least since 1936[1]) and has been revived periodically, mainly, in the opinion of the author, for the following three reasons: it is intuitive, versatile, and can be solved without perturbation theory. The network model was originally formulated for the investigation of conjugated molecules (see for example Platt[2]) and was extended to crystals by Coulson.[3] In the free electron model of a crystal the electron moves as a free particle along wires of a network which is fitted to the crystal lattice. Despite the apparent naivety of a model where wires represent bonds and nodes atoms the resulting spectrum compares favorably with those obtained from tight binding and linear combinations of atomic orbitals models.

The model can be made more realistic by putting potentials on the lines so that each node lies in the center of a well.[4,5] In addition to the investigation of bulk crystalline properties, the model has been used to investigate surface properties,[6] and localization in disordered systems.[7]

The present revival is a reformulation of the lattice network model in terms of restricted random walks. The network model is unusual in quantum mechanics because the system is multiply connected. In a multiply connected system there is no unique self-adjoint extension of the Hamiltonian.[8] The extension proposed by Griffeth,[9] explained in Sec. 1, is only one of many.

Dowker[10] describes how to do quantum mechanics systematically on a multiply connected space. Quantum mechanics is first considered on the covering space; mechanics on the base space is then described by summing over those points identified under the covering. To see just what points are identified by the covering requires a study of homotopic paths in the base space. This is explained in Sec. 2 by means of a simple example. This example will act as a model for the reformulation of the lattice network and occurs as a special case of the final result.

The reformulation of the lattice network model is explained in Sec. 3; the covering space of the network is identified as a Cayley tree. It is shown how to calculate the Green function for an electron on a Cayley tree. The Green function for an electron on the lattice is then given directly as a sum over restricted Polya walks, the distinct homotopic paths. The reformulation makes quantitative the critical role of the topology (which manifests itself in terms of closed loops) in the success of the network model (c.f. Budgor[11]).

The calculation of the number of restricted walks is described in Sec. 4. As an example of the calculation of a Green function, the average density of states per unit cell of the lattice network is calculated with the machinary developed. The modifications to the spectrum which a limited class of extensions of the boundary conditions allows, is examined.

The reformulation of the model is shown to be suitable for the investigation of topological disorder in Sec. 5. Previous authors[7] who use the network model to study localization in disordered systems consider a completely disordered network, and because Bloch's theorem is no longer available to them, resort to statistical arguments. They compare the motion of an electron with the trajectories of particles in a perfect gas and by neglecting closed circuits (the lattice forms a Cayley tree) derive a Boltzman equation for the system. By way of contrast, the present investigation calculates the exact Green function for a Cayley tree. The Green function for the lattice is found by summing this over all closed circuits.

### 1. The nonessential self-adjointness of the network model

The formulation of the quantum network model of a lattice[3] is as follows: Consider a lattice in which lattice sites are connected to nearest neighbors by wires (line segments) which represent bonds. (Pictorial representations will always depict the square lattice, Fig. 1.) An electron is allowed to move along the wires. Let $i \in I$ index the line segments each of which is considered a closed interval $0 \leqslant x_i \leqslant b_i$ of the real line. The Hilbert space for quantum mechanics is $\oplus_{i\in I} L^2(0,b_i)$. In the free electron model the wave functions $\psi_i$ on each segment satisfy the free particle Schrödinger

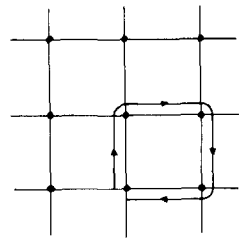

FIG. 1. Portion of a square lattice with a nontrivial loop indicated

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equation

$$H_i\psi_i = -\partial^2\psi_i/\partial x_i^2 = i\partial\psi_i/\partial t\,,$$

so that the Hamiltonian $H = \oplus_{i\in I} H_i$, where the domain

$$D(H_i) = \{\psi_i \in L^2(0,b_i): \partial^2\psi_i/\partial x_i^2 \in L^2(0,b_i)\}\,.$$

If $\{\phi_i\}_{i\in I}$ and $\{\psi_i\}_{i\in I}$ are two sets of wave functions in the domain of $H$, the Hamiltonian differs from being symmetric by

$$\sum_{i\in I}\left[-\phi_i^*\partial\psi_i/\partial x_i + \partial\phi_i^*/\partial x_i\psi_i\right]_0^{b_i}. \tag{1.2}$$

The Hamiltonian will be symmetric if the domain is further restricted to wave functions with zero boundary conditions. The Hamiltonian, however, is not self-adjoint as the domain of $H^*$ is larger than that of $H$ (there is no restriction on the boundary values). Any extension of the domain of $H$ which gives a self-adjoint operator is called a self-adjoint extension. If there is a unique self-adjoint extension the operator is said to be essentially self-adjoint.

The extension proposed by Griffeth[9] is the following:

(i) The wave function $\psi$ should be single valued and continuous at a node. For the next condition a slight change of notation is convenient. Let $p\in P$ label the sites and $0\leqslant x_{pq}\leqslant b_{pq}$ label a point on a line segment joining site $p$ to one of its nearest neighbors $q$.

(ii) With condition (i) satisfied the current will be conserved at each node $p$ if and only if

$$\sum_{n\cdot nq}\partial\psi_{pq}/\partial x_{pq}|_0 = 0\,,$$

where the sum is over all nearest neighbors $q$ to $p$.

(iii) For quantum mechanics on a lattice network, Coulson[3] supplements these two conditions by Bloch's theorem

$$\psi(\mathbf{r}+\mathbf{R}) = \exp(i\mathbf{k}\cdot\mathbf{R})\psi(\mathbf{r})\,,$$

where $\mathbf{R}$ is a lattice vector. (The notation has been changed again for the concise statement of this condition: $\psi$ is assumed defined over all Euclidian $d$ dimensional space, $\mathbf{r}\in R^d$, but takes only nonzero values on the line segments.)

An operator defined on a multiply connected space is not essentially self-adjoint.[8] A space $M$, is said to be simply connected if all loops (continuous paths with initial and final points the same) can be continuously deformed into one another.[12]

In particular, they can be deformed into the constant loop whose image is one point. If this cannot be done the space is said to be multiply connected. (As can be seen from Fig. 1, the loop depicted cannot be shrunk to a point without breaking it.) When a space is multiply connected there is the possibility of multivalued wave functions. The boundary conditions described above are thus not unique, in particular the first condition of Griffeth, and in fact it will be shown that there are countably infinitely many one-parameter extensions.

## 2. QUANTUM MECHANICS ON A BENZENE RING

To exemplify some of the statements in Sec. 1, quantum mechanics on the most elementary nonsimply connected network will be examined. This consists of a ring of wire (unit radius) with a single node on it. Other nodes can be added without affecting the arguments, and so this model could be considered to describe a benzene ring.

In a multiply connected space the classes of loops which can be deformed into one another are called homotopy classes. For the ring or circle, $S^1$, these correspond to classes of paths which wind around the circle continuously in one direction a specific number of times. It is intuitively clear that two loops which wind around the ring a different number of times cannot be deformed into one another.

In general two loops can be composed to give a third by traversing the first loop and then the second. It can be shown that this gives rise to a group structure in the homotopy classes called the fundamental group which is denoted $\pi_1(M)$. For the circle $\pi_1(S^1) = Z$, the additive integers, is just the winding number; it is clear that the composition of two loops results in the addition of the winding numbers. (Loops which wind around the circle anticlockwise correspond to, say, positive integers; those which wind around the circle clockwise correspond to negative integers; those which can be deformed into the constant loop correspond to zero.

The circle or one sphere $S^1$ is closely related to the real line $R$, locally they are indistinguishable. The relation is given by rolling the circle without slipping along the real line so that it prints out copies of itself. Analytically this relation is given by the projection $x\in R\to S^1\ni\exp(ix)$ so that points which are related by a $2\pi$ translation $x\to x+2\pi n$, $n\in Z$, are projected onto the same point in $S^1$. The circle can be thought of as the real line modulo $2\pi$; that is $S^1$ is the quotient of $R$ by the group $Z$, of translations by multiples of $2\pi$; this is denoted $S^1 = R/Z$. It is no coincidence that the translation group is isomorphic to fundamental group (there is one point in $R$ above each point in $S^1$ for each element of the fundamental group) so that $S^1 = R/\pi_1(S^1)$. The real line and the circle look locally the same, the difference between them is global; $R$ is simply connected so that $\pi_1(R) = 0$ consists of only the identity element. The real line is the universal covering space of the circle.

The above is true in general; for each multiply connected space $M$ there is a universal covering space $\widetilde{M}$ which is locally like $M$ but which is simply connected. For each point in $M$ there is one inverse image in $\widetilde{M}$ for each element of the fundamental group. The fundamental group $\pi_1(M)$ acts like a translation group on $\widetilde{M}$ and $\widetilde{M}/\pi_1(M) = M$. (Note in the example $\pi_1(M)$ is commutative, but this is not true in general.)

The systematic description of quantum mechanics on a multiply connected space is given in terms of quantum mechanics on its universal covering space.[10] Let $\psi(\tilde{x})$ be a wave function on $\widetilde{M}$. This will define a multivalued wave function on $M$ by $\psi(\gamma\tilde{x})$, $\gamma\in\pi_1(M)$. For physical reasons, since $\gamma\tilde{x}$ and $\tilde{x}$ describe the same point, $\psi(\gamma\tilde{x})$ must represent the same probability density:

$$\psi(\gamma\tilde{x}) = \exp(i\alpha(\gamma))\psi(\tilde{x}).$$

It is easy to see that the phase factors must form an abelian representation of $\pi_1(M)$. If $K_{\widetilde{M}}(\tilde{x},\tilde{x}';t)$ is the propagator on $\widetilde{M}$, the propagator on $M$ is given by

$$K_M(\tilde{x},\tilde{x}';t) = \sum_{\gamma\in\pi_1(M)} \exp(i\alpha(\gamma))K_M(\gamma\tilde{x},\tilde{x}';t)\,. \qquad (2.1)$$

Rather than finding the propagator on the circle, the prescription (2.1) will be used to find the Green function, the time-energy Fourier transform or the propagator. The prescription will be the same because the Fourier transform is linear. The Green function on the covering space $R$, the real line, of a free electron is

$$G_R(x,x';E) = -\tfrac{1}{2}(-E)^{-1/2}\exp(-(-E)^{1/2}|x-x'|)\,,$$

for $E>0$. (Positive energies are given by analytic continuation.)

Since the phase factors form a representation of $Z$, the group of integers, $\alpha(n)=\alpha n$, where $\alpha$ is an arbitrary real constant. Then

$$\begin{aligned} G_{S^1}(x,x';E) = {} & -\tfrac{1}{2}(-E)^{-1/2} - \tfrac{1}{2}(-E)^{-1/2}\sum_{n=1}^{\infty}\exp(i\alpha n) \\ & \times\exp\{-(-E)^{1/2}(2\pi n + |x-x'|)\} \\ & -\tfrac{1}{2}(-E)^{-1/2}\sum_{n=1}^{\infty}\exp(-i\alpha n) \\ & \times\exp\{-(-E)^{1/2}(2\pi n - |x-x'|)\} \end{aligned}$$

for $|x-x'|<2\pi$. It is written in this rather long way for later consideration so that it appears as a sum over nonhomotopic paths on the base space $S^1$. Every time the electron passes through the node in an anticlockwise[clockwise] direction it picks up a factor $\exp(i\alpha)$[$\exp(-i\alpha)$]. The spectrum of the system is given by the singularities of

$$\begin{aligned} G_{S^1}(x,x;E) = {} & -\tfrac{1}{2}(-E)^{-1/2}\sinh(2\pi(-E)^{1/2})/ \\ & \{\cosh(2\pi(-E)^{1/2}\} - \cos\alpha\}\,, \end{aligned}$$

which has poles at $\cos(2\pi E^{1/2}) = \cos\alpha$ for $E>0$.

The situation of quantum mechanics of a point particle on a unit circle is the same as a particle on a line segment of length $2\pi$. Symmetry of the Hamiltonian, $-\partial^2/\partial x^2$, requires that

$$\phi^*\partial\psi/\partial x|_0^{2\pi} - \partial\phi^*/\partial x\psi|_0^{2\pi} = 0$$

for two wave functions $\phi$ and $\psi$ in its domain. This will be true if the wave functions have zero boundary conditions, but the Hamiltonian is not then self-adjoint. If the wave functions satisfy the extended boundary conditions $\psi(x) = \exp(i\alpha)\psi(x+2\pi)$, where $\alpha$ corresponds to the parameter introduced above, the Hamiltonian will then be self-adjoint. The presence of the parameter affects the spectrum of the system. A physical interpretation of this is the Aharonov–Bohm effect,[8] where the splitting of degenerate states ($\alpha=0$) is due to a magnetic field.

## 3. REFORMULATION OF THE NETWORK MODEL

In order to incorporate some of the above freedom in the network model it will be formulated as a problem on a multiply connected space and evaluated as a sum over nonhomotopic paths. The covering space of the lattice network is obtained by eliminating all closed loops. Locally the lattice and its cover look the same. It is clear that the covering space of a lattice is an infinite or Cayley tree.

The propagator on a Cayley tree is obtained as follows.

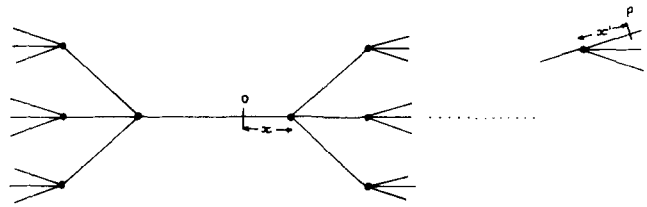


FIG. 2. Portions of the covering space of the square lattice in Fig. 1.

Suppose at time $t=0$ the electron can be located at a particular point $O$ on one of the line segments of the tree. The electron wave function on this line segment for time $t>0$ is the free particle propagator

$$\psi = (4\pi it)^{-1/2}\exp(iy^2/4t)\,,$$

where distance $y$ is measured from the initial point $O$. The electron diffuses outward from this initial point. At a node the wave function is required to vary continuously, but the current divides equally down the remaining $q-1$ branches ($q$ the number of nearest neighbors). The wave function $\psi$ and $(q-1)^{-1}\partial\psi/\partial x$ evaluated at the node act as initial conditions for the wave function in the next $q-1$ segments. These are Griffeth's boundary conditions but in this new situation the network, an infinite tree, is simply connected. The same procedure occurs at the next node and so on.

As with the example in Sec. 2, rather than deal with the propagator, the Green function will be calculated between two points $O$ and $P$ a distance $x$ and $x'$ from a node as indicated by Fig. 2. In the initial line segment the Green function is

$$-\tfrac{1}{2}(-E)^{-1/2}\exp(-(-E)^{1/2}|y|)\,.$$

(Again the energy is taken to be negative. Positive energies are obtained by analytic continuation.) In each segment the Green function satisfies

$$-\partial^2 G_i/\partial x_i = EG_i\,,$$

the general solution to which, written in what will prove to be a convenient form, is

$$(\exp(-\omega x_i),\exp(\omega x_i))\begin{pmatrix}A_i\\B_i\end{pmatrix},$$

where $\omega=(-E)^{1/2}$, $A_i$ and $B_i$ arbitrary constants. The boundary values of $G_i$, $(q-1)^{-1}\partial G_i/\partial x_i$ are initial conditions for the next segment. The relationship between coefficients in consecutive segments is given by

$$\begin{pmatrix}A_{i+1}\\B_{i+1}\end{pmatrix} = Z(b_i)\begin{pmatrix}A_i\\B_i\end{pmatrix},$$

where $b_i$ is the length of the segment and $Z(b)$ is the matrix

$$\tfrac{1}{2}(q-1)^{-1}\begin{pmatrix}q\exp(-\omega b) & (q-2)\exp(\omega b)\\ (q-2)\exp(-\omega b) & q\exp(\omega b)\end{pmatrix}.$$

Thus the Green function between two points $O$ and $P$ represented in Fig. 2 which are separated by $N$ nodes is given by

$$\begin{aligned} G_T(P,O;E) = {} & (\exp(-\omega x'),\exp(\omega x')) \\ & \times Z(b_{N-1})Z(b_{N-2})\ldots\ldots Z(b_1) \\ & \times Z(x)\begin{pmatrix}\tfrac{1}{2}\omega & \\ 0 & \end{pmatrix}^{-1} \end{aligned}$$

The fundamental group of a general network is the free group, one generator for each closed loop. The free group on $n$ generators is formed as follows. Take $n$ symbols $a_1,....,a_n$ called the alphabet, and supplement these with the symbols $a_1^-,a_2^-.....a_n^-$ and $e$. The set $S$ of words is formed by arranging any number of these $2n+1$ symbols in any order with repetition included. The composition of two words is given by juxtaposition. The inverse of a word is obtained by reversing the order of the symbols with the replacement $a_j \to a_j^-, e \to e$. An equivalence relation on the set of words is defined by

$$ee \sim a_j^- a_j \sim a_j a_j^- \sim e\,,$$

$$ea_j \sim a_j, ea_j^- \sim a_j^-\,.$$

The class of words form a group $F_n$, the free group on $n$ generators. For $n > 1$ the group is not commutative. If a finite network has $N$ nodes and $L$ line segments, the Euler Characteristic of the network $\chi$ is defined as $N - L$. The Euler Characteristic of a tree is 1 but in general $\chi < 1$. The fundamental group of a network is the free group on $1 - \chi$ generators. By building up a lattice from a finite network step by step, it is seen that the number of generators for the lattice network is infinite. The representation of the fundamental group of interest is abelian and so will also be a representation of $Z^Z$ (countable infinite product of the integers), the abelianised fundamental group. Thus the Hamiltonian on the lattice admits a countable infinity of one-parameter extensions.

The Green function on the lattice $G_L$ is given in terms of the Green function on the infinite tree by

$$G_L(x,x';E) = \sum_{\gamma \in \pi_1(L)} \exp(i\alpha(\gamma)) G_T(\gamma x, x';E)\,. \qquad (3.2)$$

Because of the complexity of the sum, it is difficult (if not impossible) to do in complete generality. To begin with the prescription for performing the sum for the identity representation, $\alpha(\gamma) = 0$ for all $\gamma$, will be given; some special nontrivial representations will be considered in the next section.

As with the example in Sec. 2, the sum will be over nonhomotopic paths between two given end points. In order to do the sum, the lattice will be divided into cells. A point on the lattice is associated with its nearest node. The points associated with each node constitute a cell. (Points on the cell boundary are equidistant from two nodes but these points only form a set of measure zero.) A point in a cell can then be labelled by a triple $\mathbf{l},\mathbf{X},x$, where $\mathbf{l}$ labels the node, $\mathbf{X}$ the direction of the bond on which the point lies, and $x$ the distance along the bond from the node (Fig. 3). The homotopic paths

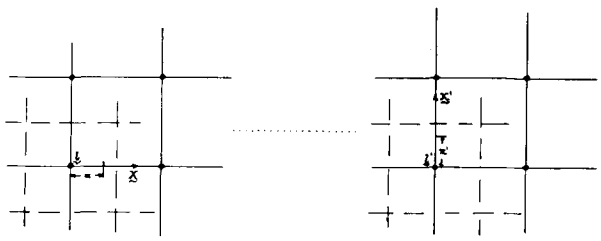

FIG. 3. Decomposition of the lattice into cells

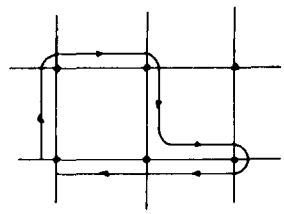

FIG. 4. The homotopic restriction imposed on Polya walks.

implied in the sum (3.2) can then be considered as Polya walks between two lattice cells $\mathbf{l}$ and $\mathbf{l}'$. The walks are not completely random but are restricted. A walk such as in Fig. 4 is not allowed because it is contractible. The homotopic representative of this walk is shown in Fig. 1. The walks are thus restricted in that immediate reversals are not allowed.

The contribution from a $n$-step walk will depend on the initial and final directions. Let $M^{\mathbf{L}}_{n\mathbf{F}}(\mathbf{l})$ be the number of restricted walks from the origin $\mathbf{O}$ to a site $\mathbf{l}$ with initial step in the $\mathbf{F}$ direction and final step in the $\mathbf{L}$ direction. (The directions $\mathbf{F}$ and $\mathbf{L}$ specify the position of nearest neighbor sites to the origin.) There will be four distinct contributions to the Green function which are tabulated in Table I. The contribution of the 0-step walk is $-\frac{1}{2}\omega^{-1}$.

## 4. RESTRICTED WALKS ON A LATTICE AND EXTENDED BOUNDARY CONDITIONS

To calculate the Green function in the identity representation, it remains to calculate the number of restricted walks on a lattice. The probability distribution of such walks was calculated by Domb and Fisher,[13] but for the sake of completeness a direct derivation of the number of restricted walks using the approach of Montroll will be given.

Consider a d dimensional regular lattice in which the lattice sites are labelled by integers $\mathbf{l} = (l_1,...,l_d)$, then

$$M^{\mathbf{L}}_{n+1\mathbf{F}}(\mathbf{l}) = \sum_{n.n\mathbf{X}\neq\mathbf{L}} M^{\mathbf{X}}_{n\mathbf{F}}(\mathbf{l}-\mathbf{L})\,, \qquad (4.1)$$

where the sum is over nearest neighbor sites (n.n). Defining

$$M_{n\mathbf{F}}(\mathbf{l}) = \sum_{n.n\mathbf{L}} M^{\mathbf{L}}_{n\mathbf{F}}(\mathbf{l})\,,$$

the number of walks starting at the origin (all directions) and finishing in a direction $\mathbf{F}$ at site $\mathbf{l}$, and iterating (4.1) gives:

$$M^{\mathbf{L}}_{n+1\mathbf{F}}(\mathbf{l}) = M_{n\mathbf{F}}(\mathbf{l}-\mathbf{L}) - M_{n-1\mathbf{F}}(\mathbf{l}) + M^{\mathbf{L}}_{n-1\mathbf{F}}(\mathbf{l})\,. \qquad (4.2)$$

Define the generating function

$$M^{\mathbf{L}}_{\mathbf{F}}(\mathbf{l},z) = \sum_{n=1}^{\infty} M^{\mathbf{L}}_{n\mathbf{F}}(\mathbf{l}) z^n$$

TABLE I. Breakdown of contributions to the Green function.

| L | F | Multiplicity | Contribution |
|---|---|---|---|
| $\neq \mathbf{X}$ | $\neq -\mathbf{X}'$ | $\sum_{n.n\mathbf{L}\neq} M^{\mathbf{L}}_{n\mathbf{F}}(l'-l)\Big]$ | $(\exp(-\omega x'),\exp(\omega x'))Z^{n}(b)Z(x)\begin{pmatrix}-\frac{1}{2}\omega^{-1}\\0\end{pmatrix}$ |
| $\neq \mathbf{X}$ | $-\mathbf{X}'$ | $\sum_{n.n\mathbf{F}\neq} M^{\mathbf{L}}_{n\mathbf{F}}(l'-l)$ | $(\exp(-\omega(b-x')),\exp(\omega(b-x')))Z^{n-1}(b)Z(x)\begin{pmatrix}-\frac{1}{2}\omega^{-1}\\0\end{pmatrix}$ |
| $\mathbf{X}$ | $\neq -\mathbf{X}'$ | $\sum_{n.n\mathbf{L}\neq -\mathbf{X}'} M^{\mathbf{L}}_{n\mathbf{F}}(l'-l)$ | $(\exp(-\omega x'),\exp(\omega x'))Z^{n-1}(b)Z(b-x)\begin{pmatrix}-\frac{1}{2}\omega^{-1}\\0\end{pmatrix}$ |
| $\mathbf{X}$ | $-\mathbf{X}'$ | $M_{n\,\mathbf{X}'\mathbf{X}}(l'-l)$ | $(\exp(-\omega(b-x')),\exp(\omega(b-x')))Z^{n-2}(b)Z(b-x)\begin{pmatrix}\frac{1}{2}\omega^{-1}\\0\end{pmatrix}$ |

by introducing a parameter $z$. Multiplying (4.2) by $z^{n+1}$ and summing from $n=2$ to infinity, the generating functions are related by

$$(1-z^2)M^{\mathbf{L}}_{\mathbf{F}}(\mathbf{l},z) = z^2M^{\mathbf{L}}_{2\mathbf{F}}(\mathbf{l}) + zM^{\mathbf{L}}_{1\mathbf{F}}(\mathbf{l}) + zM_{\mathbf{F}}(\mathbf{l}-\mathbf{L},z) - z^2M_{1\mathbf{F}}(\mathbf{l}-\mathbf{L}) - z^2M_{\mathbf{F}}(\mathbf{l},z)\,. \tag{4.3}$$

Define the Fourier transform

$$H^{\mathbf{L}}_{\mathbf{F}}(\boldsymbol{\phi},z) = \sum_{\text{all }\mathbf{l}} \exp(i\boldsymbol{\phi}.\mathbf{l})M^{\mathbf{L}}_{\mathbf{F}}(\boldsymbol{\phi},z)$$

and $H_{\mathbf{F}}(\boldsymbol{\phi},z)$ correspondingly, with the sum over all sites $\mathbf{l}$; this can be inverted

$$M^{\mathbf{L}}_{\mathbf{F}}(\mathbf{l},z) = (2\pi)^{-d}\int_{-\pi}^{\pi} d^{d}\phi\, H^{\mathbf{L}}_{\mathbf{F}}(\boldsymbol{\phi},z)\exp(-i\boldsymbol{\phi}.\mathbf{l})\,.$$

Multiplying (4.3) by $\exp(i\boldsymbol{\phi}.\mathbf{l})$ and summing over all $\mathbf{l}$ with $M^{\mathbf{L}}_{1\mathbf{F}}(\mathbf{l}) = \delta_{\mathbf{l},\mathbf{F}}\delta_{\mathbf{L},\mathbf{F}}$ and $M^{\mathbf{L}}_{2\mathbf{F}}(\mathbf{l}) = \delta_{\mathbf{l},\mathbf{L}+\mathbf{F}}(1-\delta_{\mathbf{F},-\mathbf{L}})$ gives

$$(1-z^2)H^{\mathbf{L}}_{\mathbf{F}}(\boldsymbol{\phi},z) = z\exp(i\boldsymbol{\phi}.\mathbf{F})\delta_{\mathbf{L},\mathbf{F}} - z^2\delta_{\mathbf{F},-\mathbf{L}} + (z\exp(i\boldsymbol{\phi}.\mathbf{L}) - z^2)\,H_{\mathbf{F}}(\boldsymbol{\phi},z)\,.$$

Summing $\mathbf{L}$ over nearest neighbors

$$H_{F}(\boldsymbol{\phi},z) = (z\exp(i\boldsymbol{\phi}.\mathbf{F}) - z^2)/(1 - z\lambda + (q-1)z^2)$$

with

$$\lambda = \sum_{\text{all }\mathbf{l}} M_{\mathbf{l}}(\mathbf{l})\exp(i\boldsymbol{\phi}.\mathbf{l}) = \sum_{n.n\mathbf{X}} \exp(i\boldsymbol{\phi}.\mathbf{X})$$

the characteristic function of the lattice. Substitution of this result finally gives

$$H^{\mathbf{L}}_{\mathbf{F}}(\boldsymbol{\phi},z) = (1-z^2)^{-1}\{z\exp(i\boldsymbol{\phi}.\mathbf{F})\delta_{\mathbf{L},\mathbf{F}} - z^2\delta_{\mathbf{F},-\mathbf{L}} + (z\exp(i\boldsymbol{\phi}.\mathbf{F}) - z^2)(z\exp(i\boldsymbol{\phi}.\mathbf{L}) - z^2)/(1 - z\lambda + (q-1)z^2)\}\,.$$

To calculate the Green function, Sec. 3, it is clear that what is required is the generating function of the walks $M^{\mathbf{L}}_{\mathbf{F}}(\mathbf{l},z)$ with $z$ replaced by the matrix $Z(b)$. The length of each bond will be taken to be the same. An example of such a calculation is the average density of states per unit cell:

$$\mathrm{Im}q^{-1}\pi^{-1}\sum_{n.n\mathbf{X}} \tfrac{1}{2}b^{-1}\int_{0}^{b/2} dx\, G_{L}(\mathbf{0},\mathbf{X},x;\mathbf{0},\mathbf{X},x;E^{+})\,,$$

which the above prescription gives as

$$-\mathrm{Im}\pi^{-1}(2\pi)^{-d}\int_{-\pi}^{\pi} d^{d}\phi\,\{\sinh((\omega b)/\omega q\cosh(\omega b) - \lambda) - (q-2)/2\omega\sinh(\omega b) + (q-2)/2qb\omega^2\} \tag{4.4}$$

with $\omega = (-E^{+})^{1/2}$. Only the first term of the integrand has a nonzero imaginary part and since $|\lambda| \leqslant q$ the cut is along the positive real axis and the density of states per unit cell is

$$-(2\pi)^{-d}\omega^{-1}\sinh(\omega b)\int_{-\pi}^{\pi} d^{d}\phi\,\delta(q\cosh(\omega b) - \lambda)\,.$$

The condition $q\cos(E^{1/2}b) = \lambda$ is the genalization of the dispersion relation given by Coulson[3] for specific examples. In the special case of a linear chain, $d=1$, $q=2$ and $M_{\mathbf{l}}(l) = \delta_{l,1} + \delta_{l,-1}$ the density of states reduces to that of a free particle: $\frac{1}{2}E^{-1/2}, E>0$.

The general expression (4.4) even applies to the example of a circle (Sec. 2) with $q=2$, and $M_{\mathbf{l}}(\mathbf{l}) = 2\delta_{\mathbf{l},0}$ any dimension. The extended boundary conditions for the circle can be achieved by replacing $M_{\mathbf{l}}(\mathbf{l})$ by $\exp(i\alpha)\delta_{\mathbf{l},0} + \exp(-i\alpha)\delta_{\mathbf{l},0}$ ($\lambda = 2$ is replaced by $\cos\alpha$). $M_{n}(\mathbf{l})$ is then not the restricted number of walks, but a sum of phase factors picked up at each bond on a restricted walk. This suggests the following generalization to the lattice network. Associate with each nearest neighbor bond $\mathbf{X}$ a phase $\alpha_{\mathbf{X}}$. Bonds in opposite directions are given phases of opposite sign $\alpha_{-\mathbf{X}} = -\alpha_{\mathbf{X}}$. The summation of phase factors then goes through as for the number of restricted walks above, but with the result that $\lambda$ is replaced by $\Sigma_{n.n\mathbf{X}}\exp(i\boldsymbol{\phi}.\mathbf{X})\exp(i\alpha_{\mathbf{X}})$, which is real.

For the simple cubic lattice $\lambda$ becomes $2\Sigma_{i=1}^{3}\cos(\phi_i + \alpha_i)$, but the phases $\alpha_i$ can be removed by a change of origin in the $\phi$ integration. However, for the body-centered cubic lattice three of the phases can be eliminated by a choice of origin

$$\lambda = 4\cos(\phi_1+\phi_2)\cos\phi_3 + 4\cos(\phi_1-\phi_2)\cos(\phi_3+\alpha),$$

leaving one arbitrary phase. Similarly for a face-centered cubic lattice three phases may be eliminated leaving three arbitrary phases. These correspond to more general boundary conditions than those proposed by Griffeth[9] but as is clear

from Sec. 3 they are far from being the most general. The increased freedom could perhaps represent a physical situation in which interstitial sites possess a magnetic moment.

## 5. APPLICATION TO TOPOLOGICALLY DISORDERED NETWORKS

In his conclusion Coulson[3] attributes the similarity between the network model and other models to the large extent which the geometry plays in determining the spectrum. Budgor[11] attributes the similarity to the homological structure of the network model. The present formulation in terms of restricted random walks derives the spectrum directly from the homotopic structure.

The expression for the density of states (4.4)

$$-\operatorname{Im}\pi^{-1}(2\pi)^{-d}\int_{-\pi}^{\pi} d^{d}\phi\omega^{-1}\sinh(\omega b)/(q\cosh(\omega b)-\lambda)$$

can be rewritten

$$-\operatorname{Im}\pi^{-1}q^{-1}\omega^{-1}\tanh(\omega b)\sum_{n=0}^{\infty}(q\cosh(\omega b))^{-n}N_n(0),$$

where $N_n(0)=(2\pi)^{-d}\int_{-\pi}^{\pi}d^{d}\phi\lambda^{n}$ (5.1)

is the number of unrestricted returning Polya walks on a lattice. This form may be compared with the density of states in a tight binding model with overlap $V$.

$$\operatorname{Im}\pi^{-1}\sum_{n=0}^{\infty}\{V/(E-E_0)\}^{n}N_n(0),$$

where $E_0$ determines the center of the band. This leads to the direct comparison $V\leftrightarrow -2/qb^{2}$ as noted by Coulson.[3]

The above argument shows that the only lattice dependence of the spectrum is now on the number of unrestricted returning Polya walks. Even if a nonregular lattice is chosen, such as graphite,[3] using a method similar to Thorpe,[14] block diagonalizing the connectivity matrix, the number of returning walks on a graphite layer can be found from the eigenvalues of the reduced matrix

$$\begin{pmatrix}0 & \theta\\ \theta^{*} & 0\end{pmatrix}\quad\text{where}\quad\theta=1+2\cos(\phi_1)\exp(i\phi_2).$$

A rotation of the $\phi$ coordinates puts the number of returning walks in the form

$$N_{2n}(0)=(2\pi)^{-2}\int_{-\pi}^{\pi}d^{2}\phi\,(3+2\cos\phi_1+2\cos\phi_2+2\cos(\phi_1-\phi_2))^{n},$$

$$N_{2n+1}(0)=0.$$

Substituting this into the expression (5.1) gives the density of states obtained by Coulson.[3]

In a paper by Ringwood[15] it was argued that the asymptotic form of the number of returning walks for any three-dimensional network is

$$N_n(0)=q^{n}(An^{-3/2}+B(-g)^{n}f(n)),$$

where $A$, $B$ and $g$ are positive constants

$$0.22\leqslant g\leqslant 1;\quad n^{-1/2}\leqslant f(n)\leqslant n^{-3/2}\quad n\to\infty.$$

The density of states produced by the asymptotic form of the number of returning walks

$$-\operatorname{Im}\pi^{-1}q^{-1}\omega^{-1}\tanh(\omega b)\times\lim_{N\to\infty}\sum_{N=n}^{\infty}(\cosh(\omega b))^{-n}(An^{-3/2}+B(-g)^{n}n^{-\nu})$$

gives the position and the behavior of the band edges. The function $f(n)$ has been chosen for simplicity to be $n^{-\nu}$. More complicated functions can, however, be handled.[16] Using an integral transform and summing the geometric series in its domain of convergence, the asymptotic form of the density of states is the discontinuity across the cut of

$$-\pi^{-1}q^{-1}\omega^{-1}\tanh(\omega b)\lim_{N\to\infty}(\operatorname{ch}(\omega b))^{-N}\times\int_{1}^{\infty}dy\{A(\ln y)^{1/2}/\Gamma(3/2)y^{N}(y-\operatorname{sech}(\omega b))+B(\ln y)^{\nu-1}/\Gamma(\nu)y^{N}(y+g\operatorname{sech}(\omega b))\}.$$

This function has a sequence of overlapping cuts on the positive real $E$ axis. The asymptotic density of states is

$$\tan(\sqrt{E}\,b)\{\sigma(\sec(\sqrt{E}\,b)-1)A\times\ln^{1/2}(\sec(\sqrt{E}\,b)/\Gamma(3/2)+\sigma(-g\sec(\sqrt{E}\,b)-1)B\times\ln^{\nu-1}(g\sec(\sqrt{E}\,b)/\Gamma(\nu)\}/q\sqrt{E},$$

where $\sigma$ is the Heaviside function.

Topological disorder can only affect the parameter $g$ and function $f(n)$ (a completely random walk takes the lower limits) and so gaps cannot be created in the network model by topological disorder. This finding can be contrasted with the result for the Weaire model.[15]


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# On the WKB approximation to the propagator for arbitrary Hamiltonians

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This paper presents a general expression for the WKB approximation to the propagator corresponding to an arbitrary Hamiltonian operator **H**. For example, if the correspondence rule used to pass from the classical Hamiltonian $H_c$ to **H** is such that it associates $a\mathbf{P}_i\mathbf{Q}^j + (1-a)\mathbf{Q}^j\mathbf{P}_i$ to $p_iq^j$, then the formula gives

$$K_{\mathrm{WKB}} = K_{\mathrm{VV}} \exp\left\{(\tfrac{1}{2}-a)\int_T (\partial^2 H_c/\partial q^i \partial p_i)(q_c(t),p_c(t),t)\,dt\right\},$$

where $K_{\mathrm{VV}} \equiv (2\pi i\hbar)^{-n/2}(\det M)^{1/2}\exp(iS_c/\hbar)$ is Van Vleck's well-known formula, $S_c$ being the action functional evaluated at the classical path $(q_c,p_c)$ and $M_{ij} \equiv -\partial^2 S_c/\partial q_a{}^i \partial q_b{}^j$. More generally, the formula presented here applies to any system with $n$ degrees of freedom described by a function $f(x,t)$ whose time evolution is given by $(\mathbf{H}(x,k\partial/\partial x,t) + k\partial/\partial t)f(x,t) = 0$, regardless of the form of **H**. The Schrödinger equation of quantum mechanics and the Fokker–Planck equation of diffusion are obvious examples. Many examples are discussed. This generalizes results obtained in a previous publication [J. Math. Phys. **18**, 786–90 (1977)].

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## I. INTRODUCTION

The propose of this paper is to obtain a general expression for the WKB approximation to the propagator corresponding to an arbitrary Hamiltonian operator. In an earlier publication[1] we determined a range of validity of Van Vleck's well-known formula,[2] which was known not to be universally valid.[3] The approximation derived here, generalizing Van Vleck's formula, is also valid beyond quantum-mechanical applications, as it applies to any system described by a function $f(x,t)$ whose time evolution is dictated by

$$[\mathbf{H}(x,k\partial/\partial x,t) + k\partial/\partial t]f(x,t) = 0, \tag{1}$$

such as the Fokker–Planck equation for diffusion processes.

## II. THE GENERAL WKB APPROXIMATION FORMULAS

We operate in $n$ dimensions and summation over repeated indices is implied. The following theorem summarizes our findings:

*Theorem*: Let

(i) $\mathbf{H}(\mathbf{Q},\mathbf{P},t)$ be an arbitrary Hamiltonian operator (the lack of constraints imply that it could be non-Hermitian, time-dependent, nonquadratic in **P**, etc.).

(ii) $H_c(q,p,t) \equiv \mathbf{H}(\mathbf{Q}\to q, \mathbf{P}\to p, \hbar = 0)$ be its classical counterpart.

(iii) The correspondence rule used to pass from $H_c$ to **H** be such that it makes the following associations:

$$f(q)\longleftrightarrow f(\mathbf{Q}),\quad f(p)\longleftrightarrow f(\mathbf{P}), \tag{2}$$

$$p_iq^j \longleftrightarrow a\mathbf{P}_i\mathbf{Q}^j + (1-a)\mathbf{Q}^j\mathbf{P}_i \text{ for a given } a. \tag{3}$$

[Note that (2) and (3) do not imply Hermiticity of **H**, even if $a = \frac{1}{2}$].

(iv) $[q_c(t),p_c(t)]$ be the classical solution, solving Hamilton's equations for $H_c$ such that $q_c(t_a) = q_a$ and $q_c(t_b) = q_b$,

(v) $S_c(q_b,t_b,q_a,t_a)$

$$\equiv \int_T [p_{ci}(t)\dot{q}_c^i(t) - H_c(q_c(t),p_c(t),t)]\,dt \tag{4}$$

be the classical action ($T \equiv [t_a,t_b]$, also $T \equiv t_b - t_a$).

(vi) $M_{ij}(q_b,t_b,q_a,t_a) \equiv -\partial^2 S_c/\partial q_a^i \partial q_b^j$ (5)

be the Van Vleck–Morette matrix, with determinant $\det M$.

(vii) $K(q_b,t_b,q_a,t_a)$ be the propagator corresponding to **H**, defined by

$$\left[\mathbf{H}(\mathbf{Q},\mathbf{P},t_b) - i\hbar\frac{\partial}{\partial t_b}\right]K = 0, \tag{6}$$

$$\lim_{t_b\to t_a} K = \delta(q_b - q_a), \tag{7}$$

where **Q** is represented by $q_b$ and **P** by $-i\hbar\partial/\partial q_b$.

(viii) $K_{\mathrm{WKB}}(q_b,t_b,q_a,t_a)$ be the WKB approximation to the propagator, defined by:

$$K_{\mathrm{WKB}}^{-1}[\mathbf{H}(\mathbf{Q},\mathbf{P},t_b) - i\hbar\partial/\partial t_b]K_{\mathrm{WKB}} = O(\hbar^2), \tag{8}$$

$$\lim_{t_b\to t_a} K_{\mathrm{WKB}} = \delta(q_b - q_a). \tag{9}$$

Then the WKB approximation is given by

$$W_{\mathrm{WKB}} = K_{\mathrm{VV}} \exp\left[(\tfrac{1}{2}-a)\int_{t_a}^{t_b} \frac{\partial^2 H_c}{\partial q^i \partial p_i}(q_c(t),p_c(t),t)\,dt\right], \tag{10}$$

where $K_{\mathrm{VV}}$ is Van Vleck's formula:

$$K_{\mathrm{VV}} = (2\pi i\hbar)^{-n/2}(\det M)^{1/2}\exp(iS_c/\hbar). \tag{11}$$

(The case where $\det M = 0$ is not examined here).

*More generally*, the WKB approximation is given by

$$K_{\mathrm{WKB}} = A_0 \exp(iS_c/\hbar), \tag{12}$$

where

(i) $A_0 \equiv K_0(0,t_b,0,t_a)$, (13)

(ii) $K_0(q_b',t_b,q_a',t_a)$ is the propagator corresponding to

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the Hamiltonian operator

$$\mathbf{H}_0 \equiv \tfrac{1}{2} g^{ij}(t)\mathbf{U}_{ij} + \tfrac{1}{2} f_{ij}(t)\mathbf{V}^{ij} + k_i{}^j(t)\mathbf{W}^i{}_j, \tag{14}$$

(iii)

$$g^{ij}(t) \equiv \frac{\partial^2 H_c}{\partial p_i \partial p_j}\bigg|_{\substack{q=q_c(t)\\ p=p_c(t)}}, \quad f_{ij}(t) \equiv \frac{\partial^2 H_c}{\partial q^i \partial q^j}\bigg|_{\substack{q=q_c(t)\\ p=p_c(t)}},$$

$$k_i{}^j(t) \equiv \frac{\partial^2 H_c}{\partial q^i \partial p_j}\bigg|_{\substack{q=q_c(t)\\ p=p_c(t)}}, \tag{15}$$

(iv) The correspondence rule used to pass from $H_c$ to $\mathbf{H}$ is such that it makes the following associations:

$$p_i p_j \longleftrightarrow \mathbf{U}_{ij}, \quad q^i q^j \longleftrightarrow \mathbf{V}^{ij}, \quad q^i p_j \longleftrightarrow \mathbf{W}^i{}_j. \tag{16}$$

## III. PROOF OF THE GENERAL WKB APPROXIMATION FORMULAS

Let us begin by giving a simple example illustrating the fact that the Van Vleck formula $K_{\mathrm{VV}}$ in (11) is not always equal to the WKB approximation $K_{\mathrm{WKB}}$. Let $\mathbf{H}$ be an operator such that $K_{\mathrm{VV}} = K_{\mathrm{WKB}}$. The operator

$$\mathbf{H}' \equiv F^{-1}(\mathbf{Q})\mathbf{H}F(\mathbf{Q}) \tag{17}$$

has the same $H_c$ (and hence the same $K_{\mathrm{VV}}$) as $\mathbf{H}$. Yet its WKB approximation is not $K_{\mathrm{VV}}$ but

$$K'_{\mathrm{WKB}} = F(q_a)F^{-1}(q_b)K_{\mathrm{VV}}, \tag{17a}$$

as can be verified by direct substitution.

We now prove the theorem. Formula (10) will be proved by generalizing the proof given in Ref. 1. The more general formula (12) will be proved by generalizing the method used in Ref. 4, which involves path integrals. It is presented separately because it is more on the heuristic side.

*Proof of first formula*: In Ref. 1, where we investigated the range of validity of Van Vleck's formula, we assumed that the WKB approximation was of the form:

$$K_{\mathrm{WKB}} = a(\hbar)C\exp(iB/\hbar), \tag{18}$$

where $C$ and $B$ are real functions of $q_b$, $t_b$, $q_a$, and $t_a$, independent of $\hbar$, and found that

$$\begin{aligned}
K_{\mathrm{WKB}}^{-1}\left(\mathbf{H} - i\hbar\frac{\partial}{\partial t_b}\right)K_{\mathrm{WKB}} &= \dot{B} + F(0)H_c(B',q_b,t_b) + \hbar\left[-i\frac{\dot{C}}{C} - \left(\frac{\partial^2}{\partial p_i \partial q_b^i}H_c(p,q_b,t_b)\right)_{p=B'}\left(F'(0) + \frac{i}{2}F(0)\right)\right.\\
&- \frac{iF(0)C_i'}{C}\left(\frac{\partial H_c}{\partial p_i}(p,q_b,t_b)\right)_{p=B'} - i\frac{F(0)}{2}B''_{ij}\left(\frac{\partial^2 H_c}{\partial p_i \partial p_j}(p,q_b,t_b)\right)_{p=B'}\Bigg] + \hbar^2\left\{\left[-\tfrac{1}{8}F(0)\frac{\partial^2}{\partial q_b^i \partial q_b^j}\right.\right.\\
&- F(0)\frac{C_i'}{2C}\frac{\partial}{\partial q_b^j} - F(0)\frac{C''_{ij}}{2C} - \tfrac{1}{4}F(0)B''_{ij}\frac{\partial^2}{\partial p_k \partial q_b^k} - F(0)\frac{C_k'}{2C}B''_{ij}\frac{\partial}{\partial p_k} - \tfrac{1}{8}F(0)B''_{ij}B''_{ks}\frac{\partial^2}{\partial p_k \partial p_s}\\
&- \tfrac{1}{6}F(0)B'''_{ijk}\frac{\partial}{\partial p_k} + \frac{i}{2}F'(0)\frac{\partial^2}{\partial q_b^i \partial q_b^j} + iF'(0)\frac{C_i'}{C}\frac{\partial}{\partial q_b^j} + \frac{i}{2}F'(0)B''_{ij}\frac{\partial^2}{\partial p_k \partial q_b^k} + \tfrac{1}{2}F''(0)\frac{\partial^2}{\partial q_b^i \partial q_b^j}\Bigg]\\
&\left.\times\frac{\partial^2}{\partial p_i \partial p_j}H_c(p,q_b,t_b)\right\}_{p=B'} + O(\hbar^3),
\end{aligned} \tag{19}$$

where $B''_{ij} \equiv \partial^2 B/\partial q_b^i \partial q_b^j$, etc., and $F$ is Cohen's $F$ function,[5] establishing the correspondence between $\mathbf{H}$ and $H_c$ by

$$\mathbf{H} = (2\pi\hbar)^{-2n}\int_{\mathbf{R}^{4n}} dp\,dq\,du\,dv\,F(u,v)H_c(q,p,t)\exp\{(i/\hbar)[(q-\mathbf{Q})\cdot u + (p-\mathbf{P})\cdot v]\}. \tag{20}$$

$F$ effects the generating-function correspondence

$$F(u,v)\exp[(-i/\hbar)(\mathbf{Q}u + \mathbf{P}v)] \longleftrightarrow \exp[(-i/\hbar)(qu+pv)], \tag{21}$$

and a set of $F$'s effecting a given correspondence $H_c \longleftrightarrow \mathbf{H}$ can be found by solving[6]

$$F(u,v)\int_{\mathbf{R}^{2n}} dp\,dq\,H_c(q,p,t)e^{i(qu+pv)/\hbar} = (2\pi\hbar)^n \mathrm{tr}(e^{i(\mathbf{Q}u+\mathbf{P}v)/\hbar}\mathbf{H}). \tag{22}$$

This equation for $F$, to be understood in the sense of distribution theory, may or may not have a solution, and the solution may or may not be unique if it exists.

In Ref. 1, $F$ was assumed to be a function of $u\cdot v/\hbar$ only, and this requirement is maintained here, as $u\cdot v/\hbar$ is the only dimensionless quantity one can form with $u$, $v$, and $\hbar$, and it is assumed here that $\mathbf{H}$ contains no constants (other than $\hbar$) that do not appear in $H_c$. It can be shown[7] that the fact $F$ depends on the combination $u\cdot v/\hbar$ implies that the operator $\mathbf{H}$ corresponding to $p^m q^n$ in one dimension is a linear combination of all the possible ordered arrangements of $\mathbf{P}$ $m$ times and $\mathbf{Q}$ $n$ times (true "factor ordering"). Thus, no true divisors are allowed in Cohen's scheme,[8] an important restriction since the Laplacian in curved spaces contains true divisors. We shall return to this point later.

In Ref. 1, $F$ was also assumed to be real[9] so as to insure the Hermiticity of $\mathbf{H}$. This requirement is dropped here. Therefore, equating both the real and the imaginary parts of the constant term and the term proportional to $\hbar$ to 0 in (19) yields the following four equations to be satisfied by $B$ and $C$:

$$H_c\left(q_b, \frac{\partial B}{\partial q_b}, t_b\right)\mathrm{Re}[F(0)] + \frac{\partial B}{\partial t_b} = 0, \tag{23}$$

$$H_c\left(q_b, \frac{\partial B}{\partial q_b}, t_b\right)\mathrm{Im}[F(0)] = 0, \tag{24}$$

$$\mathrm{Re}[F(0)]\frac{\partial}{\partial q_b^{\,j}}\left[C^2\frac{\partial H_c}{\partial p_j}(q_b,p,t_b)\Big|_{p=\partial B/\partial q_b}\right]$$
$$+\frac{\partial}{\partial t_b}(C^2)+2C^2\frac{\partial^2 H_c}{\partial p_i\partial q^i}(q,p,t_b)\Big|_{\substack{p=\partial B/\partial q_b\\ q=q_b}}\mathrm{Im}[F'(0)]=0, \tag{25}$$

$$\{\mathrm{Re}[F'(0)]-\tfrac{1}{2}\mathrm{Im}[F(0)]\}\left[\frac{\partial^2}{\partial p_i\partial q^i}H_c(q,p,t_b)\Big|_{\substack{p=\partial B/\partial q_b\\ q=q_b}}\right]$$
$$+\mathrm{Im}[F(0)]\left[\frac{C_i'}{C}\frac{\partial H_c}{\partial p_i}(q_b,p,t_b)+\tfrac{1}{2}B_{ij}''\frac{\partial^2 H_c}{\partial p_i\partial p_j}\right]_{p=\partial B/\partial q_b}=0, \tag{26}$$

where the third equation was rewritten in a more compact form.

First, let us translate the conditions (2) and (3) on **H** into conditions on $F$. These are:

$$F(0)=1,\quad \mathrm{Re}[F'(0)]=0,\quad \mathrm{Im}[F'(0)]=a-\tfrac{1}{2}. \tag{27}$$

[Indeed, (2) readily results from (21) with $F(0)=1$. If we differentiate (21) with respect to $v$, then set $v=0$, then do the same with $u$, we obtain

$$pq\longleftrightarrow F(0)(\mathbf{QP}+\mathbf{PQ})/2-\hbar F'(0), \tag{28}$$

which yields the two conditions on $F'(0)$.]

It is, in fact, possible to drop the requirement that the correspondence be given by an $F$ function, so that the results are valid for any **H** satisfying (2) and (3). This will be seen when we treat the more general formula (12).

Let us now solve (23)–(26) for $B$ and $C$. Since $F(0)=1$, (23) and (24) are recognized as being one of the Hamilton–Jacobi equations, yielding $B=S_c$. Note that since (23) and (24) stem from equating only the constant term to 0 in (19), an approximation to zeroth order in $\hbar$ yields $B=S_c$ and no information on $C$ other than the fact that it must be such that the boundary condition (9) is satisfied (this is not sufficient to fix $C$).

To solve (25), we note that if $\mathrm{Im}[F'(0)]=0$ ($a=\frac{1}{2}$) then $C^2=\det M$, since the (continuity) equation satisfied by the Van Vleck–Morette determinant is precisely

$$\frac{\partial}{\partial q_b^j}[\dot q_c^j(t_b)\det M]+\frac{\partial}{\partial t_b}[\det M]=0. \tag{29}$$

This leads us to write

$$C^2=N\det M, \tag{30}$$

which, when substituted in (25) and using $\mathrm{Im}[F'(0)]=a-\frac{1}{2}$ yields the equation for $N(q_b,t_b,q_a,t_a)$:

$$\frac{\partial N}{\partial t_b}+\dot q_c^j(t_b)\frac{\partial N}{\partial q_b^j}+N(2a-1)\frac{\partial^2 H_c(q,p,t_b)}{\partial q^i\partial p_i}\Big|_{\substack{q=q_b\\ p=p_c(t_b)}}=0, \tag{31}$$

with $N\to 1$ as $t_b\to t_a$ and $q_b\to q_a$, if $K_{VV}\to\delta(q_b-q_a)$ as $t_b\to t_a$.

The search for a solution of (31) is facilitated by the observation that the first two terms form the convective derivative of $N$ with respect to the final endpoint. Knowing that the convective derivative of any function $f$ of position, momentum, and time (at the classical path) with respect to either the initial or the final endpoint is 0, i.e.,

$$\left[\frac{\partial}{\partial t_b}+\dot q_c^j(t_b)\frac{\partial}{\partial q_b^j}\right]f(q_c(t),p_c(t),t)=0 \tag{32}$$

(to be proved shortly), we are led to a trial solution of the form

$$N=\exp\left[(1-2a)\int_{t_a}^{t_b}\frac{\partial^2 H_c}{\partial p_i\partial q^i}(q_c(t),p_c(t),t)\,dt\right]. \tag{33}$$

By direct substitution in (31), (33) is seen to be the correct solution [use $f=q_c$ and $f=p_c$ in (32)].

To prove (32), we first observe that it is sufficient to prove it for $f=q_c$ and $f=p_c$: the chain rule will then extend its validity to any $f$. Now, derivatives of the classical solution with respect to any parameter introduced by the boundary conditions (here, $t_a,t_b,q_a$, and $q_b$) are known to be solutions of the equation of small distrubances, obtained from the second variation of the action functional.[10–13] Since this equation is linear, its general solution is a linear combination of $2n$ linearly independent solutions. Thus, the only solution vanishing at both $t_a$ and $t_b$ must be zero everywhere. Now, the left-hand side of (32) with $f=q_c^i(t)$ is, by its very construction, a solution of the small-disturbance equation. It vanishes at $t_a$ because $q_c(t_a)=q_a$ ($a$ constant). It also vanishes at $t_b$ because

$$\frac{\partial q_c^i(t)}{\partial t_b}\Big|_{t=t_b}=\int_{t_a}^{t_b}dt\,\frac{\partial\dot q_c^i(t)}{\partial t_b}$$
$$=-\dot q_c^i(t_b)+\frac{\partial}{\partial t_b}\int_{t_a}^{t_b}\dot q_c^i(t)\,dt$$
$$=-\dot q_c^i(t_b)+\frac{\partial}{\partial t_b}(q_b^i-q_a^i)$$
$$=-\dot q_c^i(t_b), \tag{34}$$

[since $\partial/\partial t_b$ commutes with $\partial/\partial t$ when acting on $q_c(t,t_b,q_b)$]. Thus, (32) is true for $f\equiv q_c$. The case $f\equiv p_c$ is proved by observing, by substitution in the equation of small disturbances in phase space ($\mathscr{O}h=0$), that if $u$ is a parameter introduced by the boundary conditions, then

$$\partial p_{ci}(t)/\partial u=\mathbf{D}_{ij}(t)\partial q_c^j(t)/\partial u, \tag{35}$$

where

$$\mathscr{O}\equiv-\begin{pmatrix} f & k+d/dt\\ \tilde k-d/dt & g\end{pmatrix},$$
$$h\equiv\begin{pmatrix}\partial q_c(t)/\partial u\\ \partial p_c(t)/\partial u\end{pmatrix},$$
$$\mathbf{D}\equiv g^{-1}\left(\mathbf{1}\frac{d}{dt}-\tilde k\right), \tag{36}$$

and $f,g$, and $k$ are defined in (15). This completes the proof of the WKB approximation formula (10). ■

Note that (19) indicates that when $H_c$ is quadratic in both $p$ and $q$, the term proportional to $\hbar^2$ is 0 because $C$ is independent of $q_a$ and $q_b$ ($S_c$ being quadratic in $q_a$ and $q_b$), and higher-order terms are 0 because they involve third and higher derivatives of $H_c$. Thus, the WKB approximation is exact in that case. This goes beyond the well-known result

because $\mathbf{H}$ does not have to be Hermitian, so that the extra exponential term in (10) supplementing the Van Vleck formula is not constant.

Note also that in terms of the Lagrangian $L(q,\dot{q})$ we have $\partial^2 H_c(q,p)/\partial p_i \partial q^i \equiv \mathrm{tr}(H_c)_{21} = \mathrm{tr}(-L_{22}^{-1}L_{21})$.

*Proof of second formula*: Formula (12) will be proved using the path-integral approach, generalizing a method presented in Ref. 4. More details on this method and its extension to a WKB expansion of the propagator for arbitrary Hamiltonians will be presented elsewhere.

The propagator $K$ can be written as a phase space path integral as follows:

$$K(q_b,t_b,q_a,t_a) = \int_{\mathscr{P}} \left[\frac{dpdq}{h^n}\right] \exp(iS/\hbar), \tag{37}$$

where $S \equiv \int_T [p\dot{q} - H(q,p,t)]\,dt$ is the action functional and $\mathscr{P}$ is the space of paths $(q,p)$ such that $q(t_a) = q_a$ and $a(t_b) = q_b$. If $S$ is expanded around the classical path $(q_c,p_c)$, its first functional derivative vanishes by definition of the classical path and we obtain

$$K = e^{iS_c/\hbar} \int_{\mathscr{P}_0} \left[\frac{dxdy}{h^n}\right] e^{iS_c''(x,y)/\hbar} e^{-i\Omega_c(x,y)/\hbar}, \tag{38}$$

where $\mathscr{P}_0$ is the space of paths $(x,y)$ such that $x(t_a) = x(t_b) = 0$, $\Omega_c$ contains the terms beyond the second functional derivative,[13a] and the second functional derivative $S_c''$ is

$$S_c''(x,y) = \int_T dt\,[y_i(t)\dot{x}^i(t) - \tfrac{1}{2}g^{ij}(t)y_i(t)y_j(t) - \tfrac{1}{2}f_{ij}(t)x^i(t)x^j(t) - k^i_j(t)y_i(t)x^j(t)], \tag{39}$$

with $f$, $g$, and $k$ in (15).

We can define a measure $w$ on $\mathscr{P}_0$, normalized to 1 and absorbing the second variation of $S$ by:

$$dw(x,y) \equiv A_0^{-1}[dxdy/h^n]\exp(iS_c''(x,y)/\hbar), \tag{40}$$

the normalization factor being

$$A_0 \equiv \int_{\mathscr{P}_0} [dxdy/h^n]\exp(iS_c''(x,y)/\hbar). \tag{41}$$

Now, it is observed that the $S_c''$ term in (39) is in the form of an action functional corresponding to the fictitious Hamiltonian

$$H_0(x,y,t) \equiv \tfrac{1}{2}g^{ij}(t)y_iy_j + \tfrac{1}{2}f_{ij}(t)x^ix^j - k^i_j(t)y_ix^j. \tag{42}$$

Hence, (37) indicates that $A_0$ must be the propagator $K_0(q_b',t_b,q_a',t_a)$ corresponding to $H_0$, evaluated at $q_a' = q_b' = 0$. But for which Hamiltonian operator $\mathbf{H}_0$? It makes sense[6] that it should be the operator derived from $H_0$ using the same correspondence rule linking $H_c$ and $\mathbf{H}$, i.e., (14) with (16). This leaves us with

$$K = A_0 e^{iS_c/\hbar} \int_{\mathscr{P}_0} e^{-i\Omega_c(x,y)/\hbar}\,dw(x,y). \tag{43}$$

It can be shown in this general case, as was done before for special cases,[11–13] that the expansion of the $\Omega_c$ term followed by the evaluation of the path integrals (the correspondence rule being taken into account) yields a series in $\hbar$,

$$K = A_0 e^{iS_c/\hbar}(1 + \hbar K_1 + \hbar^2 K_2 + \cdots), \tag{44}$$

which identifies the constant term as the WKB approximation.■

Let us now retrieve formula (10) from this more general case. The operator $\mathbf{H}_0$ in this case is

$$\mathbf{H}_0 \equiv \tfrac{1}{2}g^{ij}(t)\mathbf{P}_i\mathbf{P}_j + \tfrac{1}{2}f_{ij}(t)\mathbf{Q}^i\mathbf{Q}^j + k^i_j(t)[a\mathbf{P}_i\mathbf{Q}^j + (1-a)\mathbf{Q}^j\mathbf{P}_i], \tag{45}$$

which can be rewritten, using $[\mathbf{Q}^i,\mathbf{P}_j] = i\hbar\delta^i_j$ as

$$\mathbf{H}_0 = \mathbf{H}_{00} + i\hbar(\tfrac{1}{2} - a)k^i_i(t), \tag{46}$$

where

$$\mathbf{H}_{00} \equiv \tfrac{1}{2}g^{ij}(t)\mathbf{P}_i\mathbf{P}_j + \tfrac{1}{2}f_{ij}(t)\mathbf{Q}^i\mathbf{Q}^j + \tfrac{1}{2}k^i_j(t)(\mathbf{P}_i\mathbf{Q}^j + \mathbf{Q}^j\mathbf{P}_i). \tag{47}$$

Now, since $\mathbf{H}_{00}$ is quadratic and Hermitian, its propagator $K_{00}$ is given exactly by Van Vleck's formula, (11). In this case, however, the $S_c$ in (11) is zero because $q_a' = q_b' = 0$. (In fact, in general $S_c = q_b'^i p_{co,i}(t_b) - q_a'^i p_{co,i}(t_a)$, where $(q_{co},p_{co})$ is the classical solution for $H_0$). Further, the "det $M$" in (11) is the same as the "det$M$" for $H_c$ because $H_0$ and $H_c$ share the same equation of small disturbances and $M_{ij}$ is a boundary value of a specific solution of that equation.[11–13] Therefore, $K_{00} = (2\pi i\hbar)^{-n/2}(\det M)^{1/2}$. Now, if $\mathbf{H}_1 = \mathbf{H}_2 + f(t)$, the propagators $K_1$ and $K_2$ are related by $K_1 = K_2 \exp[-(i/\hbar)\int_T f(s)\,ds]$. $\mathbf{H}_0$ and $\mathbf{H}_{00}$ are related in this manner. Putting all these results together gives

$$K_{\mathrm{WKB}} = (2\pi i\hbar)^{-n/2}(\det M)^{1/2} \times \exp\left\{(i/\hbar)S_c + (\tfrac{1}{2} - a)\int_T k^i_i(s)\,ds\right\}, \tag{48}$$

which is formula (10). Note that this suggests that the normalization factor $(2\pi i)^{-n/2}$ is universal and independent of $H_c$.[14]

Note in passing that it is not always easy to find out what operator $p_iq^j$ corresponds to, given the $H_c \longleftrightarrow \mathbf{H}$ correspondence, if the latter is not given by an $F$-function. Scaling tricks (replacing $\mathbf{Q}$ by $\lambda\mathbf{Q}$ in functions of $\mathbf{Q}$, then differentiating with respect to $\lambda$ and setting $\lambda$ equal to 0) sometimes help.

## IV. SOME EXAMPLES

We begin with an example pointing out that formulas (10) and (12) are not restricted to the correspondence rule being effected by an $F$-function. Consider the Hamiltonian

$$\mathbf{H} = \tfrac{1}{2}g^{-1/4}(\mathbf{Q})[\mathbf{P}_i - A_i(\mathbf{Q})]g^{1/2}(Q)g^{ij}(Q) \times [\mathbf{P}_j - A_j(\mathbf{Q})]g^{-1/4}(\mathbf{Q}) + V(\mathbf{Q}) \tag{49}$$

corresponding to

$$H_c = \tfrac{1}{2}g^{ij}(q)[p_i - A_i(q)][p_j - A_j(q)] + V(q), \tag{50}$$

where $g_{ik}g^{kj} \equiv \delta_i^j$ and $g \equiv \det(g_{ij})$. There is no $F$ in general because of the divisors.[15] Nevertheless, a direct substitution shows that Van Vleck's formula applies, and we get:

$$\begin{aligned} K_{\mathrm{VV}}^{-1}(\mathbf{H}_b - i\hbar\partial/\partial t_b)K_{\mathrm{VV}} &= \tfrac{1}{4}\hbar^2 g^{ij}(\Gamma^m_{mi}M_{,j}/M + \Gamma^l_{ij}M_{,l}/M + M_{,i}M_{,j}/2M^2 \\ &\quad - M_{,ij}/M - \tfrac{1}{2}\Gamma^m_{mi}\Gamma^l_{lj} - \Gamma^l_{ij}\Gamma^m_{ml} + \Gamma^l_{lj,i})(q_b) \\ &= O(\hbar^2), \end{aligned} \tag{51}$$

where the following properties and definitions were used:

$$M \equiv \det M,$$
$$\Gamma^i_{jk} \equiv \tfrac{1}{2} g^{ia}(g_{ja,k} + g_{ka,j} - g_{jk,a}),$$
$$g^{ij}_{,k} = -\Gamma^i_{mk} g^{mj} - \Gamma^j_{mk} g^{im},$$
$$g^{\alpha}_{,i} = 2\alpha g^{\alpha} \Gamma^l_{li}, \tag{52}$$
$$\dot{q}^j_c(t_b) = g^{jj}(t_b)[p_{ci}(t_b) - A_i(q_b)],$$
$$p_{ci}(t_b) = \partial S_c / \partial q^i_b,$$
$$\partial S_c / \partial t_b = -H_c(q_b, \partial S_c / \partial q_b),$$

as well as (29).[16]

On the other hand, (19) gives the following expression for the miss term:

$$K_{\bar{v}v}^{-1}(\mathbf{H}_b - i\hbar\partial/\partial t_b)K_{vv} = -\tfrac{1}{2}\hbar^2[\, g^{ij}_{,ij}(\tfrac{1}{4}F(0) - iF'(0) - F''(0)) + g^{ij}_{,j}(F(0) - 2iF'(0))C'_i/C + g^{ij}F(0)C''_{ij}/C\,], \tag{53}$$

an expression which cannot be matched with (51) for any $F$, for $C = M^{1/2}$. (Thus, there is no $F$).

Consider now the Fokker–Planck equation of diffusion processes:

$$\frac{\partial P}{\partial t} = \tfrac{1}{2}\frac{\partial^2}{\partial q^i \partial q^j}[D^{ij}(q,t)P] - \frac{\partial}{\partial q^i}[v^i(q,t)P], \tag{54}$$

where $D$ is the diffusion matrix and $v$ the drift vector.[17] It formally corresponds to a Hamiltonian $\mathbf{H} \equiv \mathbf{P}_i\mathbf{P}_j D^{ij}(\mathbf{Q})/2i\hbar + \mathbf{P}_i v^i(\mathbf{Q})$ with classical Hamiltonian $H_c = p_i p_j D^{ij}/2i\hbar + p_i v^i$. Since the $\mathbf{P}$ factors precede the $\mathbf{Q}$ factors, $a$ is simply equal to 1. Thus, formula (10) gives:

$$K_{\mathrm{WKB}} = (2\pi i\hbar)^{-n/2}(\det M)^{1/2} \times \exp\left[\frac{i}{\hbar}S_c - (2i\hbar)^{-1}\int_T p_{ci}(t)D^{ij}{}_{,j}(q_c(t))\,dt - \tfrac{1}{2}\int_T v^i{}_{,i}(q_c(t))\,dt\right]. \tag{55}$$

Note that the dynamical equation gives $p_{ci}(t) = i\hbar(D^{-1})_{ij}(\dot{q}^j_c - v^j)$, so that in one dimension part of the integration can be performed, yielding

$$K_{\mathrm{WKB}} = K_{vv}[D(q_b)/D(q_a)]^{-1/2} \times \exp\left(\tfrac{1}{2}\int_T ((vD' - v'D)/D)\,dt\right). \tag{56}$$

In the case of the backwards equation ($\mathbf{Q}$ precedes $\mathbf{P}$, $a = 0$), the factors $\frac{1}{2}$ are replaced by $-\frac{1}{2}$ in (56) and inside the bracket of (55).

For constant diffusion parameter ($D = 1$) and linear drift $v = -\gamma q$, one retrieves the well-known propagator[18]

$$K_{\mathrm{WKB}} = [\gamma/\pi(1 - 2e^{-2\gamma T})]^{1/2} \times \exp[-\gamma(q_b - q_a e^{-\gamma T})^2/(1 - e^{-2\gamma T})], \tag{57}$$

which, $\mathbf{H}$ being quadratic, is also exact [it satisfies (54) exactly].

It can be shown, by direct calculations, that the "miss factor" for (55) is exactly as given by (53) with $F(x) = \exp(ix/2)$.

Another interesting application is the "lognormal" process with Hamiltonian

$$\mathbf{H} = \alpha\mathbf{Q}^2\mathbf{P}^2 + \beta\,\mathbf{QP} \tag{58}$$

in one dimension, useful in modeling population growth.[19] Using formula (10) on $H_c = \alpha q^2 p^2 + \beta qp$ one gets

$$K_{\mathrm{WKB}} = (q_b/q_a)^{1-2a}K_{vv}\exp[\,\beta(a - \tfrac{1}{2})T\,], \tag{59}$$

where[20]

$$K_{vv} = (2\pi i\hbar)^{-1/2}(2\alpha T q_a q_b)^{-1/2} \times \exp\left[\frac{i}{4\hbar\alpha T}\left(\ln\frac{q_b}{q_a} - \beta T\right)^2\right]. \tag{60}$$

In our case, $a = 0$. Note that for $a = 0$ the exact propagator[21] is

$$K = K_{\mathrm{WKB}}\exp(-i\hbar\alpha T/4), \tag{61}$$

so that the expansion of the exponential gives the terms of a WKB expansion of $K$, useful for checking general formulas.

Let us also mention the elements of the WKB approximation for Hamiltonians in one dimension of the form

$$H_c = kp^m q^n, \tag{62}$$

where $k$ is a constant. The classical equation of motion is $\ddot{q}_c = (n/m)\dot{q}_c^2/q_c$ and the Lagrangian is $L = \dot{q}^{m/(m-1)} \times L = q^{-n/(m-1)}(mk)^{-1/(m-1)}$. For $m \neq n$ these elements are:

$$q_c(t) = A(t - t_0)^{m/(m-n)},$$
$$p_c(t) = [k(m-n)]^{1/(m-1)}(t - t_0)^{n/(n-m)}A^{(1-n)/(m-1)}$$
$$A \equiv q_a\left(\frac{1-\gamma}{\gamma T}\right)^{m/(m-n)},$$
$$t_0 \equiv \frac{t_a - \gamma t_b}{1 - \gamma},$$
$$\gamma \equiv (q_a/q_b)^{(m-n)/m}, \tag{63}$$
$$S_c = (m-1)(kT)^{-1/(m-1)}(m-n)^{m/(1-m)} \times (q_b^{(m-n)/m} - q_a^{(m-n)/m})^{m/(m-1)},$$
$$M = [Tk(m-n)]^{-1(m-1)}\frac{m-n}{m(m-1)}(q_a q_b)^{-n/m} \times (q_b^{(m-n)/m} - q_a^{(m-n)/m})^{(2-m)/(m-1)}.$$

For $m = n$, these elements are:

$$q_c(t) = \exp(At + B), \quad q_c(t)p_c(t) = (A/km)^{1/(m-1)},$$
$$A \equiv T^{-1}\ln(q_b/q_a), \quad B \equiv \ln[q_a(q_a/q_b)^{t_a/T}], \tag{64}$$
$$S_c = (mkT)^{-1/(m-1)}(1 - m^{-1})[\ln(q_b/q_a)]^{m/(m-1)},$$
$$M = (mkT)^{-1/(m-1)}[(m-1)q_a q_b]^{-1} \times [\ln(q_b/q_a)]^{(2-m)/(m-1)}.$$

In all cases,

$$K_{\mathrm{WKB}} = K_{vv}(q_b/q_a)^{n(1/2-a)}. \tag{65}$$

## IV. CONCLUSION

We have produced a formula to approximate the propagator corresponding to any system described by a function whose time evolution is given by a partial differential equation that is of first order in time. This approximation can be supplemented by correction terms that can be generated by path integrals, and this will be the subject of a follow-up study.[22]

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[8]"True" divisors are those that cannot be eliminated by use of the commutation relation $\mathbf{QP}-\mathbf{PQ}=i\hbar$. For example,

$$\mathbf{H}\equiv\mathbf{Q}^{1/2}\mathbf{PQPQ}^{1/2}$$

does not contain true divisors because the commutation relation $\mathbf{P}f(\mathbf{Q})-f(\mathbf{Q})\mathbf{P}=-i\hbar f'(\mathbf{Q})$ enables one to rewrite $\mathbf{H}$ as $\mathbf{PQ}^2\mathbf{P}-\frac{1}{4}\hbar^2$. We can then rewrite $-\hbar^2$ as $(\mathbf{QP}-\mathbf{PQ})^2$ and conclude that $\mathbf{H}$ is only an ordering of the factors of $p^2q^2$. However,

$$\mathbf{H}'\equiv\mathbf{Q}^{1/4}\mathbf{PQ}^{1/2}\mathbf{PQ}^{1/4}$$

does contain true divisors, because one can rewrite it as $\mathbf{PQP}+\hbar^2\mathbf{Q}^{-1}/16=\mathbf{PQP}-(\mathbf{QP}-\mathbf{PQ})^2\mathbf{Q}^{-1}/16$, which cannot be obtained simply by ordering the factors of $p^2q$. Thus, $\mathbf{H}'$ is not covered by one of Cohen's $F$ functions, but $\mathbf{H}$ is [any $F(x)$ such that $F(0)=1$, $F'(0)=0$, $F''(0)=1/8$ would do, for example $F(x)=\exp(x^2/16)$].
[9]In fact, the "Conclusion" stated at the bottom of p. 788 in Ref. 1 remains valid even if the requirement that $F$ be real is dropped.
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[13a]Specifically,

$$\Omega_c(x,y)=\sum_{n=3}^{\infty}\frac{1}{n!}\sum_{k=0}^{n}\binom{n}{k}C_{i_1\cdots i_k}{}^{i_{k+1}\cdots i_n}(t)x^{i_1}\cdots x^{i_k}y_{i_{k+1}}\cdots y_{i_n}(t)$$

where

$$C_{i_1\cdots i_k i_{k+1}\cdots i_n}(t)\equiv\left.\frac{\partial^n H_c}{\partial q^{i_1}\cdots\partial q^{i_k}\partial p_{i_{k+1}}\cdots\partial p_{i_n}}\right|_{q=q_c(t),p=p_c(t)}$$

[14]Unlike what was suggested in Ref. 1.
[15]In fact, direct use of (22) indicates that the correspondence $\frac{1}{2}g^{ij}(q)p_ip_j\longleftrightarrow\frac{1}{2}g^{\alpha}(\mathbf{Q})\mathbf{P}_ig^{-2\alpha}(\mathbf{Q})g^{ij}(\mathbf{Q})\mathbf{P}_jg^{\alpha}(\mathbf{Q})+\hbar^2\varphi(\mathbf{Q})$ is fulfilled by an $F$ function iff $\varphi(q)+\eta(q)=k\xi(q)$, where $k$ is constant, $\xi(q)\equiv\frac{1}{2}g^{ij}{}_{,ij}$, and

$$\eta(q)\equiv\tfrac{1}{8}g^{ij}[(2\alpha+\tfrac{1}{2})^2\Gamma^l_{li}\Gamma^m_{mj}+(2\alpha+\tfrac{1}{4})\Gamma^m_{ml}\Gamma^l_{ij}+\tfrac{1}{2}\Gamma^l_{is}\Gamma^s_{lj}-\tfrac{1}{4}\Gamma^l_{ij,l}-(2\alpha+\tfrac{1}{4})\Gamma^m_{mi,j}].$$

If $g^{ij}$ is such that the relation is satisfied, then any $F$ such that $F(0)=1$, $F'(0)=0$, $F''(0)=k$ will do. Weyl' rule ($F=1$) is an example for $k=0$. In particular, there is no $F$ in general for the case $\varphi=0$. In one dimension, $\eta=k\xi$ for all $g^{ij}$ of the form $g^{11}(q)=(aq+b)^c$, $a$ and $b$ being arbitrary constants and $c\equiv(\alpha+\frac{1}{4}-k)/(\alpha^2+\alpha+\frac{1}{4}-k)$.
[16]The result in (51) matches that of DeWitt in Ref. 3 for small $T$ because, using the expansion of $M$ in his Eq. (6.38) we readily get

$$K_{vv}^{-1}(\mathbf{H}_b-i\hbar\partial/\partial t_b)K_{vv}=\hbar^2[-R(q_b)/12+o(t_b-t_a)+o(q_b-q_a)],$$

where $R\equiv g^{ij}(\Gamma^l_{lj,i}-\Gamma^l_{ij,l}+\Gamma^l_{mj}\Gamma^m_{il}-\Gamma^l_{ij}\Gamma^m_{ml})$ is the Ricci scalar curvature tensor. In this case, a small-time approximation is the same as a WKB approximation.
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[18]See, e.g., F. Reif, *Fundamental of Statistical and Thermal Physics* (McGraw-Hill, 1965), p. 581.
[19]See, e.g., L. M. Ricciardi, *Diffusion Processes and Related Topics in Biology* (Springer–Verlag, Berlin 1977), p. 102; B. J. Sheeks, "Some applications of path integration using the prodistribution method", Ph.D. thesis, The University of Texas at Austin, May 1980.
[20]Note in passing that $K_{vv}$ in (60) is the exact propagator for an ordering patterned after (49), i.e., $\mathbf{H}=\alpha\mathbf{Q}^{1/2}\mathbf{PQPQ}^{1/2}+\beta(\mathbf{QP}+\mathbf{PQ})/2\equiv\alpha(\mathbf{PQ}^2\mathbf{P}-\frac{1}{4}\hbar^2)+\beta(\mathbf{QP}+\mathbf{PQ})/2$, a rare case when the WKB approximation is exact for a nonquadratic $\mathbf{H}$. Formula (53) for $F(0)=1$, $F'(0)=0$ and $F''(0)=1/8$ will confirm this.
[21]Exact propagators for Hamiltonians of the form $\mathbf{H}=\Sigma_{i=1}^{N}a_i\mathbf{Q}^i\mathbf{P}^i$ in one dimension can sometimes be found using the identity

$$\left[\sum_{i=1}^{N}a_ix^i\left(\frac{d}{dx}\right)^i\right]^m x^n=\left[\sum_{i=1}^{N}a_i\frac{n!}{(n-i)!}\theta(n-i)\right]^m x^n,$$

where $\theta(x)=0$ for $x<0$ and 1 otherwise. Thus, for $\mathbf{T}\equiv\Sigma_{i=1}^{N}a_ix^i(d/dx)^i$ one obtains

$$e^{\mathbf{T}}f(x)=\sum_{n=0}^{\infty}\frac{1}{n!}f^{(n)}(0)\exp\left[\sum_{i=1}^{N}a_i\frac{n!\theta(n-i)}{(n-i)!}\right].$$

For $N=2$, use of the integral representation

$$e^{sn^2}=(4\pi s)^{-1/2}\int_{\mathbf{R}}e^{-x^2/4s+nx}\,dx\text{gives}$$

$$e^{\mathbf{T}}f(x)=(4\pi a_2)^{-1/2}\int_{\mathbf{R}}dy\,e^{-y^2/4a_2}f(xe^{y+a_1-a_2}).$$

Changing variables to $u=x\exp(y+a_1-a_2)$ gives

$$e^{\mathbf{T}}\delta(x-x')=(x')^{-1}(4\pi a_2)^{-1/2}\times\exp[-(\ln(x'/x)+a_2-a_1)^2/4a_2].$$

Since it will be recalled, the propagator $K$ is equal to $e^{-iT\mathbf{H}/\hbar}\delta(q_b-q_a)$ when $\mathbf{H}$ is time-independent, the method can be applied here.
[22]A recent study of the correction terms in the case of the Hamiltonian in (49) can be found in F. Langouche, D. Roekaerts, and E. Tirapequi, Lett. Nuovo Cim. **25** (1979), 307–13; Physica **101 A**, 301–23 (1980); and Proc. of Workshop on Funct. Integr., Theor Appl., Louvain-la-Neuve, Nov. 6–9, 1979 (Plenum, to appear).

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# Degenerate perturbations in nonrelativistic quantum mechanics

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We investigate the effects on the discrete spectrum of an arbitrary quantum mechanical Schrödinger operator $H$, which are caused by the addition of a real rank $N$ separable potential to $H$. For such a potential the bound state energies $E_n(\lambda)$ as function of the *real* potential strength $\lambda$ are in general confined to certain *bounded* intervals. This remarkable phenomenon can be seen as a particular case of the general situation of *complex* potential strengths.

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## 1. INTRODUCTION

In this paper we shall investigate certain properties of rank $N$ separable (also called degenerate) perturbations $\lambda V_s$, in particular the effects they have on the bound-state energies of an arbitrary Schrödinger operator $H$. Many of the results we shall obtain are well known (see in particular Kato Ref. 1, Ch. IV.6, Ch. X.3, and Ch. X.4). However, a detailed study of these degenerate perturbations in a quantum mechanical language will be useful.

The behavior of the bound-state energies $E_n(\lambda)$ as functions of the *real* parameter $\lambda$ ($-\infty < \lambda < \infty$) is especially interesting. In contrast to the case of *local* perturbations, these $E_n(\lambda)$ are in general confined to certain bounded intervals, as we will see below. We have to take full account of the possibility that there are discrete eigenvalues embedded in the continuum. Such "positive eigenvalues" can occur for *local* potentials in exceptional cases only. A second complication concerns the fact that the negative eigenvalues can be degenerate. As is well known, for a regular *local* potential [in one particular partial wave space] the eigenvalues cannot be degenerate.

It may be noted that in Ref. 2 the particular case of the Coulomb potential plus the rank one Yamaguchi perturbation has been studied. Here explicit formulas containing hypergeometric functions have been given. (See also Refs. 3 and 4.)

In a subsequent paper[5] we shall consider the case of a *complex* (nonreal) coupling parameter $\lambda$.

Some preliminaries will be given in Sec. 2. In Secs. 3–6 we consider rank one perturbations. Four different cases will be distinguished here (see the classification at the end of Sec. 2). Figs. 1–4 correspond just to these four cases. The investigations of Secs. 3–6 pave the way for the general case of rank $N$ perturbations (Sec. 7). Indeed, any rank $N$ perturbation can be obtained by iteration of rank 1 perturbations. In Sec. 7 we also give certain closed formulas for rank 2 perturbations. Finally in Sec. 8 we discuss some important and interesting properties of rank $N$ perturbations.

## 2. PRELIMINARIES

We are interested in certain properties of degenerate perturbations to a given Schrödinger operator (see Ref. 6, pp. 355, 365),

$$H = H_0 + V. \tag{2.1}$$

Here $H_0$ is the kinetic energy operator. As usual we take $\hbar = 2m = 1$, so $H_0 = p^2$. We assume that $H$ is a self-adjoint operator whose essential spectrum[7] is $[0, \infty]$. Then $V$ can be, for example, a local potential $V(r)$ which vanishes for $r \to \infty$, or a separable potential. In certain cases when $H_0 + V$ is essentially self-adjoint, one obtains a self-adjoint operator in a standard fashion by taking the closure, (see e.g., Ref. 6, p. 358).

A degenerate perturbation is an operator of finite rank, also called a separable potential,

$$V_s = -\sum_{i=1}^{N} |g_i\rangle \lambda_i \langle g_i|. \tag{2.2}$$

Here $N$ is the rank, $\lambda_i$ are real numbers and $|g_i\rangle$ are called the form factors. We assume that these have a finite norm, $\langle g_i | g_i \rangle < \infty$. The operator $V_s$ is defined in a space corresponding to one particular value of the orbital angular momentum quantum number $l$. We shall restrict ourselves in this paper throughout to $l = 0$. However, all results can be generalized easily to the case of any $l > 0$.

The main purpose of this paper is to study the behavior of the nonpositive eigenvalues of $H + V_s$ as functions of the real parameters $\lambda_i$. We shall first restrict ourselves to the case $N = 1$ [Secs. 3–6]. Once this case has been fully understood, the properties of a general perturbation of rank-$N > 1$ can easily be derived, (see Sec. 7). Indeed, by including $N-1$ terms of the sum in Eq. (2.2) into $V$, the general case is reduced to the case $N = 1$. The perturbed Schrödinger operator is now

$$H_\lambda \equiv H_0 + V - \lambda |g\rangle\langle g|. \tag{2.3}$$

In Secs. 3–6 we shall study the behavior of the nonpositive eigenvalues of $H_\lambda$ as functions of $\lambda$.

We have to introduce some more notations. The (so-called outgoing) scattering states of the unperturbed Hamiltonian $H$, corresponding to the continuous spectrum, will be denoted by $|k+\rangle$. For simplicity we assume that the continuous spectrum of $H$ is absolutely continuous (see Kato, Ref. 1). Let the point spectrum of $H$ (to be distinguished from the discrete spectrum of $H$, which is the set of *isolated* eigenvalues of finite multiplicity, (see Ref. 1, p. 187 and Ref. 8, p. 2292) consist of the nonpositive eigenvalues $-\kappa_n^2$

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$(n = 1,2,...,n_n)$ and the positive eigenvalues $k_m^2$ $(m = 1,2,...,n_p)$. We denote the corresponding eigenstates by $|\kappa_n\rangle$ and $|k_m\rangle$, respectively. Then we have the following useful resolution of the identity,

$$1 = \sum_n |\kappa_n\rangle\langle\kappa_n| + \sum_m |k_m\rangle\langle k_m| + \int_0^\infty |k+\rangle\langle k+|k^2\,dk. \tag{2.4}$$

Furthermore,

$$H = -\sum_n \kappa_n^2 |\kappa_n\rangle\langle\kappa_n| + \sum_m k_m^2 |k_m\rangle\langle k_m| + \int_0^\infty k^2 |k+\rangle\langle k+|k^2\,dk \tag{2.5}$$

is the spectral resolution or spectral decomposition of $H$ (e.g. Refs. 8 and 6, pp. 252, 452 and 500). The orthonormality of the eigenstates and the scattering states is expressed by

$$\langle\kappa_n|\kappa_{n'}\rangle = \delta_{nn'},$$
$$\langle k_m|k_{m'}\rangle = \delta_{mm'},$$
$$\langle k+|k'+\rangle = k^{-2}\delta(k-k'),$$
$$\langle\kappa_n|k_m\rangle = \langle\kappa_n|k+\rangle = \langle k_m|k+\rangle = 0.$$

We shall use the Green operators or resolvents,

$$G(E) = (E-H)^{-1},$$

and

$$G_\lambda(E) = (E-H_\lambda)^{-1}.$$

From Eqs. (2.4) and (2.5) we have

$$G(E) = \sum_n \frac{|\kappa_n\rangle\langle\kappa_n|}{E+\kappa_n^2} + \sum_m \frac{|k_m\rangle\langle k_m|}{E-k_m^2} + \int_0^\infty \frac{|k+\rangle\langle k+|}{E-k^2} k^2\,dk. \tag{2.6}$$

The eigenvalues of $H_\lambda$ are just given by the poles of the resolvent $G_\lambda$. Obviously on the physical sheet $G_\lambda(E)$ has poles for *real* values of $E$ only. The following expression,

$$G_\lambda = G - \frac{G|g\rangle\langle g|G}{\lambda^{-1} + \langle g|G|g\rangle}, \tag{2.7}$$

is very useful for the study of $G_\lambda$. From Eq. (2.7) one easily obtains the interesting equality

$$\langle g|G_\lambda|g\rangle^{-1} = \lambda + \langle g|G|g\rangle^{-1}. \tag{2.8}$$

The poles of $G$ and $G_\lambda$ at some $E \leqslant 0$ are all simple poles. We note that the residue at such a pole is a projection operator. For example, when $G_\lambda$ has a pole at $E = E_n$, one easily finds

$$\lim_{E\to E_n}(E-E_n)G_\lambda(E) = |E_n\rangle_{\lambda\lambda}\langle E_n| \equiv P_n. \tag{2.9}$$

Here $|E_n\rangle_\lambda$ is the eigenstate of $H_\lambda$ corresponding to the nondegenerate eigenvalue $E_n$. If the eigenvalue $E_n$ happens to be degenerate, say $r$-fold, the projector $P_n$ is equal to

$$\sum_{i=1}^r |E_{n_i}\rangle_{\lambda\lambda}\langle E_{n_i}|.$$

In order to find the poles of $G_\lambda$, it is sufficient to investigate

(i) the poles of $G$, and
(ii) the zeros of $\lambda^{-1} + \langle g|G|g\rangle$.

This follows easily from Eq. (2.7). It is useful to distinguish degenerate and nondegenerate eigenvalues of $H$. Furthermore, it can happen accidentally that the form factor $|g\rangle$ is orthogonal to one or more of the bound state vectors $|\kappa_n\rangle$ of $H$. We shall see that the behavior of the eigenvalues of $H_\lambda$ as functions of $\lambda$ is different in this case. Therefore these different situations should be distinguished. We shall make the following classification:

I (Sec. 3) No degeneracy, all eigenvalues of $H$ are simple,

$\langle g|\kappa_n\rangle \neq 0$, for all $n$.

II (Sec. 4) No degeneracy, all eigenvalues of $H$ are simple,

$\langle g|\kappa_{n_0}\rangle = 0$, $\langle g|\kappa_n\rangle \neq 0$, for $n \neq n_0$.

III and IV At least one of the eigenvalues of $H$ is $d$-fold degenerate: $\kappa_{n_1} = ... = \kappa_{n_d}$.

III (Sec. 5) $\langle g|\kappa_{n_1}\rangle \neq 0$.

IV (Sec. 6) $\langle g|\kappa_{n_i}\rangle = 0$, for all $i = 1,2,...,d$.

## 3. CASE I: NO DEGENERACY, $\langle g|\kappa_n\rangle \neq 0$, FOR ALL $n$

In this section we assume that all eigenvalues of the unperturbed Hamiltonian $H$ are simple, and that $\langle g|\kappa_n\rangle \neq 0$ for all $n$. We shall investigate the poles of $G$ and the zeros of $\lambda^{-1} + \langle g|G|g\rangle$.

From Eq. (2.6) we see that the expression $\langle g|G(-\kappa^2)|g\rangle$ (we take $E = -\kappa^2 \leqslant 0$) has simple poles at $\kappa = \kappa_n$. Also $G$ and $G|g\rangle$ have simple poles at these values of $\kappa$. From Eq. (2.7) we have

$$\lim_{\kappa\to\kappa_n}(-\kappa^2+\kappa_n^2)G_\lambda(-\kappa^2) = |\kappa_n\rangle\langle\kappa_n| - \frac{|\kappa_n\rangle\langle\kappa_n|g\rangle\langle g|\kappa_n\rangle\langle\kappa_n|}{\langle g|\kappa_n\rangle\langle\kappa_n|g\rangle} = 0. \tag{3.1}$$

This implies that $G_\lambda$ has no pole at $\kappa = \kappa_n$. The poles of $G_\lambda$ are therefore obtained from the solutions of the equation

$$\lambda^{-1} + \langle g|G(-\kappa^2)|g\rangle = 0. \tag{3.2}$$

In this connection it is useful to recall Eq. (2.8),

$$\langle g|G_\lambda|g\rangle^{-1} = \lambda + \langle g|G|g\rangle^{-1}.$$

This equality shows in a simple way that we have to solve Eq. (3.2) since $G_\lambda$ has no pole at $\kappa = \kappa_n$. Indeed, for $\kappa = \kappa_n$ one has $\langle g|G|g\rangle^{-1} = 0$, and therefore $\langle g|G_\lambda|g\rangle^{-1} \neq 0$ when $\lambda \neq 0$.

We recast Eq. (3.2) in the form

$$\lambda^{-1} = f(\kappa). \tag{3.3}$$

The function $f$ is defined by

$$f(\kappa) \equiv \langle g|(\kappa^2 + H)^{-1}|g\rangle. \tag{3.4}$$

Differentiation with respect to $\kappa$ yields

$$\frac{d}{d\kappa}f(\kappa) = -2\kappa\langle g|(\kappa^2+H)^{-2}|g\rangle < 0, \quad \text{for } \kappa > 0. \tag{3.5}$$

Furthermore, by inserting Eq. (2.6) into Eq. (3.4) we get

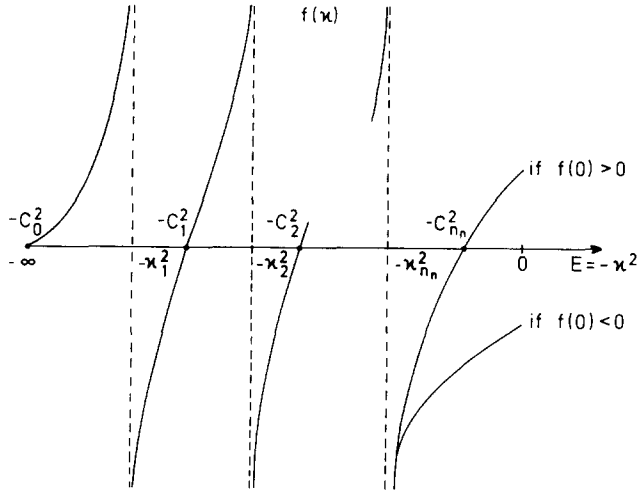


FIG. 1. The behavior of the function $f(\kappa) \equiv -\langle g|G(-\kappa^2)|g\rangle$ in case I: No degeneracy, and $\langle g|\kappa_n\rangle \neq 0$ for all $n$. The eigenvalues of $H_\lambda$ are obtained from the solutions $\kappa$ of $f(\kappa) = \lambda^{-1}$, i.e., $\kappa = f^{-1}(\lambda^{-1})$. The numbers $c_m$ are defined as the zeros of $f(\kappa)$, so $f(c_m) = 0$. Note that an eigenvalue of $H_\lambda$ can never pass any one of these numbers $c_m$.

$$f(\kappa) = \sum_n \frac{\langle g|\kappa_n\rangle\langle\kappa_n|g\rangle}{\kappa^2 - \kappa_n^2} + \sum_m \frac{\langle g|k_m\rangle\langle k_m|g\rangle}{\kappa^2 + k_m^2} + \int_0^\infty \frac{\langle g|k+\rangle\langle k+|g\rangle}{\kappa^2 + k^2} k^2\, dk. \tag{3.6}$$

From Eqs. (3.5) and (3.6) it follows that $f(\kappa)$ is a real-valued, continuous, and monotonically decreasing function of $\kappa$ on each of the following intervals,

$$0 < \kappa < \kappa_{n_n}, \ldots \ldots, \kappa_2 < \kappa < \kappa_1, \kappa_1 < \kappa < \infty. \tag{3.7}$$

The residues of $f(\kappa)$ at its poles $\kappa_n$ are all positive. Since $f(\kappa)$ decreases from $+\infty$ to $-\infty$, Eq. (3.3) has exactly one solution in each one of the intervals

$$\kappa_{n_n} < \kappa < \kappa_{n_n - 1}, \ldots \ldots, \kappa_2 < \kappa < \kappa_1,$$

for every real value of $\lambda \neq 0$. Since $f(\infty) = 0$, there is just one and only one solution for $\kappa_1 < \kappa < \infty$ if $\lambda > 0$, and there is no solution in this interval if $\lambda < 0$. (See Fig. 1.)

We can determine the nonpositive eigenvalues of $H_\lambda$ somewhat more precisely. The function $f$ has an inverse on each one of the intervals given by (3.7) since $f$ is continuous and monotonous on these intervals. We denote this inverse by $f^{-1}$. The domain of $f^{-1}$ is the whole real axis. The solutions $\kappa$ of Eq. (3.3) are given by

$$\kappa = f^{-1}(\lambda^{-1}). \tag{3.8}$$

It is useful to introduce the numbers $c_0, c_1, \ldots, c_{n_n}$. These are defined by $f^{-1}(0)$ on each one of the intervals given by (3.7). Note that $c_{n_n}$ is not defined when $f(0) < 0$. In Fig. 1 we have sketched the function $f$ as a function of the energy $E \equiv -\kappa^2$, so that it is now monotonically *increasing*. When $E = -\infty$ we have $f = 0$ and therefore $-c_0^2 = -\infty$.

Now we are in a position to discuss the behavior of the bound-state energies as functions of $\lambda$, (see Fig. 1). We start with $\lambda = 0$. The bound-state energies are then, of course, $-\kappa_n^2$, i.e., the nonpositive eigenvalues of $H_\lambda$. Let the parameter $\lambda$ now increase from 0 to $+\infty$. The eigenvalues of $H_\lambda$ then move to the left and approach the numbers $-c_n^2$ in the limit for $\lambda \to +\infty$. If $f(0) > 0$ (so that $c_{n_n}$ exists), there emerges a new eigenvalue in the interval $(-c_{n_n}^2, 0]$ for $\lambda^{-1} = f(0)$. So we see that, for positive $\lambda$, the number of nonpositive eigenvalues of $H_\lambda$ is either $n_n$ or $n_n + 1$.

On the other hand, if we let $\lambda$ decrease from 0 to $-\infty$, the eigenvalues move to the right, (see Fig. 1). The particular eigenvalue which starts at $-\kappa_{n_n}^2$ moves to $-c_{n_n}^2$ if $f(0) > 0$ (so that $c_{n_n}$ exists). However, if $f(0) < 0$, this eigenvalue moves to 0 and then disappears when $\lambda$ becomes sufficiently negative, i.e., $\lambda^{-1} > f(0)$. Therefore, the number of nonpositive eigenvalues of $H_\lambda$ is either $n_n$ or $n_n - 1$ when $\lambda$ is negative.

It is important to note that the eigenvalues can never pass the numbers $-c_n^2$. Each one of the intervals

$$(-c_0^2, -c_1^2), \ldots \ldots, (-c_{n_n - 2}^2, -c_{n_n - 1}^2) \tag{3.9}$$

contains just one and only one eigenvalue for every $\lambda \neq \pm\infty$. For $\lambda > 0$ there is also an eigenvalue in $(-c_{n_n - 1}^2, -\kappa_{n_n}^2)$, and there *can* be an eigenvalue in $(-c_{n_n}^2, 0)$. On the other hand, for $\lambda < 0$ there *can* be an eigenvalue in the interval $(-\kappa_{n_n}^2, -c_{n_n}^2)$.

So we have proved that

(i) If $f(0) = 0$, the number of nonpositive eigenvalues of $H_\lambda$ is always $n_n$, independent of $\lambda$ (finite).

(ii) If $f(0) > 0$, $H_\lambda$ has $n_n$ nonpositive eigenvalues if $\lambda < 1/f(0)$; $n_n + 1$ nonpositive eigenvalues if $\lambda \geqslant 1/f(0)$.

(iii) If $f(0) < 0$, $H_\lambda$ has $n_n$ nonpositive eigenvalues if $\lambda \geqslant 1/f(0)$; $n_n - 1$ nonpositive eigenvalues if $\lambda < 1/f(0)$.

In particular, the number of nonpositive eigenvalues cannot decrease if $f(0) > 0$, and cannot increase if $f(0) < 0$, for any finite $\lambda$.

We conclude this section with a derivation of the bound state *vectors* of $H_\lambda$ in closed form. To this end we determine the residues of $G_\lambda$ at its poles, see Eq. (2.9). With the help of Eq. (2.8) we obtain

$$\lim_{E \to E_n} (E - E_n) G_\lambda(E) = \frac{G(E_n)|g\rangle\langle g|G(E_n)}{\langle g|G^2(E_n)|g\rangle} \equiv P_n = |E_n\rangle_{\lambda\lambda}\langle E_n|. \tag{3.10}$$

Therefore the bound state vector corresponding to the negative eigenvalue $E_n$ of $H_\lambda$ is given by

$$|E_n\rangle_\lambda = G(E_n)|g\rangle(\langle g|G^2(E_n)|g\rangle)^{-1/2}. \tag{3.11}$$

It should be noted that every negative eigenvalue of $H_\lambda$ is simple. From Eqs. (2.8) and (3.11) one can easily prove that

$${}_\lambda\langle E_{n'}|E_n\rangle_\lambda = \delta_{n'n'} \tag{3.12}$$

which is the well-known orthonormality property of the bound state vectors.

## 4. CASE II: NO DEGENERACY, $\langle g|\kappa_n\rangle = 0$, FOR $n = n_0$ ONLY

In this section we shall investigate Case II. The negative eigenvalues of $H$ are nondegenerate, and $\langle g|\kappa_n\rangle = 0$ for $n = n_0$ only.

Just as in Sec. 3 we have to determine the poles of

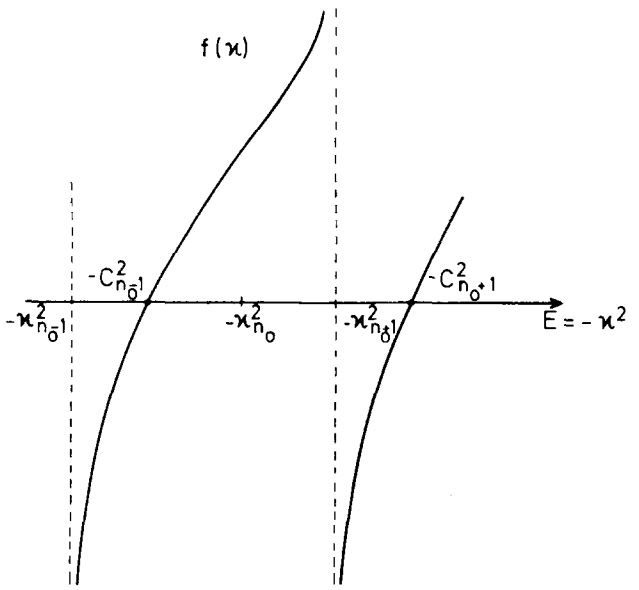


FIG. 2. The behavior of $f(\kappa)\equiv -\langle g|G(-\kappa^2)|g\rangle$ in case II. The eigenvalues of $H$ are nondegenerate, and $\langle g|\kappa_n\rangle = 0$ for $n = n_0$ only. In this case $-\kappa^2_{n_0}$ is a fixed eigenvalue of $H_\lambda$, i.e., it is independent of $\lambda$. The eigenvalues of $H_\lambda$ are obtained from the solutions $\kappa$ of the equation $f(\kappa) = \lambda^{-1}$, i.e., $\kappa = f^{-1}(\lambda^{-1})$.

$G_\lambda(E)$. It is obvious that the present case differs from Case I in one respect only. Indeed, we only have to investigate here the behavior of $f(\kappa)$ in the interval

$$-\kappa_{n_0+1} < \kappa < \kappa_{n_0-1}.$$

Because $\langle g|\kappa_{n_0}\rangle = 0$, it follows from Eq. (2.6) that $G|g\rangle$ is regular for $\kappa = \kappa_{n_0}$, for all values of $\lambda$. We see that the residues of the two terms on the right-hand side of Eq. (2.7) do not cancel. It follows that, in this case, $G_\lambda$ has a pole for $\kappa = \kappa_{n_0}$ for all values of $\lambda$. Therefore we call this pole a *fixed pole* and we call $-\kappa^2_{n_0}$ a *fixed eigenvalue* of $H_\lambda$.

The function $f(\kappa)$ has *only and only one* zero, $\kappa = c \equiv f^{-1}(0)$, between $\kappa_{n_0+1}$ and $\kappa_{n_0-1}$. According to the definition of the $c$'s, this number $c$ is $c_{n_0}$ when it lies between $\kappa_{n_0+1}$ and $\kappa_{n_0}$, so that $c_{n_0-1}$ is missing. It is $c_{n_0-1}$ when it lies between $\kappa_{n_0}$ and $\kappa_{n_0-1}$; then the number $c_{n_0}$ is missing. In Fig. 2 we have sketched the function $f$ in the vicinity of $\kappa = \kappa_{n_0}$, assuming that its zero is $c_{n_0-1}$.

When $\lambda = 0$, $H_\lambda$ has an eigenvalue $-\kappa^2_{n_0+1}$. If we let $\lambda$ increase to $+\infty$, this eigenvalue shifts to the left and approaches $-c^2_{n_0-1}$ for $\lambda\to\infty$, (see Fig. 2). Clearly it will coincide with $-\kappa^2_{n_0}$ for a certain finite value of $\lambda$. For this particular $\lambda$, $H_\lambda$ has a twofold degenerate eigenvalue $-\kappa^2_{n_0}$. We shall deduce the two corresponding eigenstates of $H_\lambda$ by evaluating the residue of $G_\lambda$ at $E = -\kappa^2_{n_0}$.

For all real $\lambda$, except one, we have

$$\lambda^{-1} + \langle g|G(-\kappa^2_{n_0})|g\rangle \neq 0. \tag{4.1}$$

By using Eq. (2.7) we easily obtain for this case,

$$\lim_{\kappa\to\kappa_{n_0}} (-\kappa^2+\kappa^2_{n_0})G_\lambda(-\kappa^2) = |\kappa_{n_0}\rangle\langle\kappa_{n_0}| \equiv P^{(1)}_{n_0}. \tag{4.2}$$

We see that the fixed eigenstate of $H_\lambda$ is identical to the eigenstate $|\kappa_{n_0}\rangle$ of $H$. This is obvious when we consider the Schrödinger equation, because $\langle g|\kappa_{n_0}\rangle = 0$.

For one particular value of $\lambda$ we have

$$\lambda^{-1} + \langle g|G(-\kappa^2_{n_0})|g\rangle = 0. \tag{4.3}$$

In this case the residue of $G_\lambda$ at $E = -\kappa^2_{n_0}$ is different from $P^{(1)}_{n_0}$. We denote this residue by the projector $P^{(2)}_{n_0}$. From Eq. (2.7) we get

$$\begin{aligned} P^{(2)}_{n_0} \equiv \lim_{\kappa\to\kappa_{n_0}} (-\kappa^2+\kappa^2_{n_0})G_\lambda(-\kappa^2) &= |\kappa_{n_0}\rangle\langle\kappa_{n_0}| \\ &\quad - G(-\kappa^2_{n_0})|g\rangle\langle g|G(-\kappa^2_{n_0}) \\ &\quad \times \lim_{\kappa\to\kappa_{n_0}} \frac{-\kappa^2+\kappa^2_{n_0}}{\lambda^{-1}+\langle g|G(-\kappa^2)|g\rangle}. \end{aligned} \tag{4.4}$$

By applying l' Hospital's theorem we obtain

$$P^{(2)}_{n_0} = |\kappa_{n_0}\rangle\langle\kappa_{n_0}| + \frac{G(-\kappa^2_{n_0})|g\rangle\langle g|G(-\kappa^2_{n_0})}{\langle g|G^2(-\kappa^2_{n_0})|g\rangle}. \tag{4.5}$$

This expression may be compared with the expression for $P_n$ in Eq. (3.10). Note that the state $G(-\kappa^2_{n_0})|g\rangle$ is indeed orthonormal to $|\kappa_{n_0}\rangle$, according to Eq. (2.6).

This shows in an explicit way that $P^{(2)}_{n_0}$ is a projector. Since $P^{(2)}_{n_0}$ projects onto a two-dimensional space, it follows that $-\kappa^2_{n_0}$ is a twofold degenerate eigenvalue of $H_\lambda$, where $\lambda$ is determined by Eq. (4.3).

We conclude this section with three remarks.

(i) If $\langle g|G(-\kappa^2_{n_0})|g\rangle = 0$, Eq. (4.3) is valid for $\lambda^{-1} = 0$ only. Therefore, the eigenvalue $-\kappa^2_{n_0}$ is nondegenerate in this case. See Fig. 2: The eigenvalue $-\kappa^2_{n_0+1}$ shifts to the left when $\lambda$ increases, and approaches $-\kappa^2_{n_0}$ for $\lambda = +\infty$. On the other hand, when $\lambda$ *de*creases from 0 to $-\infty$, the eigenvalue $-\kappa^2_{n_0-1}$ shifts to the right up to $-\kappa^2_{n_0}$.

(ii) When $|g\rangle$ is orthogonal to every eigenstate $|\kappa_n\rangle$ of $H$, the function $f(\kappa)$ is everywhere positive (i.e., for $\kappa \geqslant 0$). Obviously in this case $H_\lambda$ has only one moving eigenvalue, if and only if $\lambda \geqslant 1/f(0)$. The states $|\kappa_n\rangle$ are fixed eigenstates of $H_\lambda$.

(iii) The function $f(\kappa)$ and its derivative, $f'(\kappa) = -2\kappa\langle g|G^2(-\kappa^2)|g\rangle$, are in general smooth functions between their asymptotic values. In particular, in the case when $\langle g|\kappa_{n_0}\rangle = 0$, the behavior of $f(\kappa)$ and $f'(\kappa)$ in the vicinity of $\kappa = \kappa_{n_0}$ is in general not exceptional, cf. Fig. 2.

## 5. CASE III: $d$-FOLD DEGENERACY, $\langle g|\kappa'_{n_1}\rangle \neq 0$

In this section we shall investigate the complications which are connected with a $d$-fold degenerate eigenvalue of $H$. So we put

$$\begin{aligned} &\kappa_{n_1} = \kappa_{n_2} = \cdots = \kappa_{n_d}, \\ &H|\kappa_{n_i}\rangle = -\kappa^2_{n_1}|\kappa_{n_i}\rangle, \quad i = 1,2,\ldots,d, \end{aligned} \tag{5.1}$$

where the $|\kappa_{n_i}\rangle$ may be taken orthonormal. We assume that at least one of the numbers $\langle g|\kappa_{n_i}\rangle$ is different from zero. In Sec. 6 we shall consider the case when all $\langle g|\kappa_{n_i}\rangle$ vanish.

Following the same procedure as in Secs. 3 and 4, we obtain for the residue of $G_\lambda$ at its pole $-\kappa^2_{n_1}$ the expression,

$$\begin{aligned} &\lim_{\kappa\to\kappa_{n_1}} (-\kappa^2+\kappa^2_{n_1})G_\lambda(-\kappa^2) \\ &\quad = P - P|g\rangle\langle g|P\cdot\langle g|P|g\rangle^{-1}. \end{aligned} \tag{5.2}$$

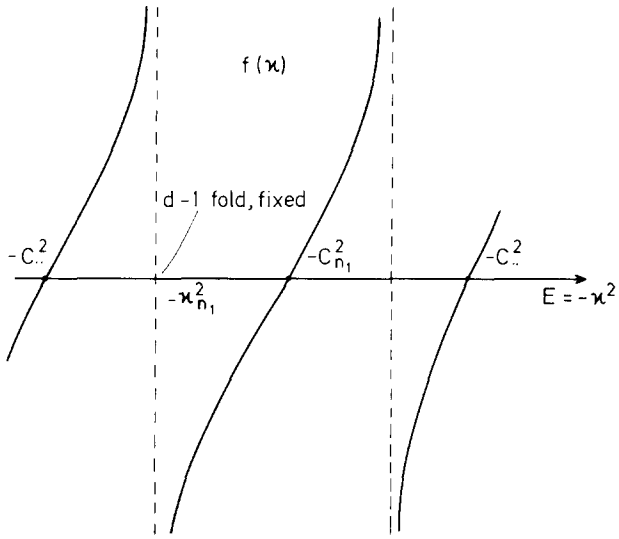


FIG. 3. The behavior of $f(\kappa)$ in case III. The eigenvalue $-\kappa_{n_1}^2$ of $H$ is $d$-fold degenerate, and $\langle g|\kappa'_{n_1}\rangle \neq 0$. It is split up by the perturbation $-\lambda\,|g\rangle\langle g|$ into $d-1$ fixed eigenvalues and 1 moving eigenvalue $E(\lambda)$ of $H_\lambda$.

Here we have used Eqs. (2.6) and (2.7). The projector $P$ is defined by

$$P \equiv \sum_{i=1}^{d} |\kappa_{n_i}\rangle\langle\kappa_{n_i}|. \tag{5.3}$$

Note that $\langle g|P\,|g\rangle^{-1}$ is a well-defined quantity, because

$$\langle g|P\,|g\rangle = \sum_{i=1}^{d} \langle g|\kappa_{n_i}\rangle\langle\kappa_{n_i}|g\rangle \tag{5.4}$$

cannot vanish. By using $P^2 = P$ one easily verifies that the expression on the right-hand side of Eq. (5.2) is a projection operator. However, the dimension of the space on which it projects is not shown.

In order to simplify the expression on the right-hand side of Eq. (5.2), we perform a basis transformation in the subspace spanned by the states $|\kappa_{n_i}\rangle$. By applying a suitable unitary operator to the $|\kappa_{n_i}\rangle$ we can obtain new basis states $|\kappa'_{n_i}\rangle$, such that

$$\begin{aligned} &\langle g|\kappa'_{n_i}\rangle \neq 0, \\ &\langle g|\kappa'_{n_i}\rangle = 0, \quad i = 2,3,\ldots,d. \end{aligned} \tag{5.5}$$

This procedure is well known from quantum mechanical perturbation theory in the case of degeneracy. Indeed, one has to diagonalize the perturbation, i.e., adjust the basis to $|g\rangle$. Since the perturbation here is one-dimensional, there is only one matrix element different from zero, namely $\langle\kappa'_{n_1}|g\rangle\langle g|\kappa'_{n_1}\rangle$. In general $|g\rangle$ is not proportional to $|\kappa'_{n_1}\rangle$.

The projection operator on the right-hand side of Eq. (5.2) has a much simpler form when expressed in terms of the $|\kappa'_{n_i}\rangle$. Indeed, by using Eq. (5.5) we get

$$\begin{aligned} \lim_{\kappa\to\kappa_{n_1}} &(-\kappa^2 + |\kappa_{n_1}^2)G_\lambda(-\kappa^2) \\ &= \sum_{i=1}^{d} |\kappa'_{n_i}\rangle\langle\kappa'_{n_i}| - |\kappa'_{n_1}\rangle\langle\kappa'_{n_1}| \\ &= \sum_{i=2}^{d} |\kappa'_{n_i}\rangle\langle\kappa'_{n_i}|. \end{aligned} \tag{5.6}$$

This is a rank-$(d-1)$ projector, which we denote by $P_{n_1}^{(d-1)}$. Clearly the multiplicity of the eigenvalue $-\kappa_{n_1}^2$ of $H_\lambda$ is $d-1$. This eigenvalue is fixed, i.e., independent of $\lambda$. In addition there is a moving eigenvalue of $H_\lambda$ which does depend on $\lambda$. It is obtained from the solution of the equation

$$\lambda^{-1} + \langle g|G(-\kappa^2)|g\rangle = 0,$$

i.e.,

$$f(\kappa) = \lambda^{-1}.$$

When $\lambda = 0$ this moving eigenvalue coincides with the $(d-1)$-fold degenerate eigenvalue $-\kappa_{n_1}^2$, (see Fig. 3).

So we see that the $d$ eigenvalues $-\kappa_{n_1}^2$ of $H$ are split up into $d-1$ fixed eigenvalues $-\kappa_{n_1}^2$ and 1 moving eigenvalue $E_n$ of $H_\lambda$. The corresponding eigenvectors of $H_\lambda$ are obtained from the residues of $G_\lambda$ at its poles. According to Eq. (5.6) the fixed eigenvectors are $|\kappa'_{n_i}\rangle$, $i = 2,3,\ldots d$ (or linear combinations). The unique eigenvector depending on $\lambda$ is given by Eq. (3.11),

$$|E_n\rangle_\lambda = G(E_n)|g\rangle\,(\langle g|G^2(E_n)|g\rangle)^{-1/2},$$

where $E_n = E_n(\lambda)$ is the corresponding eigenvalue.

## 6. CASE IV: $d$-FOLD DEGENERACY, $\langle g|\kappa_{n_i}\rangle = 0$; $i = 1,2,\ldots,d$

Just as in Sec. 5 we consider here a $d$-fold degenerate eigenvalue $-\kappa_{n_1}^2$,

$$H\,|\kappa_{n_i}\rangle = -\kappa_{n_1}^2\,|\kappa_{n_i}\rangle, \quad i = 1,2,\ldots,d. \tag{6.1}$$

In this section we assume furthermore that

$$\langle g|\kappa_{n_i}\rangle = 0, \quad i = 1,2,\ldots,d. \tag{6.2}$$

This implies that the perturbation $|g\rangle\langle g|$ is diagonal with

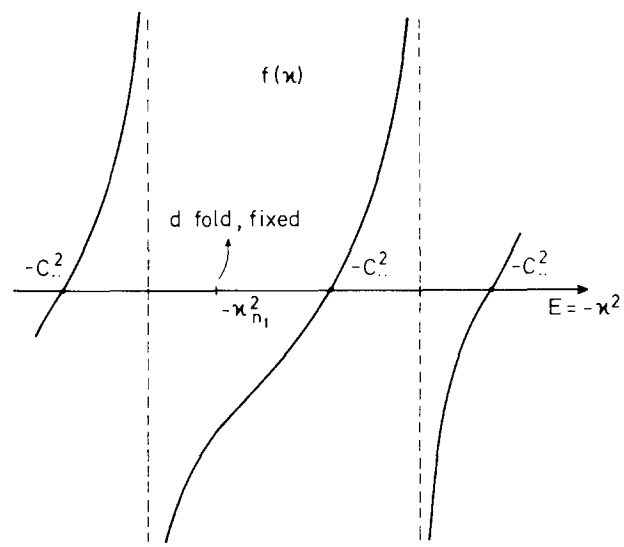


FIG. 4. The behavior of $f(\kappa)$ in case IV. The eigenvalue $-\kappa_{n_1}^2$ of $H$ is $d$-fold degenerate, and $\langle g|\kappa_{n_i}\rangle = 0$ for all $i = 1,2,\ldots,d$. This $d$-fold eigenvalue $-\kappa_{n_1}^2$ does not "feel" the perturbation $-\lambda\,|g\rangle\langle g|$ at all, i.e., it is a $d$-fold fixed eigenvalue of $H_\lambda$. There is one moving eigenvalue $E(\lambda)$ which coincides with $-\kappa_{n_1}^2$ for one particular value of $\lambda$ only [Eq. (6.5)].

respect to the basis states $|\kappa_{n_i}\rangle$ $(i = 1,2,...,d)$. Therefore no basis transformation is necessary here, in contrast to the case of Sec. 5.

From Eq. (2.6) we see that $G(-\kappa^2)|g\rangle$ is regular at $\kappa = \kappa_{n_1}$, by using Eq. (6.2). Therefore $G_\lambda(-\kappa^2)$ does have a pole at $\kappa = \kappa_{n_1}$, according to Eq. (2.7). So $-\kappa_{n_1}^2$ is an eigenvalue of $H_\lambda$. We shall now investigate the degree of degeneracy of this eigenvalue, and find that it is either $d$ or $d+1$.

For every real value of $\lambda$, except one, we have

$$\lambda^{-1} + \langle g|G(-\kappa_{n_1}^2)|g\rangle \neq 0. \tag{6.3}$$

When Eq. (6.3) holds, the residue of $G_\lambda$ at $\kappa = \kappa_{n_1}$ is given by the following projector,

$$P_{n_1}^{(d)} \equiv \lim_{\kappa \to \kappa_{n_1}} (-\kappa^2 + \kappa_{n_1}^2) G_\lambda(-\kappa^2) = \sum_{i=1}^{d} |\kappa_{n_i}\rangle\langle\kappa_{n_i}|. \tag{6.4}$$

This implies that the multiplicity of the eigenvalue $-\kappa_{n_1}^2$ is equal to $d$.

For one particular value of $\lambda$ we have

$$\lambda^{-1} + \langle g|G(-\kappa_{n_1}^2)|g\rangle = 0. \tag{6.5}$$

When Eq. (6.5) holds, we obtain the following projection operator,

$$P_{n_1}^{(d+1)} \equiv \lim_{\kappa \to \kappa_{n_1}} (-\kappa^2 + \kappa_{n_1}^2) G_\lambda(-\kappa^2) = \sum_{i=1}^{d} |\kappa_{n_i}\rangle\langle\kappa_{n_i}| + \frac{G(-\kappa_{n_1}^2)|g\rangle\langle g|G(-\kappa_{n_1}^2)}{\langle g|G^2(-\kappa_{n_1}^2)|g\rangle}. \tag{6.6}$$

So we see that the multiplicity of the eigenvalue $-\kappa_{n_1}^2$ equals $d+1$ in this case. There are $d$ fixed eigenvectors, independent of $\lambda$. These are just the eigenstates $|\kappa_{n_i}\rangle$ of $H$. The unique eigenvalue which does depend on $\lambda$ is given by

$$G(-\kappa_{n_1}^2)|g\rangle \quad (\langle g|G^2(-\kappa_{n_1}^2)|g\rangle)^{-1/2}, \tag{6.7}$$

as is easily seen from Eq. (6.6). The behavior of the function $f(\kappa) \equiv -\langle g|G(-\kappa^2)|g\rangle$ in the vicinity of $\kappa = \kappa_{n_1}$ has been sketched in Fig. 4.

## 7. ON RANK-N PERTURBATIONS

In this section we shall consider some interesting properties of a rank-$N$ perturbation. We have seen in Secs. 3–6 in which way the eigenvalues shift when a rank-1 potential is added to $H$. The eigenvalues are confined, for arbitrary strength $\lambda$, to certain intervals $(-c_n^2, -c_{n+1}^2)$, [see Eq. (3.9) and Fig. 1]. In general an eigenvalue of $H_\lambda$ cannot shift from a particular eigenvalue of $H$ to one of the two adjacent eigenvalues of $H$.

When a rank-1 potential is added to $H_\lambda$, the eigenvalues are again confined to certain intervals, different from $(-c_n^2, -c_{n+1}^2)$. It follows that, in general, any eigenvalue of $H$ plus a rank-2 potential can pass only the two adjacent eigenvalues of $H$.

By iteration we see that for a rank-$N$ perturbation, the eigenvalues can pass at most $N-1$ adjacent eigenvalues of $H$ upwards and $N-1$ adjacent eigenvalues of $H$ downwards. Exceptions to this general case occur when one (or more) of the form factors $|g_i\rangle$ is orthogonal to one or more of the bound state vectors of $H$, (cf. Sec. 4 and Fig. 2).

It is instructive to consider some explicit formulas. The Green operator corresponding to the rank-$N$ potential

$$V(\lambda_1,...,\lambda_N) = V - \sum_{i=1}^{N} |g_i\rangle\lambda_i\langle g_i| \tag{7.1}$$

is given by (cf., e.g., Sec. 5 of Ref. 9)

$$G(\lambda_1,...,\lambda_N) = G - \sum_{i,j=1}^{N} G|g_i\rangle\tau_{ij}\langle g_j|G, \tag{7.2}$$

where the matrix elements $\tau_{ij}$ follow from

$$(\tau^{-1})_{ij} = (\Lambda^{-1})_{ij} + \langle g_i|G|g_j\rangle. \tag{7.3}$$

It follows from Eq. (7.2) that, in order to find the poles of $G(\lambda_1,...,\lambda_N)$, one has to investigate the poles of $G$ and the poles of $\tau_{ij}$.

From now on we restrict ourselves to the case $N = 2$. Furthermore, we introduce the notations

$$g_{ij} \equiv \langle g_i|G|g_j\rangle \tag{7.4}$$

and

$$\tilde{\tau}_{ij} = D\tau_{ij}. \tag{7.5}$$

Here $D$ is the determinant of the $2\times 2$ matrix $\tau^{-1}$, so

$$D = (\det\tau)^{-1} = (\lambda_1^{-1} + g_{11})(\lambda_2^{-1} + g_{22}) - g_{12}^2. \tag{7.6}$$

Note that $g_{ij} = g_{ji}$ and $\tau_{ij} = \tau_{ji}$ because we restrict the energy variable $E$ to negative values. We have

$$\tilde{\tau} = \begin{pmatrix} \lambda_2^{-1} + g_{22} & -g_{12} \\ -g_{12} & \lambda_1^{-1} + g_{11} \end{pmatrix}. \tag{7.7}$$

According to Eq. (2.6), i.e.,

$$G(E) = \sum_n \frac{|\kappa_n\rangle\langle\kappa_n|}{E + \kappa_n^2} + \sum_m \cdots + \int \cdots dk,$$

$G$ has simple poles at $E = -\kappa_n^2$. We see from Eq. (7.2) that any pole $E$ of $G(\lambda_1,\lambda_2)$ is

(i) either equal to a zero of $D$

(ii) or equal to an eigenvalue $-\kappa_n^2$ of $H$. We shall investigate the latter case only.

To this end we deduce the residue of $G(\lambda_1,\lambda_2)$ at $E = -\kappa_n^2$ in closed form. By using Eq. (7.2)–(7.4) and (2.6) we obtain

$$\lim_{E \to -\kappa_n^2} (E + \kappa_n^2) G(\lambda_1,\lambda_2) = |\kappa_n\rangle\langle\kappa_n| \times \left[1 - \lim_{E \to -\kappa_n^2} \frac{\sum_{ij=1}^{N} \langle\kappa_n|g_i\rangle\tilde{\tau}_{ij}\langle g_j|\kappa_n\rangle}{(E + \kappa_n^2)D}\right]. \tag{7.8}$$

By using the explicit expressions of (7.6) and (7.7) for $D$ and $\tilde{\tau}$ we can evaluate the numerator and the denominator of the fraction in Eq. (7.8) in closed form. We obtain for both these quantities the *same* expression, namely

$$\lim_{E \to -\kappa_n^2} (E + \kappa_n^2) D = F. \tag{7.9}$$

Here $F$ is defined by

$$F \equiv (\lambda_1^{-1} + G_{11})\langle g_2|\kappa_n\rangle^2 + (\lambda_2^{-1} + G_{22})\langle g_1|\kappa_n\rangle^2 - 2G_{12}\langle g_1|\kappa_n\rangle\langle\kappa_n|g_2\rangle, \tag{7.10}$$

where the $G_{ij}$ are defined by [cf. Eq. (2.6)]

$$G_{ij} \equiv G_{ij}(-\kappa_n^2) \equiv \lim_{E \to -\kappa_n^2} \left( \langle g_i | G | g_j \rangle - \frac{\langle g_i | \kappa_n \rangle \langle \kappa_n | g_j \rangle}{E + \kappa_n^2} \right). \quad (7.11)$$

Therefore, the right-hand side of Eq. (7.8) will vanish in general,

$$\lim_{E \to -\kappa_n^2} (E + \kappa_n^2) G(\lambda_1, \lambda_2) = 0,$$

so that $G(\lambda_1, \lambda_2)$ has no pole at $E = -\kappa_n^2$. This is just what we expect: The perturbed eigenvalue differs in general from the unperturbed eigenvalue $-\kappa_n^2$. Clearly $G(\lambda_1, \lambda_2)$ *can* have a pole at $E = -\kappa_n^2$ only if

$$\lim_{E \to -\kappa_n^2} (E + \kappa_n^2) G(\lambda_1, \lambda_2) \neq 0.$$

So we see that "$F = 0$" is a *necessary* condition in order that a perturbed eigenvalue coincides with the unperturbed eigenvalue $-\kappa_n^2$.

It is interesting to consider the particular case $|g_1\rangle = |g_2\rangle$. Obviously the rank-two potential is then equal to a rank-one potential, so that our formulas must reduce to those of Secs. 3–6. Indeed we have in this case

$$F = (\lambda_1^{-1} + \lambda_2^{-1}) \langle g_1 | \kappa_n \rangle^2. \quad (7.12)$$

So $F$ can be zero only if either $\lambda_1 = -\lambda_2$ (vanishing perturbation) or if $|g_1\rangle$ is orthogonal to the eigenstate $|\kappa_n\rangle$ (in this case $-\kappa_n^2$ is a fixed eigenvalue). This is in agreement with the results of Sec. 4. On the other hand, when we let $\lambda_2$ go to zero, we see from Eq. (7.10) that $\lim_{\lambda_2 \to 0} \lambda_2 F$ can be zero only if $\langle g_1 | \kappa_n \rangle = 0$. This is again in agreement with previous results.

In general $F$ will not vanish for different $\kappa_n$'s, for fixed $\lambda_1$ and $\lambda_2$. In order to prove this, we shall work out a particular case. We take $\lambda_1 = \lambda_2 = \lambda$ fixed, and we assume that $\kappa_1 > \kappa_2 > \ldots$, and furthermore,

$$\langle g_1 | \kappa_1 \rangle \neq 0, \quad \langle g_1 | \kappa_2 \rangle \neq 0,$$
$$\langle g_2 | \kappa_1 \rangle = \langle g_2 | \kappa_2 \rangle = 0.$$

In this case $F$ reduces to

$$F(-\kappa_n^2) = (\lambda^{-1} + G_{22}(-\kappa_n^2)) \langle g_1 | \kappa_n \rangle^2. \quad (7.13)$$

By using Eq. (2.6) one easily verifies that

$$0 > G_{22}(-\kappa_1^2) > G_{22}(-\kappa_2^2).$$

Because $G_{22}(-\kappa_1^2)$ differs from $G_{22}(-\kappa_2^2)$, the equation

$$F(-\kappa_1^2) = F(-\kappa_2^2) = 0$$

cannot hold, according to Eq. (7.13).

By this example we have proved that the perturbed eigenvalues *do not all at the same time* coincide with (some of) the unperturbed eigenvalues, in general.

## 8. DISCUSSION

From the investigations of this paper we draw some interesting conclusions. Let $\Delta n_n$ denote the alteration in the number of nonpositive eigenvalues of $H$, caused by a perturbation $\lambda V$.

(i) We have proved that a rank-1 perturbation can alter the number of nonpositive eigenvalues $n_n$ (where the multiplicity is included) at most by 1:

$$|\Delta n_n| \leqslant 1.$$

By iteration one obtains from (i):

(ii) a rank-$N$ perturbation can alter $n_n$ at most by $N$:

$$|\Delta n_n| \leqslant N.$$

This fact can also be obtained from the first Weinstein–Aronszajn formula, (see Kato, Ref. 1 Ch. IV. 6, cf. Ref. 10).

For a rank-1 perturbation $-\lambda |g\rangle \langle g|$ we have proved the following interesting facts, which give more detailed information.

1. Given the Hamiltonian $H$ and the form factor $|g\rangle$, then one and only one of the following three alternatives applies:

a. Either $n_n$ increases by 1 if $\lambda$ goes from 0 to $+\infty$. In this case any finite negative $\lambda$ will not alter $n_n$. We have $f(0) > 0$, where $f$ is defined as $f(\kappa) \equiv -\langle g | G(-\kappa^2) | g \rangle$;

b. or $n_n$ decreases by 1 if $\lambda$ goes from 0 to $-\infty$. In this case any finite positive $\lambda$ will not alter $n_n$. We have $f(0) < 0$;

c. or the number of nonpositive eigenvalues is always $n_n$, independent of $\lambda$. This case applies if $f(0) = 0$.

2. The multiplicity of any nonpositive eigenvalue of $H$ can alter at most by 1 (a particular case of the Weinstein–Aronszajn formulas, see Ref. 1). A change in the multiplicity is caused by the so-called moving eigenvalues of $H_\lambda$. It is important to note that *a moving eigenvalue is always simple* (i.e., nondegenerate), except for one particular value of $\lambda$, when it coincides with some fixed eigenvalue.

3. More specifically, we have defined certain intervals with boundaries $-c_m^2$ and 0, see Figs. 1–4. The union of these intervals is just the real negative axis. When we let $\lambda$ go from $-\infty$ to $+\infty$, every moving eigenvalue shifts from the right-hand side to the left-hand side of some particular interval. Different eigenvalues move in different intervals. All moving eigenvalues are continuous and monotonically decreasing functions of $\lambda$.

Finally we consider the operator

$$H_\lambda = H - \lambda |g\rangle \langle g|$$

for $\lambda \to \pm \infty$. One might expect that every eigenvector of $H_\lambda$ will approach, in a certain sense, the form factor $|g\rangle$ when $\lambda$ goes to $+\infty$. However, only the ground-state vector of $H_\lambda$ converges to $|g\rangle$ in this case. The corresponding eigenvalue goes to $-\infty$, which means infinite binding energy. The remaining eigenvectors and eigenvalues of $H_\lambda$ have simple limits, both for $\lambda \to +\infty$ and for $\lambda \to -\infty$. We have obtained simple closed expressions:

(i) $\langle g | \kappa_n \rangle = 0$ for some $n$, then $|\kappa_n\rangle$ is not only eigenvector of $H$, but also of $H_\lambda$, with eigenvalue $-\kappa_n^2$, for all real $\lambda$.

(ii) All other eigenvectors of $H_\lambda$ have the form

$$c \cdot G(E_n) |g\rangle = \frac{c}{E_n - H} |g\rangle.$$

The eigenvalue $E_n$ is a solution $E = E_n$ of the equation,

$$\lambda^{-1} + \langle g | G(E) | g \rangle = 0.$$

Therefore, for $\lambda \to \pm \infty$, the eigenvalues $E_n$ are just given by the zeros of the quantity

$$\left\langle g \left| \frac{1}{E - H} \right| g \right\rangle.$$

So we see that $H_\lambda$ is, for $\lambda \to -\infty$, a well-defined operator, with simple eigenvectors and eigenvalues. Its essential spectrum is $[0, \infty)$, just as the essential spectrum of $H$.


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# Aharonov–Bohm scattering and the velocity operator

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It is shown that the existence of Aharonov–Bohm scattering depends upon the criteria used for establishing the stationary states. If one applies Pauli's criterion, there is no scattering. It is shown further that applying the usual criteria that the wave functions be continuous and single valued, as was done by Aharonov and Bohm, leads to stationary state wave functions which, with two exceptions, are eigenstates of the acceleration operator corresponding to eigenvalue zero. The acceleration operator is undefined for the remaining two states. Thus, only the eigenfunctions satisfying the Pauli criterion lead to well-defined, sensible physics.

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## I. INTRODUCTION

In a recent paper[1] it was argued that the total cross section for Aharonov–Bohm scattering diverges. This contradicts the well-known result of Strocchi and Wightman[2] that shows electrodynamics to be a local theory. It is this contradiction that has stimulated the investigation of the mathematical nature of Aharonov–Bohm (hereafter called AB) scattering reported here.

The author feels that it is essential to distinguish between AB scattering and the AB effect, which several investigators claim to have observed,[3–5] and which is treated in graduate textbooks, such as the one by Sakurai.[6] It must be noted that, in the past two years, papers have appeared that claim to prove the nonexistence of an AB effect[7–10]; their authors would say that the distinction being made here is superfluous. These papers will be discussed elsewhere; the only comment to be made here is that the author believes that some of the derivations of the AB effect in the literature are correct.

The claim being made here is considerably more modest than those of the papers cited above. It is shown here that the AB effect, if it exists, may not be interpreted as scattering.

AB scattering is alleged to be the scattering of electrons by a whisker of flux located along the $Z$ axis. The differential cross section was computed by AB[11] to be

$$\frac{d\sigma}{d\theta} = \frac{\sin^2(\pi\alpha)}{2\pi k \sin^2(\theta/2)}, \tag{1}$$

where $\alpha = -e\Phi/c\hbar$ and the energy of the incoming particle is $\hbar^2 k^2/2m$. This result was obtained by taking the wave function of the incident particle to be $e^{ikr\cos\theta}e^{-i\alpha\theta}$. This function gives a probability current density in the $x$ direction and is an eigenfunction of the velocity operator. It is also an energy eigenfunction, but it does not meet the commonly imposed requirement of continuity, unless $\alpha$ is an integer. It will be shown here that the criteria imposed by AB (i.e., continuity and single valuedness) are not the correct ones. The essential criterion for admissibility of wave functions was set down by W. Pauli[12,13] in 1939. Had AB subjected their energy eigenfunctions to Pauli's criterion, they would have found no scattering. This is shown below.

The Hamiltonian of the system is given by

$$H = \tfrac{1}{2}[\mathbf{P} - (e/c)\mathbf{A}(\mathbf{r})]^2, \tag{2}$$

where we put $m = \hbar = 1$. The vector potential is given by

$$A_r = 0, \quad A_\theta = \Phi/2\pi r. \tag{3}$$

The stationary state Schrödinger equation is then

$$-\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial\theta} + i\alpha\right)^2\right]\psi = \frac{k^2}{2}\psi, \tag{4}$$

## II. THE VELOCITY OPERATOR

In order to understand the physics of the scattering process, it is necessary to study the velocity operator, since changes in this quantity must be related to scattering. The velocity operator is

$$\mathbf{v} = \mathbf{P} - (e/c)\mathbf{A}(\mathbf{r}) = -i\nabla - (e/c)\mathbf{A}(\mathbf{r}). \tag{5}$$

It has components

$$v_x = \cos\theta v_r - \sin\theta v_\theta, \tag{6a}$$

$$v_y = \sin\theta v_r + \cos\theta v_\theta. \tag{6b}$$

It is convenient to introduce the operators

$$v_+ = v_x + iv_y, \tag{7a}$$

$$v_- = v_x - iv_y. \tag{7b}$$

Straightforward substitution then yields

$$v_+ = -ie^{i\theta}\frac{\partial}{\partial r} + \frac{e^{i\theta}}{r}\frac{\partial}{\partial\theta} + \frac{i\alpha e^{i\theta}}{r}, \tag{8a}$$

$$v_- = v_+^\dagger = -ie^{-i\theta}\frac{\partial}{\partial r} - \frac{e^{-i\theta}}{r}\frac{\partial}{\partial\theta} - \frac{i\alpha}{r}e^{-i\theta}. \tag{8b}$$

Equations (8) indicate that the velocity is not a vector under the spatial reflection $y \longleftrightarrow -y$. The condition $v_-(\theta) = v_+(-\theta)$ fails unless one also replaces $\alpha$ by $-\alpha$. This means that the particle velocity is a vector under spatial reflections only if one also reflects the velocities of the charges that act as the source of the magnetic flux. One notes that the Hamiltonian is also not invariant under $y \longleftrightarrow -y$ unless one puts $\alpha \longleftrightarrow -\alpha$, thus inverting the direction of the magnetic flux.

Formal computation shows that $v_+$ and $v_-$ commute, as long as no restrictions are placed upon the functions on which these operators act. The angular momentum operator is

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$$M = -i\frac{\partial}{\partial\theta}. \tag{9}$$

The operators $M$, $v_+$, and $v_-$ obey the commutation rules

$$[M,v_+] = v_+, \tag{10a}$$

$$[M,v_-] = -v_-. \tag{10b}$$

These equations lead to the results

$$[M,v_+v_-] = 0 \tag{11}$$

and

$$H = \tfrac{1}{2}v_+v_-. \tag{12a}$$

Thus, $M$ and $H$ commute, and we may use the eigenvalue $m$ of the angular momentum operator to characterize the eigenstates that comprise the basis of a Hilbert space of states having energy eigenvalue $k^2/2$. Thus if $M|m\rangle = m|m\rangle$, we find that Eq. (10a) implies that

$$Mv_+|m\rangle = (m+1)v_+|m\rangle \tag{13a}$$

and Eq. (10b) implies that

$$Mv_-|m\rangle = (m-1)v_-|m\rangle. \tag{13b}$$

$v_+$ is therefore a raising operator and $v_-$ is a lowering operator.

Let us restrict $\alpha$ to the range $0 < \alpha < 1$. Other values of $\alpha$ can be treated by making obvious changes in the discussion that follows. We are now ready to discuss solutions of the stationary state equation (4). Pauli[12,13] would argue that the appropriate energy eigenfunctions are those solutions of Eq. (4) that are square integrable and are closed under the operations $v_+$ and $v_-$. This set of functions is

$$J_\nu(kr)e^{i\nu\theta}e^{-i\alpha\theta}, \quad \nu = 0, \pm 1, \pm 2, \cdots. \tag{14}$$

This choice of stationary states leads to understandable physics, since the incident wave used by AB can be expanded in terms of these functions. Hence, there is no scattering.

It is enlightening to investigate the behavior of the AB eigenfunctions under the operations $v_+$ and $v_-$. These eigenfunctions are

$$|m\rangle = J_{|m+\alpha|}(kr)e^{im\theta}, \quad m = 0, \pm 1, \pm 2, \cdots. \tag{15}$$

One quickly sees that the operator $v_+$ can be used to generate the positive $m$ states from the eigenstate $|0\rangle$. The operator $v_-$ may similarly be used to generate the negative $m$ state from the state $|-1\rangle$. These results follow easily from the well-known recurrence relations for Bessel functions. It is clear however, that there are two distinct chains of eigenstates that are not linked to each other by $v_+$ and $v_-$.

From the recurrence relations for Bessel functions, we see that $v_-|0\rangle$ involves $J_{-1+\alpha}(kr)$; this function does not lie in the Hilbert space of AB eigenfunctions. It is infinite at the $Z$ axis, while the AB eigenfunctions all vanish there. Applying $v_-$ twice to the state $|0\rangle$ produces a function that is not square integrable over any region containing the $Z$ axis. Similarly, the function $v_+|-1\rangle$ does not lie in the AB Hilbert space. Thus in order to treat the problem using the AB eigenfunctions, one must modify the Hamiltonian to the form

$$H = \tfrac{1}{2}\sum_{m>0} v_-v_+P_m + \tfrac{1}{2}\sum_{m<0} v_+v_-P_m, \tag{12b}$$

where the $P_m$ are the projectors that project on the states $|m\rangle$. Then, on a subspace of fixed energy $k^2/2$, the operators $v_+$ and $v_-$ become multiples of isometric operators $U$ and $U^\dagger$, so that

$$v_+ = kU \quad \text{and} \quad v_- = kU^\dagger. \tag{16a,b}$$

The state $|-1\rangle$ is not in the domain of $U$ and the state $|0\rangle$ is not the domain of $U^\dagger$. The acceleration operator that gives the rate of change of $v_+$ is

$$a_+ = i[H,v_+] = ik\,[H,U]. \tag{17}$$

Similarly, we may define $a_-$ by

$$a_- = i[H,v_-] = ik\,[H,U^\dagger]. \tag{18}$$

Equations (12b), (17), and (18) show that $a_+$ and $a_-$ are zero operators when they operate on states in their respective domains of definition. The same is true of the Hermitian operators

$$a_x = \tfrac{1}{2}(a_+ + a_-) \quad \text{and} \quad a_y = (1/2i)(a_+ - a_-).$$

We therefore conclude that the AB states are all states of zero acceleration, except for the states $|0\rangle$ and $|-1\rangle$. The acceleration of the particle in these states is not defined. Thus to have well-defined observables, one must make the Pauli choice of eigenfunctions given in Eq. (14). Only this choice leads to well-defined, sensible physics.

It is well known that if a time independent Schrödinger equation has a solution $\psi^0(\mathbf{r})$, then, if a vector potential having a vanishing curl is added to the system, the corresponding energy eigenstate is given by

$$\psi(\mathbf{r}) = \psi^0(\mathbf{r})e^{(ie/\hbar c)\int^{\mathbf{S}(\mathbf{r})}\mathbf{A}(\mathbf{r}')\cdot d\mathbf{S}'}, \tag{19}$$

where $\mathbf{S}(\mathbf{r})$ is the point $\mathbf{r}$ itself. The path of integration is otherwise arbitrary. In the AB problem, $\mathbf{A}(\mathbf{r})$ is given by Eq. (3). If we take the integration path to begin at any point on the positive $x$ axis, then Eq. (19) becomes

$$\psi(\mathbf{r}) = \psi^0(\mathbf{r})e^{(ie/\hbar c)(\Phi/2\pi)\theta} = \psi^0(\mathbf{r})e^{-i\alpha\theta}. \tag{20}$$

Thus the proper eigenfunctions are related to the corresponding zero flux eigenfunctions by the usual London rule. It is therefore clear that correct discussion of the Aharonov–Bohm effect must deal with any physical consequences of this phase factor in a proper way.


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# Some models of anisotropic spheres in general relativity

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A heuristic procedure is developed to obtain interior solutions of Einstein's equations for anisotropic matter from known solutions for isotropic matter. Five known solutions are generalized to give solutions with anisotropic sources.

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## I. INTRODUCTION

The assumption of local isotropy is a common one in astrophysical studies of massive objects. However, recent theoretical work on more realistic stellar models suggests that stellar matter may be anisotropic at least in certain density ranges.[1,2] Anisotropy could be introduced by the existence of a solid core, by the presence of type $P$ superfluid, or by other physical phenomena. In this paper we do not discuss the mechanisms for inducing anisotropies. Rather, we concentrate on the following two questions:

a) What is the extent to which isotropic models differ from anisotropic ones?

b) How do we develop suitable models for anisotropic matter in the context of general relativity?

Anisotropic matter has already been considered,[3,4] and it has already been shown that some properties of anisotropic spheres may drastically differ from the properties of isotropic spheres. This paper is organized as follows:

In Sec. II we give the general conventions and the field equations. We describe the procedure for obtaining anisotropic models in Sec. III. In Sec. IV we give five examples. The last section contains a discussion of the results.

## II. THE FIELD EQUATIONS

Let us consider a static distribution of matter which is spherically symmetric but whose stress tensor may be locally anisotropic.

In Schwarzschild-like coordinates the metric can be written as:

$$ds^2 = e^{\nu}dt^2 - e^{\lambda}dr^2 - r^2d\theta^2 - r^2\mathrm{sen}^2\theta\, d\phi^2.$$

Denoting differentiation with respect to $r$ by a dash, letting $(t,r,\theta,\phi) = (0,1,2,3)$, the metric field equations read:

$$8\pi T_1^1 = -e^{-\lambda}[\nu'/r + 1/r^2] + 1/r^2, \tag{1}$$

$$8\pi T_2^2 = 8\pi T_3^3 = -e^{-\lambda}[\tfrac{1}{2}\nu'' - \tfrac{1}{4}\lambda'\nu' + \tfrac{1}{4}\nu'^2 + (\nu' - \lambda')/2r], \tag{2}$$

$$8\pi T_0^0 = e^{-\lambda}[\lambda'/r - 1/r^2] + 1/r^2, \tag{3}$$

with $T_\nu^\mu = \mathrm{diag}(\rho, -P_r, -P_\perp, -P_\perp)$, where $P_r$ and $P_\perp$ denote respectively the radial and tangential "pressure". Using (1) and (2) (or the equivalent, the conservation condition $T^\mu_{1;\mu} = 0$) the equation for hydrostatic equilibrium is found:

$$\frac{dP_r}{dr} = -(\rho + P_r)\frac{\nu'}{2} + \frac{2}{r}(P - P_r). \tag{4}$$

Integrating (3):

$$e^{-\lambda} = 1 - 2m(r)/r, \tag{5}$$

where

$$m(r) = \int_0^r 4\pi r^2\rho\, dr. \tag{6}$$

From (1) and (3):

$$\frac{\nu'}{2} = \frac{m(r) + 4\pi r^3 P_r}{r(r - 2m)}. \tag{7}$$

Obviously in the isotropic case ($P_r = P$) Eq. (4) becomes the usual Tolman–Oppenheimer–Volkov (TOV) equation for hydrostatic equilibrium.

Before trying to find specific models, we write Eq. (4) in a different form. Let

$$P_\perp - P_r = Cf(P_r,r)(\rho + P_r)r^n, \tag{8}$$

where $C$ is a parameter which measures the anisotropy; the function $f$ and the number $n$ are to be specified for each model. Taking in to account (8), Eqs. (4) becomes

$$dP_r/dr = -(\rho + P_r)\nu'/2 + 2Cf(P_r,r)(\rho + P_r)r^{n-1}. \tag{9}$$

Equation (9) can be integrated if $\rho$ is a known function of $r$ and $f(P_r,r)$ is specified. We keep the usual boundary condition $P_r(a) = 0$, where $a$ is the radius of the sphere.

## III. THE PROCEDURE

The chief question is how to choose the function $f(P_r,r)$. One approach would be to consider (9) as defining this function for arbitrary $\rho(r)$ and $P_r$. However this might produce models with strange pressure distributions and would usually not permit $C = 0$ as a subclass of a particular model. The ideal approach, of course, would be to know the relation

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between $P_r$ and $P_\perp$ on physical grounds. We shall propose a heuristic method which allows us to find a family of nonisotropic models from any isotropic model; the family will depend continuously on $C$ and permit the isotropic situation, $C = 0$, as a special case.

The procedure is as follows:

1) Take a known exact interior solution of the Einstein equations and assume the functional dependence of $\rho = \rho(r)$ of the anisotropic model is the same as that of the isotropic solution. In fact one does not expect that the presence of stresses (at least for small values of $C$) will change the matter distribution drastically.

2) Assume

$$f(P_r,r)r^{n-1} = \nu'/2. \tag{10}$$

This relation is not assumed for any specific physical reason but only because it transforms Eq. (9) into the simple form:

$$\frac{dP_r}{dr} = -h(\rho + P_r)\nu'/2, \tag{11}$$

where $h = 1 - 2C$.

The next section is devoted to the integration of Eq. (11) for different density distributions $\rho(r)$. Notice that for $h = 1$, we recover the isotropic case. $h = 0$, because of the boundary condition, implies $P_r = 0$. Such a configuration corresponds to a sphere sustained only by tangential stresses. It has been considered in a different context by Lemaître.[5]

## IV. THE MODELS

### A. Schwarzschild-like model

The first model we discuss is a generalization of the Schwarzschild interior solution. Such a generalization is already known,[3] and we can examine how our method reproduces this known solution for anisotropic matter.

Following the procedure sketched in the last section we imagine an anisotropic sphere whose density is independent of the spacelike coordinates,

$$\rho = \begin{cases} \rho_0 = \text{const}, & 0 < r < a \\ 0, & r > a \end{cases}. \tag{12}$$

Equation (6) gives

$$m(r) = \tfrac{4}{3}\pi r^3 \rho_0, \tag{13}$$

and condition (10) reads:

$$f(r,P_r)r^{n-1} = \tfrac{1}{2}\nu' = \tfrac{4}{3}\pi r(\rho_0 + 3P_r)(1 - (8\pi/3)r^2\rho_0)^{-1} \tag{14}$$

where Eq. (7) has been used. Equation (11) takes the form

$$\frac{dP_r}{dr} = -\tfrac{4}{3}\pi h(\rho_0 + P_r)(\rho_0 + 3P_r) \times (1 - (8\pi/3)\rho_0 r^2)^{-1} r. \tag{15}$$

Equation (15) can be integrated to obtain the radial pressure

$$P_r = \rho_0 \left[ \frac{(1 - \frac{8}{3}\pi r^2\rho_0)^{h/2} - (1 - \frac{8}{3}\pi a^2\rho_0)^{h/2}}{3(1 - \frac{8}{3}\pi a^2\rho_0)^{h/2} - (1 - \frac{8}{3}\pi r^2\rho_0)^{h/2}} \right] \tag{16}$$

or

$$P_r = \rho_0 \left[ \frac{(1 - 2m/r)^{h/2} - (1 - 2M/a)^{h/2}}{3(1 - 2M/a)^{h/2} - (1 - 2m/r)^{h/2}} \right], \tag{16'}$$

where $M$ is the total mass.

It is worthwhile to recall some properties of this model. For example, the critical value of the quantity $2M/a$ for which the central pressure tends to infinity is

$$2(M/a)_{\text{crit}} = 1 - (1/3)^{2/h}, \tag{17}$$

thus, the limiting case $h = 0$ ($C = 1/2$) yields $(2M/a)_{\text{crit}} = 1$ and the horizon may be reached. We recall that in the isotropic case ($h = 1$) the critical value is:

$$(2M/a)_{\text{crit}} = \tfrac{8}{9}.$$

The critical mass is

$$M_{\text{crit}} = (3/32\pi\rho_0)^{1/2}[1 - (1/3)^{2/h}]^{3/2}. \tag{18}$$

The ratio of the critical mass for the anisotropic case to the corresponding value for the isotropic case is given by

$$\frac{Ma_{\text{crit}}}{Mi_{\text{crit}}} = \tfrac{9}{8}[1 - (1/3)^{2/h}]^{3/2}. \tag{19}$$

This ratio is less than one for $h > 1$ ($C < 0$) and greater than one for $h < 1$ ($C < 0$).

Furthermore the expression (17) affects the redshift $z$ at the surface, given by

$$z = (1 - 2M/a)^{-1/2} - 1. \tag{20}$$

The critical value for the redshift is

$$z_{\text{crit}} = 3^{1/h} - 1, \tag{21}$$

thus, in principle, anisotropy is capable of explaining redshifts larger than two.

It is easy to use (16') and (7) to obtain $\nu$

$$e^{\nu} = \left[ \frac{3(1 - 2M/a)^{h/2} - (1 - 2m/r)^{h/2}}{2} \right]^{2/h}. \tag{22}$$

### B. Tolman VI-like model

The next model we shall generalize is solution VI of Tolman.[6] We recall that the equation of state of this model, for large $\rho$, approaches that for a highly compressed Fermi gas.

Using the procedure discussed above and the fact that the matter density is

$$8\pi\rho = 3/7r^2, \tag{23}$$

we get the following equation for $P_r$

$$\frac{dP_r}{dr} = -h(3/56\pi r^2 + P_r)(3/8r + 7\pi r P_r). \tag{24}$$

This equation can be integrated to obtain

$$P_r(r) = \frac{9h}{56\pi r^2}\left[\frac{1-(r/a)^{\sqrt{(4-3h)}}}{(8-3h+4\sqrt{(4-3h)})-(8-3h-4\sqrt{(4-3h)})(r/a)^{\sqrt{(4-3h)}}}\right]. \tag{25}$$

This solution restricts the values of $h$, $h<4/3$, or equivalently, $C> -1/6$. For the special case $h=4/3$, the solution is

$$P_r(r) = \frac{3}{56\pi r}\left[1-\frac{2}{2-\ln(r/a)}\right]. \tag{26}$$

Of course for the case $h=1$ we recover the Tolman VI solution. Also for $h=0$, $P_r=0$, as expected. The ratio of the central pressure to the central density is

$$P_c/\rho_c = 3h/\left(8-3h+4\sqrt{4-3h}\right). \tag{27}$$

In the case $h=1$, one gets the well-known result

$$P_c/\rho_c = \tfrac{1}{3}.$$

For the limiting value $h=4/3$, the ratio is

$$P_c/\rho_c = 1,$$

which in some sense represents a natural limiting value for the equation of state at the center of the sphere. The equation of state for the radial pressure can be written as

$$P_r(\rho) = 3h\rho\left[\frac{1-(3/56\pi)^{\sqrt{(4-3h)}/2}(\rho^{-1/2}/a)^{\sqrt{(4-3h)}}}{(8-3h+4\sqrt{(4-3h)})-(8-3h-4\sqrt{(4-3h)})(3/56\pi)^{\sqrt{(4-3h)}/2}(\rho^{-1/2}/a)^{\sqrt{(4-3h)}}}\right], \tag{28}$$

which for large values of $\rho$, becomes

$$\rho - \frac{(8-3h+4\sqrt{(4-3h)})}{3h}P_r = \left(\frac{3}{56\pi a^2}\right)^{\sqrt{(4-3h)}/2}\rho^{1-\sqrt{(4-3h)}/2}. \tag{29}$$

In the case $h=1$, we recover the expected result

$$\rho - 3P_r = \text{const}\rho^{1/2}. \tag{30}$$

For the limiting value $h=4/3$, the equation of state takes the form

$$P_r(\rho) = \left[1-\frac{4}{4-\ln(3/56\pi\rho a^2)}\right]. \tag{31}$$

Now it is not difficult to find the metric function $\nu$. Feeding (25) back into (7) and using (23)

$$e^{\nu} = \frac{4}{7}\left[\frac{(8-3h+4\sqrt{(4-3h)})-(8-3h-4\sqrt{(4-3h)})(r/a)^{\sqrt{(4-3h)}}}{8\sqrt{(4-3h)}}\right]^{1/h}\left(\frac{r}{a}\right)^{(6+\sqrt{(4-3h)})/(8-3h+4\sqrt{(4-3h)})}. \tag{32}$$

At the surface $r=a$

$$e^{\nu}\Big|_{r=a} = 1-2M/a = \tfrac{4}{7},$$

which agrees with the expression for the exterior Schwarzschild metric.

For the limiting value $h=4/3$, the metric function $\nu$ takes the form

$$e^{\nu} = \tfrac{4}{7}[(r/2a)(2-\ln(r/a))]^{3/2}. \tag{33}$$

Equation (24) has also been integrated numerically. Introduce the following dimensionless quantities

$$\hat{P} = P_r M^2, \tag{34}$$

$$z = a/r, \tag{35}$$

where $M$ is the total mass. Equation (24) becomes

$$\frac{d\hat{P}}{dz} = \tfrac{3}{4}h\hat{P}/z + 7\pi h\,(14/3)^2\hat{P}^2/z^3 + (9/7\times 64\pi)(3/14)^2 hz, \tag{36}$$

where the fact that $M/a = 3/14$ has been used. Solutions of (36) for differents values of $h$ are indicated in Fig. 1. It is worthwhile to observe that negative values of $h$ correspond to negative radial pressures. Such situations cannot be excluded *a priori* since we are not considering perfect fluids.

### C. Tolman IV-like model

Let us consider a generalization of the Tolman IV solution. We recall that the equation of state of this solution leads to results similar to those which would be obtained from the equation of state for a Fermi gas in cases of intermediate central densities. As in the preceding cases, the density is assumed to have the same functional dependence as for the isotropic case, thus

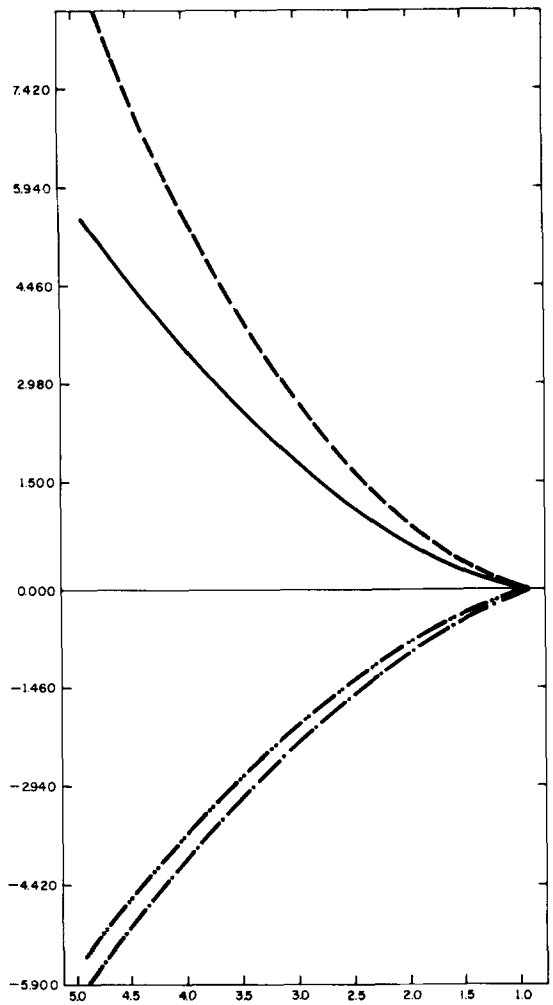


FIG. 1. The function $\hat{P} \equiv P_r M^2$ versus $z \equiv a/r$ for the Tolman VI-like model and $\epsilon = 3/14$.
a) $h = 1$ ————————
b) $h = 1.333$ ----------
c) $h = -3.1888$ -.-.-.-.-.-.-.-.-
d) $h = -2.7699$ -..-..-..-..-..-..

$$8\pi\rho = \frac{1}{A^2}\frac{(1 + 3A^2/R^2 + 3r^2/R^2)}{(1 + 2r^2/A^2)} + \frac{2}{A^2}\frac{(1 - r^2/R^2)}{A(1 + 2r^2/A^2)^2}, \tag{37}$$

where $A^2$ and $R^2$ are constants which in the isotropic case are related in a specific way through the central density and central pressure.

We calculate the function $m(r)$ and obtain

$$m(r) = r^3(R^2 + A^2 + r^2)/2R^2(A^2 + 2r^2). \tag{38}$$

Hence

$$f(r,P_r)r^{n-1} = \tfrac{1}{2}\nu' r[(R^2 + A^2 + r^2) + 8\pi R^2 P_r \times (A^2 + 2r^2)]/2(R^2 - r^2)(A^2 + r^2) \tag{39}$$

and the equilibrium equation becomes

$$8\pi\frac{dP_r}{dr} = -hr/2\left[\frac{(R^2 + 3A^2 + 3r^2)}{R^2(A^2 + 2r^2)} + \frac{2A^2(R^2 - r^2)}{R^2(A^2 + 2r^2)} + 8\pi P_r\right] \times \left[\frac{(R^2 + A^2 + r^2) + 8\pi R^2 P(A^2 + 2r^2)}{(R^2 - r^2)(A^2 + r^2)}\right]. \tag{40}$$

For $h \geqslant 3$, the integral is given by

$$\tilde{P} = 8\pi A^2 P_r(r) = \left(\frac{h}{2-h}R^2 - \frac{3-2h}{2-h}A^2 - 3r^2\right)\Big/A^2(A^2 + 2r^2). \tag{41}$$

Unfortunately, this pressure is less than zero for all real $r$ and approaches $-(3/2)A^2$ as $r \to \infty$. Hence the regime $h > 3$ cannot correspond to a bounded distribution of matter.

We did not succeed in finding an analytical solution to (40) other than (41), so that we integrated that equation numerically. In order to do that, we introduce the following dimensionless quantities:

$$\tilde{P} = 8\pi A^2 P_r,$$
$$\tilde{\rho} = 8\pi A^2 \rho,$$
$$z = 1/(y + \epsilon),$$
$$y = r/A; \quad \epsilon = M/a, \quad \kappa = A^2/R^2.$$

Thus Eq. (40) becomes

$$\frac{d\tilde{P}}{dz} = \frac{h(1 - \epsilon z)}{2z}\left[\frac{z^2(1 + 3\kappa) + 3\kappa(1 - \epsilon z)^2}{z^2 - 2(1 - \epsilon z)^2} + \frac{2z^2[z^2 - \kappa(1 - \epsilon z)^2]}{[z^2 + 2(1 - \epsilon z)^2]^2} + \tilde{P}\right] \times \left[\frac{z^2(1 + \kappa) + \kappa(1 - \epsilon z)^2 + \tilde{P}[z^2 + 2(1 - \epsilon z)^2]}{[z^2 - \kappa(1 - \epsilon z)^2][z^2 + (1 - \epsilon z)^2]}\right]. \tag{42}$$

In order to integrate this equation numerically we must specify the values of $\epsilon$, $\kappa$ and $h$; also the boundary condition $\tilde{P}(z_0) = 0$, where $z_0 = z|_{r=a}$, requires that the value of $Y_0 = a/A$ be given.

Now, from the condition

$$e^{-\lambda}|_{(r=a)} = 1 - 2M/a \tag{43}$$

we get

$$\epsilon = M/a = Y_0^2(1 + \kappa + Y_0^2)/2(1 + 2Y_0^2), \tag{44}$$

where the relation

$$e^{\lambda} = R^2(A^2 + 2r^2)/(R^2 - r^2)(A^2 + r^2)$$

has been used.

For the isotropic case ($h = 1$) we have the analytic solution

$$\tilde{P}(Y) = (1 - \kappa - 3\kappa Y^2)/(1 + 2Y^2) \tag{45}$$

and thus the boundary condition, in this case, leads to

$$Y_0^2 = (1 - \kappa)/3\kappa. \tag{46}$$

Feeding (46) back into (44) we obtain

$$\kappa = 1 - 3\epsilon. \tag{47}$$

Also, because of (44)

$$Y_0 = \left[\frac{4\epsilon - 1 - \kappa + \sqrt{((1 + \kappa)^2 - 8\epsilon + 16\epsilon^2)}}{2\kappa}\right]^{1/2}; \tag{48}$$

thus, fixing $\epsilon$, one gets uniquely the values of $Y_0$ and $\kappa$.

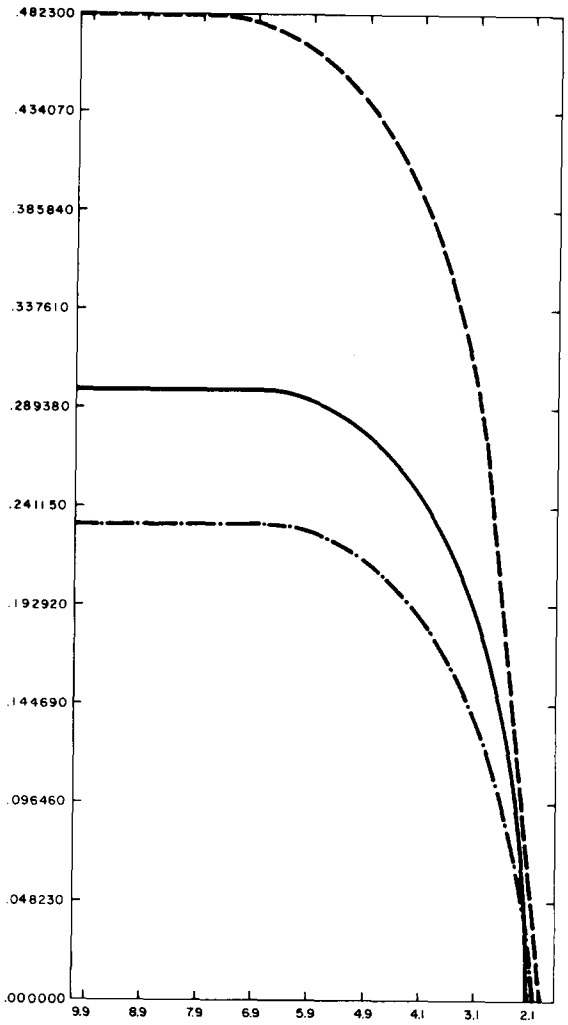


FIG. 2. The function $\hat{P} \equiv 8\pi A^2 P$, versus $z = (1/(r/A) + \epsilon)$ in the Tolman IV-like model, with $\epsilon = 0.1$ and
a) $h = 1$ ——————
$k = 0.70$
b) $h = 1.33$ - - - - - - - - - - - - - - - -
$k = 0.88$
c) $h = 0.67$
$k = 1.04$ -.-.-.-.-.-.-.-.-.-

In the nonisotropic case ($h \neq 1$) we do not have an analytic solution like (45) and so the values of $\kappa$ and $Y_0$ cannot be obtained from $\epsilon$. In order to pick values of $\kappa$ and $Y_0$ which would not lead to unphysical situations, we shall integrate for values of $h$ not very far from 1, and for $\kappa$ we shall take

$$\kappa(h) = \kappa(h = 1)[1 + |1 - h|/h]. \tag{49}$$

Fortunately Eq. (42) is "stable" with respect to a perturbation of the coefficients such as (49). Specifically we have integrated for the following cases:

1) $\epsilon = 0.1$:

| | | | |
|---|---|---|---|
| i) | $h = 1$, | $\kappa = 0.7$, | $z_0 = 2.09$, |
| ii) | $h = .67$, | $\kappa = 1.04$, | $z_0 = 2.29$, |
| iii) | $h = 1.33$, | $\kappa = 0.88$, | $z_0 = 2.20$, |

2) $\epsilon = 0.3$:

| | | | |
|---|---|---|---|
| i) | $h = 1$, | $\kappa = 0.1$, | $z_0 = 0.49$, |
| ii) | $h = 0.67$, | $\kappa = 0.15$, | $z_0 = 0.56$, |
| iii) | $h = 1.33$, | $\kappa = 0.13$, | $z_0 = 0.53$. |

The results of integration are displayed in Figs. 2 and 3. The accuracy of the numerical analysis was checked against the exact solution (for the case $h = 1$) with excellent results.

### D. Tolman V-like model

Though the Tolman V solution does not represent any interesting physical situation, we have generalized this model in order to obtain more information about the difference between the isotropic and the anisotropic case.

Following the established procedure,

$$8\pi\rho = 3/7r^2 + (10/3R^2)(r/R)^{1/3}, \tag{50}$$

$$m = (3/14)r + r^{10/3}/2R^{7/3}, \tag{51}$$

$$e^{-\lambda} = 4/7 - (r/R)^{7/3}, \tag{52}$$

where $R$ is a constant.

The condition (10) reads

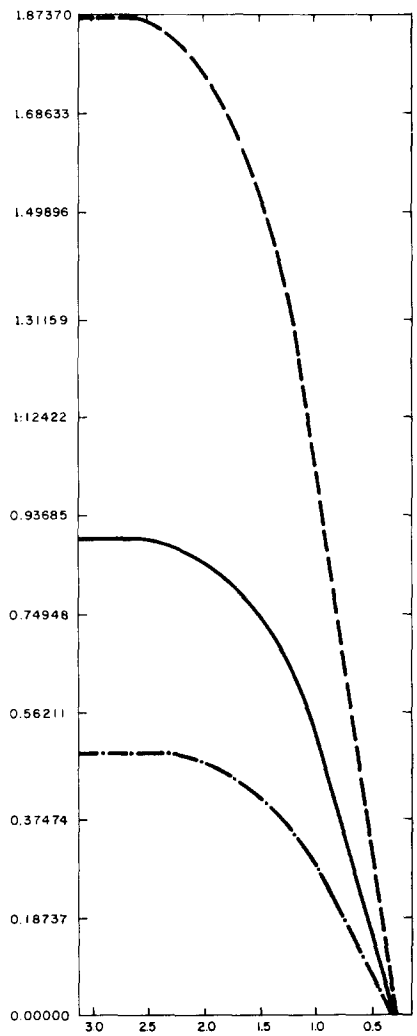


FIG. 3. The same function as in Fig. 2, with $\epsilon = 0.3$ and
$h = 1$ ——————
$k = 0.1$
$h = 1.33$ - - - - - - - - - - - - - - - -
$k = 0.13$
$h = 0.67$ -.-.-.-.-.-.-.-.-.-
$k = 0.15$

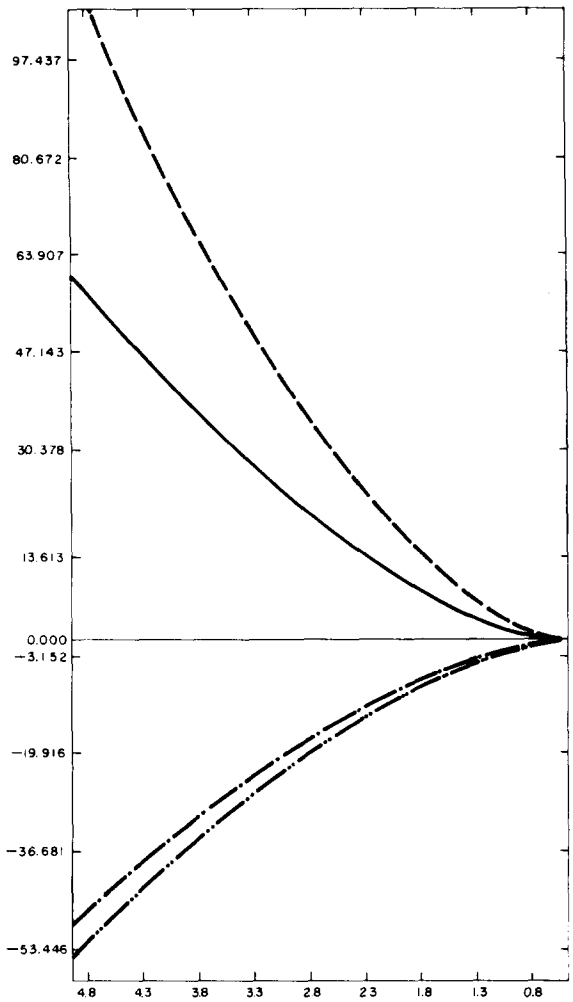


FIG. 4. The function $\hat{P} \equiv 8\pi R^2 P_r$ versus $z \equiv \epsilon R/r$ in the Tolman V-like model, with $\epsilon = 0.25$, and
$h = 1$ ——————
$h = 1.33$ ----------
$h = -2.77$ -.-.-.-.-.-.-.-.-
$h = -3.188$ -..-..-..-..-..-..-

$$f(r,P_r)r^{n-1}$$

$$= \tfrac{1}{2}\nu' = (3R^{7/3} + 7r^{7/3} + 56\pi P_r R^{7/3} r^2)/2r(4R^{7/3} - 7r^{7/3}) \tag{53}$$

so that the equilibrium equation becomes

$$8\pi \frac{dP_r}{dr} = -h\left[\, 3/7r^2 + \tfrac{10}{3}(r/R)^{1/3} + 8\pi P_r \right] \times [(3R^{7/3} + 7r^{7/3} + 56\pi P_r R^{7/3} r^2)/2r(4R^{7/3} - 7r^{7/3})]. \tag{54}$$

We could not find an analytic solution for (54), so we carried out a numerical integration. To do so, we introduce the new dimensionless variables

$$\tilde{P} = 8\pi R^2 P_r,$$

$$\tilde{\rho} = 8\pi R^2 \rho,$$

$$z = \epsilon R/r,$$

with $\epsilon = M/a$. In terms of the new variables, Eq. (54) reads

$$\left[\tfrac{4}{7}(\epsilon/z) - (\epsilon/z)^{10/3}\right](z^2/\epsilon)\frac{d\tilde{P}}{dz} = h(\epsilon/z)^2\tilde{P}^2/2 + h\left[\tfrac{3}{7} + \tfrac{13}{6}(\epsilon/z)^{7/3}\right]\tilde{P} + h\left[\tfrac{9}{98}(z/\epsilon)^2 + \tfrac{13}{14}(\epsilon/z)^{1/3} + \tfrac{5}{3}(\epsilon/z)^{8/3}\right]. \tag{55}$$

The surface of the star is defined by the value $z_0 = \epsilon R/a$; furthermore, the ratio $R/a$ can be expressed through $\epsilon$ using Eq. (51)

$$\frac{R}{a} = \left[\, 2(\epsilon - \tfrac{3}{14})\right]^{-3/7}. \tag{56}$$

In the isotropic case ($h = 1$)

$$R/a = (14)^{3/7}$$

and

$$\epsilon = \tfrac{1}{4}.$$

We have integrated for $\epsilon = 1/4$; $h = 1.33$, $h = 1$, $h = -2.77$, $h = -3.188$ and for $\epsilon = 0.3$; $h = 1.33$, $h = -3.188$, $h = -2.77$.

The solutions are shown in Figs. 4 and 5.

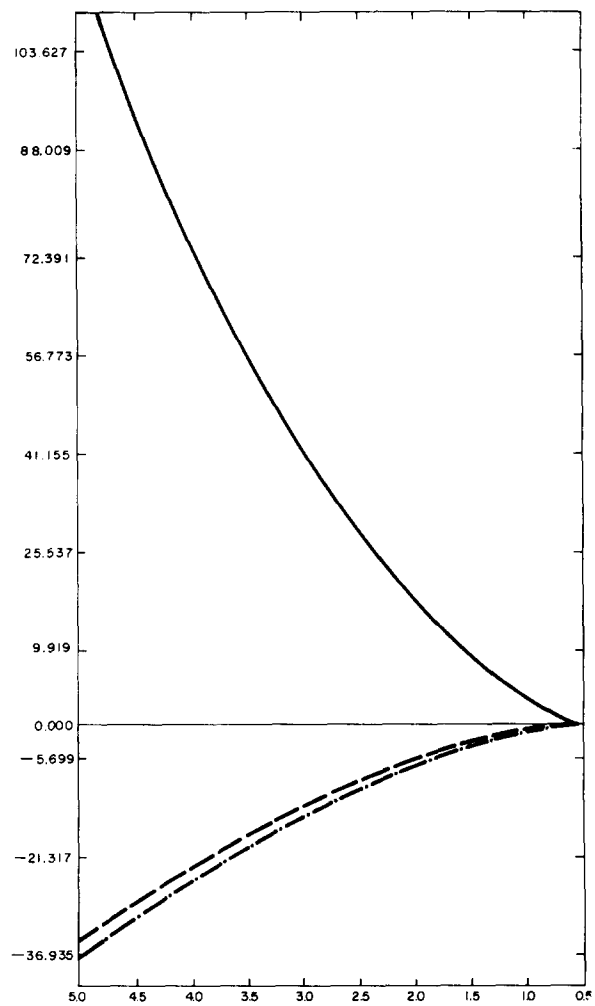


FIG. 5. Same function as before but $\epsilon = 0{,}3$ and
$h = 1.33$ ——————
$h = -2.77$ ----------
$h = -3.188$ -.-.-.-.-.-.-.-.-

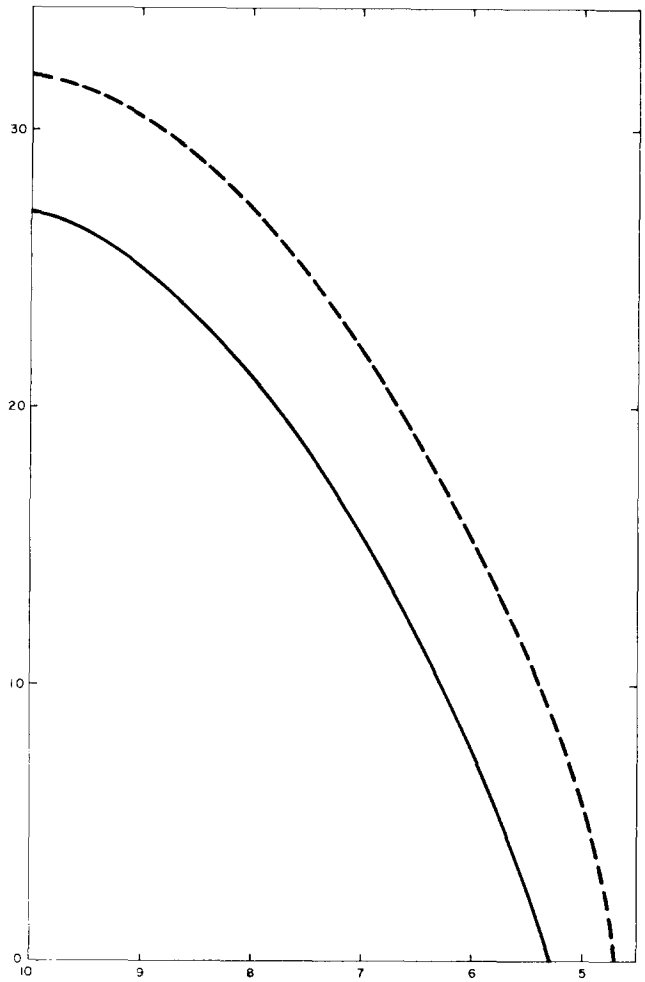


FIG. 6. The function $10^4 \times \hat{P} \equiv 10^4 8\pi P_r/\gamma$ versus $z \equiv (r\beta)^{-1/2}$ in the Adler-like model, with $\epsilon = 0.35$, and
$h = 1$ ——————
$\alpha = 0.23$
$\delta = -3.28$
$h = 1.33$
$\alpha = 0.29$ ----------
$\delta = -1.85$

### E. Adler-like model

Lastly, we shall apply our procedure to a solution found by Adler.[7] This solution is adiabatically stable, does not exhibit singularities and in principle could be used in astrophysical considerations.

The density is given by

$$8\pi\rho = 4\gamma\beta r^2/(\alpha + 3\beta r^2)^{5/3} - 3\gamma/(\alpha + 3\beta r^2)^{2/3}, \tag{57}$$

where $\gamma, \beta$ and $\alpha$ are constants. In addition,

$$m = -\gamma r^3/2(\alpha + 3\beta r^2)^{2/3}, \tag{58}$$

$$e^{-\lambda} = 1 + \gamma r^2/(\alpha + 3\beta r^2)^{2/3}, \tag{59}$$

$$f(r,P_r)r^{n-1} = \frac{\nu'}{2} = \frac{r}{2}\left[\frac{8\pi P_r(\alpha + 3\beta r^2)^{2/3} - \gamma}{(\alpha + 3\beta r^2)^{2/3} + \gamma r^2}\right] \tag{60}$$

and the equilibrium equation reads

$$8\pi \frac{dP_r}{dr} = -hr\left[\frac{4\gamma\beta r^2}{(\alpha + 3\beta r^2)^{5/3}} - \frac{3\gamma}{(\alpha + 3\beta r^2)^{2/3}} + 8\pi P_r\right] \times \left[\frac{8\pi P_r(\alpha + 3\beta r^2)^{2/3} - \gamma}{(\alpha + 3\beta r^2)^{2/3} + \gamma r^2}\right]. \tag{61}$$

In the isotropic case ($h = 1$), the solution is

$$8\pi P_r = 4\beta/(\alpha + \beta r^2) + \gamma(\alpha + 5\beta r^2)/(\alpha + \beta r^2)(\alpha + 3\beta r^2)^{2/3} \tag{62}$$

(some errors in Adler's paper have been taken into account) and

$$e^{\nu} = (\alpha + \beta r^2)^2. \tag{63}$$

Using the boundary conditions

$$P_r(a) = 0,$$

$$e_{\text{int}}^{-\lambda(r=a)} = e_{\text{int}}^{\nu(r=a)} = 1 - 2\epsilon,$$

when $\epsilon = M/a$, we find

$$\alpha = (1 - 5/2\epsilon)/(1 - 2\epsilon)^{1/2}, \tag{64}$$

$$\beta = \epsilon/2a^2(1 - 2\epsilon)^{1/2}, \tag{65}$$

$$\gamma = -2\epsilon(1 - \epsilon)^{2/3}/a^2(1 - 2\epsilon)^{1/3}. \tag{66}$$

Hence, for the isotropic case, the radial pressure can be written as

$$P_r = (\epsilon/4\pi a^2)\left[1 - 2\epsilon y^2(1 - \epsilon)^{2/3}(1 - \tfrac{5}{2}\epsilon + \tfrac{3}{2}\epsilon y^2)^{-2/3}\right] \times (1 - \tfrac{5}{2}\epsilon + \tfrac{1}{2}\epsilon y^2)^{-1} - (1 - \epsilon)^{2/3}(1 - \tfrac{5}{2}\epsilon + \tfrac{3}{2}\epsilon y^2)^{-2/3}, \tag{67}$$

with

$$y = r/a.$$

Equation (61) was integrated numerically for different values of $h$. To this end, we introduce the following variables:

$$\tilde{P} = 8\pi P_r/\gamma, \tag{68}$$

$$\tilde{\rho} = 8\pi\rho/\gamma, \tag{69}$$

$$z^2 = 1/\beta r^2, \tag{70}$$

$$\frac{d\tilde{P}}{dz} = \frac{h\delta(\alpha + 3z^{-2})^{2/3}}{z^3[(\alpha + 3z^{-2})^{2/3} + z^{-2}]}\tilde{P}^2 - \frac{h\delta(\alpha + 2z^{-2})}{[(\alpha + 3z^{-2})^{2/3} + \delta z^{-2}](\alpha + 3z^{-2})z^3}\tilde{P} + \frac{h\delta(3\alpha + 5z^{-2})}{[(\alpha + 3z^{-2})^{2/3} + \delta z^{-2}](\alpha + 3z^{-2})^{5/3}}, \tag{71}$$

where

$$\delta = \gamma/\beta.$$

In order to assign to the constants $\alpha$ and $\delta$ values which do not lead to unphysical results, we shall integrate Eq. (71) for values of $h$ close to one and assume

$$\alpha(h) = \alpha(h = 1)[1 + |1 - h|/h], \tag{72}$$

$$\delta(h) = \delta(h = 1)|1 + |1 - h|/h|. \tag{73}$$

Also for $z_0 = z(r = a)$ we get, using (67)

$$\epsilon = \delta/2z_0^2(\alpha + 3z_0^{-2})^{2/3}.$$

Figure 6 shows the solutions for $h = 1$, $h = 1.33$, with $\epsilon = 0.35$.

## V. CONCLUSIONS

We have presented a heuristic method to obtain anisotropic models in the context of general relativity.

The main virtue of the method is its simplicity and the fact that the models obtained are continuously connected with the isotropic case $h = 1$, which allows comparison with this case. Of course, whether or not these models represent physically plausible situations will depend ultimately on the agreement between relation (10) and a reasonable equation of state for the tangential pressure.


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# Observer frame rotation rates and magnetic fields in spatially homogeneous universes

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We discuss how the rotation of an observer's Cartesian reference frame is related to the precession of the shear tensor's principal axes and to the rotation vector of the fluid. An approximate solution of Einstein's equations illuminates this relationship further. In the case with a magnetic field and fluid flow a vorticity is allowed in Bianchi I cosmologies.

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## I. INTRODUCTION

In the past decade the well-known models of cosmology have been exhausted. Since an important paper by Misner,[1,2] there has been widespread consideration of anisotropic models with more complicated geometries,[3-7] referred to below as the "Maryland" universe. Simultaneously Ellis and his pupils have also developed a method for dealing with a spatially homogeneous, anisotropic cosmological model[8-10] which we shall name the "Cambridge" universe. Hawking has blended them into an hybrid.[11,12]

The models contain expanding perfect and imperfect fluids possessing shear, rotation, and acceleration of the fluid flow. In the case of perfect fluids the shear can always be diagonalized. Should there be imperfect fluids or electromagnetic fields this is not so and the off-diagonal terms in the shear tensor interact with the fluid expansion. The shear tensor precesses: Its principal axes rotate causing the temperature ellipsoid of the microwave background radiation to have an angular momentum.[2] The spin is about the observer's fluid flow vector.

This is due to another kinematical quantity which exists when imperfect fluids and electromagnetic fields are present. If the metric is of the form

$$ds^2 = -dt^2 + e^{2\alpha}e^{2\beta}{}_{ij}dx^i dx^j \tag{1}$$

with $\alpha = \alpha(t)$ and $\beta_{ij} = \beta_{ij}(t)$, a symmetric, tracefree matrix, that quantity is

$$\tau_{ij} = (e^{\beta})^{\cdot K}{}_{(i}(e^{-\beta})_{j)K}\,, \tag{2}$$

where the brackets denote the usual antisymmetry operation. It has been formally described previously as the rotation of an observer's Fermi-transported reference triad.[13,14]

The relation between these quantities can be given a more precise meaning. We shall examine that in this paper. In Sec. II the spatial tensor $\tau_{ij}$ will be shown to be the measure of the rotation of the principal axes of the coordinate shear tensor

$$\sigma_{ij} = (e^{\beta})^{\cdot K}{}_{(i}(e^{-\beta})_{j)K} \tag{3}$$

with parentheses indicating the usual symmetrization. Since the observer's reference triad vectors can be made eigenvectors of this shear tensor, $\tau_{ij}$ measures the observer's reference triad rotation. We will show this through a few simple kinematical identities.

Since $\tau_{ij}$ is a rotation, we will also examine its disentanglement from the fluid vorticity. We will show that the frame rotation and fluid rotation are proportional to each other with a Bianchi type V cosmological model as an example. This means that the universe's dynamics react back on our local reference triad.

In Sec. III we will exhibit a particular family of Bianchi I cosmologies with anisotropic stresses and give an approximate solution which shows how the shear tensor precession is truly given by the tensor $\tau_{ij}$. A formal solution which demonstrates this relation will be first given and then completed in the approximate solution.

The effect of magnetic fields will be considered in Sec. IV. There we will find two things: First, that the presence of the field allows a fluid flow to exist in Bianchi I models. Second, that those conditions allow $\tau_{ij}$ to be nonzero, which allows the vorticity to exist through the shear tensor. Again, $\tau_{ij}$ and the rotation end up proportional to each other. In this section we also give an approximate solution for all quantities. The effects of curvature in Bianchi V and IX universes is considered here.

Conclusions and suggestions for future work are summarized in the final section.

## II. REFERENCE TRIAD ROTATION AND FLUID KINEMATICAL QUANTITIES

By the Fermi transport law the Cartesian reference-frame triad vectors $\hat{e}^a$ evolve according to the equation[15,16] $d\hat{e}^a/d\tau = -\Omega^a{}_b\hat{e}^b$ where the precession tensor $\Omega$ is given by the wedge product $\Omega = -a\wedge u$ with $a$ the acceleration. This acceleration can include rotations as well as boosts. But $de^a/d\tau = \epsilon^a_{bc}\Omega^c\hat{e}^b = \epsilon^a_{bc}\epsilon^{cde}e^i{}_d e_{ei\|j}n^j\hat{e}^b$ (see Refs. 8–10), where for a fluid congruence, rather than the normal congruence, substitute $u^b$ for $n^b$.

Also from the definition of the Ricci rotation coefficients[15] $\Gamma_{abc} = e^i_a e_{ci\|j}e^j_b$ where $e^i_a$ are the tetrad components, we can formulate the relation between the Fermi transport $\Omega^a{}_b$ and $\tau_{ab}$. For a metric as in the Introduction $\Gamma_{i0j} = -\tau_{ij}$. Combining this with the first two equations

[a)]NASA-ASEE Summer Faculty Fellow, 1977–78, Marshall Space Flight Center.

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with $\hat{e}^a$ substituted for $u^a$ we easily find ($\hat{e}^i = \{e_{ci}\}$)

$$\frac{d\hat{e}^a}{d\tau} = e^i_a e_{ci\|0} e^0_b \hat{e}^c = \Gamma_{a0c}\hat{e}^c = -\tau_{ac}\hat{e}^c . \tag{4}$$

Hence $\Omega^a_c = \tau_{ac}$. By this elementary example $\tau_{ac}$ represents the rotation rate of an observer's Fermi-transported reference triad. This is amplified in the formalism of Ref. 10. The fluid flow vector is given by $u_\mu = \cosh\beta n_\mu + \sinh\beta\tilde{c}_\mu$, where $\beta$ is the hyperbolic angle of tilt between $u_\mu$ and $n_\mu$ the normal to the homogeneous hypersurfaces of constant time and $\tilde{c}_\mu$ is the projection of $u_\mu$ into these hypersurfaces. The tetrad vector commutators give the affine connection coefficients $\Gamma_{\alpha\beta\gamma}$ via $[\hat{E}_k, \hat{E}_\mu] = \gamma^\nu_{k\mu}\hat{E}_\nu$ and $\Gamma_{\alpha\beta\gamma} = \frac{1}{2}(\gamma_{\alpha\beta\gamma} + \gamma_{\gamma\alpha\beta} - \gamma_{\beta\gamma\alpha})$. In the normal basis $\hat{E}_0 = \hat{n}$, $\hat{E}_\mu = \hat{e}_\mu$, then $[\hat{n}, \hat{e}_\mu] = (\epsilon^\nu_{\mu\sigma}\Omega^\sigma - \theta^\nu{}_\mu)\hat{e}_\nu$ and $[e_k, e_\mu] = (\epsilon_{k\mu\tau}n^{\tau\nu} + \delta^\nu_\mu a_k - \delta^\nu_k a_\mu)\hat{e}_\nu$, where $\theta_{\mu\nu} = n_{(\mu\|\nu)}$ ($\|\nu \equiv$ covariant derivative) is the expansion + shear tensor of the normal congruence, $\Omega^\sigma = \epsilon^{\sigma\mu\nu}e^i_\mu e_{\nu i\|j}n^j$ is the rotation rate of $\hat{e}$ along the normal congruence, and $n^{\tau\nu}(a_k)$ is a relative tensor (vector) determining the geometry of the spacelike hypersurfaces.[10]

We now analyze this quantity according to the formalism of King and Ellis.[10] The reader should refer to their paper for the form of the main equations. Use is made of the Jacobi identities, the inertia and momentum density conservation equations, and the Einstein field equations. They give an explicit algebraic relation between the vorticity and shear in perfect-fluid, tilted, spatially homogeneous models:

$$\omega_{\alpha\beta} = \tfrac{1}{2}(\mu+\rho)^{-1}\cosh^{-1}\beta(\epsilon_{\alpha\beta\sigma}n^{\sigma k} + \delta^k_\alpha a_\beta - \delta^k_\beta a_\alpha) \times(\epsilon_{k\rho\tau}n^{\tau\nu} - 3a_\rho\delta^\nu{}_k)\sigma^\rho_\nu \tag{5}$$

which shows how $\omega_\mu$ is coupled to the peculiar velocity vector of the matter $\tilde{c}_k$ and to the shear $\sigma^\rho_\nu$. We will show from a different perspective how $\tilde{\tau}$ is the the observer reference frame rotation. A specific example will show a direct relationship between $\Omega^\tau$ and $\omega_{\mu\nu}$. In a model of Bianchi type V we can take $a_k = a\delta^1_k$ and $\tilde{c}_k = c\delta^3_k$. The tetrad vectors are

$$\begin{aligned}
\hat{e}_0 &= \frac{\partial}{\partial t},\\
\hat{e}_1 &= X^{-1}(t)\left(\frac{\partial}{\partial x^1} + f(t,x^1,x^3)\frac{\partial}{\partial x^2} + g(t,x^1)\frac{\partial}{\partial x^3}\right),\\
\hat{e}_2 &= Y^{-1}(t)e^{A_0x^1}\frac{\partial}{\partial x^2},\\
\hat{e}_3 &= Z^{-1}e^{A_0x^1}\left(\frac{\partial}{\partial x^3} + K(t)\frac{\partial}{\partial x^2}\right).
\end{aligned} \tag{6}$$

The Jacobi identities and (13) (23) field equations give $a = A_0x^{-1}$, $\sigma_{13} = \Sigma^0_{13}(YZ^2)^{-1}$, $\sigma_{23} = \Sigma^0_{23}(XY^2)^{-1}$, and establish consistency conditions to fix $K = -2\int\Sigma_{23}Z(XY^2)^{-1}\,dt$. The conservation equations are $d\ln(wl^3\times\cosh\beta)/dt = 0$ and $d\ln(r\sinh\beta)/dt = -Z^{-1}c^2\partial_t Z$. The Jacobi identities and (02) (13) field equations fix the triad rotation $\Omega_3 = \sigma_{12} = 0$, $\Omega_2 = -\sigma_{13}$, and $\Omega_1 = -\sigma_{23}$. The remaining field equations and dynamics need not concern us here, save that they can be consistently solved as in King and Ellis.[10] The relative connecting vector $X^a$ between two points can be aligned with the reference triad vector $\hat{e}^a$. It evolves then according to[9]: $dX^a/dt = \theta^a{}_bX^b$ to first order. If $\theta^a{}_b$ is diagonal we have only expansion of the components of $X^a$. But if $\sigma_{13} = -\Omega_2 \neq 0$ and $\sigma_{23} = -\Omega_1 \neq 0$, then the vector itself will rotate. Hence $\hat{e}^a$ will rotate with it. Equation(5) establishes the relation between the triad rotation and the fluid rotation. The fluid rotation is $\omega_{13} = \frac{3}{2}(\mu+p)^{-1}\cosh^{-1}\beta\,\sigma^1_3$. Then by the Jacobi identity and (02) (13) field equations $\Omega^2 = -\sigma_{13}$ and for the triad rotation tensor $\Omega_{\mu\nu} = \epsilon_{\mu\pi\nu}\Omega^\pi$ we find $\Omega_{13} = -\frac{2}{3}(\mu+p)\cosh\beta\,\omega_{13}$. Now if we may assume an equation of state $p = \gamma\mu$, the conservation law gives $\cosh\beta = W_0l^{-3}\mu^{-1-\gamma}$, where $W_0$ is a constant and is

$$\Omega_{13} = -\tfrac{2}{3}(1+\gamma)W_0l^{-3}\mu^{-\gamma}\omega_{13} . \tag{7}$$

Now $2(1+\gamma)W_0/3$ is a constant, hence the difference between $\Omega_{13}$ and $\omega_{13}$ is contained in the $l^{-3}\mu^{-\gamma}$ term. Neglecting the effects of $\cosh\beta$ on the fluid expansion we have that $\mu$ varies as $l^{-3}$ to $l^{-6}$ as $\gamma$ ranges 0 to 1 as a first-order approximation. Then, with an allowed rescaling of $\omega_{13}$ so that $2(1+\gamma)W_0/3 = 1$, it is possible for $\Omega_{13} = -\omega_{13}$ in certain circumstances. We discuss the meaning of this below.

## III. DEMONSTRATION BY AN APPROXIMATE SOLUTION OF EINSTEIN'S EQUATIONS

We now consider the nature of this phenomenon within the context of the Maryland universe[1-7] in particular with regard to the nature of $\tau_{ij}$. The initial discussion shall be concerned with the simplest spatial geometry of Bianchi type I.

The metric is of the form $ds^2 = -dt^2 + e^{2\alpha}e^{2\beta}_{ij}dx^idx^j$, where $\alpha = \alpha(t)$ and $\beta_{ij}$ is a symmetric $3\times3$ traceless matrix. The affine connection and Einstein tensors are well known. The connection coefficients are $\Gamma_{ij0} = -\Gamma_{0ij} = \dot{\alpha}\delta_{ij} + \sigma_{ij}$, $\Gamma_{i00} = -\Gamma_{00i} = \Gamma_{ijk} = 0$, and $\Gamma_{i0j} = -\tau_{ij}$, where $\dot{} = \partial/\partial t$, $\sigma_{ij} = (e^\beta)^K_{(i}\dot{e}^{-\beta}_{K|j)}$ and $\tau_{ij} = (e^\beta)^K_{[i}\dot{e}^{-\beta}_{K|j]}$. The Ricci tensor components are $R^0_0 = 3\ddot{\alpha} + 3\dot{\alpha}^2 + \sigma_{ij}\sigma_{ij}$, $R^0_i = 0$, $R_{ij} = [\ddot{\alpha} + 3\dot{\alpha}^2]\delta_{ij} + \sigma_{ij} + 3\dot{\alpha}\sigma_{ij} + [\sigma,\tau]_{ij}$, and $R = 6\ddot{\alpha} + 12\dot{\alpha}^2 + \sigma_{ij}\sigma_{ij}$. The field equations are

$$\begin{aligned}
&3\dot{\alpha}^2 - \tfrac{1}{2}\sigma_{ij}\sigma_{ij} = T^{00},\\
&\sigma_{ij} + 3\dot{\alpha}\sigma_{ij} + [\sigma,\tau]_{ij} = T_{ij} - \tfrac{1}{3}\delta_{ij}T^K_K ,\\
&-6\ddot{\alpha} - 9\dot{\alpha}^2 - \tfrac{3}{2}\sigma_{ij}\sigma_{ij} = T_{KK} .
\end{aligned} \tag{8}$$

We shall explicitly solve Eqs. (8) for a universe containing a general fluid with a magnetic field. The matrix $\beta_{ij}$ will have block diagonal form wherein $\beta_{23} \neq 0$. The magnetic field will have the components $B_\mu = B_2\delta^2_\mu + B_3\delta^3_\mu$. The pertinent field equations read

$$\begin{aligned}
&\dot{\sigma}_{11} + 3\dot{\alpha}\sigma_{11} = \pi_{11},\\
&\dot{\sigma}_{22} + 3\dot{\alpha}\sigma_{22} + 2\sigma_{23}\tau_{32} = \pi_{22},\\
&\dot{\sigma}_{33} + 3\dot{\alpha}\sigma_{33} + 2\sigma_{32}\tau_{23} = \pi_{33},\\
&\dot{\sigma}_{23} + 3\dot{\alpha}\sigma_{23} + \sigma_{22}\tau_{23} - \tau_{23}\sigma_{33} = \pi_{23},\\
&\dot{\sigma}_{32} + 3\dot{\alpha}\sigma_{32} + \sigma_{33}\tau_{32} - \tau_{32}\sigma_{22} = \pi_{32} .
\end{aligned} \tag{9}$$

The trace-free stresses $\pi_{\alpha\beta}$ may be due to viscous stresses and Maxwell stresses,

$$\pi_{\alpha\beta} = -\lambda\sigma_{\alpha\beta} - \tfrac{1}{4}B_\alpha B_\beta + \tfrac{1}{12}B^2\delta_{\alpha\beta} . \tag{10}$$

Their exact form will not be important in the formal solution

we are seeking. Maxwell's equations and the hydrodynamic equations could give us the functional relations of $B$, $\sigma_{\alpha\beta}$, $\alpha$, etc., required.

We subtract the second and third of Eqs. (9) from each other and sum the fourth and fifth of Eqs. (9). We also make use of the trace-free property of $\beta_{ij}$ and $\sigma^i_i = 0$. These give

$$\begin{aligned}
&(\sigma_{22} - \sigma_{33})^{\cdot} + 3\dot{\alpha}(\sigma_{22} - \sigma_{33}) + 4\sigma_{23}\tau_{32} = \pi_{22} - \pi_{33}\,,\\
&2\dot{\sigma}_{23} + 6\dot{\alpha}\sigma_{23} - 2(\sigma_{22} - \sigma_{33})\tau_{32} = 2\pi_{23}\,,\\
&(\sigma_{22} + \sigma_{33})^{\cdot} + 3\dot{\alpha}(\sigma_{22} + \sigma_{33}) = -\pi_{11}\,.
\end{aligned} \tag{11}$$

These can be solved completely. First let $\Sigma = e^{3\alpha}(\sigma_{22} - \sigma_{33})$, $\Sigma_{23} = 2\sigma_{23}e^{3\alpha}$, $\Pi = (\pi_{22} - \pi_{33})e^{3\alpha}$, and $\Pi_{23} = 2\pi_{23}e^{3\alpha}$. Then the first two of Eqs. (11) are $\Sigma^{\cdot} + 2\tau_{32}\Sigma_{23} = \Pi$ and $\Sigma_{23} - 2\tau_{32}\Sigma^{\cdot} = \Pi_{23}$, which can be combined on multiplying the second equation by $i = \sqrt{-1}$ into $(\Sigma + i\Sigma_{23})^{\cdot} = 2i\tau_{32}(\Sigma + i\Sigma_{23}) + (\Pi + i\Pi_{23})$. The general solution is $(\Sigma + i\Sigma_{23}) = (\Sigma^0 + i\Sigma^0_{23})e^{2i\int\tau_{32}dt} + e^{2i\int\tau_{32}dt}\int(\Pi + \Pi_{23}) \times e^{-2i\int\tau_{32}dt}\,dt$. Using this with the last of Eq. (11) for $(\sigma_{22} + \sigma_{33})$ we find for the components of the shear (superscript zero indicates a constant):

$$\sigma_{11}e^{3\alpha} = \sigma^0_{11} + \int \pi_{11}e^{3\alpha}\,dt\,, \tag{12}$$

$$\begin{aligned}
2\sigma_{22}e^{3\alpha} = {}& \sigma^0_{22}(1 + \cos\phi) + \sigma^0_{33}(1 - \cos\phi) - 2\sigma^0_{23}\sin\phi\\
&+ \cos\phi\int[(\pi_{22} - \pi_{33})\cos\phi + 2\pi_{23}\sin\phi\,]e^{3\alpha}\,dt\\
&+ \sin\phi\int[(\pi_{22} - \pi_{33})\sin\phi - 2\pi_{23}\cos\phi\,]e^{3\alpha}\,dt\\
&- \int\pi_{11}e^{3\alpha}\,dt\,,
\end{aligned} \tag{13}$$

$$\begin{aligned}
2\sigma_{33}e^{3\alpha} = {}& \sigma^0_{33}(1 + \cos\phi) + \sigma^0_{22}(1 - \cos\phi) + 2\sigma^0_{23}\sin\phi\\
&- \cos\phi\int[(\pi_{22} - \pi_{33})\cos\phi - 2\pi_{23}\sin\phi\,]e^{3\alpha}\,dt\\
&- \sin\phi\int[(\pi_{22} - \pi_{23})\sin\phi - 2\pi_{23}\cos\phi\,]e^{3\alpha}\,dt\\
&- \int\pi_{11}e^{3\alpha}\,dt\,,
\end{aligned} \tag{14}$$

$$\begin{aligned}
2\sigma_{23}e^{3\alpha} = {}& 2\sigma^0_{23}\cos\phi + (\sigma^0_{22} - \sigma^0_{33})\sin\phi\\
&+ \cos\phi\int[(2\pi_{23}\cos\phi - (\pi_{22} - \pi_{33})\sin\phi\,]e^{3\alpha}\,dt\\
&+ \sin\phi\int[(\pi_{22} - \pi_{33})\cos\phi + 2\pi_{23}\sin\phi\,]e^{3\alpha}\,dt\,,
\end{aligned} \tag{15}$$

where $\phi = 2\int\tau_{32}\,dt$. If viscous stresses are present it is more straightforward to replace the factor $e^{3\alpha}$ by $e^{3\alpha + \lambda t}$ in Eqs. (12)–(15) with the contribution to $\pi_{\alpha\beta}$ coming from the magnetic fields.

We now make the solution more explicit. In the case of vanishing viscosity and magnetic field the evolution of the shear would be just $\sigma_{ij} = \sigma^0_{ij}e^{-3\alpha}$. We will therefore take Eqs. (12)–(15) as giving the effects of viscosity and magnetic fields as small perturbations to the simplest possible anisotropic background. Maxwell's equations would give $B_2 \cong B^0_2 e^{-2\alpha}$ and $B_3 \cong B^0_3 e^{-2\alpha}$. Dimensional analysis of the shear evolution equations shows that $\tau_{ij}$ must be close to the form $\tau_{ij} \cong \tau^0 t^{-1}$ where $\tau^0$ is a constant or very slowly varying function of time. Then to this order of approximation $\cos\phi = \cos[2\tau^0\ln(t/t^0)]$. The inertial density conservation equations give that the inertia density evolves as $\rho = \rho^0 e^{-3\gamma\alpha}$, where the speed of sound $V_S$ in the equation of state relating pressure $p$ to the inertia density $\rho$, $p = (\gamma - 1)\rho$, is $V_S = (\gamma - 1)^{1/2}$. Then to the lowest order (isotropic universe) $e^{\alpha} = [(3\gamma\rho_0/2\sqrt{3})t]^{2/3\gamma}$, which is usually written $e^{\alpha} = At^{2/3\gamma}$ with $A$ a constant.

To evaluate the shear we use Eq. (13) as an example and evaluate the shear component $\sigma_{22}$. It will have integrals in it of the form

$$\int Ct^{2/3\gamma}\cos[2\tau^0\ln(t/t_0)]\,dt \tag{16}$$

which is the very first in Eq. (13) with $C = (A/4)\times(B^{0^2}_3 - B^{0^2}_2)$. We use the gauge freedom allowed by general covariance to set $\tau^0 = \frac{1}{2}$. This means that all rotation and precession rates of frames or fluid components are scaled by the rotation rate of observer reference frames. Using the substitution $x = \ln(t/t_0)$. The integral passes over to the well-known form $D\int e^{(2/3\gamma + 1)x}\cos x\,dx$ with $D = Ct_0^{2/3\gamma + 1}$. The $\sigma_{22}$ shear component is then

$$\begin{aligned}
\sigma_{22} = {}& \frac{t^{-2/\gamma}}{2A^3}\{\sigma^0_{22}[1 + \cos\ln(t/t_0)] + \sigma^0_{33}[1 - \cos\ln(t/t_0)] - 2\sigma^0_{23}\sin\ln(t/t_0)\} + \frac{t^{-4/3\gamma + 1}}{4A^2}\\
&\times\left(\frac{(B^0_3)^2 - (B^0_2)^2(2/3\gamma + 1)/2 + B^0_2B^0_3}{[(2/3\gamma + 1)^2 + 1]} - \frac{(B^0_2)^2 + (B^0_3)^2}{6(2/3\gamma + 1)}\right)
\end{aligned} \tag{17}$$

or in terms of $\alpha$,

$$\sigma_{22} = \frac{e^{-3\alpha}}{2}\left[\sigma^0_{22}\left(1 + \cos\frac{3\gamma\alpha}{2A}\right) + \sigma^0_{33}\left(1 - \cos\frac{3\gamma\alpha}{2A}\right) - 2\sigma^0_{23}\sin\frac{3\gamma\alpha}{2A}\right] + e^{-(4\gamma - 3/2)\alpha}\{E\}\,, \tag{18}$$

where $\{E\}$ is the constant term in the brackets in Eq. (17). The full set of shear terms are listed in the Appendix. The shear terms may be inserted into the $T^{00}$ Einstein equation (8) using either Eq. (17) or (18) above to yield information about the expansion.

Since we are obviously using the small shear approxi-

mation we add a disturbance $\epsilon$ to $\alpha$ where $\epsilon^2 \ll 1$. Then the $T^{00}$ Einstein equation is

$$\dot{\alpha}^2 + 2\,\dot{\alpha}\dot{\epsilon} = T^{00} - \tfrac{1}{2}\sigma_{ij}\sigma_{ij}\,. \tag{19}$$

Inspection of the shear terms in the Appendix shows that the equation becomes

$$\begin{aligned}\dot{\epsilon} = \frac{3\gamma t}{4}\Big(& t^{-4/\gamma}\sum_{n=0}^{n=2}(M'_n\cos^n\phi + N'_n\sin^n\phi) \\ &+ t^{-10/3\gamma+1}\sum_{n=0}^{n=1}(0'_n\cos^n\phi + P'_n\sin^n\phi) \\ &+ t^{-4/\gamma}Q'\sin\phi\cos\phi + t^{-8/3+2}R'\Big)\,,\end{aligned} \tag{20}$$

where the primed case letters are all constants. This can be transformed to

$$\begin{aligned}\dot{\epsilon} = {} & e^{-(6-3\gamma/2)\alpha}\sum_{n=0}^{n=2}\left[M_n\cos^n\left(\frac{3\gamma\alpha}{2A}\right) + N_n\sin^n\left(\frac{3\gamma\alpha}{2A}\right)\right] \\ &+ e^{-(5-3\gamma)\alpha}\sum_{n=0}^{n=1}\left[0_n\cos^n\left(\frac{3\gamma\alpha}{2A}\right) + P_n\sin^n\left(\frac{3\gamma\alpha}{2A}\right)\right] \\ &+ e^{-(6-3\gamma/2)\alpha}Q\cos\left(\frac{3\gamma\alpha}{2A}\right)\sin\left(\frac{3\gamma\alpha}{2A}\right) + e^{-(4-3\gamma)\alpha}R\,,\end{aligned} \tag{21}$$

$$\begin{aligned}\epsilon = {} & \frac{2A}{3\gamma}e^{a\alpha}\Bigg[\sum_{n=0}^{n=2}\frac{M_n\cos^{n-1}x}{a^2+n^2}\left(a\cos x + n\sin x + \frac{n(n-1)}{a}\right) \\ &+ \sum_{n=0}^{n=2}\frac{N_n\sin^{n-1}x}{a^2+n^2}\left(a\sin x - n\cos x + \frac{n(n-1)}{a}\right)\Bigg] \\ &+ \frac{2A}{3\gamma}e^{b\alpha}\Bigg[\sum_{n=0}^{n=1}\frac{0_n\cos^{n-1}x}{a^2+n^2}(a\cos x + n\sin x) \\ &+ \sum_{n=0}^{n=1}\frac{P_n\sin^{n-1}x}{a^2+n^2}(a\sin x - n\cos x)\Bigg] \\ &- \frac{2AR}{3(4-3\gamma)\gamma}e^{-(4-3\gamma)\alpha} + \frac{2A}{3\gamma}\int e^{a\alpha}\cos x\,\sin x\,dx\,,\end{aligned} \tag{22}$$

where $a = -(6-3\gamma)2A/3\gamma$, $x = 3\gamma\alpha/2A$, and $b = -(5-4\alpha/2)2A/3\gamma$. This completes the approximate solution. The expansion is altered by a complicated oscillatory pattern superimposed on it in response to the shear. Overall, we see that the precession rate of the observer reference frames is controlled by the shear tensor strictly by the terms in $\cos\ln(t/t_0)$ and $\sin\ln(t/t_0)$. If $\tau^0 = 0$ the effects of these terms vanish and there is no spin of the observer reference frame.

It is clear that while $\sigma_{11}$ stands alone there is a great deal of mixing of $\sigma_{22}$, $\sigma_{33}$, and $\sigma_{23}$. The contributions due to $\sigma^0_{33}$ and $\sigma^0_{22}$ affect $\sigma_{22}$ and $\sigma_{33}$ in the same way, while their effect on $\sigma_{23}$ depends only on their difference. The important variable is the phase angle $\phi = 2\int\tau_{32}\,dt$; $\sigma_{22}$ decreases as $-2\sigma^0_{23}\sin\phi$ while $\sigma_{33}$ increases as $+2\sigma^0_{23}\sin\phi$. One may also examine the contributions due to the inhomogeneous terms in the differential equations, i.e., due to the trace-free stresses.

Consider an observer's reference triad to be a shear eigenvector and sight on a sample distant galaxy with position vector $\hat{e}_G = \delta\hat{e}_2 + \epsilon\hat{e}_3$. Then as the shear evolves, (say) $\sigma_{33}$ increases with respect to $\sigma_{22}$, and we find the 3-component of $\hat{e}_G$ increasing while the 2-component decreases. The reference frame "rotates" toward the 3-direction. Another way of viewing this is that $\sigma_{23}$ decreases as the reference frame precesses with the shear tensor. Dynamically, this means that the evolution of the universe tends to diagonalize the shear tensor, so that one of the principal axes will end up aligned with the magnetic field. Once the reference triad is aligned with the shear principal directions, it rotates with their precession. The angle of this rotation is given by $\phi = 2\int\tau_{32}\,dt$, $\tau_{32}$ being a measure of the rotation rate of the reference triad.

Cosmological observations would be altered in an interesting way by these effects. Proper motions of distant objects as formulated by Kristian and Sachs[17] furnish a good example. The evolution of the image direction cosine $e^\mu$ is given by

$$\begin{aligned}\frac{de^\mu}{dt} = {} & e^\beta(\sigma_{\mu\beta} + \omega_{\mu\beta}) \\ &+ r[e^\beta(\sigma_{\gamma\beta} + \omega_{\gamma\beta})U_{\mu\|\gamma} - e^\beta E_{\mu\beta}]\end{aligned} \tag{23}$$

where $\omega_{\mu\beta}$ is the vorticity tensor and $U_{\mu\|\gamma}$ is the total velocity gradient $U_{\mu\|\gamma} = \theta_{\mu\gamma} + \omega_{\mu\gamma}$. The Newman–Penrose identities[18] give the optical scalar equations which we may use to find $E_{\mu\nu}$,

$$E_{\mu\nu} = \dot{\sigma}_{\mu\nu} - 2\sigma_{\mu\nu}\theta\,. \tag{24}$$

Using Eqs. (17), (18), and (22) one finds the precession rate, $de^\mu/dt$ as a quadrupole pattern on the celestial sphere. However, the direction cosine is the direction vector $\hat{e}^\mu$ in the observer rotation frame which is spinning, in a sense opposite to the velocity as shown in Sec. II. Thus, one would conclude that the proper motion was much greater than it really was.

If a flow, or peculiar velocity, were imparted to the fluid in the form $U_\mu = U_0\delta_\mu{}^0 + U_2\delta_\mu{}^2$, the $T^{0i} = 0$ field equations would normally constrain it so that $U_2 = 0$. With a magnetic field $B_a = B_2\delta_a{}^2 + B_3\delta_a{}^3$ present, this is not the case. For then we have an electric field $E_1 = U_0U_2B_3$ and a Poynting vector $P_2 = U_0E_1B_3$. The $T^{0i}$ equation then reads

$$\gamma\rho U_2U_0 = P_2\,. \tag{25}$$

The shear equations then include terms containing the Reynolds stresses $\pi^R{}_{ij}$,

$$\pi_{ij}{}^R = \gamma\rho(U_iU_j - \delta_{ij}U_KU^K/3) \tag{26}$$

The conservation equations for the momentum density are no longer trivial and give a lowest order solution of $U_2 = U^0_2\exp[-\alpha - (\gamma-1)\ln\rho/\gamma]$ for nondissipative fluids. The Reynolds stress terms are therefore of the form $f\gamma\rho_0e^{-3\gamma\alpha}(U^0_2)^2e^{-[2-6(\gamma-1)]\alpha}$, where $f = +\frac{2}{3}, -\frac{1}{3}$, which finally contains terms of the order $e^{(3\gamma-8)\alpha}$ or $A^{(3\gamma-8)}\times t^{(6\gamma-16)/3\gamma}$. The additive contribution to the $\sigma_{22}$ shear component is then of the form

$$\frac{f\gamma\rho_0(U^0_2)^2A^{3\gamma-8}(t/t_0)^{(6\gamma-16)/3\gamma+1}}{2-[(6\gamma-16)/3\gamma+1\ ]}\,. \tag{27}$$

This is a heavy contribution to the shear.

The vorticity vector is given by $\omega^a = \frac{1}{2}\eta^{abcd}U_bU_{c\|d}$ where $\eta^{abcd}$ is the four-dimensional alternating object. One finds in this case that $\omega^1 = (U_2{}^2 + \frac{1}{2})\sigma_{23}$. Collins[19] has shown that Bianchi type I models with a magnetic field can evolve like a Bianchi II model. Batakis[20] has shown that type II

models can have vorticity if electromagnetic fields are present in addition to the perfect fluid. It is almost as though the field endows the manifold with a spatial curvature. The presence of a spatial curvature is necessary if a perfect fluid is to have a peculiar velocity. The velocity then provides "curvature" terms to react back on the field via Maxwell's equations. One of Maxwell's equations in this case[21] $B^a{}_{\|a} - B^a U_a - 2\omega^a E_a = 0$ which gives $B_2 U_2 = -2(U_2^2 + \frac{1}{2})\sigma_{23} U_2 B_3$. The equation for $B_3$ gives $B_3 \sim B_3{}^0 e^{-2\alpha} U_0{}^{-1/6}$ and $B_2$ is found algebraically. Note the additional term $U_0{}^{-1/6}$ which is $(1 - U_2{}^2)^{-1/2}$, affecting the field's dynamics because $U_2 \neq 0$.

In more general geometries the spatial curvature of the homogeneity surfaces $R^*_{ij}$ enters the field equations with the extra terms $R^*/2, R^*_{ij} - R^*/3\delta_{ij}$, and $R^*/2$ in the last of the three Eqs. (8). The $T_{0i}$ Einstein equation is no longer trivial, being

$$e^{-\alpha}[(e^{-\beta}\sigma e^{\beta})_{ba} C^a{}_{bc} (e^{-\beta})_{ci} - \sigma_{ij}(e^{-\beta})_{jc} C^a{}_{ac}] = T^{0i}, \quad (28)$$

linking the nondiagonal $\sigma, \beta$, and group structure constants $C^a{}_{bc}$ to the matter currents. The group structure constants are given by the spatial triad commutation relations.

In Bianchi type V spaces $C^2{}_{21} = C^3{}_{31} = 1$ and type IX $C^a{}_{bc} = \epsilon_{abc}$ (the permutation operator).

These two types correspond to open and closed Friedman universes. In type V the space curvature is isotropic so $R^*_{ij} - (1/3)R^*\delta_{ij} = 0$ and $\tau_{ij}$ affects dynamics the same way as in type I. Things are more complicated in type IX since there $(1/2)R^*_{ij} = (3e^{-2\alpha}/4)(V_g - 1)$ and $R_{ij} - \frac{1}{3}R^*\delta_{ij} = (3e^{-2\alpha}/4)\partial V_g/\partial\beta_{ij}$ with $V_g = (1/3)\mathrm{Tr}\,[e^{4\beta} - 2e^{-2\beta})_{ij} + \delta_{ij}]$.

The spatial rotation of the fluid in these cases is

$$\omega^a = e^{-3\alpha}\epsilon_{abc}[1/2 C^d{}_{bc} u_d u^0 + u_b \dot{u}_c] \quad (29)$$

for a stress tensor with components $T_{0i} = (\rho + p)u_0 u_i$. Equation (28) is solved for the velocity $u_i$ and then inserted in Eq. (29) to determine the vorticity, in terms ultimately of the noncommuting elements of $(e^{\beta})^{ij}$ and $(e^{-\beta})_{ij}$.

In type V Eq. (28) reads $3\sigma_{1i} = \rho_0 e^{-3\alpha} u_i$, hence $u_i = (3/\rho_0)e^{3\alpha}\sigma_{1i}$ for dust (pressure-free matter). Hence $\omega^a = (3/\rho_0)\epsilon_{abc} C^i{}_{bc}\sigma_{1i}/2 + (3/\rho_0)^2 \epsilon_{abc} e^{-3\alpha}\sigma_{1b}(e^{3\alpha}\sigma_{1c})$. In this case, let $\beta_{ij}$ have the block diagonal form with $\beta_{12} \neq 0$ so that $\tau_{12}$ replaces $\tau_{32}$ in the previous discussion. Then there can only be spatial velocity components $u_1$ and $u_2$ by the $T^{0i}$ equation ($u_3 = 0$). The vorticity vector only has $\omega^3 \neq 0$ while $\omega^1 = \omega^2 = 0$. Then we have competition between $\omega_{12}$ and $\tau_{12}$ which must be disentangled if we are to understand certain of the observations. We have $\omega^3 = (3/\rho_0)\sigma_{12} e^{-\alpha - \beta_{11}} + (3/\rho_0)^2 e^{3\alpha}[\sigma_{11}(\sigma_{12})^{\cdot} - \sigma_{12}(\sigma_{11})^{\cdot}]$. This expression may be used for the former expression, inserting $(e^{3\alpha}\sigma_{11})^{\cdot} = (\Pi_{11} - 2\sigma_{12}\tau_{21})e^{3\alpha}$ and $(e^{3\alpha}\sigma_{12})^{\cdot} = (\Pi_{12} - \sigma_{11}\tau_{12} + \tau_{12}\sigma_{22})e^{3\alpha}$ from the trace-free space–space Einstein equations, Eqs. (9) with the $\beta_{12} \longleftarrow \beta_{23}$ substitution.

In type IX the $T^{0i}$ equation reads $\frac{1}{2}\epsilon_{ijk} e^{-\alpha}[e^{2\beta}, \sigma]_{jk} = T_{0i}$. Again we restrict ourselves to the block diagonal form for $\beta_{ij}$, taking $\beta_{23} \neq 0$ in the preceding equation and the vorticity vector by Eq. (29) has only the $\omega^1$ component as then again a rotation tensor $\omega_{23}$ is mixed with a triad spin tensor $\tau_{23}$. In solving the shear equations (9) we have to deal with the space curvature anisotropy. If we consider that it may become an additive part to the trace-free stresses,[4] viz. $\Pi_{ij} \to \Pi_{ij} - R^*_{ij} + (1/3)R^*\delta_{ij}$, then formally the effect of $\tau_{ij}$ is the same on the dynamics. Certainly nothing is changed qualitatively in this behavior. The rotation of the universe has been discussed with no reference to the metric tensor's principal axes.[11,12] But in others[4–6] the fluid rotation is defined by the rotation of the metric's principal axes. A certain portion of an observer's perception of rotation in proper motion and distortion measurements in these type IX models[4–6] (and in other types[11,12]) would be in the precession of his reference triad as eigenvectors of the shear tensor (aligned with its, hence the metric's, principal directions).

In the more general tumbling (and possibly "mix master") models the relation of $\tau_{ij}$ to the dynamics and to the vorticity is difficult to display without making approximations. Using the results of perturbation theory[4,11] the behavior of $\tau_{ij}$ is easily calculated for comparison with $\omega_{ij}$. The results are in accord with this discussion. One possible interpretation is that the evolving shear tensor represents a gravitational wave of wavelength greater than the horizon distance; then $\tau_{ij}$ represents the angular momentum or spin tensor of that wave's circularly polarized component.

More study of the role of magnetic fields is needed, particularly in magnetohydrodynamic models such as those of Tupper and Dunn.[22] If we expect a high-temperature plasma to conduct electricity, then certainly we should include the dissipative Joule heating and Ampere forces in our analysis.

## IV. CONCLUSIONS

We have examined the rotation of an observer's reference triad in currently accepted formalism for treating spatially homogeneous cosmologies. An observer's triad rotation is affected by the shear dynamics through Einstein's equations. The quantity $\tau_{ij} = (e^{\beta})^{\cdot K}{}_{[i}(e^{-\beta})_{j]K}$ is the triad rotation tensor. The role of the magnetic field is most important.

Confusion can arise between an observer's triad rotation and the rotation of the cosmological fluid in proper motion measurements. The observations must be very carefully examined, then, to be sure of the role played by the various kinematical quantities. The confusion varies with Bianchi type, as shown by the $\tau_{ij} \to \omega_{ij}$ relations discussed. In particular a precessing shear tensor may appear to be due to a rotating fluid when the cause is partially a rotating quadrupole distortion much like a circularly-polarized long wavelength gravitational wave.

It may be that the upper limits on the cosmological vorticity can be further reduced if a component due to the rotation of our own reference triad can be identified. Other observations, such as the distortion and proper motion effects,[17] and number counts, may possibly allow separate limits to be fixed for each quantity, so that more precise limits, including possible lower limits, may be determined. It is certain anyway that $\tau_{ij}$ is an important entity, both in Einstein's equations and in observations. Most interesting

will be the issue of whether one group type will mimic another model's behavior upon inclusion of fluid flows, electromagnetic fields, and magnetocurrents. For then the universe will be a confusing place indeed.


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## APPENDIX

The full forms of the rate of shear tensor's $\sigma_{ij}$ components are given here. The most general trace-free stress tensor $\pi_{ij}$ in the spatial hypersurfaces is given by

$$\pi_{ij} = -\lambda\sigma_{ij} - [\tfrac{1}{4}B_iB_j - \tfrac{1}{12}B^2\delta_{ij}] + \gamma\rho(U_iU_j - U^2\delta_{ij}/3), \tag{A1}$$

where $\lambda, B_i, U_i, \gamma$, and $\rho$ are the kinematic viscosity, magnetic induction, fluid velocity, equation of state index, and inertial density. The parts of $\pi_{ij}$ are the viscous stresses, Maxwell stresses, and Reynolds' stresses. We will consider mainly Maxwell stresses here. The formal solutions to Einstein's equation for the shear are Eqs. (12)–(15) in this paper. Using the analysis immediately following those equations one finds

$$\sigma_{11} = \frac{\sigma_{11}{}^0}{A^3}\left(\frac{t}{t_0}\right)^{-2/\gamma} + \frac{(B_2{}^0)^2 + (B_3{}^0)^2}{12A^2(2/3\gamma+1)}\left(\frac{t}{t_0}\right)^{-4/3\gamma+1} \tag{A2a}$$

$$= \sigma_{11}^0 e^{-3\alpha} + \frac{(B_2{}^0)^2 + (B_3{}^0)^2}{12(4/3\gamma+1)} e^{-(4\gamma-3/2)} \tag{A2b}$$

$$\sigma_{22} = \frac{(t/t_0)^{-2/\gamma}}{2A^3}\{\sigma_{22}{}^0[1+\cos\ln(t/t_0) + \sigma_{33}{}^0(1-\cos\ln(t/t_0)) - 2\sigma_{23}{}^0\sin\ln(t/t_0)\} + \frac{(t/t_0)^{-4/3\gamma+1}}{4A^2}$$
$$\times\left(\frac{[(B_3{}^0)^2 - (B_2{}^0)^2](2/3\gamma+1)/2 + B_2{}^0B_3{}^0}{[(2/3\gamma+1)^2+1]} - \frac{(B_2{}^0)^2+(B_3{}^0)^2}{6(2/3\gamma+1}\right) \tag{A3a}$$

$$= \frac{e^{-3\alpha}}{2}\left[\sigma_{22}{}^0\left(1+\cos\frac{3\gamma\alpha}{2A}\right)\right] + \sigma_{33}{}^0\left(1-\cos\frac{3\gamma\alpha}{2A}\right) - 2\sigma_{23}{}^0\sin\frac{3\gamma\alpha}{2A} + e^{-(4\gamma-3/2)\alpha}\{E\}, \tag{A3b}$$

$$\sigma_{33} = \frac{(t/t_0)^{-2/\gamma}}{2A^3}\{\sigma_{33}{}^0[1+\cos\ln(t/t_0) + \sigma_{22}{}^0(1-\cos\ln(t/t_0)) + 2\sigma_{33}{}^0\sin\ln(t/t_0)\} - \frac{(t/t_0)^{-4/3\gamma+1}}{4A^2}$$
$$\times\left(\frac{(B_3{}^0)^2 - (B_2{}^0)^2(2/3\gamma+1)/2 + B_2{}^0B_3{}^0}{[(2/3\gamma+1)^2+1]} + \frac{(B_2{}^0)^2+(B_3{}^0)^2}{6(2/3\gamma+1)}\right) \tag{A4a}$$

$$= \frac{e^{-3\alpha}}{2}\left\{\sigma_{33}\left(1+\cos\ln\frac{3\gamma\alpha}{2A}\right) + \sigma_{22}{}^0\left[1-\cos\ln\left(\frac{3\gamma\alpha}{2A}\right)\right] + 2\sigma_{33}{}^0\sin\frac{3\gamma\alpha}{2A}\right\} - e^{-(4\gamma-3/2)\alpha}\{F\}, \tag{A4b}$$

$$\sigma_{23} = \frac{\sigma_{23}{}^0}{A^3}(t/t_0)^{-2\gamma}\cos\ln(t/t_0) + \frac{(t/t_0)^{-2/\gamma}}{2A^3}(\sigma_{22}{}^0 - \sigma_{33}{}^0)\sin\ln(t/t_0)$$
$$- \frac{(t/t_0)^{-4/3\gamma+1}}{4A^2}\left(\frac{B_2{}^0B_3{}^0(2/3\gamma+1) + [(B_2{}^0)^2 - (B_3{}^0)^2]/2}{[(2/3\gamma+1)^2+1]}\right) \tag{A5a}$$

$$\left[\sigma_{23}{}^0e^{-3\alpha}\cos\ln\frac{3\gamma\alpha}{2A} + \frac{e^{-3\alpha}}{2}(\sigma_{22}{}^0 - \sigma_{33}{}^0)\sin\ln\frac{3\gamma\alpha}{2A} - e^{-(4\gamma-3/2)\alpha}\{G\}\right]. \tag{A5b}$$

These may be used in the $T^{00}$ Einstein equations to determine the evolution of $\alpha$ in either form, depending on the desired type of approximation being used.

If viscous stresses are present, then all terms should include a factor of $e^{-\lambda t}$ to show the effects of viscous dissipation of shear.

When Reynolds' stresses are present, say for a peculiar velocity $U_2 \neq 0$, then the new terms in $\pi_{ij}$ are

$$\pi_{11} = -\gamma\rho U_2{}^2/3, \tag{A6a}$$

$$\pi_{22} = 2\gamma\rho U_2{}^2/3, \tag{A6b}$$

$$\pi_{33} = -\gamma\rho U_2{}^2/3. \tag{A6c}$$

The lowest-order evolution of $\rho$ and $U_2$ are $\rho = \rho_0 e^{-3\gamma\alpha}$ and $U_2 = U_2{}^0 e^{(3\gamma-4)\alpha}$. The Reynolds's stresses then assume the

form

$$\pi_{11} = -\tfrac{1}{3}\gamma\rho_0(U_2^0)^2 e^{(3\gamma-8)\alpha} \tag{A7a}$$

$$= -\tfrac{1}{3}\gamma\rho_0(U_2^0)^2 A^{3\gamma-8} t^{2(3\gamma-8)/3\gamma}, \tag{A7a'}$$

$$\pi_{22} = \tfrac{2}{3}\gamma\rho_0(U_2^0)^2 e^{(3\gamma-8)\alpha} \tag{A7b}$$

$$= \tfrac{2}{3}\gamma\rho_0(U_2^0)^2 A^{3\gamma-8} t^{2(3\gamma-8)/3\gamma}, \tag{A7b'}$$

$$\pi_{33} = \pi_{11}. \tag{A7c}$$

The Reynolds' stress contributions to the rate of shear ${\sigma_{ij}}^R$ are then easily found:

$${\sigma_{11}}^R$$

$$= -\frac{\gamma\rho_0(U_2^0)^2 A^{3\gamma}}{3A^8[(6\gamma-16)/3\gamma+1]}(t/t_0)^{(6\gamma-16)/3\gamma+1} \tag{A8a}$$

$$= -\frac{\gamma\rho_0(U_2^0)^2 A^{-3/2} e^{[(9\gamma-24)/3\gamma+3/2]\alpha}}{3A^{8-8\gamma}[(6\gamma-16)/3\gamma+1]}, \tag{A8b}$$

$${\sigma_{22}}^R$$

$$= +\frac{\gamma\rho_0(U_2^0)^2 A^{3\gamma}}{6A^8}\frac{(t/t_0)^{(6\gamma-16)/3\gamma+1}[6\gamma-16)/3\gamma+1]}{\{[(6\gamma-16)/3\gamma+1]^2+1\}} - \tfrac{1}{2}{\sigma_{11}}^R \tag{A9a}$$

$$= +\frac{\gamma\rho_0(U_2^0)^2 A^{3\gamma}}{6A^{8-8\gamma}}\frac{e^{[(9\gamma-24)/3\gamma+3/2]\alpha}}{\{[(6\gamma-16)/3\gamma+1]^2+1\}} - \tfrac{1}{2}{\sigma_{11}}^R \tag{A9b}$$

$$= {\sigma_{22}}^{-R} - \tfrac{1}{2}{\sigma_{11}}^R, \tag{A9c}$$

$${\sigma_{33}}^R = -{\sigma_{22}}^{-R} - \tfrac{1}{2}{\sigma_{11}}^R, \tag{A10}$$

$${\sigma_{23}}^R = \frac{\gamma\rho_0(U_2^0)^2 A^{3\gamma}}{6A^8}\frac{(t/t_0)^{(6\gamma-16)/3\gamma+1}}{\{[(6\gamma-16)/3\gamma+1]^2+1\}} \tag{A11a}$$

$$= +{\sigma_{22}}^{-R}[(6\gamma-16)/3\gamma+1]^{-1}. \tag{A11b}$$

The full shear tensor may then be constructed ${\sigma_{ij}}^{EM} + {\sigma_{ij}}^R$ for computation.

The full shear tensor may then be constructed ${\sigma_{ij}}^{EM} + {\sigma_{ij}}^R$ for computation.


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# On the Hoenselaers–Kinnersley–Xanthopoulos spinning mass fields

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The metrics of the Hoenselaers–Kinnersley–Xanthopoulos family of spinning mass solutions with arbitrary positive number distortion parameter $\delta$ and with twin rotation-reflection parameters besides mass parameter are studied. When values of two parameters are unequal or equal, the metrics are asymmetric or symmetric with respect to the reflection at the equatorial plane, respectively. The metrics for any distortion parameter $\delta$ contain no event horizon.

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## 1. INTRODUCTION

On the problem of the stationary axisymmetric, asymptotically flat exact Einstein vacuum field Hoenselaers, Kinnersley, and Xanthopoulos[1] (H–K–X) found, through their study of the symmetry transformations leaving the gravitational field equations invariant, a family of spinning mass solutions with arbitrary positive number distortion parameter $\delta$ and with two parameters besides mass parameter. They have given the solutions in the form of the Ernst complex function[2] $\epsilon$.

The purpose of the present paper is to give the metric functions $f$, $\omega$, and $\gamma$ [see Eq. (4) for the definition], to clarify the physical meaning of two parameters $\lambda$ ( $=\alpha_1$ in H–K–X notation) and $\mu$ ( $=\alpha_2$ in H–K–X notation), and to study the property of the H–K–X metrics. This family of solutions has four parameters, i.e. mass parameter $m$, positive number distortion parameter $\delta$, and twin rotation-reflection parameters $\lambda$ and $\mu$. The angular momentum $J$ about the symmetry axis ($z$ axis) is

$$\begin{aligned} J &= \frac{\kappa^2(\lambda+\mu)}{(1-\lambda\mu)^2}\,[(\mu-\lambda)\sin\tau] \\ &\quad + \{2\delta+1-(2\delta+3)\lambda\mu\}\cos\tau] \\ &= m^2(\lambda+\mu)\{(\delta(1-\lambda\mu)-2\lambda\mu)^2+(\mu-\lambda)^2\}^{-3/2} \\ &\quad \times[(\mu-\lambda)^2+(1+\lambda\mu)(\delta(1-\lambda\mu)-2\lambda\mu) \\ &\quad + 2(\delta(1-\lambda\mu)-2\lambda\mu)^2], \end{aligned} \tag{1}$$

where the unit of distance $\kappa$ is

$$\kappa = m(1-\lambda\mu)\{(\delta(1-\lambda\mu)-2\lambda\mu)^2+(\mu-\lambda)^2\}^{-1/2}, \tag{2}$$

and the angle $\tau$ is

$$\tan\tau = (\mu-\lambda)(\delta(1-\lambda\mu)-2\lambda\mu)^{-1} \tag{3}$$

[consult Eqs. (33), (32), and (31) for the derivation of the angular momentum $J$ about the symmetry axis ($z$ axis), the unit of distance $\kappa$, and the angle $\tau$, respectively]. The angle $\tau$ is the parameter of the NUT–Geroch transformation with respect to the timelike Killing vector, which is necessary in order to have the asymptotic flatness. When $\lambda \neq \mu$ or $\lambda = \mu$, the metrics are asymmetric or symmetric with respect to the reflection at the equatorial plane, respectively. The metrics with any distortion parameter $\delta$ contain no event horizon.

In the latter half of this section the notation will be explained along the way to give convenient expressions of the gravitational field equations for sources with axial symmetry and angular momentum. In Sec. 2 the metric functions of the H–K–X family of spinning mass solutions with arbitrary positive number distortion parameter $\delta$ will be given. Finally, in Sec. 3 the property of the metrics obtained will be studied.

The line element is written in the form

$$ds^2 = f^{-1}\{e^{2\gamma}(dz^2+d\rho^2)+\rho^2\,d\phi^2\} - f(dt-\omega\,d\phi)^2, \tag{4}$$

where $z$, $\rho$, and $\phi$ are the Weyl–Papapetrou coordinates and the three metric functions $f$, $\omega$, and $\gamma$ are functions of $z$ and $\rho$ only. Prolate spheroidal coordinates $x$ and $y$ are introduced as

$$\rho = \kappa(x^2-1)^{1/2}(1-y^2)^{1/2} \text{ and } z = \kappa xy,$$

where the unit of distance $\kappa$ is given in Eq. (2) [consult Eq. (32) for the derivation of $\kappa$]. The notations $a = x^2-1$ and $b = y^2-1$ are also introduced. The Einstein vacuum field equations are

$$\nabla(f^{-1}\nabla f+\omega f^2\rho^{-2}\nabla\omega) = 0, \tag{5}$$

$$\nabla(f^2\rho^{-2}\nabla\omega) = 0, \tag{6}$$

$$\gamma_z - 2^{-1}f^{-2}\rho(f_z f_\rho+\Omega_z\Omega_\rho) = 0, \tag{7}$$

$$\gamma_\rho + 4^{-1}f^{-2}\rho((f_z)^2+(\Omega_z)^2-(f_\rho)^2-(\Omega_\rho)^2) = 0, \tag{8}$$

where Eqs. (9) are used in advance and, for example, $\gamma_z = \partial\gamma/\partial z$. It follows from Eqs. (6) and (5) that there are potentials $\Omega$ and $P$, respectively, which satisfy

$$\begin{aligned} &\rho^{-2}f^2\omega_y = -\kappa^{-1}b^{-1}\Omega_x \quad \text{and} \\ &\rho^{-2}f^2\omega_x = -\kappa^{-1}a^{-1}\Omega_y, \end{aligned} \tag{9}$$

$$f^{-1}f_x+\rho^{-2}\omega f^2\omega_x = -\kappa^{-1}a^{-1}(\omega\Omega)_y + a^{-1}P_y,$$

$$f^{-1}f_y+\rho^{-2}\omega f^2\omega_y = -\kappa^{-1}b^{-1}(\omega\Omega)_x + b^{-1}P_x. \tag{10}$$

$A$, $B$, $H$, $I$, and $G$ are defined by the relations

$$f = A/B,\ \Omega = 2I/B,\ B = A+2H+2G,$$

and

$$H^2+I^2 = AG+G^2.$$

The Ernst $\epsilon$ and $\xi$ functions[2] are $\epsilon = (A+i2I)/B$ and $\xi = (H+iI)/G$. Then Eqs. (9) and (10) become

$$\begin{aligned} &2aA^{-2}(H(A+2G)_x-(A+2G)H_x) = P_y, \\ &2bA^{-2}(H(A+2G)_y-(A+2G)H_y) = P_x, \end{aligned} \tag{11}$$

$$\begin{aligned} &2aA^{-2}(I(A+2G)_x-(A+2G)I_x) = Q_y, \\ &2bA^{-2}(I(A+2G)_y-(A+2G)I_y) = Q_x, \end{aligned} \tag{12}$$

$$\begin{aligned} &4aA^{-2}(IH_x-HI_x) = R_y, \\ &4bA^{-2}(IH_y-HI_y) = R_x, \end{aligned} \tag{13}$$

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and

$$\omega = -\kappa(Q + R) + \text{const.} \tag{14}$$

Three potentials $P$, $Q$, and $R$ are transformed linearly among them under the operation of three generators of the SU(1,1) Ehlers group. Under the operation of one of three generators (parameter is $\tau$) $A$, $H$, $I$, $G$, $P$, $Q$, and $R$ are transformed as

$$\begin{aligned} &A' = A, H' = H\cos\tau + I\sin\tau, \\ &I' = -H\sin\tau + I\cos\tau, \\ &G' = G, P' = P\cos\tau + Q\sin\tau, \\ &Q' = -P\sin\tau + Q\cos\tau, \text{ and } R' = R. \end{aligned} \tag{15}$$

This is the NUT–Geroch transformation with respect to the timelike Killing vector [see Eqs. (3) and (31) for detail]. Equations (11)–(13) are the gravitational field equations for sources with axial symmetry and angular momentum.[3]

## 2. METRIC FUNCTIONS

The metric functions $f, \omega$, and $\gamma$ of the H–K–X family of spinning mass solutions, which satisfy Eqs. (11)–(13), are

$$f = A/B, \tag{16}$$

$$\omega = -\kappa(Q + R - 2(\lambda + \mu)(1 - \lambda\mu)^{-1}), \tag{17}$$

$$\kappa = m(1 - \lambda\mu)\{(\delta(1 - \lambda\mu) - 2\lambda\mu)^2 + (\mu - \lambda)^2\}^{-1/2}, \tag{18}$$

$$e^{2\gamma} = Aa^{\delta(\delta-1)}/(1 - \lambda\mu)^2(a - b)^{\delta^2+4\delta+4}, \tag{19}$$

$$\begin{aligned} A = {} & a^\delta(a - b)^{4\delta+4} + \lambda^2 a^{3\delta+1} b(x + y)^{4\delta+4} \\ & + \mu^2 a^{3\delta+1} b(x - y)^{4\delta+4} \\ & - 2\lambda\mu a^{3\delta+1}(a - b)^{2\delta+3} + \lambda^2\mu^2 a^{5\delta+4}, \end{aligned} \tag{20}$$

$$B = A + 2H + 2G, \tag{21}$$

$$H = \bar{H}\cos\tau + \bar{I}\sin\tau, \quad I = -\bar{H}\sin\tau + \bar{I}\cos\tau, \tag{22}$$

$$\tan\tau = (\mu - \lambda)(\delta(1 - \lambda\mu) - 2\lambda\mu)^{-1}, \tag{23}$$

$$\begin{aligned} \bar{H} = {} & (\tfrac{1}{4})(a - b)^{4\delta+4}\{(x + 1)^{2\delta} - (x - 1)^{2\delta}\} \\ & + (\tfrac{1}{4})\lambda^2 a^{2\delta}(x + y)^{4\delta+4}\{(y - 1)^2(x + 1)^{2\delta+2} \\ & - (y + 1)^2(x - 1)^{2\delta+2}\} \\ & + (\tfrac{1}{4})\mu^2 a^{2\delta}(x - y)^{4\delta+4}\{(y + 1)^2(x + 1)^{2\delta+2} \\ & - (y - 1)^2(x - 1)^{2\delta+2}\} \\ & - (\tfrac{1}{2})\lambda\mu a^{2\delta}(a - b)^{2\delta+3}\{(x + 1)^{2\delta+2} \\ & - (x - 1)^{2\delta+2}\} \\ & + (\tfrac{1}{4})\lambda^2\mu^2 a^{4\delta+2}\{(x + 1)^{2\delta+4} - (x - 1)^{2\delta+4}\}, \end{aligned} \tag{24}$$

$$\begin{aligned} \bar{I} = {} & -\lambda a^{2\delta}(a - b)^{2\delta+3}(x + y)^{2\delta+1} \\ & + \mu a^{2\delta}(a - b)^{2\delta+3}(x - y)^{2\delta+1} \\ & + \lambda^2\mu a^{4\delta+2}(x + y)^{2\delta+3} - \lambda\mu^2 a^{4\delta+2}(x - y)^{2\delta+3}, \end{aligned} \tag{25}$$

$$\begin{aligned} G = {} & (\tfrac{1}{4})(a - b)^{4\delta+4}\{(x + 1)^\delta - (x - 1)^\delta\}^2 \\ & + (\tfrac{1}{4})\lambda^2 a^{2\delta}(x + y)^{4\delta+4}\{(y - 1)(x + 1)^{\delta+1} \\ & - (y + 1)(x - 1)^{\delta+1}\}^2 \\ & + (\tfrac{1}{4})\mu^2 a^{2\delta}(x - y)^{4\delta+4}\{(y + 1)(x + 1)^{\delta+1} \\ & - (y - 1)(x - 1)^{\delta+1}\}^2 \\ & - (\tfrac{1}{2})\lambda\mu a^{2\delta}(a - b)^{2\delta+3}\{(x + 1)^{\delta+1} - (x - 1)^{\delta+1}\}^2 \\ & + (\tfrac{1}{4})\lambda^2\mu^2 a^{4\delta+2}\{(x + 1)^{\delta+2} - (x - 1)^{\delta+2}\}^2, \end{aligned} \tag{26}$$

$$P = \bar{P}\cos\tau + \bar{Q}\sin\tau, \quad Q = -\bar{P}\sin\tau + \bar{Q}\cos\tau, \tag{27}$$

$$\begin{aligned} \bar{P}A = {} & 2\delta y a^\delta(a - b)^{4\delta+4}, \\ & + 2\lambda^2 a^{3\delta+1} b(x + y)^{4\delta+4}(-x + (\delta + 1)y) \\ & + 2\mu^2 a^{3\delta+1} b(x - y)^{4\delta+4}(x + (\delta + 1)y) \\ & - 4\lambda\mu(\delta + 1)y a^{3\delta+1}(a - b)^{2\delta+3} \\ & + 2\lambda^2\mu^2(\delta + 2)y a^{5\delta+4}, \end{aligned} \tag{28}$$

$$\begin{aligned} \bar{Q}A = {} & -\lambda a^\delta(a - b)^{2\delta+3}(x + y)^{2\delta+1}\{(y - 1)(x + 1)^{2\delta+1}, \\ & + (y + 1)(x - 1)^{2\delta+1}\} \\ & + \mu a^\delta(a - b)^{2\delta+3}(x - y)^{2\delta+1}\{(y + 1)(x + 1)^{2\delta+1} \\ & + (y - 1)(x - 1)^{2\delta+1}\} \\ & + \lambda^2\mu a^{3\delta+1}(x + y)^{2\delta+3}\{(y - 1)(x + 1)^{2\delta+3} \\ & + (y + 1)(x - 1)^{2\delta+3}\} \\ & - \lambda\mu^2 a^{3\delta+1}(x - y)^{2\delta+3}\{(y + 1)(x + 1)^{2\delta+3} \\ & + (y - 1)(x - 1)^{2\delta+3}\}, \end{aligned} \tag{29}$$

and

$$\begin{aligned} RA = {} & -\lambda a^\delta(a - b)^{2\delta+3}(x + y)^{2\delta+1}\{(y - 1)(x + 1)^{2\delta+1} \\ & - (y + 1)(x - 1)^{2\delta+1}\} \\ & + \mu a^\delta(a - b)^{2\delta+3}(x - y)^{2\delta+1}\{(y + 1)(x + 1)^{2\delta+1} \\ & - (y - 1)(x - 1)^{2\delta+1}\} \\ & + \lambda^2\mu a^{3\delta+1}(x + y)^{2\delta+3}\{(y - 1)(x + 1)^{2\delta+3} \\ & - (y + 1)(x - 1)^{2\delta+3}\} \\ & - \lambda\mu^2 a^{3\delta+1}(x - y)^{2\delta+3}\{(y + 1)(x + 1)^{2\delta+3} \\ & - (y - 1)(x - 1)^{2\delta+3}\}. \end{aligned} \tag{30}$$

The four parameters are mass $m$, positive number distortion parameter $\delta$, and twin rotation-reflection parameters $\lambda$ and $\mu$.

## 3. PROPERTY OF METRICS

Equations (20), and (28)–(30) show that, when $x$ tends to infinity, $x \to \infty$, the leading behavior of $A$, $\bar{P}$, $\bar{Q}$, and $R$ are

$$\begin{aligned} &A \sim (1 - \lambda\mu)^2 x^{10\delta+8}, \\ &\bar{P}A \sim 2(1 - \lambda\mu)\{\delta(1 - \lambda\mu) - 2\lambda\mu\} y x^{10\delta+8} + 0x^{10\delta+8}, \\ &\bar{Q}A \sim 2(1 - \lambda\mu)(\mu - \lambda) y x^{10\delta+8} + 0x^{10\delta+8}, \\ &RA \sim 2(1 - \lambda\mu)(\lambda + \mu) x^{10\delta+8}. \end{aligned} \tag{31}$$

In order to have the asymptotic flatness, i.e., in order to have the vanishing metric function $\omega = -\kappa(Q + R) + \text{const}$ when $x$ tends to infinity, the NUT–Geroch transformation with respect to the timelike Killing vector given in Eqs. (15) is introduced, on the one hand, to eliminate $y x^{10\delta+8}$ terms from $QA = (-\bar{P}\sin\tau + \bar{Q}\cos\tau)A$, and the integration constant in Eq. (14) on the metric function $\omega$ is used, on the other hand, to eliminate $x^{10\delta+8}$ terms from $RA$. Therefore one gets $\tau$, $Q$, and $\omega$ given in Eqs. (3), (27), and (17), respectively.

The unit of distance $\kappa$ is defined to be the inverse of the coefficient of the term $-2m/x$ in the leading behavior

$$f \sim 1 - 2m/\kappa x \tag{32}$$

for $x \to \infty$. Then $\kappa$ given in Eq. (2) comes from Eqs. (16), (20)–(26), and (32). The angular momentum $J$ about the symmetry axis, the $z$ axis, is defined to be the coefficient of the term $2b/\kappa x$ in the leading behavior

$$\omega \sim J\, 2b/\kappa x \tag{33}$$

for $x \to \infty$. Then $J$ given in Eq. (1) comes from Eqs. (17), (18), (23), (27)–(30), and (33).

Equations (20), (24)–(26), and (28)–(30) on the metric functions $A, \bar{H}, \bar{I}, G, \bar{P}, \bar{Q}$, and $R$ show that the $y$-dependence of $A, \bar{H}, G, \bar{Q}$, and $R$ is always via the factors, i.e., $(\mu - \lambda)y$ multiplied by the even power of $y$, and that the $y$-dependence of $\bar{I}$ and $\bar{P}$ is not via these factors. When the parameter $\lambda$ is not equal to the parameter $\mu$, the metrics with arbitrary distortion parameter $\delta$ are asymmetric with respect to the reflection at the equatorial plane $y = 0$. When $\lambda = \mu$, the NUT–Geroch parameter $\tau$ vanishes and the metrics with arbitrary distortion parameter $\delta$ are symmetric with respect to the reflection at the equatorial plane of symmetry $y = 0$. From this and from Eq. (1) defining the angular momentum $J$ about the $z$ axis, the parameters $\lambda$ and $\mu$ are named as twin rotation-reflection parameters.

Equations (7) and (8) on the metric function $\gamma$ become

$$\gamma_x = -bA^{-2}(a-b)^{-1}(x(aK+bL) - yaM),$$

and

$$\gamma_y = -aA^{-2}(b-a)^{-1}(y(bL+aK) - xbM), \tag{34}$$

where $K$, $L$, and $M$ are defined as

$$K = (H_x)^2 + (I_x)^2 - (G_x)^2 - A_x G_x,$$

$$L = (H_y)^2 + (I_y)^2 - (G_y)^2 - A_y G_y,$$

and

$$M = 2H_x H_y + 2I_x I_y - 2G_x G_y - A_x G_y - G_x A_y.$$

$K$, $L$, and $M$ are invariants of the NUT–Geroch transformation with respect to the timelike Killing vector given in Eqs. (15). $K$, $L$, and $M$ of the H–K–X family of solutions with arbitrary distortion parameter $\delta$ do not vanish except in the case of $\lambda = \mu = 0$ ($K \neq 0$, and $L = M = 0$ when $\lambda = \mu = 0$). By contrast, $M$ of the Kerr–Tomimatsu–Sato family of spinning mass solutions with arbitrary positive integer distortion parameter $\delta$ always vanishes.[3] Both $aK + bL$ and $M$ are factorized by $A$. From Eqs. (34) we obtain the metric function $\gamma$ given in Eq. (19).

The proper area $\Sigma$ of the surface $x = 1$ is

$$\Sigma = 4\pi\kappa \int_0^1 (-e^{2\gamma}\omega^2)^{1/2}\, dy. \tag{35}$$

It follows that $\omega(x=1) \sim$ finite and $e^{2\gamma}(x=1) \sim 0$. The proper area $\Sigma$ with arbitrary distortion parameter $\delta$ vanishes. Therefore the H–K–X family of spinning mass solutions with arbitrary positive number distortion parameter $\delta$ contains no event horizon.

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# On stationary axially symmetric Einstein–Maxwell scalar and Brans–Dicke–Maxwell fields

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A particular type of exact solutions of Einstein–Maxwell massless scalar field equations corresponding to stationary axially symmetric fields is presented here. The solutions are linear combinations of static fields with constant coefficients. Further, by a proper choice of conformal transformation the solutions have been transformed to the Brans–Dicke fields coupled with source-free electromagnetic fields. Finally these solutions have been transformed to a general form through unit transformations.

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## 1. INTRODUCTION

The study of scalar meson fields has attracted the attention of many workers. Brahmachary[1] considered the massive whereas Bergmann and Leipnik[2] considered the massless scalar fields coupled to spherically symmetric gravitational fields. Janis *et al.*[3] have further considered the problem from the point of view of singularities and Gautreau,[4] Singh,[5] and Buchdahl[6] have extended the study to the case of nonspherical Weyl and plane symmetric fields. Later on the workers in the field, with a few exceptions (Stephenson[7]), have directed their efforts to the study of massless scalar fields coupled to gravitational and electromagnetic fields (Refs 8–11). The generalization of the Reissner–Nördstrom solution in the presence of a massless scalar field was obtained by Penny.[12] Janis *et al.*[13] obtained the solutions of the Einstein scalar and Brans–Dicke field equations for static space–time and also gave a procedure to generate static solutions of the coupled Einstein–Maxwell scalar field equations and the Brans–Dicke scalar tensor theory (Brans and Dicke[14]). Recently, the solutions of axially symmetric Einstein–Maxwell scalar field equations have been given by Eris and Gurses[15] and the Brans–Dicke–Maxwell fields have been studied by Singh and Rai.[16]

In Sec. 2 we obtain solutions to the stationary axially symmetric gravitational field coupled to massless scalar and source-free electromagnetic fields following the method first introduced by Lewis[17] to obtain the solutions for the axially symmetric gravitational fields. Using Weyl-like canonical coordinates we give here a special class of solutions obtained from the linear combinations of Weyl's static fields.[18] The solution admits a very simple interpretation, similar to Arbex and Som (Refs. 19 and 20), that an observer in canonical space $(r,\theta,z)$ describes the static fields of the canonical space $(r',\theta',z')$ using a reference system which rotates with constant angular speed $\Omega$ whose measure is given by $|\Omega| < 1$. Although some of the steps are parallel to Arbex and Som,[19,20] we have written the steps in full because of certain changes due to corrections of the calculation errors of these papers. For vanishing rotation one gets the static field. According to Dicke,[21] by a proper choice of conformal factor and scaling the metric as well as the field quantities suitably, the Brans–Dicke–Maxwell scalar fields coupled with source-free electromagnetic fields reduce to the Einstein–Maxwell massless scalar fields and *vice versa*. Thus, in Sec. 3 we have obtained solutions for Brans–Dicke–Maxwell fields. Further, in Sec. 4 we have used the unit transformations given by Morganstern[22] and the above solutions have been transformed to a more general form. Some concluding remarks are given in Sec. 5.

## 2. SOLUTIONS OF THE FIELD EQUATIONS

We consider a stationary axially symmetric space–time where the sources of the geometry are massless scalar and source-free electromagnetic fields. The field equations are

$$R_{\mu}^{\nu} = -K\,[V_{,\mu}V^{,\nu} + E_{\mu}^{\nu}], \tag{2.1}$$

with

$$E_{\mu}^{\nu} = -F_{\mu\alpha}F^{\nu\alpha} + \tfrac{1}{4}\delta_{\mu}^{\nu}F^{\rho\lambda}F_{\rho\lambda}, \tag{2.2}$$

$$g^{\mu\nu}V_{;\mu\nu} = 0, \tag{2.3}$$

$$F_{;\nu}^{\mu\nu} = 0, \tag{2.4}$$

$$F_{[\mu\nu;\alpha]} = 0, \tag{2.5}$$

where $V$ is a scalar field and the semicolon denotes covariant derivative.

We take the stationary axially symmetric line element in the form

$$ds^2 = f\,dt^2 - e^{2\psi}(dr^2 + dz^2) - l\,d\phi^2 + 2m\,d\phi\,dt, \tag{2.6}$$

where $f$, $\psi$, $l$, and $m$ are functions of $r$ only. We shall number the coordinates $r,z,\phi,t$ as 1,2,3,4, respectively. On account of the stationary character of the field we can take the surving components of $F^{\mu\nu}$ to be $F^{31}(=-F^{13})$ and $F^{41}(=-F^{14})$ only. Then from Eqs. (2.1) and (2.2) it follows that

$$R_4^4 + R_3^3 = 0. \tag{2.7}$$

One can now introduce Weyl-like canonical coordinates[23] such that

$$fl + m^2 = r^2. \tag{2.8}$$

If one makes a linear transformations of the coordinate differentials[17] such as

$$\begin{aligned} dt &= dt'\cosh u - d\phi'\sinh u, \\ d\phi &= d\phi'\cosh u - dt'\sinh u, \end{aligned} \tag{2.9}$$

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with

$$f = F\cosh^2 u - L\sinh^2 u, \quad l = L\cosh^2 u - F\sinh^2 u, \tag{2.10}$$

$$m = \tfrac{1}{2}(L - F)\sinh 2u,$$

the metric (2.6) transforms into

$$ds^2 = F\,dt'^2 - e^{2\psi}(dr^2 + dz^2) - L\,d\phi'^2 \tag{2.11}$$

in Weyl's canonical system.

In general, the transformation (2.9) is purely local. In our case, we choose $u$ as constant. Now let

$$\cosh u = \gamma \quad \text{and} \quad \sinh u = \gamma\Omega, \tag{2.12}$$

where $\gamma$ and $\Omega$ are constants such that

$$\gamma = (1 - \Omega^2)^{-1/2}. \tag{2.13}$$

From Eqs. (2.8) and (2.10) we have

$$fl + m^2 = r^2 = FL. \tag{2.14}$$

We now choose

$$F = e^{2\alpha} \quad \text{and} \quad L = r^2 e^{-2\alpha}, \tag{2.15}$$

where $\alpha$ is a function of $r$ only. Then Eq. (2.10) takes the form

$$f = \gamma^2(e^{2\alpha} - \Omega^2 r^2 e^{-2\alpha}), \quad l = \gamma^2(r^2 e^{-2\alpha} - \Omega^2 e^{2\alpha}),$$
$$m = \gamma^2\Omega(r^2 e^{-2\alpha} - e^{2\alpha}). \tag{2.10a}$$

The field equations may now be explicitly written as

$$r\psi_{11} - \psi_1 - 2\alpha_1(1 - r\alpha_1) = \sqrt{(-g)}\,K\,[e^{-2\psi}V_{,1}^2 + \tfrac{1}{2}(F^{41}F_{41} + F^{31}F_{31})], \tag{2.16}$$

$$r\psi_{11} + \psi_1 = -\sqrt{(-g)}\,\frac{K}{2}(F^{41}F_{41} + F^{31}F_{31}), \tag{2.17}$$

$$\gamma^2\frac{\partial}{\partial r}[1 - r\alpha_1(1 + \Omega^2)] = -\sqrt{(-g)}\,\frac{K}{2}(F^{41}F_{41} - F^{31}F_{31}), \tag{2.18}$$

$$\gamma^2\frac{\partial}{\partial r}[r\alpha_1(1 + \Omega^2)] = \sqrt{(-g)}\,\frac{K}{2}(F^{41}F_{41} - F^{31}F_{31}), \tag{2.19}$$

$$-(\gamma^2\Omega)\frac{\partial}{\partial r}[(1 - 2r\alpha_1)] = \sqrt{(-g)}\,KF^{41}F_{31}, \tag{2.20}$$

$$(\gamma^2\Omega)\frac{\partial}{\partial r}[(1 - 2r\alpha_1)] = \sqrt{(-g)}\,KF^{31}F_{41}, \tag{2.21}$$

$$\gamma = k - n\log r, \tag{2.22}$$

$k$ and $n$ being constants of integration. From Eqs. (2.20) and (2.21) one obtains

$$-\frac{F^{31}}{F^{41}} = \frac{F_{31}}{F_{41}} = \beta, \tag{2.23}$$

where $\beta$ is a constant.

We consider now two cases:

$$\text{(i)}\ \beta = 1/\Omega$$
$$\text{(ii)}\ \beta = \Omega. \tag{2.24}$$

*Case (i)* $\beta = 1/\Omega$: In this case the observer in canonical space $(r,\phi,z)$ describes the pure static magnetic field in canonical space $(r',\phi',z')$ using a reference frame which rotates with angular speed $\Omega$.

From Eq. (2.4) we have

$$\sqrt{(-g)}\,F^{31} = A, \tag{2.25}$$

where $A$ is a constant.

From Eqs. (2.20), (2.21), (2.23), and (2.25) we have

$$e^{2\alpha}\left[\alpha_{11} + \frac{\alpha_1}{r}\right] = \left(-\frac{K}{2}\right)\frac{A^2}{\gamma^2},$$

which on integration gives

$$e^{2\alpha} = \{(r)^{1+b} - a(r)^{1-b}\}^2, \tag{2.26}$$

where $a$ and $b$ are constants of integration satisfying the relation

$$a = A^2K/8b^2\gamma^2. \tag{2.27}$$

From Eqs. (2.17), (2.20), (2.21), and (2.25) one obtains

$$r\psi_{11} + \psi_1 = -\frac{1}{2}\frac{\partial}{\partial r}[(1 - 2r\alpha_1)] = \frac{\partial}{\partial r}(r\alpha_1),$$

which on integration gives

$$\psi = \alpha + B\log r + D, \tag{2.28}$$

$B$ and $D$ being constants of integration.

Using the value of $\alpha$ from Eq. (2.26) in Eq. (2.16), we get

$$B = \left(b^2 - \frac{Kn^2}{2} - 1\right). \tag{2.29}$$

Substituting $\alpha$ in expression (2.10a), we have

$$f = \gamma^2[\{(r)^{1+b} - a(r)^{1-b}\}^2 - \Omega^2 r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2}],$$
$$l = \gamma^2[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \Omega^2\{(r)^{1+b} - a(r)^{1-b}\}^2],$$
$$m = \gamma^2\Omega\,[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \{(r)^{1+b} - a(r)^{1-b}\}^2], \tag{2.10b}$$

and from Eqs. (2.26), (2.28), and (2.29)

$$e^{2\psi} = r^{2[b^2 - (Kn^2/2) - 1]}\{(r)^{1+b} - a(r)^{1-b}\}^2.$$

*Case (ii)* $\beta = \Omega$: In this case the static field in the canonical space $(r',\phi',z')$ is a purely radial electrostatic field. From Eq. (2.4) one gets

$$\sqrt{(-g)}\,F^{41} = B, \tag{2.30}$$

where $B$ is a constant. Equations (2.20), (2.21), (2.23), and (2.30) yield

$$e^{-2\alpha}[r^2\alpha_{11} + r\alpha_1] = -\frac{KB^2}{2\gamma^2}. \tag{2.31}$$

On integration we get

$$e^{2\alpha} = \{(r)^d + c(r)^{-d}\}^{-2}, \tag{2.32}$$

where $c$ and $d$ are integration constants satisfying the relation

$$c = B^2K/8d^2\gamma^2. \tag{2.33}$$

From Eqs. (2.17), (2.20), (2.21), and (2.30) one obtains

$$r\psi_{11} + \psi_1 = \frac{1}{2}\frac{\partial}{\partial r}[(1 - 2r\alpha_1)] = -\frac{\partial}{\partial r}(r\alpha_1),$$

which on integration gives

$$\psi = -\alpha + M\log r + N, \tag{2.34}$$

where $M$ and $N$ are constants of integration.

Substituting the value of $\alpha$ from Eq. (2.32) in Eq. (2.16), we get

$$M = \left(d^2 - \frac{Kn^2}{2}\right). \tag{2.35}$$

Substituting $\alpha$ in expression (2.10a), we get

$$\begin{aligned} f &= \gamma^2[\{(r)^d + c(r)^{-d}\}^{-2} - \Omega^2 r^2\{(r)^d + c(r)^{-d}\}^2], \\ l &= \gamma^2[r^2\{(r)^d + c(r)^{-d}\}^2 - \Omega^2\{(r)^d + c(r)^{-d}\}^{-2}], \\ m &= \gamma^2\Omega\,[r^2\{(r)^d + c(r)^{-d}\}^2 - \{(r)^d + c(r)^{-d}\}^{-2}], \end{aligned} \tag{2.10c}$$

and from Eqs. (2.32), (2.34), and (2.35)

$$e^{2\psi} = r^{2[d^2 - (Kn^2/2)]}\{(r)^d + c(r)^{-d}\}^2,$$

when $n = 0$, the solutions (2.10b) and (2.10c) immediately go to the solutions of Arbex and Som[19,20] (with some corrections), which further reduces to Lewis' solution[17] when $A$ and $B$ are set equal to zero.

## 3. SOLUTION FOR BRANS–DICKE–MAXWELL SCALAR FIELDS

As pointed out in the Introduction, the Brans–Dicke scalar electromagnetic fields are conformal to the coupled zero-mass scalar and source-free electromagnetic fields of Einstein's gravitational theory. A similar result in the case of vacuum Brans–Dicke fields has been established by Peters[24] and Tabensky and Taub.[25] It has been shown that the conformal transformation

$$\exp\left\{\frac{\sqrt{2}V}{(\omega + \frac{3}{2})^{1/2}}\right\} = \Phi_{\rm BD}, \tag{3.1a}$$

$$(\Phi_{\rm BD})^{-1} g_{\mu\nu} = \underset{\rm BD}{g}_{\mu\nu}, \tag{3.1b}$$

where $\Phi_{\rm BD}$ and $\underset{\rm BD}{g}_{\mu\nu}$ are the quantities occurring in the Brans–Dicke theory, reduces the Brans–Dicke vacuum fields to zero-mass scalar fields of Einstein's gravitational theory and *vice versa*. The above transformation works again when the source-free electromagnetic field is also present in addition to the scalar fields.

In this case we consider a new stationary axially symmetric metric

$$ds^2 = \bar{f}\,dt^2 - e^{\overline{2\psi}}(dr^2 + dz^2) - \bar{l}\,d\phi^2 + 2\,\bar{m}\,d\phi\,dt, \tag{3.2}$$

with $\bar{f}$, $\bar{\psi}$, $\bar{l}$, and $\bar{m}$ as functions of $r$ only. After conformal transformation we get the values of $\bar{f}$, $\bar{\psi}$, $\bar{l}$, and $\bar{m}$.

(i) *For pure static magnetic field*, we consider the solution (2.10b). Applying the conformal transformation (3.1a) and (3.1b), we obtain

$$\Phi_{\rm BD} = \exp\left\{\frac{\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{3.3a}$$

$$\begin{aligned} \bar{g}_{11} = \bar{g}_{22} &= -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[b^2 - (Kn^2/2) - 1]}\{(r)^{1+b} - a(r)^{1-b}\}^2, \\ \bar{g}_{33} &= -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \Omega^2\{(r)^{1+b} - a(r)^{1-b}\}^2], \\ \bar{g}_{44} &= \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2[\{(r)^{1+b} - a(r)^{1-b}\}^2 - \Omega^2 r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2}], \\ \bar{g}_{34} = \bar{g}_{43} &= \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2\Omega\,[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \{(r)^{1+b} - a(r)^{1-b}\}^2]. \end{aligned} \tag{3.3b}$$

(ii) *For purely radial electrostatic field*, we consider the solution (2.10c). Applying the conformal transformation (3.1a) and (3.1b) we obtain

$$\Phi_{\rm BD} = \exp\left\{\frac{\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{3.4a}$$

$$\begin{aligned} \bar{g}_{11} = \bar{g}_{22} &= -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[d^2 - (Kn^2/2)]}\{(r)^d + c(r)^{-d}\}^2, \\ \bar{g}_{33} &= -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2[r^2\{(r)^d + c(r)^{-d}\}^2 - \Omega^2\{(r)^d + c(r)^{-d}\}^{-2}], \\ \bar{g}_{44} &= \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2[\{(r)^d + c(r)^{-d}\}^{-2} - \Omega^2 r^2\{(r)^d + c(r)^{-d}\}^2], \end{aligned}$$

$$\bar{g}_{34} = \bar{g}_{43} = \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\gamma^2\Omega\,[r^2\{(r)^d + c(r)^{-d}\}^2 - \{(r)^d + c(r)^{-d}\}^{-2}]. \tag{3.4b}$$

Let us now consider a static axially symmetric line element

$$ds^2 = \bar{F}\,dt'^2 - e^{2\bar{\psi}}(dr^2 + dz^2) - \bar{L}\,d\phi'^2, \tag{3.5}$$

with $\bar{F}$, $\bar{\psi}$, and $\bar{L}$ as functions of $r$ only. After conformal transformation we get the values of $\bar{F}$, $\bar{\psi}$, and $\bar{L}$.

(i) *For pure static magnetic field*, we consider the solution corresponding to Eq. (2.11). Applying the conformal transformation (3.1a) and (3.1b) we get

$$\Phi_{BD} = \exp\left\{\frac{\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{3.6a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[b^2 - (Kn^2/2) - 1]}\{(r)^{1+b} - a(r)^{1-b}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2},$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\{(r)^{1+b} - a(r)^{1-b}\}^2. \tag{3.6b}$$

(ii) *For purely radial electrostatic field*, we consider the solution corresponding to Eq. (2.11). After conformal transformation we get

$$\Phi_{BD} = \exp\left\{\frac{\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{3.7a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[d^2 - (Kn^2/2)]}\{(r)^d + c(r)^{-d}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^2\{(r)^d + c(r)^{-d}\}^2,$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}\{(r)^d + c(r)^{-d}\}^{-2}. \tag{3.7b}$$

when $\Omega = 0$, the solution in case (i) reduces to a Brans–Dicke analog of the axially symmetric magnetic field given by Ghosh and Sengupta.[26] For $\Omega = 0$, the solution of case (ii) becomes an analog of the solution for a static, cylindrically symmetric radial electrostatic field obtrained by Mukherjee,[27] Bonnor,[28] and Raychaudhuri.[29]

## 4. GENERAL FORM OF THE SOLUTIONS

We consider, without loss of generality, the scalar $\Phi$ as a specific function $\Lambda$, viz., $\Phi = \Phi_0\Lambda$, in the original Brans–Dicke equations and subsequently scale the length, time, and reciprocal mass by the common factor $[\Lambda(x)]^{(1-\theta)/2}$; then

$$\bar{g}_{ij} \to \bar{\bar{g}}_{ij} = \Lambda^{1-\theta}\bar{g}_{ij}, \tag{4.1a}$$

$$\Phi \to \bar{\Phi} = \Phi_0\Lambda^{\theta}, \tag{4.1b}$$

where $\theta$ is a parameter.

We consider the stationary axially symmetric metric

$$ds^2 = \bar{\bar{f}}\,dt^{\bar{\bar{2}}} - e^{2\psi}(dr^2 + dz^2) - \bar{l}\,d\phi^2 + 2\bar{m}\,d\phi\,dt, \tag{4.2}$$

where $\bar{\bar{f}}$, $\bar{\psi}$, $\bar{l}$, and $\bar{m}$ as functions of $r$ only. After unit transformation we get the values of $\bar{\bar{f}}$, $\bar{\psi}$, $\bar{l}$, and $\bar{m}$.

(i) *For pure static magnetic field*, application of the unit transformation (4.1) on the solution (2.10b) yields

$$\Phi \to \bar{\Phi} = \Phi_0\Lambda^{\theta} = \exp\left\{\frac{\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\},$$

where

$$\Lambda = \exp\left\{\frac{\sqrt{2}(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}$$

and we have assumed $\Phi_0 = 1$ for simplicity. Thus, the solution in the present case is given by

$$\bar{\Phi} = \exp\left\{\frac{\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{4.3a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[b^2 - (Kn^2/2) - 1]}\{(r)^{1+b} - a(r)^{1-b}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \Omega^2\{(r)^{1+b} - a(r)^{1-b}\}^2],$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2[\{(r)^{1+b} - a(r)^{1-b}\}^2 - \Omega^2 r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2}],$$

$$\bar{g}_{34} = \bar{g}_{43} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2\Omega\,[r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2} - \{(r)^{1+b} - a(r)^{1-b}\}^2]. \tag{4.3b}$$

(ii) *For purely radial electrostatic field*, through similar steps the solution (2.10c), after unit transformation, turns into

$$\bar{\Phi} = \exp\left\{\frac{\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{4.4a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2\{d^2 - (Kn^2/2)\}}\{(r)^d + c(r)^{-d}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2[r^2\{(r)^d + c(r)^{-d}\}^2 - \Omega^2\{(r)^d + c(r)^{-d}\}^{-2}],$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2[\{(r)^d + c(r)^{-d}\}^{-2} - \Omega^2 r^2\{(r)^d + c(r)^{-d}\}^2],$$

$$\bar{g}_{34} = \bar{g}_{43} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \gamma^2\Omega\,[r^2\{(r)^d + c(r)^{-d}\}^2 - \{(r)^d + c(r)^{-d}\}^{-2}]. \tag{4.4b}$$

Let us again consider a static axially symmetric line element

$$ds^2 = \bar{F}\,dt'^2 - e^{2\bar{\psi}}(dr^2 + dz^2) - \bar{L}\,d\phi'^2, \tag{4.5}$$

with $\bar{F}$, $\bar{\psi}$, and $\bar{L}$ as functions of $r$ only. Under unit transformation we get the values of $\bar{F}$, $\bar{\psi}$, and $\bar{L}$.

(i) *For pure static magnetic field*, we consider the solution for Eq. (2.11). Under unit transformation (4.1), we get

$$\bar{\Phi} = \exp\left\{\frac{\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{4.6a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[b^2 - (Kn^2/2) - 1]}\{(r)^{1+b} - a(r)^{1-b}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^2\{(r)^{1+b} - a(r)^{1-b}\}^{-2},$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \{(r)^{1+b} - a(r)^{1-b}\}^2. \tag{4.6b}$$

(ii) *For purely radial electrostatic field*, in a similar manner the solution for (2.11), after unit transformation, turns into

$$\bar{\Phi} = \exp\left\{\frac{\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\}, \tag{4.7a}$$

$$\bar{g}_{11} = \bar{g}_{22} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^{2[d^2 - (Kn^2/2)]}\{(r)^d + c(r)^{-d}\}^2,$$

$$\bar{g}_{33} = -\exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} r^2\{(r)^d + c(r)^{-d}\}^2,$$

$$\bar{g}_{44} = \exp\left\{\frac{-\sqrt{2}\theta(k - n\log r)}{(\omega + \frac{3}{2})^{1/2}}\right\} \{(r)^d + c(r)^{-d}\}^{-2}. \tag{4.7b}$$

If we put $\theta = 1$, we get the solutions of Sec. 3.

## 5. CONCLUDING REMARKS

We have considered only two classes of exact solutions of the Einstein–Maxwell scalar and Brans–Dicke–Maxwell fields corresponding to the observer's two modes of description of the static field—either the static axially symmetric magnetic field (2.10b) or the static axially symmetric radial electrostatic field (2.10c). Of course, another class of solutions may be obtained when $\beta$ is different from $\Omega$. In this case the solution would correspond to the observer's descriptions of the static axial magnetic field as well as the radial electrostatic field.


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# The quantum equivalence principle and finite particle creation in expanding universes

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A formulation of the equivalence principle in quantum field theory is introduced. The quantum equivalence principle yields implementable Bogolyubov transformations. In this way we find a theory for a scalar field in curved space–time where particle creation is finite for every value of the coupling constant. In the particular case of conformal coupling the initial conditions of positive and negative frequency wave functions coincide with the ones of a first order WKB approximation. The coefficients of the Bogolyubov transformations are exactly computed and the created energy density is also finite.

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## 1. INTRODUCTION

The problem of quantizing a scalar field on a curved background has been treated in several ways. We will consider only two of these techniques:

(1) the "in-out" theory and

(2) the Green's function general theory.

Although the first one can be considered as a particular case of the second one, this last theory is older because it was always considered as the natural way to generalize the field formalism to curved space–time. If one can find some natural generalization of the flat space Green's functions: $\Delta(x-x')$ and $\Delta_1(x-x')$ to curved space–time, one can also find the positive and negative frequency parts of the field and construct a reasonable quantum theory. One can find a straightforward generalization of $\Delta(x-x')$, that we shall call $G(x,x')$, but it can be shown (cf. Ref. 1) that it is not always possible to find an unique generalization of $\Delta_1(x-x')$; i.e., $G_1(x,x')$ (unless space–time is static). The difficulty can be overcome if we suppose that each Cauchy surface $S$ of the universe (that normally is a globaly hyperbolic manifold) has its own $G_1^{(S)}(x,x')$, and therefore it has its own splitting into positive and negative frequency solutions, i.e., its own representation of the C.C.R. This implies the existence of a Bogolyubov transformation between the positive and negative frequency wave functions of two Cauchy surfaces. This implies also that particles are created and/or annihilated when we go from one surface to another. This is a reasonable phenomena because if the gravitational field (the curved background) is not static there must be a variation on the number of particles. One the contrary if the gravitational field is static $G_1(x,x')$ is unique and the particle number is constant.

The problem is to find a way to define the correct $G_1^{(S)}(x,x')$ for each Cauchy surface. In our opinion the solution must fulfill two necessary conditions:

(1) It must be based on physical principles.

(2) The number of particles created must be finite, i.e., the Bogolyubov transformation between the different operator algebras must be implementable.

Since canonical quantization based on diagonalization of the instantaneous Hamiltonian yields nonimplementable Bogolyubov transformations (cf. Refs. 2 an 3) a lot of work has been done in the "in-out" theory where the quantum fields are studied in some particular universes which are asymptotically static. In the "in-out" asymptotic states of these universes $G_1^{\text{in(out)}}(x,x')$ is unambiguously defined and the Bogolyubov transformation among them can be computed yielding the number of particles created. The restricted theory can be considered fairly satisfactory in many cases (as in the Hawking effect).

But the real universal is not asymptotically static. Moreover if we restrict ourselves to the "in-out" theory we shall never be able to see how the particle creation reacts in the universe evolution, i.e., to formulate a cosmology that takes into account the quantum phenomena.

For this reason we have tried to find a solution in the general case. Our point of view is that this solution must be based on the two cornerstones of general relativity: covariance and equivalence so we have developed a covariant formalism in the sense that the quantization is defined through covariant objects like the $G(x,x')$ and $G_1(x,x')$. (Therefore, it is not an analogy of canonical quantization in a privileged coordinate system.) If some coordinates (as $t$) seem to be privileged it is because they have some physical meaning (e.g., the proper time of a fluid of particles that fills the universe). We base our solution on a version of the strong equivalence principle that we call the quantum equivalence principle. The strong equivalence principle states that in every point of space–time there exists a system of coordinates where the inertial-gravitational forces vanish. In this system space–time behaves locally as if it were flat. We suppose that the biscalar $G_1(x,x')$ behaves like $\Delta_1(x,x')$ when $x \to x'$. However this condition cannot be imposed when $x \to x'$ along every direction, and at every point, in space–time (cf. Ref. 1). So

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we demand that $G_1^{(S)}(x,x')$ behaves like $\Delta_1(x,x')$ when $x \to x'$ on the Cauchy surface $S$. This is our quantum equivalence principle that allows us to define the $G_1^{(S)}(x,x')$.

With these tools we find a self-consistent answer to our problem.

The nicest features of our solution are the following:

(1) It is implementable for every value of the coupling constant (we even have found a general class of implementable theories that contain ours; cf. Sec. 5) so the particle creation is finite.

(2) In the case of conformal coupling ( $\xi = \frac{1}{6}$) the boundary conditions of our positive and negative frequency wave functions coincide with the boundary conditions of similar functions found with a first order WKB approximation. Therefore, our particle model at each time is an exact solution of the Klein–Gordon equation that satisfies at that time the boundary conditions of a first order WKB approximation. This model combines two important features of the flat space free particles. In fact flat space wave functions are solutions of the Klein–Gordon equation and are a first order WKB approximation, of course, in flat space the first order WKB approximation turns out to be exact.

(3) The coefficients of the Bogolyubov transformation can be exactly computed directly from the wave function with really simple formulas [cf. Eq. (6.21)].

(4) The most logical generalization to our theory of the energy of the field in flat space–time, namely

$$E = \int_S \langle T^0{}_0 \rangle \, d\sigma ,$$

where $S$ is a Cauchy surface and $d\sigma$ is the element of area in $S$, is also finite in the case of conformal coupling (cf. Sec. 7).

The generalization of our method to fields with higher spin as well as to the case of a curved spatial metric will be considered elsewhere. The cosmological implications of the particle creation predicted by our model will be the subject of a subsequent publication.

## 2. DEFINITIONS AND NOTATION

In this Section we state well-known results, that will be useful later on, using the notation of Ref. 1. We will work in a space–time $V_4$ endowed with a Robertson–Walker metric,

$$ds^2 = dt^2 - a^2(t)\delta_{\alpha\beta}dx^\alpha dx^\beta , \quad \alpha,\beta = 1, 2, 3 , \tag{2.1}$$

that we shall call an expanding universe even in the case where $a(t)$ is not monotonically increasing. $\delta_{\alpha\beta}$ is Kronecker's function.

We will study the quantization of a neutral scalar field $\phi(x)$, that is, a real valued function on $V^4$ that satisfies the Klein–Gordon equation

$$(\Delta - \mu^2 - \xi R)\phi = 0 , \tag{2.2}$$

where $\Delta = -g^{ij}\nabla_i\partial_j$ is the *Laplace* operator, $\mu$ is the mass, and

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{(\dot{a})^2}{a^2}\right), \quad \dot{a} = \frac{da}{dt}$$

is the curvature scalar. The coupling constant $\xi$ can take any real value. The case $\xi = 0$ is the "minimal coupling" and $\xi = \frac{1}{6}$ is the "conformal coupling."

We want to generalize the notions of positive and negative frequency solutions of Eq. (2.2), from flat space–time to $V_4$, using the kernels $G(x,x')$ and $G_1(x,x')$, i.e., the generalizations of the usual kernels

$$\Delta(x - x') = \frac{1}{(2\pi)^3}\int \frac{\sin w_p(x^0 - x'^0)}{w_p} \times \exp[-i\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')]d^3\mathbf{p} , \tag{2.3a}$$

$$\Delta_1(x - x') = \frac{1}{(2\pi)^3}\int \frac{\cos w_p(x^0 - x'^0)}{w_p} \times \exp[-i\mathbf{p}\cdot(\mathbf{x} - \mathbf{x}')]d^3\mathbf{p} , \tag{2.3b}$$

where

$$p = |\mathbf{p}^2| , \quad w_p = (\mu^2 + p^2)^{1/2} , \text{ a = const.}$$

We remark tht the real physical lengths are $a(t)x^\alpha$ and that the physical momentum $p^\alpha$ is canonically conjugated to these physical coordinates. We shall call $k^\alpha$ the momentum conjugated to $x^\alpha$ that is related to the $p^\alpha$ as $k^\alpha = a(t)p^\alpha$.

$G(x,x')$, the generalization of the commutator $\Delta(x - x')$, has been found a long time ago by Lichnerowicz (cf. Ref. 4) for all globally hyperbolic manifolds. In particular for our $V_4$ with metric (2.1). This $G(x,x')$ has locally all the properties of the $\Delta(x - x')$; i.e., it is real and

$$G(x, x') = -G(x, x') , \quad (\Delta_x - \mu^2 - R\xi)G(x, x') = 0 . \tag{2.4}$$

It provides too the solution of the Cauchy problem for Eq. (2.2) with Cauchy data: $\phi_S$, $\dot{\phi}_S$ on a Cauchy surface $S$,

$$\phi(x') = \int_S [G(x', x)\dot{\phi}_S(x) - \phi(x)n^i\partial_i G(x, x')] \, d\sigma . \tag{2.5}$$

$G(x,x')$ satisfies the boundary conditions

$$G(x, x') = 0 \quad \text{if } x, x' \in S , \tag{2.6}$$

$$n^i\partial_i G(x, x') = \delta_S(x, x') \quad \text{if } x, x' \in S , \tag{2.7}$$

where $\delta_S(x,x')$ is the dirac $\delta$ on the surface $S$ and $n^i$ is the unitary vector normal to $S$ pointing towards the future.

The support ${}_{x'}G(x, x')$ lies in the interior of the light conoid with vertex $x$. There is a unique and well defined $G(x,x')$ that fulfills all these conditions.[4]

On the contrary there are infinitely many $G_1(x,x')$ that generalize $\Delta_1(x,x')$ having its usual properties, i.e., such that $G_1$ is real and

$$G_1(x, x') = G_1(x', x) , \tag{2.8}$$

$$(\Delta_x - \mu^2 - \xi R)G_1(x, x') = 0 , \tag{2.9}$$

$$G(x, x') = \int_S \left[\left(\frac{\partial}{\partial t_y}G_1(x', y)\right)G_1(x, y) - G_1(x', y)\frac{\partial}{\partial t_y}G_1(x, y)\right] d\sigma_y . \tag{2.10}$$

Since $G(x,x')$ and $G_1(x,x')$ define the solutions of positive and negative frequency (cf. Ref. 1) there are infinitely many possible quantizations, each one corresponding to a particular choice of $G_1(x,x')$. (This phenomenon is the ambiguity first stated by Parker.[5])

Our point of view (as it was introduced in Ref. 6) is that there exists a different $G_1^{(S)}(x,x')$ for each Cauchy surface of $V_4$ [in particular a different $G_1^{(\tau)}(x,x')$ for each surface

$t = \tau = \text{const}$ of $V_4$]. These different $G_1$ produce different definitions of positive and negative frequency and cause particle creation or annihilation when we go from one time $\tau$ to another $\tau'$. The $G_1^{(\tau)}(x,x')$ must be defined by reasonable initial conditions based on physical principles.

The functions $\phi(x)$, $G(x,x')$, and $G_1(x,x')$ can be expanded as follows: Let us introduce an inner product in the space of complex solutions of Eq. (2.2),

$$\langle u, v\rangle = i\int_S [(\partial_i u^*)v - u^*(\partial_i v)]n^i\, d\sigma\,. \tag{2.11}$$

If $u$ and $v$ are solutions of the Klein–Gordon equation (2.2), the inner product (2.11) is independent of the Cauchy surface $S$ on which the integration is performed. This inner product is Hermitian so $\langle u,u\rangle$ is real number, but it is not positive defined. Then we can classify the complex solutions of Eq. (2.2) as *positive*, if $\langle u,u\rangle > 0$, *negative*, if $\langle u,u\rangle < 0$, and *degenerated* if $\langle u,u\rangle = 0$.

Let $\{\phi_{\mathbf{k}}\}\cup\{\phi_{\mathbf{k}}^*\}$ be a base of the space of complex solutions of Eqs. $\mathbf{k}\in R$ is a set of three continuous parameters that label the solutions [as we said we reserve symbol $\mathbf{p}$ for the usual momentum as in Eq. (2.3)]. This base will be called an *orthonormal base* if

$$\begin{aligned}
&\langle \phi_{\mathbf{k}}, \phi_{\mathbf{h}}\rangle = -\delta(\mathbf{k}-\mathbf{h})\,,\\
&\langle \phi_{\mathbf{k}}^*, \phi_{\mathbf{h}}^*\rangle = \delta(\mathbf{k}-\mathbf{h})\,,\\
&\langle \phi_{\mathbf{k}}, \phi_{\mathbf{h}}^*\rangle = 0\,,
\end{aligned} \tag{2.12}$$

where $\delta(k)$ is Dirac's distribution. So vectors $\phi_{\mathbf{k}}^*$ are positive and vectors $\phi_{\mathbf{k}}$ are negative. We can go from one orthonormal base to another via a Bogolyubov transformation. We can develope $\phi(x)$, $G_1(x,x')$, and $G_1(x,x')$ on the orthonormal base,

$$\phi(x) = \int [a_{\mathbf{k}}\phi_{\mathbf{k}}(x) + a_{\mathbf{k}}^+\phi_{\mathbf{k}}^*(x)]\, d^3k\,, \tag{2.13}$$

$$G(x,x') = i\int [\phi_{\mathbf{k}}(x)\phi_{\mathbf{k}}^*(x') - \phi_{\mathbf{k}}(x')\phi_{\mathbf{k}}^*(x)]\, d^3k\,, \tag{2.14}$$

$$G_1(x,x') = \int [\phi_{\mathbf{k}}(x)\phi_{\mathbf{k}}^*(x') + \phi_{\mathbf{k}}(x')\phi_{\mathbf{k}}^*(x)]\, d^3k\,. \tag{2.15}$$

But while Eq. (2.14) is invariant under Bogolyubov transformations because $G(x,x')$ is unique (and can also be verified directly) Eq. (2.15) is not invariant, therefore $G_1(x,x')$ *depends on the base* $\{\phi_{\mathbf{k}}\}\cup\{\phi_{\mathbf{k}}^*\}$ we use. We shall call the subspace of positive (resp. negative frequency) solutions the space spanned by the $\{\phi_k^*\}$ (resp. $\{\phi_k\}$). It can be easily shown that if we know $G_1(x,x')$ we can find the subspaces of positive and negative solutions and vice versa (cf. Ref. 1).

As $\phi_{\mathbf{k}}$ can be defined by its Cauchy data on a surface $t = \tau = \text{const}$ [that we shall call $\phi_{\mathbf{k}}^{(\tau)}(x)$, $\dot\phi_{\mathbf{k}}^{(\tau)}(x)$], the $G_1^{(\tau)}(x,x')$ is defined by its Cauchy data and so are the subspaces of positive and negative frequency. Then we must search for reasonable $\phi_{\mathbf{k}}^{(\tau)}$, $\dot\phi_{\mathbf{k}}^{(\tau)}$, or equivalently for reasonable $G_1^{(\tau)}(x,x')$ and $(d/dt)G_1^{(\tau)}(x,x')$ at each time $\tau$, in order to have the base of the subspace of positive (resp. negative) frequency solutions [that we shall call $\{\phi_{\mathbf{k}}^{*(\tau)}\}$ (resp. $\{\phi_{\mathbf{k}}^{(\tau)}\}$)] well defined at each time $\tau$. Once we have these bases we can develop $\phi(x)$ at two different times:

$$\phi(x) = \int [a_{\mathbf{k}}^{(\tau)}\phi_{\mathbf{k}}^{(\tau)} + a_{\mathbf{k}}^{+\,(\tau)}\phi_{\mathbf{k}}^{*(\tau)}]\, d^3k\,, \tag{2.16a}$$

$$\phi(x) = \int [a_{\mathbf{k}}^{(\tau')}\phi_{\mathbf{k}}^{(\tau')} + a_{\mathbf{k}}^{+\,(\tau')}\phi_{\mathbf{k}}^{*(\tau')}]\, d^3k\,. \tag{2.16b}$$

The base functions at times $\tau$ and $\tau'$ are related by a Bogolyubov transformation

$$\begin{aligned}
&\phi_{\mathbf{k}}^{(\tau)} = \alpha_{\mathbf{k}}\phi_{\mathbf{k}}^{(\tau')} + \beta_{\mathbf{k}}\phi_{\mathbf{k}}^{*(\tau')}\,,\\
&\phi_{\mathbf{k}}^{*(\tau')} = \alpha_{\mathbf{k}}^*\phi_{\mathbf{k}}^{*(\tau')} + \beta_{\mathbf{k}}^*\phi_{\mathbf{k}}^{(\tau')}\,,\\
&|\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1\,.
\end{aligned} \tag{2.17}$$

The corresponding annihilation and creation operators are related by

$$a_{\mathbf{k}}^{(\tau')} = \alpha_{\mathbf{k}}a_{\mathbf{k}}^{(\tau)} + \beta_{\mathbf{k}}^*\mathbf{a}_{\mathbf{k}}^{*(\tau)}\,, \tag{2.18}$$

$$a_{\mathbf{k}}^{*(\tau')} = \beta_{\mathbf{k}}\mathbf{a}_{\mathbf{k}}^{(\tau)} + \alpha_{\mathbf{k}}^*a_{\mathbf{k}}^{*(\tau)}\,. \tag{2.19}$$

Let us assume that at time $\tau$ the universe is in the vacuum state at that time $|0\rangle_{(\tau)}$, i.e.,

$$N_{\mathbf{k}}^{(\tau)}|0\rangle_{(\tau)} = a_{\mathbf{k}}^{*(\tau)}a_{\mathbf{k}}^{(\tau)}|0\rangle_{(\tau)} = 0\,. \tag{2.20}$$

Then the mean number of particle density in mode $\mathbf{k}$ at time $\tau'$ will be

$$\begin{aligned}
{}_{(\tau)}\langle 0|N_{\mathbf{k}}^{(\tau')}|0\rangle_{(\tau)} &= {}_{(\tau)}\langle 0|a_{\mathbf{k}}^{*(\tau')}a_{\mathbf{k}}^{(\tau')}|0\rangle_{(\tau)}\\
&= |\beta_{\mathbf{k}}|^2\,.
\end{aligned} \tag{2.21}$$

This implies that the average number of particle density at time $\tau'$ is

$$N(\tau') = \int d^3\mathbf{k}\,{}_{(\tau)}\langle 0|N_{\mathbf{k}}^{(\tau')}|0\rangle_{(\tau)} = \int d^3\mathbf{k}\,|\beta_k|^2\,. \tag{2.22}$$

So if the universe is in the vacuum state at time $\tau$ the necessary and sufficient condition in order that the average number of particles at time $\tau'$ is finite is that

$$\int |\beta_k|^2\, d^3\mathbf{k} < \infty\,. \tag{2.23}$$

This is also the necessary and sufficient condition in order that the Bogolyubov transformation (2.18), (2.19) is implementable.[7] So we must search our boundary conditions among the ones that produce a finite average number of particles from the vacuum or equivalently yields an implementable Bogolyubov transformation.

## 3. THE QUANTUM EQUIVALENCE PRINCIPLE

We shall prove that the solution of our problem can be based on an adequate interpretation of the strong equivalence principle. One of its versions states that at every event of space–time there exists a coordinate system where all gravitational forces vanish. We assume that locally in such an event (that can be taken as the origin of coordinates) and in such a system of coordinates there is a box of side $2\rho$ (our laboratory) and a time interval $2\Theta$ (the length of our experiment) where, since there is no gravitational field, we can use flat space–time quantum field theory. This statement is only approximately true but becomes more and more correct as $\Theta, \rho \to 0$. We shall call this assumption the "quantum equivalence principle" and we shall study its consequences.

Therefore, we shall place our space–time laboratory with its time axis parallel to the curves $x^\alpha = 0 =$ contant $t =$ variable of the above mentioned coordinate system and with its plane $t = 0$ tangent to the $t = 0 =$ constant, $x^\alpha$ = variable surfaces. The covariant derivative of the curve $x^\alpha = 0, t =$ variable vanish at the origin so it is locally a geodesic. In this way we are sure that there are no gravitational forces and we locally have a free falling laboratory, that we shall call a Galilean laboratory.

Let $s$ be the space–time interval between 0 and an event $x$ placed outside the light conoid of 0 but inside our laboratory and our experiment's time. Based on our principle we can say that when $\Theta, \rho \to 0$

$$G_1^{(0)}(0, x) = \Delta_1(s), \tag{3.1}$$

whre $\Delta_1(s)$ is the flat space $\Delta_1$ [Eq. (2.3.2)] that, because of Lorentz invariance is only a function of $s$, the length of the universal interval between 0 and $x$. We shall see how we can deduce from Eq. (3.1) the correct initial conditions for $G_1^{(\tau)}$ (in the case $\tau = 0$ because of our particular choice of the origin). We restrict ourselves to the system of coordinates where the metric takes the form (2.1). Then we have a spherical spatial symmetry and we can consider only the coordinates $(T,R)$ of event $x$, where $T$ is the time interval between 0 and $x$, and $R = [x_1^2 + x_2^2 + x_3^2]^{1/2}$. Of course $T < \Theta$, $R < \rho$.

Let us compute $s = s(0,x)$ using a straight line from 0 to $x$ in the laboratory coordinates.[8] We have:

$$s = \int_0^T (a^2 dr^2 - dt^2)^{1/2} = \int_0^T \left(\frac{R^2}{T^2} a^2(t) - 1\right)^{1/2} dt . \tag{3.2}$$

Afterwards we shall take $T \to 0$ leaving $R \neq 0$ constant, so we can develop the square root, and we obtain

$$s = \frac{R}{T}\int_0^T a(t)\, dt - \frac{1}{2}\frac{T}{R}\int_0^T \frac{dt}{a(t)} - \frac{1}{8}\frac{T^3}{R^3}\int_0^T \frac{dt}{a^3(t)} . \tag{3.3}$$

We shall also need:

$$\frac{\partial s}{\partial T} = \frac{R}{T^2}\left[Ta(T) - \int_0^T a(t)dt\right] - \frac{1}{2R}\left(\int_0^T \frac{dt}{a(t)} + \frac{T}{a(T)}\right) - \cdots . \tag{3.4}$$

When $T \to 0$ we can compute the limits of Eqs. (3.3) and (3.4),

$$\lim_{T\to 0} s = Ra(0) , \quad \lim_{T\to 0} \frac{\partial s}{\partial T} = \tfrac{1}{2}R\dot{a}(0) . \tag{3.5}$$

Now we need to compute $d\Delta_1/ds$. From Eq. (2.3b) it follows (notice that because of Lorentz invariance $\Delta_1$ is only a function of $s$)

$$\Delta_1 = -\frac{\mu^2}{4\pi}\,\mathrm{Im}\frac{H_1^{(1)}(i\mu s)}{i\mu s} = \frac{\mu^2}{4\pi}\,\mathrm{Re}\frac{H_1^{(1)}(i\mu s)}{\mu s} \tag{3.6}$$

so we have that

$$\frac{d\Delta_1}{d(\mu s)} = -\frac{\mu^2}{4\pi}\,\mathrm{Re}\, i\frac{H_2^{(1)}(i\mu s)}{\mu s} = -\frac{\mu^2}{4\pi}\,\mathrm{Re}\left(\frac{2}{(\mu s)^2}H_1^{(1)}(i\mu s) - \frac{i}{\mu s}H_0^{(1)}(i\mu s)\right)$$

$$= -\frac{2}{\mu s}\Delta_1 + \frac{\mu^2}{4\pi}\frac{1}{\mu s}\,\mathrm{Re}[iH_0^{(1)}(i\mu s)] . \tag{3.7}$$

Therefore,

$$\frac{d\Delta_1}{ds} = -\frac{2}{s}\Delta_1 - \frac{\mu^2}{4\pi s}\,\mathrm{Im}[H_0^{(1)}(i\mu s)] . \tag{3.8}$$

From (3.1), (3.5), (3.6), and (3.8) we have that when $T \to 0$,

$$G_1(0, x) = \Delta_1(Ra(0)) , \tag{3.9a}$$

$$\frac{\partial G_1(0, x)}{\partial T} = -\frac{\dot{a}(0)}{a(0)}\left\{\Delta_1(Ra(0)) + \frac{\mu^2}{8\pi}\,\mathrm{Im}[H_0^{(1)}(i\mu Ra(0))]\right\} . \tag{3.9b}$$

These equations are only true for $\Theta \to 0, \rho \to 0$. $\Theta \to 0$ is already taken into account as we have taken $T \to 0$. $\rho \to 0$ implies that Eqs. (3.9) are only valid for $R \to 0$.

We really want to find the boundary conditions of $G_1^{(0)}(0,x)$ on the whole surface $t = \tau = 0$. Now we know that these conditions are given by Eq. (3.9) when $R \to 0$ (i.e., for small spacelike distances between 0 an $x$) if we want to satisfy the quantum equivalence principle. Therefore, when $R$ is large this principle tells us only the first term in an expansion of the boundary condition in powers of $R$, but nothing about the other terms.

Nevertheless the 3-surface $t =$ constant $x^\alpha =$ variable, are spatially flat and can be considered crowded with Galilean laboratories. All points of this 3-surface are in free fall following the geodesics $x^\alpha =$ constant $t =$ variable, so we can consider each 3-surface as a huge quasi-Galilean laboratory. Certainly we can say that Eq. (3.1) is valid in our quasi-Galilean laboratory, because its only difference with a real Galilean laboratory is that it is expanding. So instantaneously we can assure that both (3.9a) and (3.9b) are satisfied, because the expansion of the quasi-Galilean laboratory has been taken into account through the definition of Eq. (3.2) and the computation of the time derivatives Eq. (3.4).

So let us adopt an extended version of the quantum equivalence principle and state that Eqs. (3.9) are valid in all the 3-surface $t = 0$, $x^\alpha =$ variable. So we forget the limit $\rho \to 0$ and we adopt (3.9) as the initial conditions that $G_1^{(\tau)}(x,x')$ [$G_1^{(0)}(0,x)$ with our particular choice of the origin] must satisfy on the 3-surface, i.e., we neglect, for the moment, all the terms in the expansion of $G_1$ and $(d/dT)G_1$, but the first ones, In fact: As we are dealing only with a first order theory, then we can suppose that all the neglected terms are of higher order. (This statement can be rigorously proved in the context of the exact theory.)

Of course, to make sure that (3.9) are allowed initial conditions we must prove that they satisfy Eq. (2.10), as we shall see further on.

## 4. POSITIVE AND NEGATIVE FREQUENCY SOLUTIONS

To find an expansion of the initial conditions (3.9) that yields to definition of positive and negative frequency solutions it is necessary to expand the last term in the rhs of Eq. (3.9b). To do so we take Eq. (3.6) and compute;

$$\frac{d\Delta_1}{d\mu} = \frac{2}{\mu}\frac{\mu^2}{4\pi}\,\mathrm{Re}\,\frac{H_1^{(1)}(i\mu s)}{\mu s} + \frac{\mu^2}{4\pi}\left(\frac{d}{d\mu s}\,\mathrm{Re}\,\frac{H_1^{(1)}(i\mu s)}{\mu s}\right)s \tag{4.1}$$

and using (3.7) we get

$$\frac{d\Delta_1}{d\mu} = -\frac{\mu}{4\pi}\,\mathrm{Im}[H_0^{(1)}(i\mu s)]\,. \tag{4.2}$$

If we call $H = a(0)/\dot{a}(0)$, i.e., the Hubble coefficient, we have

$$-\frac{H\mu^2}{8\pi}\,\mathrm{Im}[H_0^{(1)}(i\mu s)] = H\mu^2\frac{d}{d\mu^2}\Delta_1 \tag{4.3}$$

so the initial conditions (3.9) become:

$$G_1^{(\tau)}(x, x') = \Delta_1\,, \tag{4.4a}$$

$$\frac{dG_1^{(\tau)}(x, x')}{dt} = -H\Delta_1 + H\mu^2\frac{d}{d\mu^2}\Delta_1\,, \tag{4.4b}$$

if $x,x'\in S(\tau)$, i.e., the surface $t = \tau$ = constant. Now it is easy to find the expansion of all the terms in (4.4).

First we try to solve Eq. (2.2) by separation of variables

$$\phi(x) = \phi_{\mathbf{k}}(t)e^{-i\mathbf{k}\cdot\mathbf{x}}\,. \tag{4.5}$$

The differential equation for $\phi_{\mathbf{k}}(t)$ is

$$\ddot{\phi}_{\mathbf{k}}(t) + 3\frac{\dot{a}}{a}\dot{\phi}_{\mathbf{k}}(t) + (\mu^2 + \xi R + k^2/a^2)\phi_{\mathbf{k}} = 0\,. \tag{4.6}$$

From Eq. (2.3b) we know that $\Delta_1(x,x')$ and its derivative are

$$\begin{aligned}\Delta_1(x,x') &= (2\pi a)^{-3}\int\frac{\cos w_k(t-t')}{w_k}\\ &\quad\times\exp[-i\mathbf{k}(\mathbf{x}-\mathbf{x}')]\,d^3\mathbf{k}\,,\\ \frac{d\Delta_1(x,x')}{d\mu^2} &= -\frac{(2\pi a)^{-3}}{2}\int\left(\frac{\cos w_k(t-t')}{w_k^3}\right.\\ &\quad\left.+\frac{\sin w_k(t-t')}{w_k}(t-t')\right)\\ &\quad\times[\exp - i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')/a]\,d^3\mathbf{k}\,,\end{aligned} \tag{4.7}$$

where $w_k = (\mu^2 + a^{-2}\mathbf{k}^2)^{1/2}$ and we have changed variable of integration from $\mathbf{p}$ to $\mathbf{k} = a\mathbf{p}$, and the physical lengths $ax$ for the coordinate variables $x$.

When $t = t' = \tau$ we have:

$$\begin{aligned}\Delta_1(x, x') &= (2\pi a)^{-3}\int\frac{\exp[-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')/a]}{w_k}\,d^3\mathbf{k}\,,\\ \frac{d\Delta_1(x, x')}{d\mu^2} &= -\frac{(2\pi a)^{-3}}{2}\int\frac{\exp[-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')/a]}{w_k^3}\,d^3\mathbf{k}\,.\end{aligned} \tag{4.8}$$

As we have solved (2.2) by separation of variables the initial conditions for the $\phi_{\mathbf{k}}$ will be in general:

$$\phi_{\mathbf{k}}^{(\tau)}(\tau, x) = A_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}\,,\quad \dot{\phi}_{\mathbf{k}}^{(\tau)}(\tau, x) = B_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}\,, \tag{4.9}$$

where $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$ are arbitrary numbers. In this way we can find all possible and negative frequency splittings. But as $\phi_{\mathbf{k}}^{(\tau)}$, $\phi_{\mathbf{k}}^{*(\tau)}$ will be used to define the $G$ and $G_1$ through Eqs. (2.14) and (2.15) we can multiply the $\phi_{\mathbf{k}}$ by a complex number of unit modulus, $e^{i\theta}$, without any changes in $G$ and $G_1$. As the kernels define the subspaces of positive and negative frequency solutions, these subspaces will also be invariant under this change. So we can take the $A_{\mathbf{k}}$ as a real number without any loss of generality.

Then the $G_1(x,x')$ at $S(\tau)$ will be [cf. Eq. (2.15)]

$$G_1(x, x') = \int\{A_{\mathbf{k}}^2\exp[i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')] + A_{\mathbf{k}}^2\exp[i\mathbf{k}\cdot(\mathbf{x}'-\mathbf{x})]\}\,d^3\mathbf{k}\,. \tag{4.10}$$

If we make the change $k^\alpha \to -k^\alpha$ in the first term, nothing will change because the $A_{\mathbf{k}}$ are real functions of $\mathbf{k}^2$ due to the spherical spacelike symmetry, so

$$G_1(x, x') = 2\int A_{\mathbf{k}}^2\exp[-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')]\,d^3\mathbf{k}\,. \tag{4.11}$$

Then to satisfy (4.4a) we must have

$$A_k = (2\pi a)^{-3/2}(2w_k)^{-1/2}\,. \tag{4.12}$$

The derivative of $G_1(x,x')$ at $S(\tau)$ will be

$$\frac{d}{dt}G_1(x, x') = \int(B_{\mathbf{k}}^* A_{\mathbf{k}} + A_{\mathbf{k}}B_{\mathbf{k}})\times\exp[-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')]\,d^3\mathbf{k}\,, \tag{4.13}$$

where we have used the same argument to perform the change $k^\alpha \to -k^\alpha$. If we put

$$B_{\mathbf{k}} = a_{\mathbf{k}} + ib_{\mathbf{k}}\,, \tag{4.14}$$

where $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are real numbers and we try to satisfy Eq. (4.4b) using Eq. (4.12), we have

$$a_{\mathbf{k}} = -H(2\pi a)^{-3/2}(2w_k)^{1/2}\left(\frac{1}{2w_k} + \frac{1}{4}\frac{\mu^2}{w_k^3}\right). \tag{4.15}$$

Finally, to satisfy Eq. (2.10) it is necessary and sufficient that in expansions (2.14) and (2.15), the base $\{\phi_{\mathbf{k}}^{*(\tau)}\}\cup\{\phi_{\mathbf{k}}^{(\tau)}\}$ fulfills Eqs. (2.12).

But

$$\begin{aligned}&\langle\phi_{\mathbf{k}}^{*(\tau)}, \phi_{\mathbf{h}}^{*(\tau)}\rangle\\ &\quad= ia^3\int\left[\left(\frac{d}{dt}\phi_{\mathbf{k}}^{(\tau)}\right)\phi_{\mathbf{k}}^{*(\tau)} - \phi_{\mathbf{k}}^{(\tau)}\frac{d}{dt}\phi_{\mathbf{h}}^{*(\tau)}\right]d^3\mathbf{x}\\ &\quad= ia^3(B_{\mathbf{k}}A_{\mathbf{h}} - A_{\mathbf{k}}B_{\mathbf{h}}^*)\int\exp[-i\mathbf{x}\cdot(\mathbf{k}-\mathbf{h})]\,d^3\mathbf{x}\\ &\quad= (2\pi a)^3 i(B_{\mathbf{k}}A_{\mathbf{h}} - A_{\mathbf{k}}B_{\mathbf{h}}^*)\delta(\mathbf{k}-\mathbf{h})\,.\end{aligned} \tag{4.16}$$

So to satisfy Eq. (2.12) we must have

$$A_{\mathbf{k}}(B_{\mathbf{k}} - B_{\mathbf{k}}^*) = -i(2\pi a)^{-3}\,, \tag{4.17}$$

therefore

$$b_k = -(2\pi a)^{-3/2}(w_k/2)^{1/2}\,. \tag{4.18}$$

From (4.12), (4.15), and (4.18) we can state the initial conditions of the negative frequency solutions of mode $\mathbf{k}$:

$$\phi_{\mathbf{k}}^{(\zeta)}(\zeta, x) = (2\pi a)^{-3/2}(2w_k)^{-1/2}e^{-i\mathbf{k}\cdot\mathbf{x}}\,, \tag{4.19}$$

$$\dot{\phi}_{\mathbf{k}}^{(\tau)}(\tau, x) = (2\pi a)^{-3/2}\left[-i\left(\frac{w_k}{2}\right)^{1/2} - (2w_k)^{1/2}\times\left(\frac{1}{2w_k} + \frac{\mu^2}{4w_k^3}\right)H\right]e^{-i\mathbf{k}\cdot\mathbf{x}}\,. \tag{4.19b}$$

The positive frequency solutions will have, of course, the complex conjugated initial values.

Now we will prove that with these initial conditions the Bogolyubov transformation (2.18), (2.19) is implementable for all real values of the coupling constant $\xi$.

## 5. IMPLEMENTABILITY

To prove the implementability of our theory we use the rigorous results on the estimation of the error in the WKB approximation due to Olver.[9,10] Olver's results have previously been used by Fulling[11] to prove the implementability of his model.

Let us make a change of variable $t \to \eta$ and of the field $\phi \to \psi$ in order to put Eq. (4.6) in the standard form:

$$\eta = \int_0^t a(t')^{-1}\, dt', \tag{5.1}$$

$$\phi_{\mathbf{k}}(t) = a^{-1}(t)\psi_{\mathbf{k}}(t). \tag{5.2}$$

We emphasize that these changes have only a *mathematical purpose* and have little to do with the physics of the problem.

With these changes Eq. (4.6) becomes

$$\psi_{\mathbf{k}}'' + \{\mathbf{k}^2 + a^2[\mu^2 + (\xi - \tfrac{1}{6})R]\}\psi_{\mathbf{k}} = 0, \tag{5.3}$$

where

$$\psi_{\mathbf{k}}' = \frac{d\psi_{\mathbf{k}}}{d\eta}.$$

Now we can use Olver's theory in the equation

$$\frac{d^2\psi}{d\eta^2} + k^2 p(k,\eta)\psi = 0 \tag{5.4}$$

[cf. Ref. 9, p. 800, Eq. (4.7), Theorem IV, and Ref. 10], where $p(k,\eta)$ is a strictly positive $C^2$ function of $\eta$. We identify Eqs. (5.3) and (5.4) making

$$p(k,\eta) = 1 + k^{-2}a^2[\mu^2 + (\xi - \tfrac{1}{6})R] = \frac{a^2}{k^2}[w_k^2 + (\xi - \tfrac{1}{6})R]. \tag{5.5}$$

We see that $p(k,\eta) > 0$ for $k$ large enough.

This is the only case in which we are interested since we must prove (2.23).

Equation (5.4) has the following solution,[9]

$$\psi(k,\eta) = (2k)^{-1/2}p^{-1/4} \times \left[\exp\left(-ik\int_0^\eta p^{1/2}d\eta'\right) + \epsilon(k,\eta)\right] \tag{5.6}$$

and its derivative,

$$\frac{d\psi}{d\eta} = -i\left(\frac{k}{2}\right)^{1/2}p^{1/4}\left[\exp\left(-ik\int_0^\eta p^{1/2}\,d\eta'\right) - \frac{i}{4k}p^{-3/2}\frac{dp}{d\eta}\left[\exp\left(-ik\int_0^\eta p^{1/2}\,d\eta'\right) + \epsilon\right] \times + i\delta(k,\eta)\right], \tag{5.7a}$$

$$\delta(k,\eta) = \frac{i}{k}\frac{d\epsilon}{d\eta}\frac{1}{p^{1/2}}, \tag{5.7b}$$

$$|\epsilon|, |\delta| \leqslant \exp\frac{F}{k} - 1, \tag{5.8}$$

$$F(k,\eta) = \int_0^\eta |p^{-1/4}\frac{d^2p^{-1/4}}{d\eta^2}|\, d\eta'. \tag{5.9}$$

But as $p(k,\eta)$ has the form

$$p(k,\eta) = 1 + k^{-2}\tilde{p}(\eta), \tag{5.10}$$

where

$$\tilde{p}(\eta) = a^2[\mu^2 + (\xi - \tfrac{1}{6})R], \tag{5.11}$$

from Eqs. (5.8) and (5.9) we can easily deduce

$$|\epsilon|, |\delta|, k^{-1}p^{-3/2}\left|\frac{dp}{d\eta}\right| = O(k^{-3}) \tag{5.12}$$

where $k \to \infty$.

Now let $\psi^{(0)}(k,\eta)$ and $\psi^{(\zeta)}(k,\eta)$ be the solution of Eqs. (5.4) that satisfies the following initial conditions:

$$\sqrt{2}\bar{\psi}^{(0)}(k,0) = k^{-1/2}\pi^{-1/4}(k,0), \quad i\sqrt{2}\bar{\psi}'^{(0)}(k,0) = k^{1/2}\pi'^{1/4}(k,0), \tag{5.13}$$

$$\sqrt{2}\bar{\psi}^{(\zeta)}(k,\zeta) = k^{-1/2}\pi^{-1/4}(k,\zeta), \quad i\sqrt{2}\bar{\psi}'^{(\zeta)}(k,\zeta) = k^{1/2}\pi'^{1/4}(k,\zeta), \tag{5.14}$$

where $\zeta = \int_0^\tau a(t')^{-1}\, dt'$, and where $\pi(k,\eta)$ and $\pi'(k,\eta)$ are functions to be determined later on in such a way that the Bogolyubov transformation between the $\psi^{(0)}$, $\psi^{*(0)}$ and the $\psi^{(\zeta)}$ $\psi^{*(\zeta)}$ is implementable. We assume that $\pi(k,\eta)$ is always different from zero and that $\pi^{-1/4}$ and $\pi'^{1/4}$ remain bounded when $k \to \infty$.

Let the functions $\psi(k,\eta)$ and $\psi^*(k,\eta)$ be the solutions of Eq. (5.4) that satisfy the following initial conditions [cf. Eqs. (5.6) and (5.7)]:

$$\sqrt{2}\bar{\psi}(k,0) = k^{-1/2}p^{-1/4}(k,0), \tag{5.15}$$

$$i\sqrt{2}\bar{\psi}'(k,0) = k^{1/2}p^{1/4}(k,0)\left(1 - \frac{i}{4k}p^{-3/2}(k,0)\frac{dp(k,0)}{d\eta}\right). \tag{5.16}$$

Notice that[9]

$$\epsilon(k,0) = \delta(k,0) = 0.$$

So we have

$$\psi^{(0)}(k,\eta) = A_k^{(0)}\psi(k,\eta) + B_k^{(0)}\psi^*(k,\eta). \tag{5.17}$$

We must compute $A_k^{(0)}$ and $B_k^{(0)}$ in such a way that the initial conditions (5.13) are satisfied. We obtain

$$A_k^{(0)} = \frac{1}{2}\left[\left(\frac{\pi(k,0)}{p(k,0)}\right)^{-1/4} \times \left(1 + \frac{i}{4k}p^{-3/2}(k,0)\frac{dp}{d\eta}(k,0)\right) + \left(\frac{\pi'(k,0)}{p(k,0)}\right)^{1/4}\right], \tag{5.18}$$

$$B_k^{(0)} = \frac{1}{2}\left[\left(\frac{\pi(k,0)}{p(k,0)}\right)^{-1/4} \times \left(1 - \frac{i}{4k}p^{-3/2}(k,0)\frac{dp}{d\eta}(k,0)\right) - \left(\frac{\pi'(k,0)}{p(k,0)}\right)^{1/4}\right].$$

In a similar way

$$\psi_k^{(\zeta)}(\eta) = A_k^{(\zeta)}\psi(k,\eta) + B_k^{(\zeta)}\psi^*(k,\eta). \tag{5.19}$$

Therefore, to satisfy the initial conditions (5.14) at $\eta = \zeta$ we have

$$A_k^{(\zeta)} = \frac{1}{2}\left[\left(\frac{\pi(k,\zeta)}{p(k,\zeta)}\right)^{-1/4}\left(1+\frac{i}{4k}p(k,\zeta)^{-3/2}\frac{dp}{d\eta}(k,\zeta)\right)+\left(\frac{\pi'(k,\zeta)}{p(k,\zeta)}\right)^{1/4}\right]$$
$$\times\exp ik\int_0^\zeta p^{1/2}(k,\eta)\,d\eta + O(\epsilon)+O(\delta)\,, \tag{5.20}$$

$$B_k^{(\zeta)} = \frac{1}{2}\left[\left(\frac{\pi(k,\zeta)}{p(k,\zeta)}\right)^{-1/4}\left(1-\frac{i}{4k}p(k,\zeta)^{-3/2}\frac{dp}{d\eta}(k,\zeta)\right)-\left(\frac{\pi'(k,\zeta)}{p(k,\zeta)}\right)^{1/4}\right]$$
$$\times\exp\left(-ik\int_0^\zeta p^{1/2}(k,\eta)\,d\eta\right)+O(\epsilon)+O(\delta)\,.$$

Now, between $\psi_k^{(0)}$ and $\psi_k^{(\tau)}$ there must be a relation like Eq. (2.17) (with $\tau'\to 0$, $\tau\to\zeta$) so

$$\psi_k^{(\zeta)} = \tilde\alpha_k\psi_k^{(0)} + \tilde\beta_k\psi_k^{*(0)}\,. \tag{5.21}$$

Then we must have:

$$A_k^{(\zeta)} = A_k^{(0)}\tilde\alpha_k + B_k^{*(0)}\tilde\beta_k\,, \tag{5.22}$$

$$B_k^{(\zeta)} = B_k^{(0)}\tilde\alpha_k + A_k^{*(0)}\tilde\beta_k\,. \tag{5.23}$$

We can compute $\tilde\alpha_k$ and $\tilde\beta_k$ from this system. Its determinant is

$$\Delta_k = \left(\frac{\pi(k,0)}{p(k,0)}\right)^{-1/4}\left(\frac{\pi'(k,0)}{p(k,0)}\right)^{1/4}. \tag{5.24}$$

Therefore, $\tilde\beta_k$ is

$$\tilde\beta_k = 2i\left\{\frac{[\pi'(k,\zeta)/p(k,\zeta)]^{1/4}}{[\pi(k,0)/p(k,0)]^{-1/4}} - \frac{[\pi(k,\zeta)/p(k,\zeta)^{-1/4}]}{[\pi'(k,0)/p(k,0)]^{1/4}}\right\}$$
$$\times\sin k\int_0^\zeta p^{1/2}(k,\eta)\,d\eta + 2\left\{\frac{[\pi(k,\zeta)/p(k,\zeta)]^{-1/4}}{[\pi(k,0)/p(k,0)]^{-1/4}} - \frac{[\pi'(k,\zeta)/p(k,\zeta)]^{1/4}}{[\pi'(k,0)/p(k,0)]^{1/4}}\right\}$$
$$\times\cos k\int_0^\zeta p^{1/2}(k,\eta)\,d\eta + O(\epsilon)+O(\delta)+O\left(k^{-1}p^{-3/2}(k,0)\frac{dp}{d\eta}(k,0)\right)+O\left(k^{-1}p^{-3/2}(k,\zeta)\frac{dp}{d\eta}(k,\zeta)\right). \tag{5.25}$$

A sufficient condition in order that our Bogolyubov transformation (2.18), (2.19) be implementable is that $|\tilde\beta_k| = O(1/k^{3/2+\epsilon})$, $\epsilon>0$ when $k\to\infty$.

In fact, from Eqs. (5.2) and (5.21) we have

$$a(t)\phi_k^{(\zeta)} = \tilde\alpha_k a(t)\phi_k^{(0)} + \tilde\beta_k a(t)\phi_k^{*(0)} \tag{5.26}$$

where $\tau$ is such that $\zeta = \int_0^\tau a^{-1}(t')\,dt'$. Comparing with Eq. (2.17) (with $\tau'=0$) we have

$$\alpha_{\mathbf{k}} = \tilde\alpha_k\,,\quad \beta_{\mathbf{k}} = \tilde\beta_k\,. \tag{5.27}$$

Therefore, if $\beta_{\mathbf{k}}$ behaves like $O(k^{-(3/2+\epsilon)})$ when $k\to\infty$, the integral (2.23) is convergent,

$$\int|\beta_{\mathbf{k}}|^2\,d^3k = 4\pi\int_0^\infty|\beta_{\mathbf{k}}|^2k^2\,dk<\infty\,. \tag{5.28}$$

From Eq. (5.12) we see that there is no problem with the last four terms of Eq. (5.25). Now let $\pi$ and $\pi'$ be written as

$$\pi(k,\eta) = p(k,\eta)Q^4(k,\eta)\,, \tag{5.29a}$$

$$\pi'(k,\eta) = p(k,\eta)Q'^4(k,\eta)\,. \tag{5.29b}$$

Then in order that $|\beta_k|$ behaves like $O(k^{-(3/2+\epsilon)})$ we need

$$\left|\frac{Q(k,0)Q'(k,0)Q(k,\eta)Q'(k,\eta)-1}{Q(k,\eta)Q'(k,0)}\right| = O\left(\frac{1}{k^{3/2+\epsilon}}\right), \tag{5.30a}$$

$$\left|\frac{Q(k,0)Q'(k,0)-Q(k,\eta)Q'(k,\eta)}{Q(k,\eta)Q'(k,0)}\right| = O\left(\frac{1}{k^{3/2+\epsilon}}\right). \tag{5.30b}$$

For example if for some constant $C>0$,

$$Q(k,\eta) = C + P(k,\eta)\,, \tag{5.31a}$$

$$Q'(k,\eta) = \pm 1/C + P'(k,\eta)\,, \tag{5.31b}$$

$$|P(k,\eta)| = O(1/k^{3/2+\epsilon})\,, \tag{5.32a}$$

$$|P'(k,\eta)| = O(1/k^{3/2+\epsilon})\,, \tag{5.32b}$$

(5.30a) and (5.30b) will be satisfied.

Now it is easy to verify that our initial conditions (4.19) are included in this general class of boundary conditions from all possible implementable theories. In fact if we make the transformations (5.1) and (5.2) we have:

$$\psi_k^{(\eta)}(\eta) = (2\pi)^{-3/2}[2a(\eta)w_k]^{-1/2}\,, \tag{5.33}$$

$$\frac{d\psi_k^{(\eta)}(\eta)}{d\eta} = (2\pi)^{-3/2}\left[-i\left(\frac{a(\eta)w_k}{2}\right)^{1/2} - [2a(\eta)w_k]^{1/2}\frac{\mu^2H(\eta)}{4w_k^3}\right].$$

We can write $k^{1/2}p^{1/4}(k,\eta)$ as

$$k^{1/2}p^{1/4}(k,\eta) = (aw_k)^{1/2}\left|1+w_k^{-2}(\xi-\tfrac{1}{6})R\right|^{1/4} \tag{5.34}$$

and

$$(aw_k)^{1/2} = k^{1/2}p^{1/4}\left|1-a^2(\xi-\tfrac{1}{6})R/k^2p\right|^{1/4}. \tag{5.35}$$

So if we put the initial conditions (5.33) in the form of Eq. (5.14),

$$\pi = p(2\pi)^6\left(1-a^2\frac{(\xi-\frac{1}{6})R}{k^2p}\right), \tag{5.36a}$$

$$\pi' = \frac{p}{(2\pi)^6}\left(1-a^2\frac{(\xi-\frac{1}{6})R}{k^2p}\right)\left(1-\frac{i\mu^2H}{2w_k^3}\right)^4. \tag{5.36b}$$

Then in the notation of Eqs. (5.29) and (5.31)

$$C = (2\pi)^{3/2}\,, \tag{5.37a}$$

$$P = (2\pi)^{3/2}\left[\left(1-a^2\frac{(\xi-\frac{1}{6})R}{k^2p}\right)^{1/4}-1\right], \tag{5.37b}$$

$$P' = \frac{1}{(2\pi)^{3/2}}\left[\left(1-a^2\frac{(\xi-\frac{1}{6})R}{k^2p}\right)^{1/4}\left(1-\frac{i\mu^2H}{2w_k^3}\right)-1\right], \tag{5.37c}$$

and it is now straightforward to see that (5.32a) and (5.32b)

are satisfied, so our transformation is implementable and we have the creation of a finite number of particles for every real value of the coupling constant $\xi$.

*Remarks*:

(1) If we choose the naïve initial conditions

$$G_1^{(\tau)}(x, x') = \Delta_1(x, x'), \tag{5.38a}$$

$$\frac{d}{dt} G_1^{(\tau)}(x, x') = 0, \tag{5.38b}$$

the Bogolyubov transformation is not implementable (this was proven in Refs. 2 and 3). These initial conditions are widely used (see Ref. 6 for example). They were thought to be the most natural generalization of the flat space–time conditions, besides these conditions diagonalize the Hamiltonian. But if we compare Eq. (5.38) with the present initial conditions (4.4) we see that in (5.38) the expansion of the universe is neglected [i.e., to obtain (5.38b) we make $H = 0$ in (4.4b)].

(2) If we eliminate the term

$$-(2\pi a)^{-3/2}(2w_k)^{1/2}(\mu^2/4w_k^3)H$$

in (4.19b) [or equivalently, the second term in the rhs of Eq. (4.4b)] we have Fulling's initial conditions (cf. Ref. 11) that yields a implementable theory. But it seems to us that there is no physical reason to adopt these initial conditions. (As a matter of fact, Ref. 11 anticipates that all the initial conditions differing in terms $\sim k^{-3}$ are essentially equivalent. So we can say that the quantum equivalence principle picks the right one.)

(3) If in Fulling's theory we choose the vacuum state $|0\rangle$ as the state of the universe at time $t = 0$ and we use the time evolution $a(t) = a_0 t^q$ we arrive a the Mamaev, Mostepanenko, and Starobinskiĭ theory (cf. Ref. 12) that is, of course, also implementable, but in our opinion also deserves the same criticism. The initial condition of these theories are only conditions that resemble the flat space ones in coordinates $\eta$ and field $\psi$. But the change of coordinates and the change of field are only made for mathematical convenience, and we think that a theory cannot be based on this resemblance.

## 6. COMPUTATION OF α AND β WITH CONFORMAL COUPLING

From now on we shall only study the conformal coupling, i.e., we make $\xi = \frac{1}{6}$. Then we can have an idea of the relevant phenomena predicted by the theory in the easiest way. Besides, in Sec. 7 we shall see that there is a good physical reason to prefer the conformal coupling: The energy is also finite.

From Eq. (5.5) we see that in this case

$$p(k, \eta) = 1 + \mu^2 a^2(\eta)/k^2 = (a^2/k^2)w_k^2 . \tag{6.1}$$

We first remark that with this $p$, Eqs. (5.15), (5.16) become

$$\psi(k, \eta) = (2aw_k)^{-1/2}, \tag{6.2}$$

$$\frac{d\psi}{d\eta}(k, \eta) = -i\left(\frac{aw_k}{2}\right)^{1/2}\left(1 - \frac{i\mu^2 H}{2w_k^3}\right),$$

i.e., exactly the boundary condition (5.33) if we disregard the unimportant factor $(2\pi)^{-3/2}$. Therefore, in the conformal coupling case the boundary conditions (5.33) obtained from the quantum equivalence principle are the boundary conditions that we would find if we take the first approximation of the WKB method [multiplied by $(2\pi)^{-3/2}$]:

$$\psi^{(\eta)}(k, \lambda) = (2\pi)^{-3/2}(2k)^{-1/2}p^{-1/4}\exp\left(-ik\int_0^\lambda p^{1/2}\, d\eta'\right), \tag{6.3}$$

[cf. Eq. (5.6) with $\epsilon(k,\lambda) = 0$] and its first derivative

$$\frac{d\psi^{(\eta)}}{d\lambda}(k, \lambda) = (2\pi)^{-3/2}(-i)\left(\frac{k}{2}\right)^{1/2}p^{1/4}\left(1 - \frac{i}{4k}p^{-3/2}\frac{dp}{d\lambda}\right) \times \exp(-ik)\int_0^\lambda p^{1/2}\, d\eta') \tag{6.4}$$

[cf. Eq. (5.7) with $\epsilon(k,\lambda) = \delta(k,\lambda) = 0$].

Therefore our particle model at each time is an exact solution of the Klein–Gordon equation that satisfies, at that time, the boundary conditions of a first approximation of the WKB method. This model combines two important features of the flat space-free particles. In fact, their wave functions are solutions of the Klein–Gordon equation and the WKB approximation, only that in that case the first approximation turns out to be exact.

Let us define[9] the following new variable $x$, and field $W$:

$$x = \int_0^\eta [p(k, \eta')]^{1/2}\, d\eta' = \frac{1}{k}\int_0^\eta aw_k\, d\eta' = \frac{1}{k}\int_0^t w_k\, dt', \tag{6.5a}$$

$$W = (2k)^{1/2}p^{1/4}\psi \tag{6.5b}$$

(we modify the definition of $W$ in Ref. 9 with a new constant factor $(2k)^{1/2}$ for our convenience). Then Eq. (5.4) becomes

$$\frac{d^2W}{dx^2} + [k^2 - f(k, x)]W = 0, \tag{6.6}$$

where

$$f(k, x) = \left[4p\frac{d^2p}{d\eta^2} - 5\left(\frac{dp}{d\eta}\right)^2\right]\Big/16p = -p^{-3/4}\frac{d^2}{d\eta^2}p^{1/4} = \frac{1}{2}\frac{\mu^2k^2}{w_k^4}\left(2 - \frac{5}{2}\frac{\mu^2}{w_k^2} - q\right)H^2, \tag{6.7}$$

where $q$ is the deacceleration parameter

$$q = -(\ddot{a}/a)H^{-2}.$$

It follows from (6.5b) and (5.6) that

$$W(k, x) = e^{-ik\cdot x} + \epsilon. \tag{6.8}$$

Moreover from (5.7b),

$$\delta(k, \eta) = \frac{1}{k}\frac{\partial\epsilon}{\partial x}\frac{1}{p^{1/2}} \tag{6.9}$$

and since (6.5a) implies

$$\frac{\partial\epsilon}{\partial\eta} = \frac{\partial\epsilon}{\partial x}\frac{1}{p^{1/2}} \tag{6.10}$$

we have

$$\delta = \frac{1}{k}\frac{\partial\epsilon}{\partial x}. \tag{6.11}$$

Now we are ready to find $\alpha_k$ and $\beta_k$. As we have shown, function (6.9) multiplied by $(2\pi)^{-3/2}$ satisfies our boundary condition (5.33) at $\eta = 0$. Therefore, $A_k^{(0)} = (2\pi)^{-3/2}$ and $B_k^{(0)} = 0$ in (5.17).

Then from Eqs. (5.19), (5.22), and (5.23) we have

$$\psi_k^{(\eta)}(\lambda) = (2\pi)^{-3/2}[\alpha_k\psi(k,\lambda) + \beta_k\psi^*(k,\lambda)]. \tag{6.12}$$

This function must also satisfy the boundary condition (5.33) at $\lambda = \eta$. So we have

$$\begin{aligned}\alpha_k[\exp(-ikx) + h] + \beta_k[\exp(ikx) + h^*] &= 1 - \left[\alpha_k\left(\exp(-ikx) + \frac{i}{k}\frac{dh}{dx}\right)\right.\\ &\quad - \beta_k\left(\exp(ikx) - \frac{i}{k}\frac{dh^*}{dx}\right)\\ &\quad \left. - \frac{i\mu^2 H}{2w_k^3}[\alpha k\exp(-ikx) + h] + \beta_k[\exp(ikx) + h^*]\right]\\ &= \left[\left(1 - \frac{i}{2}\frac{\mu^2 H}{w_k^3}\right)\right].\end{aligned} \tag{6.13}$$

That yields the system

$$\begin{aligned}(e^{-ikx} + \epsilon)\alpha_k + (e^{ikx} + \epsilon^*)\beta_k &= 1,\\ \left(e^{-ikx} + \frac{i}{k}\frac{d\epsilon}{dx}\right)\alpha_k - \left(e^{ikx} - \frac{i}{k}\frac{d\epsilon^*}{dx}\right)\beta_k &= 1.\end{aligned} \tag{6.14}$$

Now, let us observe that the Wronskian of Eq. (5.4) is a constant, which we can find with the initial conditions (6.2),

$$\begin{aligned}\psi\frac{d\psi^*}{d\eta} - \psi^*\frac{d\psi}{d\eta} &= \frac{i}{2}\left(2 + \epsilon e^{ixk} + \epsilon^* e^{-ixk} + \frac{i}{k}\frac{\partial\epsilon}{\partial x}e^{ixk}\right.\\ &\quad \left. - \frac{i}{k}\frac{\partial\epsilon^*}{\partial x}e^{-ixk} + \frac{i\epsilon^*}{k}\frac{\partial\epsilon}{\partial x} - \frac{i\epsilon}{k}\frac{\partial\epsilon^*}{\partial x}\right) = i.\end{aligned} \tag{6.15}$$

So we have that

$$\begin{aligned}\epsilon e^{ikx} + \epsilon^* e^{-ikx} + \frac{i}{k}\frac{\partial\epsilon}{\partial x}e^{ixk} - \frac{i}{k}\frac{\partial\epsilon^*}{\partial x}e^{-ikx}\\ + \frac{i\epsilon^*}{k}\frac{\partial\epsilon}{\partial x} - \frac{i\epsilon}{k}\frac{\partial\epsilon^*}{\partial x} = 0.\end{aligned} \tag{6.16}$$

Now if we compute the determinant $\Delta_k'$ of the system (6.14) and use (6.16) we find

$$\Delta_k' = -2. \tag{6.17}$$

Therefore, $\alpha_k$ and $\beta_k$ are

$$\alpha_k = e^{ixk} + \frac{1}{2}\left(\epsilon^* - \frac{i}{k}\frac{\partial\epsilon^*}{\partial x}\right), \tag{6.18a}$$

$$\beta_k = -\frac{1}{2}\left(\epsilon - \frac{i}{k}\frac{\partial\epsilon}{\partial x}\right). \tag{6.18b}$$

Again using (6.16) we can easily verify that $(\alpha_k)^2 - (\beta_k)^2 = 1$.

These are very simple formulas, but the real nice thing is that we can even compute directly the $\alpha_k$ and $\beta_k$ from the function $W$.

From Eq. (6.8) we have

$$\epsilon = W - e^{-ikx}, \tag{6.19}$$

$$\frac{\partial\epsilon}{\partial x} = \frac{dW}{dx} + ike^{-ikx}, \tag{6.20}$$

that, with Eq. (6.18), yield

$$\begin{aligned}\alpha_k &= \frac{1}{2}\left(W^* - \frac{i}{k}\frac{dW^*}{dx}\right),\\ \beta_k &= -\frac{1}{2}\left(W - \frac{i}{k}\frac{dW}{dx}\right).\end{aligned} \tag{6.21}$$

We also have an integral representation of $\alpha_k$ and $\beta_k$. In fact, the recurrence relation of the sequence of approximations of $\epsilon$ is [cf. Ref. 9, Eq. (2.26)]

$$\begin{aligned}\epsilon_n(k,x) = \frac{1}{k}\int_0^x \sin k(x-y)f(k,y)\\ \times[\epsilon_{n-1}(k,y) + e^{-iky}]\,dy, \quad n \geqslant 1.\end{aligned} \tag{6.22}$$

If we take the limit $n \to \infty$, since the sequence converges uniformly, we have the exact integral equation

$$\epsilon(k,x) = \frac{1}{k}\int_0^x \sin k(x-y)f(k,y)[\epsilon(k,y) + e^{-iky}]\,dy. \tag{6.23}$$

Then from Eqs. (6.18) and (6.19) we have

$$\alpha_k = e^{ikx}\left(1 - \frac{i}{2}\int_0^{kx} e^{-i\theta}W^* G\,d\theta\right), \tag{6.24}$$

$$\beta_k = \frac{i}{2}e^{ikx}\int_0^{kx} e^{-i\theta}WG\,d\theta, \tag{6.25}$$

where the integration variable is $\theta = kx$ and

$$G(k,x) = k^{-2}f(k,x) = \frac{1}{2}\frac{\mu^2}{w_k^4}\left(2 - \frac{5}{2}\frac{\mu^2}{w_k^2} - q\right)H^2, \tag{6.26}$$

## 7. THE ENERGY DENSITY

Of course energy is not a well-defined notion in curved space–time. Strictly speaking, energy is the zero component of the momentum, a global 4-vector that we cannot define in this case.

The best thing we can do is to compute the (0,0) component of the energy–momentum tensor of the field, obtained from the Lagrangian that corresponds to the field equations (2.2) and integrate in a $t$ = constant surface. The (0,0) component of the energy–momentum tensor is given by[13,14]

$$\begin{aligned}T^0{}_0 = \tfrac{1}{2}(\partial_t\phi)^2 + 6\xi H\phi\partial_t\phi + \frac{1}{2a^2}(\nabla\phi)^2\\ + \tfrac{1}{2}\mu^2\phi^2 + 3\xi H^2\phi^2 - \frac{2\xi}{a^2}\sum_{j=1}^{3}\partial_j(\phi\partial_j\phi).\end{aligned} \tag{7.1}$$

The total energy density operator at time $t = \tau$ will be

$$E(\tau) = \int_S T^0{}_0\,d\sigma, \tag{7.2}$$

where $d\sigma$ is the area element of the Cauchy surface, $S$, $t = \tau =$ etc.

Using Eq. (2.13) and the boundary conditions (4.19) we obtain

$$E(\tau) = \int d^3\mathbf{k}\left[w_k + (\tfrac{1}{2} - 3\xi)\frac{H^2}{w_k}\left(1 + \frac{\mu^2}{w_k^2}\right) + \frac{H^2\mu^4}{8w_k^5}\right] a_{\mathbf{k}}^{*(\tau)} a_{\mathbf{k}}^{(\tau)}$$
$$+ \int d^3\mathbf{k}\left[(\tfrac{1}{2} - 3\xi)\frac{H^2}{2w_k}\left(1 + \frac{\mu^2}{w_k^2}\right) + \frac{1}{16}\frac{H^2\mu^4}{w_k^5} + i\frac{H}{2}\left(1 + \frac{\mu^2}{2w_k^2} - 6\xi\right)\right]$$
$$\times a_{\mathbf{k}}^{(\tau)} a_{-\mathbf{k}}^{(\tau)} + \int d^3\mathbf{k}\left[(\tfrac{1}{2} - 3\xi)\frac{H^2}{2w_k}\left(1 + \frac{\mu^2}{w_k^2}\right) + \frac{1}{16}\frac{\mu^4 H^2}{w_k^5} - \frac{iH}{2}\left(1 + \frac{\mu^2}{2w_k^2} - 6\xi\right)\right] a_{\mathbf{k}}^{*(\tau)} a_{-\mathbf{k}}^{*(\tau)}, \tag{7.3}$$

where we have taken the usual prescription of normal ordering.

As before, we assume that at time $\tau$ the universe is in the vacuum state $|0\rangle_{(\tau)}$. The mean value of the energy density at time $\tau'$ will be, in the conformal case ($\xi = \frac{1}{6}$)

$$_{(\xi)}\langle 0|E(\tau')|0\rangle_{(\tau)} = \int d^3\mathbf{k}\, e(k)|\beta_{\mathbf{k}}|^2, \tag{7.4}$$

where

$$e(k) = w_k + (\tfrac{1}{2} - 3\xi)\frac{H^2}{w_k}\left(1 + \frac{\mu^2}{w_k^2}\right) + \frac{H^2\mu^2}{8w_k^5}. \tag{7.5}$$

To derive (7.5) we have used (2.18), (2.19), and (7.3). Clearly

$$|e(k)| \leqslant C|\mathbf{k}|, \tag{7.6}$$

for some constant $C$. It follows from (5.25), (5.29), (5.31), and (5.37) that

$$|\beta_k| = O\left(\frac{1}{k^3}\right), \quad k \to \infty.$$

Then in the conformal case the integral (7.4) is convergent, and then the energy of the created particles in finite.


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# Percolation theory on pairs of matching lattices

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An important magnitude in percolation theory is the critical probability, which is defined as the supremum of those values of the occupation-probability $p$, for which only finite clusters occur. In 1964 Sykes and Essam obtained the relation $P_c^{(s)}(L) + P_c^{(s)}(L^*) = 1$, where $L$ and $L^*$ are a pair of matching lattices and $P_c^{(s)}$ denotes the critical probability (site-case). The proof was not complete, but based on certain assumptions about the mean number of clusters. Though Sykes and Essam suggested that the above relation holds for all mosaics (i.e., multiply-connected planar graphs) and decorated mosaics, we have constructed a counterexample. Subsequently, for a more restricted class of graphs, an alternative derivation of the Sykes–Essam relation is given, this time based on the usual assumption that below the critical probability the mean cluster size is finite. The latter assumption is also used to prove for some nontrivial subgraphs of the simple quadratic lattice $S$, that their critical probability is equal to $P_c^{(s)}(S)$. Finally, for a certain class of lattices, sequences of numbers are constructed, which converge to the critical probability. In the case of the site process on $S$, the number with highest index we found, is $0.5925 \pm 0.0002$, which seems to be a reasonable estimate of $P_c^{(s)}(S)$.

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## 1. INTRODUCTION

Percolation problems arise in many branches of science and engineering. Concerning physics, the most interesting example is the dilute ferromagnet, where the concentration of magnetic particles is $p$ and the concentration of nonmagnetic impurites is $1 - p$. Below a certain value of $p$, the so-called critical concentration $P_c$, there are only finite clusters of magnetic particles and therefore no spontaneous magnetism occurs at any temperature. On the other hand, if $p > P_c$, spontaneous magnetism will occur below a certain temperature.

Generally, percolation can be described mathematically as follows. A graph $G$ consists of abstract points, called vertices (or sites or atoms) and connections between some of these points, called bonds. These bonds may be oriented, in which case they connect in only one direction, or nonoriented. In this paper we only deal with nonoriented graphs, i.e., graphs of which all bonds are nonoriented.

With the graph $G$ we now relate a so-called random coloring as follows: Each vertex of $G$ has, independently of all other vertices, a fixed probability $p$ of being colored black, and $q = 1 - p$ of being colored white. For such a realization of this random coloring we distinguish two section-graphs of $G$, one, called $G_b$, containing all black, and the other, $G_w$, containing all white vertices of $G$.

Percolation theory studies the properties of $G_b$ and $G_w$. Especially, in the case that $G$ is infinite, we are interested in the critical value $P_c$ of $p$, above which infinite black clusters appear.

A related model is that in which the bonds of $G$, instead of the vertices, are randomly colored. This model and the model above are known as the bond- and the site-percolation process respectively. It appears that the site process is the more general one, because the bond process on a graph $G$ is, in a certain sense, equivalent with the site process on the covering graph $G^c$ of $G$. Therefore, quite often certain results are proved for the site- and then translated to the bond-case.

In 1964 Sykes and Essam[1] published some interesting results for two-dimensional percolation processes. We shall use much of their terminology. A more general introduction to the subject is to be found in, e.g., Refs. 2 and 3.

*Remark*: In this article we shall only deal with lattices which are mosaics or decorated mosaics.

One of the main results of Sykes and Essam is the relation

$$P_c^{(s)}(L) + P_c^{(s)}(L^*) = 1, \tag{1}$$

where $L$ and $L^*$ are a pair of matching lattices and $P_c^{(s)}$ denotes the critical probability for the site-percolation process. This relation follows from the fact that the mean number of black $L$ clusters per vertex differs from the mean number of white $L^*$ clusters per vertex by a finite polynomial $\phi(p)$ (where $p$ is, as it will be throughout this article, the probability of a given vertex being black), in formula:

$$k(p;L) = k(1-p;L^*) + \phi(p). \tag{2}$$

Now Sykes and Essam derive (1) immediately from (2) by the assumption (which has not been proved) that in the domain $0 \leqslant p \leqslant 1$ the function $k$ is singular at $P_c^{(s)}$ and nowhere else.

Next they remark that the triangular lattice $T$ is self-matching, which implies, by (1), that:

$$P_c^{(s)}(T) = \tfrac{1}{2}, \tag{3}$$

and that (3) more generally holds for any lattice of which all faces are triangular. However, it is easy to construct such a lattice for which (3) is not true, as follows.

Figure 1(a) shows a sequence of triangles $A_0, A_1, A_2, \cdots$, each of which (except $A_0$) has six vertices on its perimeter,

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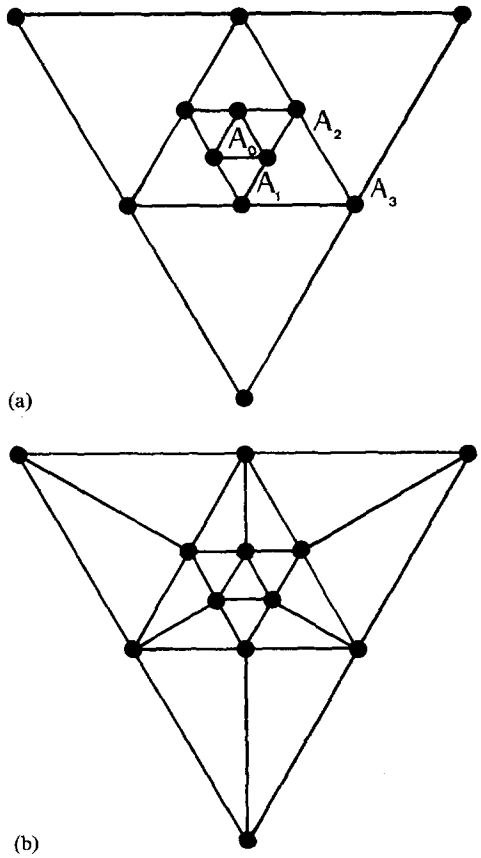


FIG. 1(a) Lattice, consisting of a sequence of nested triangles $A_0, A_1, A_2, \cdots$. (b) The lattice obtained by triangulation of the lattice in (a). It appears that the critical probability (site-case) of this lattice is, in contrast with the Sykes–Essam relation, not $\frac{1}{2}$ but 1.

one at each corner and one at the center of each of its edges.

The fully triangulated graph $G$ in Fig. 1(b) is obtained by drawing a bond in every nontriangular face of Fig. 1(a).

Considering the site-percolation process on $G$, we note that, if $p < 1$, for each $i > 0$ the probability of the event that all six vertices of $A_i$ are white is $q^6 > 0$. Further, we observe that any pair of the triangles with odd indices $A_1, A_3, A_5, \cdots$, has no common vertex, hence the number of white vertices on the perimeter of one of these triangles is independent of that on the others. But then it follows from a well-known law of probability theory that there is with probability 1 at least one such $A_i$ of which all six vertices are white. It is obvious that such a triangle blocks all possible black walks starting in one of the corners of $A_0$. This is the case for every $p < 1$, so we may conclude that for this graph, which obviously is a mosaic, $P_c^{(s)} = 1$, so that (3) and therefore (1) does not hold.

In Sec. 2 relation (1) will be derived for a restricted class of lattices in a way that is totally different from that of Sykes and Essam. The proof is based on the following assumption:

*Assumption* 1: If $p < P_c^{(s)}$ then the mean number of vertices that can be reached from a given vertex via black walks (i.e., the mean size of black clusters) is finite.

Though not proved, this assumption is not unusual. It is even the main idea behind the method of estimating the critical probability by means of cluster-size expansion (see Domb, Sykes[4]).

It will appear that, besides (1), the assumption has other interesting consequences. In Sec. 3, e.g., we shall use it to prove for a certain class of subgraphs of the simple quadratic lattice $S$, that their critical probability is the same as for $S$ itself. In Sec. 4 assumption 1, combined with a theorem of Hammersley, leads to another mathematical approach of a method to estimate the critical probability for certain lattices. This method is rather similar to the renormalization group method used by Reynolds *et al.*[5,6]

## 2. AN ALTERNATIVE DERIVATION OF: $P_c^{(s)}(L) + P_c^{(s)}(L^*) = 1$.

We shall first discuss some definitions and arguments which lead to Lemma 1. Then we are ready to prove (1) for certain lattices.

Let $v$ be a vertex of some graph $G$.

$N^n(v)$ denotes the set of all vertices of $G$ that can be reached from $v$ in $n$ or fewer steps.

Further we define:

$$B^0(v) = N^0(v) = \{v\},$$

$$B^n(v) = N^n(v) \backslash N^{n-1}(v).$$

We shall call $B^n(v)$ the sphere with center $v$ and radius $n$. Now consider the site-percolation process on $G$ of which every vertex is colored black with probability $p$ and white with probability $1-p$. Let $S(p;v)$ be the mean number of vertices that can be reached from $v$ by black walks, and denote by $S_n(p;v)$ the mean number of such vertices which lie in $B^n(v)$, $n = 0,1,2,\cdots$. It is clear that

$$S(p;v) = \sum_{n=0}^{\infty} S_n(p;v). \tag{4}$$

Further let $P_n(p;v)$ be the probability of the event that at least one vertex outside $N^n(v)$ can be reached from $v$ by a black walk.

Every walk from $v$ to a vertex outside $N^n(v)$ obviously visits some vertex of $B^n(v)$ and the probability that at least one vertex of the latter kind can be reached from $v$ by a black walk is not larger than $S_n(p;v)$, so that

$$P_n(p;v) < S_n(p;v); \tag{5}$$

this, combined with (4) and assumption 1 gives:

*Lemma* 1: If $p < P_c^{(s)}$, then $\Sigma_{n=0}^{\infty} P_n(p;v) < \infty$.

For reasons of simplicity we shall first study as an example the site-process on the simple quadratic lattice $S$, for which with the help of Lemma 1 we shall prove (1). Afterwards the results will be generalized. Because for this lattice the functions $S_n$, $S$, and $P_n$ do not depend on $v$, we shall omit this parameter.

For $p < P_c^{(s)}(S)$, it follows, by Lemma 1, that the series $\Sigma P_n(p)$ converges and so, for some $M \in \mathbb{N}$ and positive real number $r$:

$$\sum_{n=M+1}^{\infty} P_n(p) = r < 1. \tag{6}$$

Denote by $W_\infty$, $W$, and $C$ the events that the vertex $0 = (0,0)$ belongs to an infinite white $S^*$ cluster, that all vertices $(0,0), (0,-1),\ldots,(0,-M)$ are white, and that the vertex

0 is black or surrounded by a black $S$ circuit, respectively.

From the matching–property (see Appendix 1 of Ref. 1 for a proof) it follows that either $W_\infty$ or $C$ occurs. We also note the following: If all vertices (0,0), (0, −1),...,(0, − $M$) are white, then the event $C$ can only occur if there is a black $S$ walk from a vertex on the $Y$ axis below (0, − $M$) to a vertex on the $Y$ axis above 0. Further, for each positive $n$, all vertices on the positive $Y$ axis lie outside $N^n((0, -n))$, so that the probability of the event that at least one of these vertices can be reached from (0, − $n$) by a black walk is smaller than $P_n(p)$. Therefore, if for events $E_1$ and $E_2$ $\Pr\{E_1|E_2\}$ denotes the conditional probability of $E_1$, given $E_2$, it follows for $p < P_c^{(s)}(S)$:

$$\Pr\{C\,|\,W\} < \sum_{n=M+1}^{\infty} P_n(p) = r < 1, \tag{7}$$

and hence

$$\Pr\{W_\infty\} \geqslant \Pr\{W\}\,\Pr\{W_\infty\,|\,W\}$$
$$= q^{M+1}(1 - \Pr\{C\,|\,W\}) > q^{M+1}(1 - r) > 0. \tag{8}$$

So we have proved that, for $p < P_c^{(s)}(S)$, there is a positive probability that a given vertex belongs to an infinite white $S^*$ cluster. In other words, if $p < P_c^{(s)}(S)$, then $1 - p > P_c^{(s)}(S^*)$. This immediately yields, by taking $p = P_c^{(s)}(S) - \epsilon$, with $\epsilon$ positive and arbitrarily small:

$$P_c^{(s)}(S) + P_c^{(s)}(S^*) \leqslant 1. \tag{9}$$

Fisher,[7] generalizing Harris' method,[8] proved that for a certain class of lattices, to which $S$ belongs, $P_c^{(b)}(L) + P_c^{(b)}(L^D) \geqslant 1$, where $L^D$ is the dual lattice of $L$ and $P_c^{(b)}$ denotes the critical probability for the bond-percolation process. This result can be extended to the site-case, so that we have, for $S$,

$$P_c^{(s)}(S) + P_c^{(s)}(S^*) \geqslant 1, \tag{10}$$

which, combined with (9), yields the wanted relation:

$$P_c^{(s)}(S) + P_c^{(s)}(S^*) = 1. \tag{11}$$

When we call two vertices $v_1$ and $v_2$ equivalent if, for all $n$ and $p$, $S_n(p;v_1) = S_n(p;v_2)$, then we can generalize the above result as follows:

*Theorem* 1: Let $L$ be a lattice which has only a finite number of classes of equivalent vertices and which possesses a pair of orthogonal symmetry-axes. Then

$$P_c^{(s)}(L) + P_c^{(s)}(L^*) = 1.$$

The proof of Theorem 1 is similar to that of the special case of the simple quadratic lattice (see also Fisher[7]).

## 3. SOME NONTRIVIAL SECTION-GRAPHS OF $S$ WITH CRITICAL PROBABILITY $P_c^{(s)}(S)$.

In this section it will first be shown that $P_c^{(s)}(S(\frac{1}{2}\pi)) = P_c^{(s)}(S)$, where $S(\frac{1}{2}\pi)$ denotes the quadrant of $S$ with vertex-set $\{(n,m)|n,m \geqslant 0\}$. Analogously $S^*(\frac{1}{2}\pi)$ will denote the quadrant of $S^*$ with the same vertex-set as $S(\frac{1}{2}\pi)$.

From the matching-property (see Ref. 1) it follows that the vertex 0 = (0,0) belongs to an infinite white cluster of $S^*(\frac{1}{2}\pi)$ if and only if there is no black walk in $S(\frac{1}{2}\pi)$ from some vertex $(n,0)$ to some vertex $(0,m)$,$n,m \geqslant 0$. It is trivial that the probability of the latter event is smaller than the probability of the corresponding event for $S$, which, in the case that $p < P_c^{(s)}(S)$, can be proved (in a similar way as in Sec. 2) to be smaller than 1. So we have that, for $p < P_c^{(s)}(S)$ (which, by (11), is equivalent with $1 - p > P_c^{(s)}(S^*)$, $1 - p \geqslant P_c^{(s)}(S^*(\frac{1}{2}\pi))$. Hence it follows that

$$P_c^{(s)}(S^*(\tfrac{1}{2}\pi)) \leqslant P_c^{(s)}(S^*). \tag{12}$$

On the other hand, because $S^*(\frac{1}{2}\pi)$ is a subgraph of $S^*$, it is clear that the critical probability of the first cannot be smaller than that of the second; hence

$$P_c^{(s)}(S^*(\tfrac{1}{2}\pi)) = P_c^{(s)}(S^*). \tag{13}$$

The analog of (13) for $S$ is obtained by changing the roles of $S$ and $S^*$.

In the same way we can prove the following theorem:

*Theorem* 2: Let $u$ be a positive real number and let $S'$ be a connected subgraph of $S$ containing the section-graph of $S$ with vertex-set

$$\{(n,m)|0 \leqslant n; 0 \leqslant m \leqslant un\},$$

then

$$P_c^{(s)}(S') = P_c^{(s)}(S).$$

*Remark*: It is noted that similar results hold for many other lattices, particularly for the triangular and the honeycomb lattice.

## 4. ESTIMATES OF THE CRITICAL PROBABILITY

In this section for a certain class of lattices we shall construct sequences of numbers which converge to the critical probability. As in the last two sections, we shall first take as an example the simple quadratic lattice $S$.

Let $K(n)$ be the so-called "box" with $(n+1)\times(n+1)$ vertices (see Fig. 2).

By the upper, the lower, the left, and the right side of $K(n)$ we mean the sets $\{(0,n),(1,n),...,(n,n)\}$, $\{(0,0),(1,0),...,(n,0)\}$, $\{(0,0),(0,1),...,(0,n)$, and $\{(n,0),(n,1),...,(n,n)\}$, respectively.

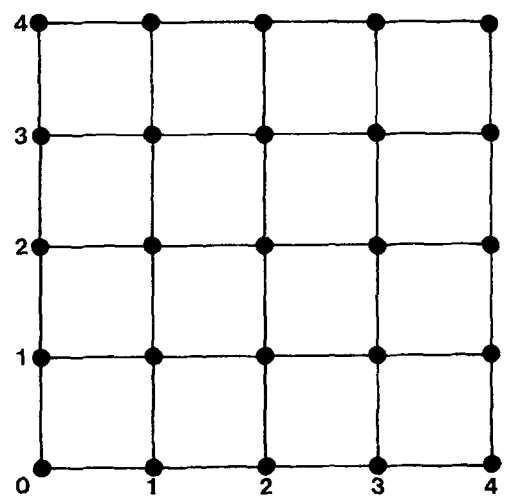


FIG. 2. The box $K(4)$ of the simple quadratic lattice.

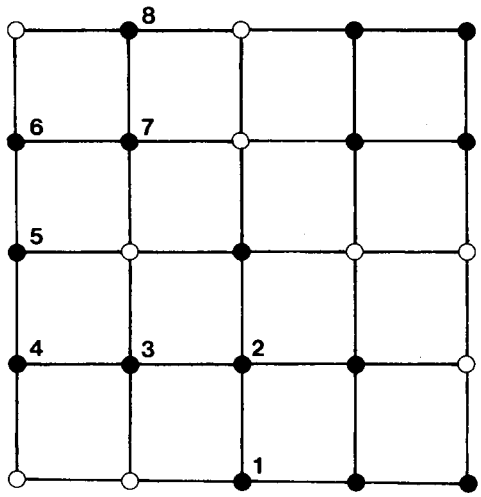


FIG. 3. Example of a coloring of the box in Fig. 2. In this example the event $B_4$ and not $W_4^*$ occurs. The numbered vertices mark a black $S$ walk from the lower to the upper side.

Let $B_n(W_n)$ be the event that there is a black (white) $S$ walk, entirely lying in $K(n)$, from the lower to the upper side of the box.

Analogously $B_n^*(W_n^*)$ denotes the event that there is a black (white) $S^*$ walk, entirely lying in $K(n)$, from the left to the right side.

Further we define:

$$f_n(p) = \Pr\{B_n\}; f_n^*(p) = \Pr\{B_n^*\}. \tag{14}$$

From this definition and the fact that the probability that a vertex is white is $1-p$, it follows that

$$\Pr\{W_n\} = f_n(1-p); \Pr\{W_n^*\} = f_n^*(1-p). \tag{15}$$

Because of the matching-property either $B_n$ or $W_n^*$ takes place (see e.g., Fig. 3). Hence, by (14) and (15):

$$f_n(p) = 1 - f_n^*(1-p). \tag{16}$$

It will be shown that, for $p < P_c^{(s)}(S)$, the sequence $f_n(p)$ tends to zero. Analogously, if $p < P_c^{(s)}(S^*)$, then $f_n^*(p)$ tends to zero. For this we shall first state a stronger version of Lemma 1.

Consider the site-percolation process on a graph $G$. Let $v$ be a vertex of $G$. Define the following functions [with $B^n(v)$ as defined in Sec. 2]: $E_n(p;v) \equiv$ the mean number of vertices in $B^n(v)$ that can be reached from $v$ by at least one black walk of which all vertices, except the last one [which, of course, is in $B^n(v)$], are in $N^{n-1}(v)$. Further,

$$F_n(p) \equiv \sup_v E_n(p;v).$$

In the case that $G$ is a so-called medium[9] the following holds: If, for certain $n$ and $p$, $F_n(p) = \lambda < 1$, then, for each nonnegative integer $m$ and each vertex $v$:

$$F_m(p;v) < \lambda^{[m/n]}, \tag{17}$$

where $[m/n]$ denotes the integer part of $(m/n)$ and with $P_m(p;v)$ as defined in Sec. 2. This theorem, which is due to Hammersley,[10] was formulated and proved by him for the bond-case,[11] but it is easily seen that also the above site-version holds.

Now if the medium $G$ contains only a finite number of classes of equivalent vertices (equivalent used in the same sense as in Sec. 2), then it follows from assumption 1 that in the case that $p$ is smaller than the critical probability, for each vertex $v$, $\Sigma_{m=0}^{\infty} E_m(p;v) < \infty$. Hence, (because of the finite number of equivalence classes) in that case there will be some $n$ such that $F_n(p) < 1$. Next, application of Hammersley's theorem leads to the following lemma:

*Lemma* 2: If $p < P_c^{(s)}(G)$, then there exists a $\lambda(p) < 1$, such that for all $m$ and all vertices $v$:

$$P_m(p;v) < \lambda^m(p).$$

*Remark*: If, in Hammersley's theorem, $[m/n]$ would be replaced by $(m/n)$, then Lemma 2 follows trivially from the above reasonings (take $\lambda(p) = \lambda^{1/n}$), with $\lambda$ as in Hammersley's theorem). The presence of the [ ]-function makes only a slight change of the proof necessary.

We are now ready to prove the statement about the limiting behavior of $f_n(p)$: From the definition it is clear that $f_n(p)$ is smaller than the probability of the event that there is a black $S$ walk, not necessarily lying entirely in the box $K(n)$, from some vertex $(i,0)$ to some vertex $(j,n)$ $(0 \leqslant i, j \leqslant n)$. Further, for each $i$ and $j$, the vertex $(j,n)$ lies outside $N^{n-1}((i,0))$ so that, for $p < P_c^{(s)}(S)$, it follows from Lemma 2 that

$$f_n(p) \leqslant \sum_{i=0}^{n} P_{n-1}(p;(i,0)) < (n+1)\lambda^{n-1}(p), \tag{18}$$

so that $f_n(p) \to 0$ for $n \to \infty$.

Of course the same arguments hold for $S^*$, i.e., if $p < P_c^{(s)}(S^*)$ then, for $n \to \infty$,

$$f_n^*(p) \to 0. \tag{19}$$

But, from (11), $p < P_c^{(s)}(S^*)$ is equivalent with

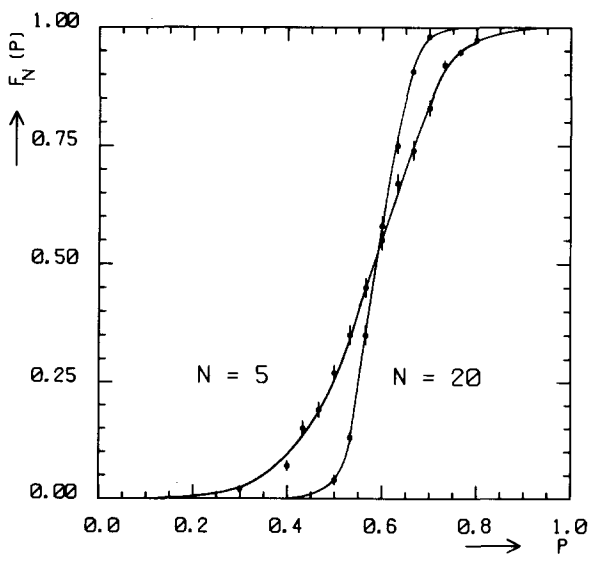


FIG. 4. The function $f_n(p)$ for $n = 5$ and $n = 20$.

$1-p > P_c^{(s)}(S)$. Hence, by combining (16), (18), and (19), we have the following theorem.

*Theorem* 3: Denote by $f_n(p)$ the probability of the event that there is a black $S$ walk, which connects the lower and the upper side of the box $K(n)$ and which does not leave this box. Then, for $n \to \infty$

$$f_n(p) \to 0, \text{ for } p < P_c^{(s)}(S),$$
$$f_n(p) \to 1, \text{ for } p > P_c^{(s)}(S).$$

Of course, by symmetry, an analogous theorem holds for $S^*$.

*Remark*: The substance of this theorem is already mentioned in earlier papers, e.g., by Reynolds *et al.*[5,6] (who show even more, namely that the "unstable" fixed points of the $f_n$'s converge to the critical probability), but our proof is new. Their theory is based on scaling-arguments, which are very interesting but rather heuristic. On the other hand, our approach does not give insight in the theory of critical exponents. The interested reader is also referred to work by Kirkpatrick.[12]

Though Theorem 3 says nothing about the limiting-behavior of $f_n(p)$ in the case that $p = P_c^{(s)}(S)$, we do have the following theorem:

*Theorem* 4: Let $r$ be any real number in the open interval (0,1) and let $g_n : [0,1] \to [0,1]$ be the inverse function of $f_n$, then:

$$\lim_{n \to \infty} g_n(r) = P_c^{(s)}(S).$$

This theorem follows from Theorem 3 and the fact that every $f_n(p)$ is continuous (it is a polynomial) and increasing in $p$, while, for each $n$, $f_n(0) = 0$ and $f_n(1) = 1$.

Every polynomial $f_n$ is computable (because for every $n$ there is only a finite number of ways in which the vertices of $B(n)$ can be colored black and white); hence Theorem 4 indeed provides sequences of numbers which converge to the critical probability. Unfortunately, even for rather small $n$, it takes very much time to calculate $f_n$. For various values of $n$ and $p$, estimates of $f_n(p)$ are made by Monte Carlo simulations (see e.g., Fig. 4). These values lead to estimates of $g_n(r)$. Though every number between 0 and 1 is allowed, we made the most natural choice and took $r = \frac{1}{2}$.

TABLE I.

| | $f_n(p)$ | 0.590 | 0.591 | 0.592 | 0.593 | 0.594 | 0.595 |
|---|---|---|---|---|---|---|---|
| | 80 | 0.454 ± 0.009 | | | | | 0.560 ± 0.009 |
| $n$ ↕ | 120 | 0.433 ± 0.012 | 0.462 ± 0.012 | 0.495 ± 0.012 | 0.527 ± 0.012 | 0.533 ± 0.012 | 0.567 ± 0.012 |
| | 160 | 0.405 ± 0.012 | 0.450 ± 0.012 | 0.477 ± 0.012 | 0.526 ± 0.012 | 0.539 ± 0.012 | 0.584 ± 0.012 |

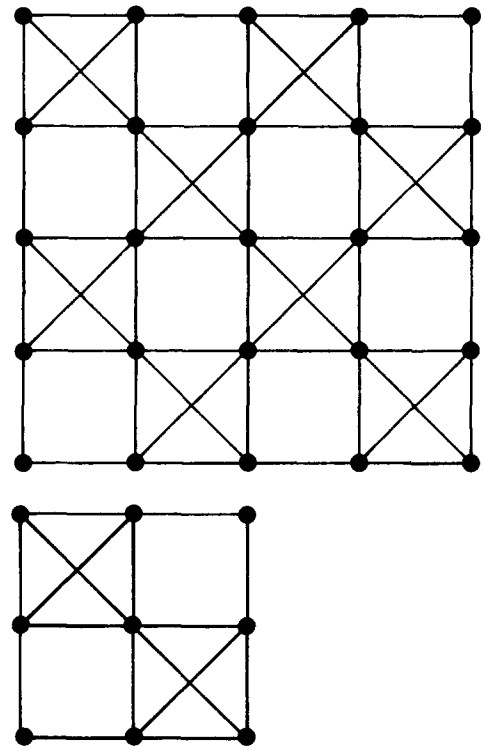

FIG. 5(a) The box $K(2)$ of the covering-lattice of $S$. (b) Unit-cell of the lattice in (a).

Linear interpolation in the intervals $[p_{n,1}, p_{n,2}]$, where $p_{n,1}(p_{n,2})$ is the largest (smallest) $p$ in Table 1 such that the uncertainty region of $f_n(p)$ lies entirely below (above) $\frac{1}{2}$ (that is: $p_{120,1} = 0.591$, $p_{120,2} = 0.593$; $p_{160,1} = 0.592$, $p_{160,2} = 0.593$), yields:

$$g_{80}(\tfrac{1}{2}) = 0.5922 \pm 0.0003,$$
$$g_{120}(\tfrac{1}{2}) = 0.5922 \pm 0.0003, \quad (20)$$
$$g_{160}(\tfrac{1}{2}) = 0.5925 \pm 0.0002.$$

The results (20) give the impression that the last value, $0.5925 \pm 0.0002$, is a reasonable estimate for the critical probability. This estimate is within the uncertainty region of the less precise result of Sykes *et al.*,[13] who obtained $P_c^{(s)}(S) = 0.593 \pm 0.002$, and a little smaller than the estimate of Reynolds *et al.*,[6] who found $0.5935^{+0.0005}_{-0.0010}$.

Finally it should be remarked that analogs of Theorems 3 and 4 hold for many other lattices, specifically for those

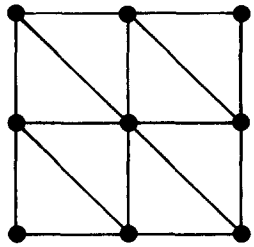

FIG. 6. By drawing one diagonal in each face of the simple quadratic lattice, we obtain this lattice, which is isomorphic with the regular triangular lattice.

which have a pair of orthogonal symmetry-axes and are regularly built up of rectangular unit-cells (see e.g., Fig. 5). In these cases we take for $K(n)$ the box consisting of $n \times n$ unit-cells.

Remarkable cases are those of the lattice in Fig. 5, which is the covering-lattice of the simple quadratic lattice, and of the triangular lattice $T$, which is isomorphic with the lattice formed by drawing one diagonal in each face of the simple quadratic lattice (see Fig. 6).

From the self-matchingness of these lattices and the symmetry of their boxes it follows that in these cases $f_n(p) = f_n^*(p)$, which, by (16), yields for all $n$ and $p$:

$$f_n(p) + f_n(1-p) = 1, \tag{21}$$

and hence

$$f_n(\tfrac{1}{2}) = \tfrac{1}{2}. \tag{22}$$

But, for these lattices, $\frac{1}{2}$ is exactly the value of $P_c(S)$, so that $f_n(p)$ is constant at the critical probability.

From (22) it also follows that, for all $n$

$$g_n(\tfrac{1}{2}) = P_c(S). \tag{23}$$

So if we take $r = \frac{1}{2}$ then, for these lattices, Theorem 4 yields an exact result.

*Added in proof*: In Sec. 4 a theorem of Hammersley is used to prove that, for $p < P_c^{(s)}(S)$, $\lim_{n\to\infty} (n+1)P_{n-1}(p;v) = 0$ and hence $\lim_{n\to\infty} f_n(p) = 0$ [see Lemma 2 and (18)]. It is possible to derive this result directly, i.e., without using Hammersley's theorem, namely as follows: $P_n(p;v)$ (see definition in Sec. 2) is obviously decreasing in $n$. Further, if $p < P_c^{(s)}(S)$, then, by Lemma 1 (Sec. 2), $\Sigma P_n(p;v) < \infty$. Hence, if $p < P_c^{(s)}(S)$, then, with $[n/2]$ denoting the integer part of $n/2$:

$$0 \leqslant nP_n(p;v) < 2\sum_{n/2}^{n} P_m(p;v) \to 0, \text{ for } n \to \infty.$$


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# Solution of the inverse problem in multigroup transport theory [a)]

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A solution is given for the (inverse) problem of determining the scattering laws for a multigroup, anisotropically scattering medium, in terms of the boundary fluxes corresponding to finite slabs.

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## I. INTRODUCTION

The problem of determining the scattering law for a medium by measuring and processing the results of one-dimensional experiments has been considered in a number of recent articles.[1-15] In much of this work, the angular fluxes on the boundaries of and within the system must be measured to obtain a solution. From the experimental point of view, it is preferable to have to measure only the incident and outgoing fluxes. Pahor's solution[1] does require just the measurements of these boundary fluxes, but his solution is approximate and applicable only for thin slabs.

Siewert[9,10] and McCormick,[11] however, have recently derived exact solutions for one-group, anisotropic scattering problems in a finite slab, in which only the boundary fluxes need to be measured. Siewert's first solution [Ref. 9, Eq. (12)] is based on the assumption of a two-term (linearly anisotropic) scattering law, and is derived by manipulating Chandrasekhar's $X$ and $Y$ functions.[16] Siewert[10] later extended this result to a three-term scattering law and reduced the derivation to direct manipulations of the transport equation. McCormick[11] then found a solution for a general $(N+1)$-term scattering law. McCormick's analysis makes use of azimuthally asymmetric fluxes and leads to a linear "triangular" system of equations, whereas Siewert's analysis makes use of only the azimuthally symmetric flux and leads to a nonlinear set of equations. In spite of these differences, McCormick's analysis[11] is similar to that of Siewert,[10] and both analyses give the same result for isotropic $(N=0)$ scattering.

More recently, Siewert and Maiorino[12] and McCormick[13] have solved inverse problems for Rayleigh-scattering atmospheres. Also, McCormick and Sanchez have studied various numerical solutions of inverse transport problems,[14] and have developed solutions for more general inverse problems.[15]

In this note we consider multigroup transport in an anisotropically scattering, finite slab medium. We require that the number $G$ of energy groups and the number $N+1$ of Legendre moments in the scattering law are given and finite, and that the total cross sections for each group are known. (Actually, it suffices to know the total cross section for only one group.) We then derive linear equations from which the scattering laws can be determined by performing $G^2(N+1)$ slab geometry experiments and measuring only the boundary angular fluxes. Our method is similar to that of Siewert[10] and McCormick,[11] although we do not make use of the azimuthally asymmetric fluxes, as McCormick did. (If we had followed McCormick's treatment of the azimuthally asymmetric fluxes, the number of necessary slab experiments would be reduced to $G^2$, but the algebra would become more difficult. Such a solution could be less sensitive to experimental error; however we shall not develop this solution here.) Finally, we show that our solution reduces to the appropriate parts of McCormick's[11] and Siewert's[10] solutions for the special cases of one-group scattering with an $(N+1)$- and a three-term scattering law, respectively.

## II. ANALYSIS

We shall consider forward transport problems of the following form:

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\Sigma\cdot\psi(x,\mu)=\tfrac{1}{2}\sum_{n=0}^{N}P_n(\mu)\mathsf{C}_n\cdot\psi_n(x),\quad 0<x<a, \tag{2.1}$$

$$\psi_n(x)=\int_{-1}^{1}P_n(\mu')\psi(x,\mu')\,d\mu', \tag{2.2}$$

$$\psi(0,\mu)=\mathbf{f}_L(\mu),\quad 0<\mu\leqslant 1, \tag{2.3}$$

$$\psi(a,\mu)=\mathbf{f}_R(\mu),\quad -1\leqslant\mu<0. \tag{2.4}$$

Here $P_n(\mu)$ are the Legendre polynomials, $\Sigma$ is a known diagonal $G\times G$ matrix, $\mathsf{C}_n$ are unknown $G\times G$ matrices, and the angular and incident fluxes $\psi$, $\mathbf{f}_L$, $\mathbf{f}_R$ are $G\times 1$ vectors. We shall also consider adjoint transport problems of the form

$$-\mu\frac{\partial}{\partial x}\psi^*(x,\mu)+\psi^*(x,\mu)\cdot\Sigma=\tfrac{1}{2}\sum_{n=0}^{N}P_n(\mu)\psi_n^*(x)\cdot\mathsf{C}_n,\quad 0<x<a, \tag{2.5}$$

$$\psi_n^*(x)=\int_{-1}^{1}P_n(\mu')\psi^*(x,\mu')\,d\mu', \tag{2.6}$$

$$\psi^*(0,\mu)=\mathbf{f}_L^*(\mu),\quad -1\leqslant\mu<0, \tag{2.7}$$

$$\psi^*(a,\mu)=\mathbf{f}_R^*(\mu),\quad 0<\mu\leqslant 1. \tag{2.8}$$

In these equations, $\psi^*$, $\mathbf{f}_L^*$, and $\mathbf{f}_R^*$ are $1\times G$ vectors.

To begin, we multiply Eq. (2.1) on the left by $\partial\psi^*/\partial x$ and integrate over $\mu$. This gives

$$\int_{-1}^{1}\mu\left(\frac{\partial}{\partial x}\psi^*\right)\cdot\left(\frac{\partial}{\partial x}\psi\right)d\mu+\int_{-1}^{1}\left(\frac{\partial}{\partial x}\psi^*\right)\cdot\Sigma\cdot\psi\,d\mu=\tfrac{1}{2}\sum_{n=0}^{N}\left(\frac{d}{dx}\psi_n^*\right)\cdot\mathsf{C}_n\cdot\psi_n\,. \tag{2.9}$$

[a)] Research performed under the auspices of the U.S. Department of Energy.

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Next we multiply Eq. (2.5) on the right by $\partial\psi/\partial x$ and integrate over $\mu$. This gives

$$-\int_{-1}^{1}\mu\left(\frac{\partial}{\partial x}\psi^*\right)\cdot\left(\frac{\partial}{\partial x}\psi\right)d\mu+\int_{-1}^{1}\psi^*\cdot\Sigma\cdot\left(\frac{\partial}{\partial x}\psi\right)d\mu$$
$$=\tfrac{1}{2}\sum_{n=0}^{N}\psi_n^*\cdot\mathsf{C}_n\cdot\left(\frac{\partial}{\partial x}\psi_n\right). \tag{2.10}$$

Now we add Eqs. (2.9) and (2.10) and get

$$\frac{d}{dx}\int_{-1}^{1}\psi^*\cdot\Sigma\cdot\psi\,d\mu=\frac{d}{dx}\frac{1}{2}\sum_{n=0}^{N}\psi_n^*\cdot\mathsf{C}_n\cdot\psi_n\,. \tag{2.11}$$

Finally, we integrate Eq. (2.11) over $0\leqslant x\leqslant a$ to obtain the main result:

$$\int_{-1}^{1}\psi^*(0,\mu)\cdot\Sigma\cdot\psi(0,\mu)\,d\mu-\int_{-1}^{1}\psi^*(a,\mu)\cdot\Sigma\cdot\psi(a,\mu)\,d\mu$$
$$=\tfrac{1}{2}\sum_{n=0}^{N}\left[\psi_n^*(0)\cdot\mathsf{C}_n\cdot\psi_n(0)-\psi_n^*(a)\cdot\mathsf{C}_n\cdot\psi_n(a)\right]. \tag{2.12}$$

This equation relates the boundary values of any pair of forward and adjoint angular fluxes to the unknown matrices $\mathsf{C}_n$, $0\leqslant n\leqslant N$. There are $G^2(N+1)$ unknowns in these matrices, and there is no restriction on the boundary conditions given by Eqs. (2.3), (2.4), (2.7), and (2.8). Thus, if boundary conditions for $G^2(N+1)$ distinct pairs of forward and adjoint problems can be prescribed such that the outgoing angular fluxes and the incident adjoint angular fluxes can be measured by experiment, then Eq. (2.12) would provide a set of linear $G^2(N+1)$ equations for the same number of unknowns. These unknowns could then be determined by solving this linear system. [It is clear that if only one total cross section were known, then the remaining cross sections and the scattering law could be detemined by performing $G^2(N+1)+G-1$ experiments.]

As an example, let us consider an experimental situation in which measuring devices are situated on both sides of a slab, and beams of neutrons are incident on one or both sides of the slab. Then for $G^2(N+1)$ different incident angular fluxes, one can measure the outgoing angular fluxes, and thereby obtain $G^2(N+1)$ distinct sets of angular fluxes defined on the boundaries of the slab. In order to make use of these functions in Eq. (2.12), it suffices to obtain just one solution of the adjoint problem (2.5)–(2.8) which can be measured experimentally. Such a solution exists if we prescribe

$$\psi_g^*(0,\mu)=1,\quad -1\leqslant\mu<0,\quad 1\leqslant g\leqslant G, \tag{2.13}$$
$$\psi_g^*(a,\mu)=1,\quad 0<\mu\leqslant 1,\quad 1\leqslant g\leqslant G. \tag{2.14}$$

Then $\psi^*$ has the following physical (and measurable) interpretation at $x=0$ and for $0<\mu\leqslant 1$:

$\psi_g^*(0,\mu)=$ the total current exiting the slab due to a unit incident beam at $(0,\mu)$ in group $g$. (2.15)

Also,

$$\psi^*(a,\mu)=\psi^*(0,-\mu),\quad -1\leqslant\mu<0. \tag{2.16}$$

To verify this, we consider the following forward transport problem for a function $\Psi(x,\mu;g_0,\mu_0)$:

$$\mu\frac{\partial}{\partial x}\Psi+\Sigma\cdot\Psi=\tfrac{1}{2}\sum_{n=0}^{N}P_n(\mu)\mathsf{C}_n\cdot\Psi_n, \tag{2.17}$$

$$\Psi_n(x,g_0,\mu_0)=\int_{-1}^{1}P_n(\mu')\Psi(x,\mu';g_0,\mu_0)\,d\mu', \tag{2.18}$$
$$\Psi_g(0,\mu;g_0,\mu_0)=\mu^{-1}\delta(\mu,-\mu_0)\delta_{gg_0},\quad 0<\mu\leqslant 1, \tag{2.19}$$
$$\Psi_g(a,\mu;g_0,\mu_0)=0,\quad -1\leqslant\mu<0. \tag{2.20}$$

Multiplying Eq. (2.17) on the left by the solution $\Psi^*$ of the problem (2.5), (2.6), (2.13), and (2.14), and integrating over $\mu$ and $x$, we easily obtain

$$\psi_{g_0}^*(0,\mu_0)=\sum_{g=1}^{G}\left\{\int_0^1\mu\Psi_g(a,\mu;g_0,\mu_0)\,d\mu-\int_{-1}^{0}\mu\Psi_g(0,\mu;g_0,\mu_0)\,d\mu\right\},$$
$$1\leqslant g_0\leqslant G,\quad 0<\mu_0\leqslant 1. \tag{2.21}$$

This verifies the interpretation (2.15), and Eq. (2.16) follows by symmetry.

Thus, suitable boundary values of $\psi^*$ can be determined by performing the same type of experiments for the forward angular flux as described earlier, measuring the outgoing currents, and then introducing these currents into Eq. (2.21).

The above formulas simplify if the matrices $\mathsf{C}_n$ are *a priori* known to be symmetric. Then for any solution $\psi(x,\mu)$ of the forward transport equation, a corresponding solution of the adjoint equation is

$$\psi^*(x,\mu)=\psi^{\mathrm{T}}(x,-\mu), \tag{2.22}$$

where T denotes "transpose." Since the Legendre polynomials satisfy

$$P_n(-\mu)=(-1)^nP_n(\mu), \tag{2.23}$$

then Eq. (2.22) and (2.23) give

$$\psi_n^*(x)=(-1)^n\psi_n^{\mathrm{T}}(x). \tag{2.24}$$

With the choice of $\psi^*$, Eq. (2.12) reduces to

$$\int_0^1\psi^{\mathrm{T}}(0,-\mu)\cdot\Sigma\cdot\psi(0,\mu)\,d\mu-\int_0^1\psi^{\mathrm{T}}(a,\mu)\cdot\Sigma\cdot\psi(a,\mu)\,d\mu$$
$$=\tfrac{1}{4}\sum_{n=0}^{N}(-1)^n\left[\psi_n^{\mathrm{T}}(0)\cdot\mathsf{C}_n\cdot\psi_n(0)-\psi_n^{\mathrm{T}}(a)\cdot\mathsf{C}_n\cdot\psi_n(a)\right]. \tag{2.25}$$

In this situation, only the forward angular fluxes on the boundary need to be measured.

In the special case of one-group scattering and the change of notation $\Sigma_{11}=\sigma$, $(C_n)_{11}=\sigma c_n$, Eq. (2.25) reduces, after dividing out $\sigma$, to

$$\int_0^1\psi(0,-\mu)\psi(0,\mu)\,d\mu-\int_0^1\psi(a,-\mu)\psi(a,\mu)\,d\mu$$
$$=\tfrac{1}{4}\sum_{n=0}^{N}(-1)^nc_n\left[\psi_n^2(0)-\psi_n^2(a)\right]. \tag{2.26}$$

This equation has been derived by McCormick,[11] and for the special case $N=2$ was derived earlier by Siewert.[10]


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# Thermodynamics. II. The extended thermodynamic system

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The algebraic theory of thermodynamics developed in a previous paper is extended to include the algebraic structure that arises from the introduction of a physical body into the theory. The extension is based on very general definitions of both the thermodynamic states of a body and subsystems of that body. The algebraic analysis, which includes bodies in nonuniform states, shows that the set of all thermodynamic states of a body has the same algebraic structure as the set of thermodynamic states and that composite systems are induced by the algebraic structure of thermodynamic states. The analysis also justifies a variational treatment of thermodynamic bodies in uniform as well as nonuniform states. The variational calculation includes all conventional methods of calculation as special cases and helps to illuminate the origin and interpretation of the electrochemical potential.

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## INTRODUCTION

Thermodynamics has long enticed scientists from diverse disciplines to its service with the twin attractants of utility and simplicity. While the utility was always there in abundance, the proffered simplicity was often evanescent. I examined the mathematical structure of thermodynamics in a recent paper[1] with the intent of stripping it of those assumptions and notions which are inessential for its development and which only seem to obfuscate the underlying simplicity. It proved possible to construct an algebraic theory of thermodynamics which was devoid of partitions, composite systems, and the zeroth law of thermodynamics, independent of any particular brand of mechanics, and had a global character in the set of thermodynamic states. Surprisingly, it was never necessary to mention what is the essence of any physical theory: a physical body to which the theory is applied. In this paper I shall remedy this hiatus in the theory and focus on the algebraic structure that arises when this aspect of a physical theory is brought into play.

The inclusion of a physical body in a thermodynamic analysis can complicate the theory considerably because it forces one to choose a suitable definition for the thermodynamic states of such a body. This inevitably makes the theory dependent on the structure of that body to some extent. Traditionally thermodynamic states of bodies have been taken to be uniform over the body. The chief virtue of such a definition is that it effectively makes the states of the body coincide with the abstract set of thermodynamic states, a fact I alluded to in my first paper (p. 1595). The greatest deficiency of such a definition is the restriction it imposes on the applicability of thermodynamic analysis to real world problems. Physical bodies in the real world are seldom in uniform states and this is especially true when electromagnetic and gravitational fields are present. More often bodies exhibit large gradients in properties and it would be advantageous to be able to treat bodies in such nonuniform states by thermodynamic analysis. The primary purpose of the analysis described in this paper is to extend the algebraic analysis of the first paper to include nonuniform states within the scope of thermodynamic analysis. The algebraic approach will be global relative to the thermodynamic states of a body and it will lead to results which will be applicable to bodies which can be characterized as being in local equilibrium states.

The paper will not be confined only to working out the algebraic details associated with the introduction of a body into the formalism. Some space will also be devoted to the development of a continuum realization of the algebraic formalism. There are three objectives which will guide this development. One objective is to give a more equitable treatment of constitutive relations in deriving a realization of the first law. The second objective is to demonstrate that the formalism contains conventional thermodynamics as a special case. The final objective is to use the formalism for the thermodynamical treatment of systems in the presence of electromagnetic and gravitational fields and thus to shed some light on the origin and interpretation of the electrochemical potential and the related gravitational function.

This paper will rely heavily on the results contained in the paper which preceded it and I shall presuppose a knowledge of that paper's contents. The notation to be used here will be identical to that used there insofar as that is possible. When it becomes necessary to refer to a specific result from the first paper, such as an equation or a theorem, the reference will be preceded by the letter A. For example, Theorem A.I.42 is Theorem I.42 from that paper.

Since the publication of the first paper I have found some minor typographical errors and these are corrected in the Appendix. Also to be found in the Appendix is the proof of an extended version of Theorem A.I. 42 from the first paper.

## I. ALGEBRAIC CONSIDERATIONS

As in the first paper, I shall adopt the approach of subdividing the algebraic analysis into two parts. The first of these will be devoted to developing those algebraic ideas which are necessary for a complete thermodynamics but which were not needed in my previous paper. The treatment is largely confined to establishing an order on a collection of the partitions of a given set. In the second portion of this section I shall look at the enriched structure of algebraic

thermodynamics that is a consequence of a physical body's presence and the interaction of the body's algebraic structure with the algebraic structure on $\Sigma$.

### A. Some algebraic preliminaries

Partitions of sets will play an important role in the further development of those aspects of algebraic thermodynamics to be examined in this paper. A partition of a non-null set is any collection of its disjoint, non-null subsets whose union is the given set. There is a direct connection between equivalence relations and partitions because every equivalence relation on a set induces a partition of that set and conversely. Several cases of partitions induced by equivalence relations were described in the first paper. Here we shall be concerned, not with the origin of a particular partition, but with the relationship of one partition to another. The partitions themselves will arise in a natural way from the thermodynamic discussion. We shall now begin to establish an order structure on a collection of partitions.

*Definition* I.1: Let $X$ be a nonempty set and $\mathsf{P}(X)$ a collection of its partitions. Define relations $\leqslant_P$ and $=_P$ on $\mathsf{P}(X)$ by the prescription that if $P_1 = \{P_1(\alpha)|\alpha\in\Delta\}\in\mathsf{P}(X)$ and $P_2 = \{P_2(\lambda)|\lambda\in\Lambda\}\in\mathsf{P}(X)$ then (1) $P_1\leqslant_P P_2$ iff $\forall\,\alpha\in\Delta\ \exists$ some $\lambda\in\Lambda$ such that $P_1(\alpha)\subset P_2(\lambda)$, and (2) $P_1 =_P P_2$ iff $P_1\subset P_2$ and $P_2\subset P_1$. If $P_1\leqslant_P P_2$ then $P_1$ is said to be a refinement of $P_2$ or $P_2$ is said to be a coarsening of $P_1$. If $P_1 =_P P_2$ then $P_1$ is said to be equal to $P_2$.

Figure 1 shows the Venn diagrams of three partitions of a given set. The partition $P_1$ is obtained by further partitioning the elements of the partition $P_2$ and therefore $P_1$ is clearly a refinement of $P_2$. On the other hand, the partition $P_3$ is neither a refinement of $P_1$ or $P_2$ nor are they refinements of $P_3$. If we anticipate that $(\mathsf{P}(X), \leqslant_P, =_P)$ will be shown to be a partially ordered set, then we realize that $\mathsf{P}(X)$ will not necessarily be a chain, that is, $\leqslant_P$ may not be a linear order on $\mathsf{P}(X)$.

*Theorem* I.2: The triplet $(\mathsf{P}(X), \leqslant_P, =_P)$ is a partially ordered set and $P_1 = P_2$ iff $P_1 =_P P_2$ iff $P_1\leqslant_P P_2$ and $P_2\leqslant_P P_1$.

*Proof*: The relation $=_P$ is an equivalence relation on $\mathsf{P}(X)$ because it is obvious from its definition that $=_P$ is nothing more than the usual equivalence relation of set equality. That is, $P_1 =_P P_2$ iff $P_1 = P_2$. The relation $\leqslant_P$ is (1) reflexive because $P_1(\alpha)\subset P_1(\alpha)\forall\alpha\in\Delta$ and thus $P_1\leqslant_P P_1$. It is (2) antisymmetric for, suppose that $P_1\leqslant_P P_2$ and $P_2\leqslant_P P_1$. Then this $\Rightarrow\forall\alpha\in\Delta\ \exists$ some $\lambda\in\Lambda$ such that $P_1(\alpha)\subset P_2(\lambda)$ and $\forall\lambda\in\Lambda\ \exists$ some $\alpha'\in\Delta$ such that $P_2(\lambda)\subset P_1(\alpha')$ and so we see that

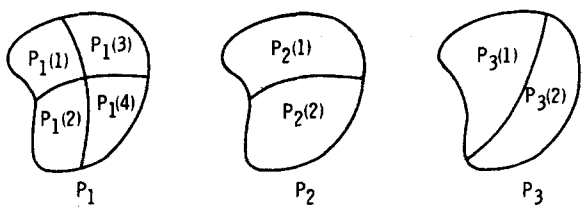


FIG. 1. An example of three partitions of a set $X$ illustrating $P_1\leqslant_P P_2$ and $P_2\not\leqslant_P P_3$.

$P_1(\alpha)\subset P_2(\lambda)\subset P_1(\alpha')$. But then $P_1(\alpha)\subset P_1(\alpha')$ and $P_1(\alpha)\cap P_1(\alpha')\neq\emptyset$ which $\Rightarrow P_1(\alpha') = P_1(\alpha)$ because $P_1$ is a partition of $X$ and therefore $P_1(\alpha)\subset P_2(\lambda)\subset P_1(\alpha') = P_1(\alpha)$. Thus we see that $P_1(\alpha) = P_2(\lambda)$ and therefore $P_1\subset P_2$. In exactly the same way we see that $\forall\lambda\in\Lambda\ \exists$ some $\alpha'\in\Delta$ such that $P_2(\lambda)\subset P_1(\alpha')$ and $\forall\alpha'\in\Delta\ \exists$ some $\lambda'\in\Lambda$ such that $P_1(\alpha')\subset P_2(\lambda')$. Now $P_2(\lambda)\subset P_1(\alpha')\subset P_2(\lambda')\Rightarrow P_2(\lambda)\cap P_2(\lambda')\neq\emptyset\Rightarrow P_2(\lambda') = P_2(\lambda)\Rightarrow\forall\lambda\in\Lambda\ \exists$ some $\alpha'\in\Delta$ such that $P_2(\lambda) = P_1(\alpha')\Rightarrow P_2\subset P_1$. But since $P_1\subset P_2$ and $P_2\subset P_1$ we have $P_1 = P_2\Longleftrightarrow P_1 =_P P_2$. The relation $\leqslant_P$ is also (3) transitive for suppose $P_1\leqslant_P P_2$ and $P_2\leqslant_P P_3$. This implies that $[\forall\alpha\in\Delta\ \exists$ some $\lambda\in\Lambda$ such that $P_1(\alpha)\subset P_2(\lambda)]$ and $[\forall\lambda\in\Lambda\ \exists$ some $\gamma\in\Gamma$ such that $P_2(\lambda)\subset P_3(\gamma)]\Rightarrow\forall\alpha\in\Delta\ \exists$ some $\gamma\in\Gamma$ such that $P_1(\alpha)\subset P_3(\gamma)\Rightarrow P_1\leqslant_P P_3$. There still remains the simple chore of proving the converse of the antisymmetry property. $P_1 =_P P_2$ iff $P_1 = P_2$ iff $P_1\subset P_2$ and $P_2\subset P_1$ iff $[\forall\alpha\in\Delta\ \exists$ some $\lambda\in\Lambda$ such that $P_1(\alpha) = P_2(\lambda)\Rightarrow P_1(\alpha)\subset P_2(\lambda)\Rightarrow P_1\leqslant_P P_2]$ and $[\forall\lambda\in\Lambda\ \exists$ some $\alpha\in\Delta$ such that $P_2(\lambda) = P_1(\alpha)\Rightarrow P_2(\lambda)\subset P_1(\alpha)\Rightarrow P_2\leqslant_P P_1]$. If this result is combined with the antisymmetry property, then $P_1\leqslant_P P_2$ and $P_2\leqslant_P P_1$ iff $P_1 =_P P_2$.

*Corollary* I.3: Let $(\mathsf{P}(X), \leqslant_P, =_P)$ be a partially ordered collection of partitions of $X$ and define a relation $<_P$ on $\mathsf{P}(X)$ by $P_1 <_P P_2$ iff $P_1\leqslant_P P_2$ and $P_1\neq_P P_2$. Then $(\mathsf{P}(X), <_P)$ is a strictly ordered set and $<_P$ is the strict order induced by $\leqslant_P$ and $=_P$.

*Proof*: The proof is an immediate consequence of the preceding theorem and Theorem A.I.21(1).

As a general rule, it is not necessary for a partially ordered set to have either a largest or a smallest element nor is it necessary for its subsets to possess upper and lower bounds. But in the case of the triplet $(\mathsf{P}(X), \leqslant_P, =_P)$ it is easy to show that each subset possesses both an upper and a lower bound and may contain a smallest or a largest element.

*Theorem* I.4: Let $(\mathsf{P}(X), \leqslant_P, =_P)$ be a partially ordered collection of partitions of $X$, $P^0 = \{X\}$, and $P_0 = \{\{x\}|x\in X\}$. Then (1) $P^0$ is an upper bound for every subset of $\mathsf{P}(X)$, (2) $P_0$ is a lower bound for every subset of $\mathsf{P}(X)$, and (3) $\mathsf{P}(X)$ contains a maximal element. (4) If $P^0, P_0\in\mathsf{P}(X)$ they are the largest and smallest elements, respectively, of $\mathsf{P}(X)$.

*Proof*: The collection $\mathsf{P}(X)$ can be regarded as a subset of the collection of all partitions of $X$ and clearly, $P_0$ and $P^0$ are partitions of $X$. Because every subset $X'$ of $X$ satisfies $X'\subset X$ it is true that $P_1\leqslant_P P^0\forall P_1\in\mathsf{P}(X)$ and therefore $P^0$ is an upper bound for $\mathsf{P}(X)$ and each of its subsets. The elements of the partition $P_0$ are one element sets and there can be no further refinement of $P_0$. Hence, $P_0\leqslant_P P_1\forall P_1\in\mathsf{P}(X)$ and therefore $P_0$ is a lower bound for $\mathsf{P}(X)$ and each of its subsets. Since every subset of $\mathsf{P}(X)$ has an upper bound then every chain of $\mathsf{P}(X)$ has an upper bound and, by Zorn's lemma A.I.25, $\mathsf{P}(X)$ contains a maximal element. Clearly if $P_0, P^0\in\mathsf{P}(X)$ they are the smallest and largest elements of $\mathsf{P}(X)$.

The next two results explore the relationship between comparable elements of the partially ordered set $(\mathsf{P}(X), \leqslant_P, =_P)$. Specifically, I shall show that if $P_1$ is a refinement of $P_2$ then every element of $P_2$ is expressible as a union of elements of $P_1$. This is equivalent to the statement that every refine-

ment of $P_2$ can be generated by partitioning the elements of $P_2$. A similar result will also be obtained for the situation where $P_1 \leqslant_P P_2$ and $P_1 \leqslant_P P_3$.

*Theorem* I.5: Let $(\mathsf{P}(X), \leqslant_P, =_P)$ be a partially ordered collection of partitions of $X$, and $P_1 \leqslant_P P_2$. If $P_1 = \{P_1(\alpha) | \alpha \in \Delta\}$ and $P_2 = \{P_2(\lambda) | \lambda \in \Lambda\}$ then, $\forall \lambda \in \Lambda$, $P_2(\lambda) = \cup_{\alpha \in \Delta(\lambda)} P_1(\alpha)$ where $\Delta \supset \Delta(\lambda) \equiv \{\alpha | \alpha \in \Delta\}$ and $P_1(\alpha) \subset P_2(\lambda)\} \neq \emptyset$.

*Proof*: From $P_1 \leqslant_P P_2$ and the definition of $\leqslant_P$ given in Definition I.1(1) it follows that $\Delta(\lambda) \neq \emptyset$. From the definition of $\Delta(\lambda)$ it follows that $\cup_{\alpha \in \Delta(\lambda)} P_1(\alpha) \subset P_2(\lambda)$. Next suppose $\exists x \in P_2(\lambda)$ and $x \notin \cup_{\alpha \in \Delta(\lambda)} P_1(\alpha)$. But since $P_1$ is a partition $x \in P_1(\alpha')$ for some $\alpha' \in \Delta$ and because $P_1 \leqslant_P P_2 \exists$ a $\lambda' \in \Lambda$ such that $P_1(\alpha') \subset P_2(\lambda')$ and therefore $x \in P_2(\lambda')$. Hence, $x \in P_2(\lambda) \cap P_2(\lambda') \neq \emptyset$ and because $P_2$ is a partition it follows that $P_2(\lambda') = P_2(\lambda) \Rightarrow P_1(\alpha') \subset P_2(\lambda') = P_2(\lambda) \Rightarrow \alpha' \in \Delta(\lambda)$ $\Rightarrow x \in \cup_{\alpha \in \Delta(\lambda)} P_1(\alpha)$ and hence $P_2(\lambda) \subset \cup_{\alpha \in \Delta(\lambda)} P_1(\alpha)$. Thus we have established that $P_2(\lambda) = \cup_{\alpha \in \Delta(\lambda)} P_1(\alpha)$.

*Corollary* I.6: Let $(\mathsf{P}(X), \leqslant_P, =_P)$ be a partially ordered collection of partitions of $X$, $P_1 \leqslant_P P_2$ and $P_1 \leqslant_P P_3$ where $P_1 = \{P_1(\alpha) | \alpha \in \Delta\}$, $P_2 = \{P_2(\lambda) | \lambda \in \Lambda\}$ and $P_3 = \{P_3(\gamma) | \gamma \in \Gamma\}$. If $\Delta(\lambda) = \{\alpha | \alpha \in \Delta \text{ and } P_1(\alpha) \subset P_2(\lambda)\}$ and $\Delta(\gamma) = \{\alpha | \alpha \in \Delta \text{ and } P_1(\alpha) \subset P_3(\gamma)\}$ then $P_2(\lambda) \cap P_3(\gamma) = \cup_{\alpha \in \Delta(\lambda) \cap \Delta(\gamma)} P_1(\alpha) \forall \lambda \in \Lambda$ and $\gamma \in \Gamma$.

*Proof*: By Theorem I.5 $P_2(\lambda) = \cup_{\alpha' \in \Delta(\lambda)} P_1(\alpha')$ and $P_3(\gamma) = \Sigma_{\alpha'' \in \Delta(\gamma)} P_1(\alpha'')$. By applying the distributive law for set intersections we see that $P_2(\lambda) \cap P_3(\gamma)$ $= P_2(\lambda) \cap (\cup_{\alpha'' \in \Delta(\gamma)} P_1(\alpha'')) = \cup_{\alpha'' \in \Delta(\gamma)} (P_2(\lambda) \cap P_1(\alpha''))$ $= \cup_{\alpha' \in \Delta(\lambda)} \cup_{\alpha'' \in \Delta(\gamma)} (P_1(\alpha') \cap P_1(\alpha''))$. But $P_1$ is a partition and $P_1(\alpha') \cap P_1(\alpha'') = \emptyset$ unless $P_1(\alpha') = P_1(\alpha'')$ and therefore $P_2(\lambda) \cap P_3(\gamma) = \cup_{\alpha \in \Delta(\lambda) \cap \Delta(\gamma)} P_1(\alpha)$.

I shall require some algebraic properties of real valued functions and their integrals for some of the discussions to be given later in the paper. Those properties which I shall need are generally available in numerous textbooks on abstract algebra, real analysis, and measure theory, but for convenience I shall simply list, without proof, the few properties which I will use. The proofs of the measure theoretic results, for example, can be found in the textbook by Royden.[2]

*Theorem* I.7(a): Let $(R, +, \cdot, \leqslant, =)$ be the extended real number system with the usual order and $\mathcal{F}(X, R)$ be the collection of all real valued function on a set $X$. Extend addition, multiplication, and order from $R$ to $\mathcal{F}(X, R)$ in a pointwise manner. Thus if $f, g, h \in \mathcal{F}(X, R)$ then

(1) $h = f + g$ iff $h(x) = f(x) + g(x) \forall x \in X$, (2) $h = f \cdot g$ iff $h(x) = f(x) \cdot g(x) \forall x \in X$, (3) $f \leqslant g$ iff $f(x) \leqslant g(x) \forall x \in X$, and (4) $f = g$ iff $f(x) = g(x) \forall x \in X$. Then $(\mathcal{F}(X, R), +, \cdot, \leqslant, =)$ is a paritally ordered ring and $f = g$ iff $f \leqslant g$ and $g \leqslant f$.

*Theorem* I.7(b): Suppose $\mathsf{B}$ is a $\sigma$-algebra of subsets of $X$, that is, $\mathsf{B}$ is a collection of subsets of $X$ which is an algebra of sets and is closed under a countable union of the elements of $\mathsf{B}$. Further, suppose that $\nu: \mathsf{B} \to R$ is a real valued function on $\mathsf{B}$. The triplet $(X, \mathsf{B}, \nu)$ is a complete measure space iff (1) $\nu(E) \geqslant 0 \forall E \in \mathsf{B}$, (2) $\nu(\emptyset) = 0$, (3) if $\{E_i \in \mathsf{B} | i \in N\}$ is a disjoint sequence in $\mathsf{B}$ then $\nu(\cup_{i=1}^{\infty} E_i) = \Sigma_{i=1}^{\infty} \nu(E_i)$, and (4) if $E \in \mathsf{B}$, $\nu(E) = 0$ and $A \subset E$, then $A \in \mathsf{B}$. The function $\nu$ is called a measure.

*Theorem* I.7(c): Suppose $f, g \in \mathcal{F}(X, R)$ are measurable with respect to $\mathsf{B}$ and denote the integral of $f$ over $E \in \mathsf{B}$ with respect to the complete measure space $(X, \mathsf{B}, \nu)$ by $\int_E f \, d\nu$. Then (1) if $f \geqslant 0$ then $\int_E f \, d\nu \geqslant 0$ and also $\int_E f \, d\nu = 0$ iff $f = 0$ almost everywhere with respect to $\nu$, that is, everywhere except on a set of $\nu$-measure zero. (2) Suppose $E$ is the union of a disjoint sequence $\{E_i \in \mathsf{B} | i \in N\}$ in $\mathsf{B}$ and either $f \geqslant 0$ or $f$ is integrable over $E$. Then $\int_E f \, d\nu = \Sigma_{k=1}^{\infty} \int_{E_k} f \, d\nu$. If $f$ and $g$ are integrable over $E$ and $r_1, r_2 \in R$ then (3) $\int_E (r_1 f + r_2 g) \, d\nu$ $= r_1 \int_E f \, d\nu + r_2 \int_E g \, d\nu$, and (4) if $f \leqslant g$ almost everywhere then $\int_E f \, d\nu \leqslant \int_E g \, d\nu$.

*Theorem* I.7(d): Suppose $m \in \mathcal{F}(X, R)$, $m \geqslant 0$ and define a function $\mu: \mathsf{B} \to R$ by $\mu(E) = \int_E m \, d\nu \forall E \in \mathsf{B}$. Then $\mu$ is a measure and is absolutely continuous with respect to the measure $\nu$ since $\nu(E) = 0 \Rightarrow \mu(E) = 0$.

We can now draw an interesting conclusion about chains of integrable functions in $\mathcal{F}(X, R)$ with these facts at our disposal.

tions, integrable over $X \in \mathsf{B}$ with respect to a complete measure space $(X, \mathsf{B}, \nu)$, and let $G$: $\{f | f \in \mathcal{F}(X, R)$ and $f$ integrable$\} \to R$ be a map defined by $G(f) = \int_X f \, d\nu$. Then $G | C$ is an order isomorphism and $G(r_1 f + r_2 g) = r_1 G(f) + r_2 G(g)$.

*Proof*: We begin by establishing a preliminary result which depends only on the fact that $C$ is a chain. Obviously $f \leqslant g \Rightarrow f \leqslant g$ almost everywhere and $f = g \Rightarrow f = g$ almost everywhere. To establish the converse suppose $f = g$ almost everywhere and $f \neq g$. But $f \neq g \Rightarrow f < g$ or $g < f \Rightarrow f < g$ almost everywhere or $g < f$ almost everywhere $\Rightarrow f \neq g$ almost everywhere which is a contradiction. Thus $f = g$ iff $f = g$ almost everywhere. Finally, suppose $f \leqslant g$ almost everywhere and $f \nleqslant g$. But $f \nleqslant g \Rightarrow g \leqslant f \Rightarrow g \leqslant f$ almost everywhere $\Rightarrow f = g$ almost everywhere $\Rightarrow f = g \Rightarrow f \leqslant g$. Hence, we have that $f \leqslant g$ iff $f \leqslant g$ almost everywhere. We are now ready to establish the properties of the map $G$. The relation $G(r_1 f + r_2 g)$ $= r_1 G(f) + r_2 G(g)$ is an immediate consequence of Theorem I.7(c.3). Now $f = g \Rightarrow f - g = 0$ and therefore $0 = G(0) = G(f - g) = G(f) - G(g)$. Hence, $f = g \Rightarrow G(f) = G(g)$. Conversely, suppose $G(f) = G(g)$. Then $0 = G(f) - G(g) = G(f - g)$ and also $0 = G(g) - G(f) = G(g - f)$. But $C$ is a chain and therefore $f \leqslant g$ or $g \leqslant f \Rightarrow g - f \geqslant 0$ or $f - g \geqslant 0$ and by Theorem I.7(c.1) $g - f = 0$ or $f - g = 0$ almost everywhere iff $f = g$. Thus, $G(f) = G(g)$ iff $f = g$ and $G | C$ is a 1–1 function. We still need to establish that $G | C$ is a homomorphism. By Theorem I.7(c.4) $f \leqslant g$ iff $f \leqslant g$ almost everywhere $\Rightarrow G(f) \leqslant G(g)$. Conversely, suppose $G(f) \leqslant G(g)$ and $f \nleqslant g$. But since $C$ is a chain $f \nleqslant g \Rightarrow g \leqslant f \Rightarrow G(g) \leqslant G(f)$ and thus $G(f) = G(g)$ iff $f = g$ $\Rightarrow f \leqslant g$. Therefore, $f \leqslant g$ iff $G(f) \leqslant G(g)$ and $G | C$ is an order isomorphism.

*Corollary* I.9: Let $C$ and $G$ be as in Theorem I.8. If $C$ has a maximal element, it is unique, is the largest element of $C$, and the map, $\delta: C \to \mathcal{F}(X, R)$ defined by $\delta(g) = g - f^0$, where $f^0$ is the maximal element, is an order isomorphism and $G | \operatorname{Im} \delta$ is an order isomorphism.

*Proof*: Suppose $f^0$ and $g^0$ are maximal elements of $C$. Then $f^0 \leqslant g^0$ or $g^0 \leqslant f^0 \Rightarrow g^0 = f^0$ or $f^0 = g^0$ and thus if a maximal element exists it is unique. We know that $g \leqslant f^0$ or $(f^0 \leqslant g \Rightarrow g = f^0 \Rightarrow g \leqslant f^0) \forall g \in C$ and therefore $g \leqslant f^0 \forall g \in C$ and hence $f^0$ is the largest element. Now $\delta(g_1) \leqslant \delta(g_2)$ iff $g_1 - f^0 \leqslant g_2 - f^0$ iff $g_1 \leqslant g_2$. From this it follows that

$\delta(g_1) = \delta(g_2)$ iff $\delta(g_1) \leqslant \delta(g_2)$ and $\delta(g_2) \leqslant \delta(g_1)$ iff $g_1 \leqslant g_2$ and $g_2 \leqslant g_1$ iff $g_1 = g_2$. Hence, $\delta$ is an order isomorphism. Now $G[\delta(g_1)] \leqslant G[\delta(g_2)]$ iff $G(g_1 - f^0) \leqslant G(g_2 - f^0)$ iff $G(g_1) - G(f^0) \leqslant G(g_2) - G(f^0)$ iff $G(g_1) \leqslant G(g_2)$ iff $g_1 \leqslant g_2$. From this it follows that $G[\delta(g_1)] = G[\delta(g_2)]$ iff $g_1 = g_2$. Thus the range of $G \mid \mathrm{Im}\delta$ is order isomorphic to $C$ which, as was just shown, is order isomorphic to $\mathrm{Im}\delta$ and thus $\mathrm{Im}\delta$ is order isomorphic to the range of $G \mid \mathrm{Im}\delta$.

From the foregoing it should be clear that if we were to define a map $\bar{\delta}$: $\mathrm{Im}\, G \mid C \to R$ by $\bar{\delta}[G(g)] = G(g) - G(f^0)$ then we have the situation depicted in Fig. 2 and the relationship $(G \mid \mathrm{Im}\,\delta) \circ \delta = \bar{\delta} \circ (G \mid C)$. Of course, the set $\mathrm{Im}\,\delta$ is order isomorphic to the $\mathrm{Im}\,\bar{\delta}$ by virtue of the order isomorphism $G \mid \mathrm{Im}\,\delta$. We have that $\mathrm{Im}\,\delta = \{\delta(g) = g - f^0 \mid g \in C, f^0$ maximal in $C\}$ and it is clear that $\delta(g) \leqslant 0 \forall g \in C$ and $\delta(g) = 0$ iff $g$ is the unique maximal element of $C$. Similarly, we have $\mathrm{Im}\bar{\delta} = \{\bar{\delta}[G(g)] \mid g \in C, f^0$ maximal in $C\}$ and by isomorphism $\bar{\delta}[G(g)] \leqslant 0 \forall g \in C$ and $\delta[G(g)] = 0$ iff $g$ is the unique maximal element. To clarify the relationship between the set $\mathrm{Im}\,\delta$ and the set $\mathrm{Im}\,\bar{\delta}$ we observe that $\bar{\delta}[G(g)] = G(g) - G(f^0) = G(g - f^0) = G[\delta(g)]$ and using the definition of $G$ this becomes

$$\bar{\delta}\left[\int_X g\, dv\right] = \int_X \delta(g)\, dv.$$

Thus we have here a situation similar to that encountered in the calculus of variations. The set $C$ is analogous to the space of competing functions while $\mathrm{Im}\,\delta$ is analogous to the space of admissible variations. Note, however, that the analogy is not exact. In the calculus of variations both the space of competing functions and the space of admissible variations are required to be subsets of a normed linear space over $R$ and the space of admissible variations also must be a normed linear space over $R$. These conditions were not necessary for Corollary I.9 and Theorem I.8.

### B. Algebraic thermodynamics of extended thermodynamic systems

We are now in a position to extend, in a relatively simple and direct manner, the algebraic theory of thermodynamics from a theory constructed only on $\Sigma$ to a theory which takes into account not only $\Sigma$ but also the physical body which is to be described by the rules of thermodynamics. It is the combination of body and states which is the essence of physical theory. That is, in a physical theory we are dealing with two primitive, and hence undefined, abstract concepts: the notion of a body and the notion of states. We are constrained to learn about the properties of the two only by studying their combination. A nonpedestrian analog is easily constructed from a set of automobiles and a collection of roadways for those automobiles together with their synthesis into traffic. Certainly, in this example, we could study separately the automobiles and the roadways. But the analog to physical science in this example is what can be learned about automobiles and roadways by studying only their combination in traffic. Thus a physical theory may be though of as an amalgamation of the mathematical structure of the body with the mathematical structure of those states used to describe the body. The explicit inclusion of the body in the formalism of the theory is essential if the theory is to be a physically meaningful one for it is precisely the behavior of the body that we seek to describe by the mathematics. Without a body a theory cannot have a physical expression and so would be devoid of physical meaning even though names with a physical connotation were given to elements of the mathematical structure. All tests of a physical theory are performed by carrying out measurements on the body. In this sense the introduction of a body can be interpreted as a realization of the abstract theory of states.

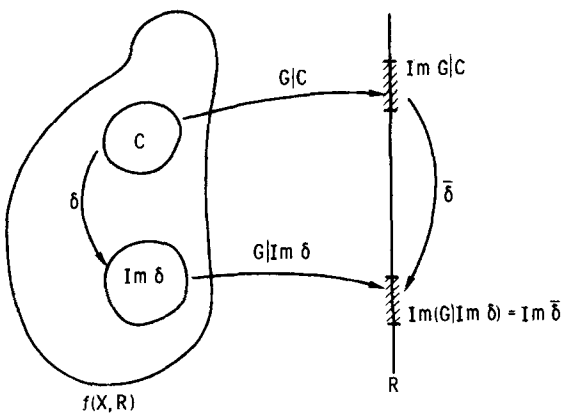


FIG. 2. Interrelationship among the isomorphisms of Theorem I.8 and Corollary I.9.

To begin the development we must first introduce the body and define the manner in which it is to be described thermodynamically.

*Axiom* I.10: There exists a set $U$ called the universe.

*Definition* I.11: Any subset $B \subset U$ is called a body in the universe. A body is said to be a thermodynamic body iff $\exists$ a function $\sigma$: $B \to \Sigma$. The function $\sigma$ is said to be an extended thermodynamic state (or simply a thermodynamic state) of $B$. The collection of all thermodynamic states of $B$, namely the set of all $\Sigma$-valued functions on $B$, $\mathscr{f}(B, \Sigma)$, is called an extended thermodynamic system.

The body $B$ will not vary but will remain fixed for the balance of the paper and we can simplify the notation a little by suppressing $B$ as a label. Henceforth, $\mathscr{f}(\Sigma)$ will be used in place of $\mathscr{f}(B, \Sigma)$. From Definition I.11 we see that the thermodynamic state of a body is specified by assigning a thermodynamic state to each of its points. This pointwise definition of a state of $B$ immediately suggests the pointwise extension of relations on $\Sigma$ to relations on $\mathscr{f}(\Sigma)$. That is, the relations on $\Sigma$ can be used to induce relations on $\mathscr{f}(\Sigma)$ in exactly the same way that the relations on $R$ were used to induce relations on $\mathscr{f}(X, R)$ in Theorem I.7(a). This procedure will be applied to the relations induced by a collection of simple processes (Definitions A.I. 17 and A.I. 31).

*Definition* I.12: Define relations on $\mathscr{f}(\Sigma)$ as follows: $\forall \sigma, \sigma' \in \mathscr{f}(\Sigma)$ (1) $\sigma \overset{\mathscr{B}}{=} \sigma'$ iff $\sigma(b) \overset{\mathscr{B}}{=} \sigma'(b) \forall b \in B$, (2) $\sigma =_{\mathscr{B}} \sigma'$ iff $\sigma(b) =_{\mathscr{B}} \sigma'(b) \forall b \in B$, and (3) $\sigma \leqslant_{\mathscr{B}} \sigma'$ iff $\sigma(b) \forall b \in B$ where $\mathscr{B}$ is either $\mathscr{P}$ or $\mathscr{A}$.

A great advantage to this natural pointwise extension of mathematical structure is the fact that the relations on $\mathscr{f}(\Sigma)$

inherit all the properties of the corresponding relations on $\Sigma$. For example, we know that $\forall x, x' \in \Sigma$, $x =_{\mathscr{A}} x'$ iff $x \leqslant_{\mathscr{A}} x'$ and $x' \leqslant_{\mathscr{A}} x$. But then from this we see that $\sigma =_{\mathscr{A}} \sigma'$ iff $\sigma(b) =_{\mathscr{A}} \sigma'(b) \forall b \in B$ iff $\sigma(b) \leqslant_{\mathscr{A}} \sigma'(b)$ and $\sigma'(b) \leqslant_{\mathscr{A}} \sigma(b) \forall b \in B$ iff $\sigma \leqslant_{\mathscr{A}} \sigma'$ and $\sigma' \leqslant_{\mathscr{A}} \sigma$. In a similar way all the algebraic structure of $\Sigma$ is passed on to $\mathscr{f}(\Sigma)$ intact and we may restate all theorems for $\Sigma$ as theorems for $\mathscr{f}(\Sigma)$ without the necessity for reproving them in the new context. We must only make sure that the definitions in $\Sigma$ and $\mathscr{f}(\Sigma)$ are compatible and use similar notation. As an example, we used $[x]$ as the notation for the equivalence classes of $=_{\mathscr{A}}$ in $\Sigma$; in $\mathscr{f}(\Sigma)$ the equivalence classes of $=_{\mathscr{A}}$ could be written as $[\sigma]$. For completeness and clarity I shall restate the theorems and definitions from $\Sigma$ as theorems and definitions for $\mathscr{f}(\Sigma)$. Accompanying each restated theorem or definition will be the number of its counterpart in $\Sigma$ shown in parentheses.

*Definition* I.13: (Definition A.I. 34) A process **P** on $B$ is a map from $B$ to the set of all processes on $\Sigma$, $\mathbf{P}: B \to \{P \mid P \text{ a process on } \Sigma\}$. A process **P** on $B$ is said to be (1) a physical process or $\mathscr{P}$-process iff $P \in \mathbf{ImP} \Rightarrow P$ is a $\mathscr{P}$-process on $\Sigma$, (2) an adiabatic process or an $\mathscr{A}$-process iff $P \in \mathbf{ImP} \Rightarrow P$ is an $\mathscr{A}$-process on $\Sigma$, (3) a reversible process or a $\mathscr{P} \cap \mathscr{P}^*$-process iff $P \in \mathbf{ImP} \Rightarrow P$ is a $\mathscr{P} \cap \mathscr{P}^*$-process on $\Sigma$, and (4) a reversible adiabatic process or an $\mathscr{A} \cap \mathscr{A}^*$-process iff $P \in \mathbf{ImP} \Rightarrow P$ is an $\mathscr{A} \cap \mathscr{A}^*$-process on $\Sigma$.

*Theorem* I.14: (Theorem A.I.36) The relations $\underset{\sim}{\mathscr{A}}$, $=_{\mathscr{A}}$, $\underset{\sim}{\mathscr{P}}$, and $=_{\mathscr{P}}$ are equivalence relations on $\mathscr{f}(\Sigma)$ and, furthermore, (1) each equivalence class of $=_{\mathscr{A}}$ ($=_{\mathscr{P}}$) is a subset of some equivalence class of $\underset{\sim}{\mathscr{A}}$ ($\underset{\sim}{\mathscr{P}}$) and (2) the relation $\underset{\sim}{\mathscr{P}}$ possesses only one equivalence class, namely $\mathscr{f}(\Sigma)$ itself.

*Definition* I.15: (Definition A.I. 37) If $\sigma \underset{\sim}{\mathscr{A}} \sigma'$, then $\sigma$ and $\sigma'$ are said to be adiabatically equivalent. The equivalence classes of $\underset{\sim}{\mathscr{A}}$ are called the adiabatic components and denoted by $\Gamma_\lambda$, $\lambda \in \Lambda$ and $\Lambda$ is an index set. If $\sigma =_{\mathscr{A}} \sigma'$, then $\sigma$ and $\sigma'$ are said to be adiabatically equal. The equivalence classes of $=_{\mathscr{A}}$ are denoted by $[\sigma]$, $\sigma \in \mathscr{f}(\Sigma)$.

*Theorem* I.16: (Theorem A.I. 38) The triplet $(\mathscr{f}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ is a nonbranching partially ordered set whose maximal chains partition the adiabatic components. For each $\sigma \in \mathscr{f}(\Sigma)$, $[\sigma]$ is a subset of some maximal chain, and $\forall \sigma$, $\sigma' \in \mathscr{f}(\Sigma)$, $\sigma =_{\mathscr{A}} \sigma'$ iff $\sigma \leqslant_{\mathscr{A}} \sigma'$ and $\sigma' \leqslant_{\mathscr{A}} \sigma$.

*Theorem* I.17: (Theorem A.I.39) Let $\mathscr{S} = \{[\sigma] \mid \sigma \in \mathscr{f}(\Sigma)\}$ be the collection of equivalence classes of the relation $=_{\mathscr{A}}$ on $\mathscr{f}(\Sigma)$. If $=$ is the equivalence relation of ordinary equality in $\mathscr{S}$ and if $[\sigma] \leqslant [\sigma']$ iff $\sigma \leqslant_{\mathscr{A}} \sigma'$, then $(\mathscr{S}, \leqslant, =)$ is a nonbranching partially ordered set whose maximal chains partition $\mathscr{S}$. Let $\Gamma = \{\Gamma_\lambda \mid \lambda \in \Lambda\}$ be the collection of adiabatic components of $\mathscr{f}(\Sigma)$ and $\mathscr{S}_\lambda = \{[\sigma] \mid \sigma \in \Gamma_\lambda\}$. Then (1) $\{\mathscr{S}_\lambda \mid \lambda \in \Lambda\}$ is a partition of $\mathscr{S}$, (2) the maximal chains of $\mathscr{S}$ partition $\mathscr{S}_\lambda$, and (3) $\mathscr{C} = \{[\sigma] \mid \sigma \in \mathbb{C}, \mathbb{C} \text{ a chain in } \mathscr{f}(\Sigma)\}$ is a maximal chain in $\mathscr{S}$ iff $\mathbb{C}$ is a maximal chain in $\mathscr{f}(\Sigma)$.

*Corollary* I.18: (Corollary A.I.40) There exists a 1-1 correspondence between the maximal chains in $\mathscr{S}$ and the maximal chains in $\mathscr{f}(\Sigma)$.

*Definition* I.19: (Definition A.I.41) Let $\mathbb{C}$ be a chain, not necessarily maximal, in $(\mathscr{f}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. A thermodynamic body $B$ is said to be in an equilibrium state with respect to $\mathbb{C}$ iff its thermodynamic state is a maximal element of $\mathbb{C}$.

Only Definition I.13 and Definition I.19, in the string of theorems and definitions following Definition I.12, contain new ideas. The others are mere restatements of results for $\Sigma$ in the context of $\mathscr{f}(\Sigma)$. Definition I.13 introduces the new idea of a process on $B$ by relating it to processes on $\Sigma$, which were previously defined, while Definition I.19 defines an equilibrium state for a body. I have elected to define relations on $\mathscr{f}(\Sigma)$ as extensions of relations on $\Sigma$ rather than define them by means of processes on $B$ which would be analogous to the procedure used to define relations on $\Sigma$. Consequently, we must establish the relationship between processes on $B$ and relations on $\mathscr{f}(\Sigma)$ by a theorem. The definition of an equilibrium state for $B$ given in Definition I.19 does not mention the previous definition of an equilibrium state of a chain in $\Sigma$, Definition A.I.41, and this naturally raises questions about their consistency. The following theorems deal with these two matters.

*Theorem* I.20: (Definition A.I.31 and Definition A.I.17) If $\sigma, \sigma' \in \mathscr{f}(\Sigma)$ then (1) $\sigma \leqslant_{\mathscr{B}} \sigma'$ iff $\sigma \xrightarrow{\mathbf{P}} \sigma'$ and **P** a $\mathscr{B}$-process on $B$, (2) $\sigma =_{\mathscr{B}} \sigma'$ iff $\sigma \xrightarrow{\mathbf{P}} \sigma'$ and **P** a $\mathscr{B} \cap \mathscr{B}^*$-process on $B$, and (3) $\sigma \sim_{\mathscr{B}} \sigma'$ iff $\sigma \xrightarrow{\mathbf{P}} \sigma'$ and **P** a $\mathscr{B} \cup \mathscr{B}^*$-process on $B$ where $\mathscr{B}$ is either $\mathscr{P}$ or $\mathscr{A}$.

*Proof*: To establish (1) we need only observe that $\sigma \leqslant_{\mathscr{B}} \sigma'$ iff $\sigma(b) \leqslant_{\mathscr{B}} \sigma'(b) \forall b \in B$ iff $\sigma(b) \xrightarrow{\mathbf{P}(b)} \sigma'(b) \forall b \in B$ and $\mathbf{P}(b)$ a $\mathscr{B}$-process on $\Sigma$ iff $\sigma \xrightarrow{\mathbf{P}} \sigma'$ and **P** a $\mathscr{B}$-process on $B$. I used in succession Definition I.12, Definition A.I.31, and Definition I.13. Analogous proofs hold for (2) and (3) if Definition A.I. 17 is substituted for Definition A.I.31.

*Definition* I.21: Let $\mathbb{C}$ be a subset of $\mathscr{f}(\Sigma)$. The collection of subsets of $\Sigma$, $\mathscr{C}(\mathbb{C})$, induced by $\mathbb{C}$ is defined by $\mathscr{C}(\mathbb{C}) \equiv \{C(b) \mid b \in B\}$, where $C(b) \equiv \{x \mid x = \sigma(b) \text{ and } \sigma \in \mathbb{C}\}$.

*Theorem* I.22: Let $\mathbb{C}$ be a subset of $\mathscr{f}(\Sigma)$. Then $\mathbb{C}$ is a chain in $(\mathscr{f}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ iff $\mathscr{C}(\mathbb{C})$ is a collection of chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$.

*Proof*: We know that $\mathbb{C}$ is a chain iff $\forall \sigma_1, \sigma_2 \in \mathbb{C}$, $\sigma_1 \leqslant_{\mathscr{A}} \sigma_2$ or $\sigma_2 \leqslant_{\mathscr{A}} \sigma_1$ iff $\sigma_1(b) \leqslant_{\mathscr{A}} \sigma_2(b)$ or $\sigma_2(b) \geqslant \sigma_1(b) \forall b \in B$ iff $C(b)$ is a vhain in $\Sigma$ $\forall b \in B$.

*Theorem* I.23: (Theorem A.I.42, see Appendix of this paper) Let $\mathbb{C}$ be a chain in $(\mathscr{f}(\Sigma), \leqslant_{\mathscr{A}} =_{\mathscr{A}})$ and $\mathscr{C}(\mathbb{C})$ be the induced collection of chains in $\Sigma$. Then $\epsilon$ is an equilibrium state of $B$ with respect to $\mathbb{C}$ iff $\epsilon(b)$ is an equilibrium state of $C(b) \forall b \in B$. Further, $\epsilon(b') \in [\epsilon(b)] \cap C(b) \forall b' \in B$ such that $C(b') = C(b)$.

*Proof*: By Definition I.19 $\epsilon$ is an equilibrium state of $B$ iff it is maximal in $\mathbb{C}$ iff $\epsilon \leqslant_{\mathscr{A}} \sigma \Rightarrow \sigma =_{\mathscr{A}} \epsilon \forall \sigma \in \mathbb{C}$ iff $\epsilon(b) \leqslant_{\mathscr{A}} \sigma(b) \Rightarrow \sigma(b) =_{\mathscr{A}} \epsilon(b) \forall b \in B$ and $\forall \sigma \in \mathbb{C}$ iff $\epsilon(b)$ is an equilibrium state of $C(b) \forall b \in B$. If $C(b') = C(b)$ then the maximal elements at $b'$ coincide with the maximal elements at $b$, that is, $[\epsilon(b')] \cap C(b') = [\epsilon(b)] \cap C(b)$ and by the version of Theorem A.I.42 given in the Appendix of this paper $\epsilon(b') \in [\epsilon(b)] \cap C(b)$.

I have already pointed out that the basic algebraic structures of $(\mathscr{f}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ and $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ are identical by virtue of the definition of relations on $\mathscr{f}(\Sigma)$ as pointwise extensions of relations on $\Sigma$. This made it possible to transfer a number of results from $\Sigma$ directly to $\mathscr{f}(\Sigma)$. But certainly the two partially ordered sets are not identical in all of their properties. What is the precise relationship between these two sets? The next theorem demonstrates that $\mathscr{f}(\Sigma)$ contains an order isomorphic copy of $\Sigma$ embedded in it.

*Theorem* I.24: The partially ordered set $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ is order isomorphically embedded in $(\mathscr{P}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$.

*Proof*: Define a function $h: \Sigma \xrightarrow{\text{into}} \mathscr{P}(\Sigma)$ by the prescription that $h(x) = \sigma$ where $\sigma$ is the constant function on $B$ whose range is the one element set $\{x\}$. Then, obviously, $h(x_1) \leqslant_{\mathscr{A}} h(x_2)$ iff $\sigma_1 \leqslant_{\mathscr{A}} \sigma_2$ iff $\sigma_1(b) \leqslant_{\mathscr{A}} \sigma_2(b) \forall b \in B$ iff $x_1 \leqslant_{\mathscr{A}} x_2$. Hence, $h$ is an order homomorphism because it satisfies Definition A.I. 23(1). The second condition of Definition A.I. 23 is redundant because $=_{\mathscr{A}}$ satisfies Theorem A.I. 21(1). This redundancy was pointed out in the first paragraph following Definition A.I.23(1). Each $\sigma \in \mathrm{Im}\, h$ has only one preimage and therefore $h$ is 1-1 and an isomorphism.

The partially ordered set $(\mathscr{P}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ can be given some additional structure, not possessed by $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$, by coupling the known structure of $\Sigma$ with the one fundamentally new algebraic element accompanying the body $B$, namely the thermodynamic states of $B$. The specific components I shall use are the partition of $\Sigma$ into chains, established in the first paper, and the preimages of these chains for the thermodynamic states of $B$. This combination will enable us to define some partitions of $\mathscr{P}(\Sigma)$ which, in turn, will help in the analysis of the structure of $\mathscr{P}(\Sigma)$. The ultimate objective is a better understanding of the maximal chains in $\mathscr{P}(\Sigma)$ and their relationship to the maximal chains in $\Sigma$.

*Theorem* I.25: Let $\mathscr{C} = \{C_\alpha | \alpha \in \Delta\}$ be a partition of $\Sigma$ into chains and define a relation $\equiv_{\mathscr{C}}$, called $\Sigma$-chain equivalence, on $\mathscr{P}(\Sigma)$ by $\sigma_1 \equiv_{\mathscr{C}} \sigma_2$ iff $\sigma_1^{-1}(C_\alpha) = \sigma_2^{-1}(C_\alpha) \forall \alpha \in \Delta$. Then $\equiv_{\mathscr{C}}$ is an equivalence relation on $\mathscr{P}(\Sigma)$ and its equivalence classes are denoted by $\langle \sigma \rangle_{\mathscr{C}}$. If $\sigma_1 \equiv_{\mathscr{C}} \sigma_2$ then $\sigma_1$ and $\sigma_2$ are said to be $\Sigma$-chain equivalent with respec to $\mathscr{C}$.

*Proof*: The proof is a trivial consequence of the definition of the relation $\equiv_{\mathscr{C}}$.

*Theorem* I.26: The equivalence classes $\langle \sigma \rangle_{\mathscr{C}}$ are chains in $\mathscr{P}(\Sigma)$.

*Proof*: Suppose $\sigma_1 \equiv_{\mathscr{C}} \sigma_2$ and $b \in B$. Then because $\sigma_1^{-1}(C_\alpha) = \sigma_2^{-1}(C_\alpha) \forall \alpha \in \Delta$ we know $\forall b \in B$ that $\sigma_1(b)$, $\sigma_2(b) \in C_\alpha$ for some $\alpha \in \Delta$ and thus $\forall b \in B$, $\sigma_1(b)$ and $\sigma_2(b)$ are comparable. Hence, $\sigma_1(b) \leqslant_{\mathscr{A}} \sigma_2(b)$ or $\sigma_2(b) \leqslant_{\mathscr{A}} \sigma_1(b) \forall b \in B$ iff $\sigma_1 \leqslant_{\mathscr{A}} \sigma_2$ or $\sigma_2 \leqslant_{\mathscr{A}} \sigma_1$.

*Definition* I.27: Let $\mathsf{P}(\Sigma) \equiv \{\mathscr{C} | \mathscr{C}$ a partition of $\Sigma$ into chains$\}$ be the collection of all partitions of $\Sigma$ into chains, $P_{\mathscr{C}} \equiv \{\langle \sigma \rangle_{\mathscr{C}} | \sigma \in \mathscr{P}(\Sigma)\}$ be the partition of $\mathscr{P}(\Sigma)$ induced by the relation of $\Sigma$-chain equivalence where $\mathscr{C} \in \mathsf{P}(\Sigma)$, and $\mathsf{P}(\mathscr{P}(\Sigma)) \equiv \{P_{\mathscr{C}} | \mathscr{C} \in \mathsf{P}(\Sigma)\}$ the collection of all partitions of $\mathscr{P}(\Sigma)$ induced by the relation of $\Sigma$-chain equivalence.

*Theorem* I.28: In the partially ordered sets $(\mathsf{P}(\Sigma), \leqslant_P, =_P)$ and $(\mathsf{P}(\mathscr{P}(\Sigma)), \leqslant_P, =_P)$ we have that $\mathscr{C} \leqslant_P \mathscr{C}'$ iff $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'}$ iff $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$.

*Proof*: The theorem will be established by first showing that $\mathscr{C} \leqslant_P \mathscr{C}'$ iff $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$ and then demonstrating that $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$ iff $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'}$. Let $\mathscr{C} = \{C_\alpha | \alpha \in \Delta\}$ and $\mathscr{C}' = \{C_\lambda | \lambda \in \Lambda\}$. Then by Theorem I.5 $\mathscr{C} \leqslant_P \mathscr{C}' \Rightarrow C_\lambda = \cup_{\alpha \in \Delta(\lambda)} C_\alpha$ and using a property of inverse set functions we see that $\forall \lambda \in \Lambda$, $\sigma^{-1}(C_\lambda) = \sigma^{-1}(\cup_{\alpha \in \Delta(\lambda)} C_\alpha) = \cup_{\alpha \in \Delta(\lambda)} \sigma^{-1}(C_\alpha)$. From this result and the definition of chain equivalence given in Theorem I.25 we find that $\sigma_1 \equiv_{\mathscr{C}} \sigma_2$ iff $\sigma_1^{-1}(C_\alpha) = \sigma_2^{-1}(C_\alpha) \forall \alpha \in \Delta \Rightarrow \cup_{\alpha \in \Delta(\lambda)} \sigma_1^{-1}(C_\alpha) = \cup_{\alpha \in \Delta(\lambda)} \sigma_2^{-1}(C_\alpha) \Rightarrow \sigma_1^{-1}(C_\lambda) = \sigma_2^{-1}(C_\lambda) \forall \lambda \in \Lambda \Rightarrow \sigma_1 \equiv_{\mathscr{C}'} \sigma_2$. But if $\sigma_1 \equiv_{\mathscr{C}} \sigma_2 \Rightarrow \sigma_1 \equiv_{\mathscr{C}'} \sigma_2$ then each equivalence class of $\equiv_{\mathscr{C}}$ meets only one equivalence class of $\equiv_{\mathscr{C}'}$ and therefore $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$. Conversely, suppose $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$ and $\mathscr{C} \not\leqslant_P \mathscr{C}'$. Now $\mathscr{C} \not\leqslant_P \mathscr{C}' \Rightarrow \exists$ some $\alpha \in \Delta$ such that $C_\alpha \not\subset C_\lambda \forall \lambda \in \Lambda$. But clearly, $\exists$ some $\lambda \in \Lambda$ such that $C_\alpha \cap C_\lambda \neq \emptyset$ because $\mathscr{C}'$ is a partition of $\Sigma$. Therefore, since $C_\alpha \not\subset C_\lambda$, $\exists x \in C_\alpha$ such that $x \notin C_\lambda \Rightarrow \exists \lambda' \in \Lambda$ such that $x \in C_{\lambda'}$ and therefore $C_\alpha \cap C_{\lambda'} \neq \emptyset$. Thus, we have $\Lambda(\alpha) = \{\lambda | \lambda \in \Lambda$ and $C_\alpha \cap C_\lambda \neq \emptyset\}$ is a set with a least two members and $C_\alpha \subset \cup_{\lambda \in \Lambda(\alpha)} C_\lambda$. Suppose $\lambda, \lambda' \in \Lambda(\alpha)$ and assume $B$ has at least two elements. Then we can always partition $B$ so that $B = B_\lambda \cup B_{\lambda'}$, and $B_\lambda \cap B_{\lambda'} = \emptyset$. Define two thermodynamic states, $\sigma_1$ and $\sigma_2$, of $B$ such that $\sigma_1^{-1}(C_\alpha \cap C_\lambda) = B_\lambda \neq \emptyset$, $\sigma_1^{-1}(C_\alpha \cap C_{\lambda'}) = B_{\lambda'} \neq \emptyset$ and $\sigma_2^{-1}(C_\alpha \cap C_\lambda) = B$. Then it follows (see Fig. 3) that $\sigma_1^{-1}(C_\alpha) = B = \sigma_2^{-1}(C_\alpha)$ and $\sigma_1^{-1}(C_{\alpha'}) = \emptyset = \sigma_2^{-1}(C_{\alpha'}) \forall \alpha' \in \Delta$ and $\alpha' \neq \alpha$. Consequently, $\sigma_1 \equiv_{\mathscr{C}} \sigma_2$. But $\sigma_1^{-1}(C_\lambda) = B_\lambda \neq B$ and $\sigma_2^{-1}(C_\lambda) = B$ and, therefore, $\sigma_1 \neq_{\mathscr{C}'} \sigma_2$. Thus $\sigma_1 \in \langle \sigma_2 \rangle_{\mathscr{C}}$ and $\sigma_1 \notin \langle \sigma_2 \rangle_{\mathscr{C}'}$ and hence $\langle \sigma_2 \rangle_{\mathscr{C}} \not\subset \langle \sigma_2 \rangle_{\mathscr{C}'}$ which contradicts $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$. Therefore it follows that $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma) \Rightarrow \mathscr{C} \leqslant_P \mathscr{C}'$ if $B$ has at least two elements. Suppose $B = \{b_0\}$ has only one member. Then the elements of $\mathscr{P}(\Sigma) = \{\sigma_x | \sigma_x : B \to \Sigma$ and $\sigma_x(b_0) = x\} = \{\sigma_x | x \in \Sigma\}$. A pair of functions in $\mathscr{P}(\Sigma)$ will then be $\Sigma$-chain equivalent iff they map $b_0$ into the same chain, that is, $\sigma_x \equiv_{\mathscr{C}} \sigma_{x'}$ iff $x, x' \in C_\alpha$ for some $\alpha \in \Delta$. In this notation we have the translation $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$ iff $\forall x, x' \in \Sigma$, $\sigma_{x'} \equiv_{\mathscr{C}} \sigma_x \Rightarrow \sigma_{x'} \equiv_{\mathscr{C}'} \sigma_x$. Thus $\forall \alpha \in \Delta$ we know that $x', x \in C_\alpha \in \mathscr{C}$ iff $\sigma_{x'} \equiv_{\mathscr{C}} \sigma_x \Rightarrow \sigma_{x'} \equiv_{\mathscr{C}'} \sigma_x$ iff $x', x \in C_\lambda \in \mathscr{C}'$ for some $\lambda \in \Lambda$. Therefore, $\forall \alpha \in \Delta$ $\exists$ some $\lambda \in \Lambda$ such that $C_\alpha \subset C_\lambda$ iff $\mathscr{C} \leqslant_P \mathscr{C}'$. Hence, regardless of the cardinality of $B$, $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \Rightarrow \mathscr{C} \leqslant_P \mathscr{C}'$ and thus $\mathscr{C} \leqslant_P \mathscr{C}'$ iff $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$. To complete the proof of the theorem suppose that $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$. But then this $\Rightarrow$ that $\forall \sigma \in \mathscr{P}(\Sigma) \exists$ some $\sigma' \in \mathscr{P}(\Sigma)$, namely $\sigma' = \sigma$, such that $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma' \rangle_{\mathscr{C}'}$ and, by Definitions I.1 and I.27, $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'}$. Conversely, we know from the definition of $\leqslant_P$ that $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'}$ iff $\forall \sigma \in \mathscr{P}(\Sigma) \exists$ some $\sigma' \in \mathscr{P}(\Sigma)$ such that $\langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma' \rangle_{\mathscr{C}'}$. But then by the properties of equivalence relations $\sigma \in \langle \sigma \rangle_{\mathscr{C}} \Rightarrow \sigma \in \langle \sigma' \rangle_{\mathscr{C}'} \Rightarrow \sigma \equiv_{\mathscr{C}'} \sigma' \Rightarrow \langle \sigma \rangle_{\mathscr{C}'} = \langle \sigma' \rangle_{\mathscr{C}'}$ and thus $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'} \Rightarrow \langle \sigma \rangle_{\mathscr{C}} \subset \langle \sigma' \rangle_{\mathscr{C}'} = \langle \sigma \rangle_{\mathscr{C}'} \forall \sigma \in \mathscr{P}(\Sigma)$.

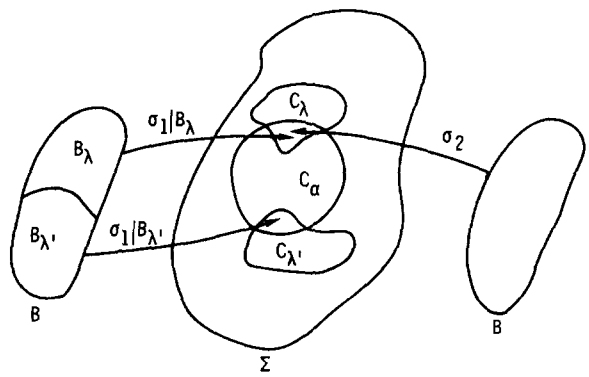


FIG. 3. Definition of functions $\sigma_1: B \to \Sigma$ and $\sigma_2: B \to \Sigma$ used in proof of Theorem I.28.

*Corollary* I.29: The partially ordered sets $(\mathsf{P}(\Sigma), \leqslant_P, =_P)$, $(\mathsf{P}(\mathscr{J}(\Sigma)), \leqslant_P, =_P)$ and $(\{\langle\sigma\rangle_{\mathscr{C}} \mid \mathscr{C} \in \mathsf{P}(\Sigma)\}, \subset, =)$, where $\sigma \in \mathscr{J}(\Sigma)$, are order isomorphic.

*Proof*: From Theorem I.2 and I.28 we see that $\mathscr{C} = \mathscr{C}'$ iff $\mathscr{C} =_P \mathscr{C}'$ iff $\mathscr{C} \leqslant_P \mathscr{C}'$ and $\mathscr{C}' \leqslant_P \mathscr{C}$ iff $P_{\mathscr{C}} \leqslant_P P_{\mathscr{C}'}$ and $P_{\mathscr{C}'} \leqslant_P P_{\mathscr{C}}$ iff $P_{\mathscr{C}} =_P P_{\mathscr{C}'}$ iff $P_{\mathscr{C}} = P_{\mathscr{C}'}$. Similarly, $\mathscr{C} = \mathscr{C}'$ iff $\mathscr{C} =_P \mathscr{C}'$ iff $\mathscr{C} \leqslant_P \mathscr{C}'$ and $\mathscr{C}' \leqslant_P \mathscr{C}$ iff $\langle\sigma\rangle_{\mathscr{C}} \subset \langle\sigma\rangle_{\mathscr{C}'}$ and $\langle\sigma\rangle_{\mathscr{C}'} \subset \langle\sigma\rangle_{\mathscr{C}}$ iff $\langle\sigma\rangle_{\mathscr{C}} = \langle\sigma\rangle_{\mathscr{C}'}$. It follows that the functions $\theta: \mathsf{P}(\Sigma) \to \mathsf{P}(\mathscr{J}(\Sigma))$ and $\theta_\sigma: \mathsf{P}(\Sigma) \to \{\langle\sigma\rangle_{\mathscr{C}} \mid \mathscr{C} \in \mathsf{P}(\Sigma)\}$ defined by $\theta(\mathscr{C}) = P_{\mathscr{C}}$ and $\theta_\sigma(\mathscr{C}) = \langle\sigma\rangle_{\mathscr{C}}$ are order isomorphisms because they are order homomorphisms by Definition A.I.23 and are 1-1.

*Corollary* I.30: Consider the partially ordered sets $(\mathsf{P}(\Sigma), \leqslant_P, =_P)$, $(\mathsf{P}(\mathscr{J}(\Sigma)), \leqslant_P, =_P)$ and $(\{\langle\sigma\rangle_{\mathscr{C}} \mid \mathscr{C} \in \mathsf{P}(\Sigma)\}, \subset, =)$. Let $\mathscr{C}^0 = \{C_\lambda \mid \lambda \in \Lambda$ and $C_\lambda$ a maximal chain in $\Sigma\}$ and $\mathscr{C}_0 = \{\{x\} x \in \Sigma\}$. Then (1) $\mathscr{C}^0$ ($\mathscr{C}_0$) is the largest (smallest) member of $\mathsf{P}(\Sigma)$, (2) $P_{\mathscr{C}^0}$ ($P_{\mathscr{C}_0}$) is the largest (smallest) member of $\mathsf{P}(\mathscr{J}(\Sigma))$, and (3) $\langle\sigma\rangle_{\mathscr{C}^0}$ ($\langle\sigma\rangle_{\mathscr{C}_0}$) is the largest (smallest) member of $\{\langle\sigma\rangle_{\mathscr{C}} \mid \mathscr{C} \in \mathsf{P}(\Sigma)\}$.

*Proof*: The set $\mathscr{C}^0$ is a member of $\mathsf{P}(\Sigma)$ because, by Theorem A.I.38, the maximal chains partition $\Sigma$. Then for any chain $C \subset \Sigma$ $\exists$ some $\lambda \in \Lambda$ such that $C \subset C_\lambda$ and therefore if $\mathscr{C}' = \{C_\alpha \mid \alpha \in \Delta\} \in \mathsf{P}(\Sigma)$ we see that $\mathscr{C}' \leqslant_P \mathscr{C}^0 \forall \mathscr{C}' \in \mathsf{P}(\Sigma)$ and, by Definition A.I.24, $\mathscr{C}^0$ is the largest element of $\mathsf{P}(\Sigma)$. The set $\mathscr{C}_0$ is also a member of $\mathsf{P}(\Sigma)$ because its members are one element chains of $\Sigma$ which partition $\Sigma$. By Theorem I.4 $\mathscr{C}_0$ is the smallest element of $\mathsf{P}(\Sigma)$. The balance of this corollary is a consequence of the isomorphism expressed by Corollary I.29.

There is an important ramification of Corollaries I.29 and I.30. From these corollaries we see that a chain in $\mathsf{P}(\Sigma)$ induces a nested collection of chains in $(\mathscr{J}(\Sigma), \leqslant_{\mathscr{C}}, =_{\mathscr{C}})$. For example, if $\mathscr{C}_1 \leqslant_P \mathscr{C}_2 \leqslant_P \mathscr{C}_3 \leqslant_P \cdots$ is a chain in $\mathsf{P}(\Sigma)$ then a corresponding chain in $\mathscr{J}(\Sigma)$ is $\langle\sigma\rangle_{\mathscr{C}_1} \subset \langle\sigma\rangle_{\mathscr{C}_2} \subset \langle\sigma\rangle_{\mathscr{C}_3} \subset \cdots$. But $\mathscr{C}^0$ is the largest member of $\mathsf{P}(\Sigma)$ and so the largest chain we could find in such a nested sequence would be $\langle\sigma\rangle_{\mathscr{C}^0}$. Is it possible that $\langle\sigma\rangle_{\mathscr{C}^0}$ is a maximal chain in $\mathscr{J}(\Sigma)$ or, equivalently, is $P_{\mathscr{C}^0}$ the partition of $\mathscr{J}(\Sigma)$ into maximal chains? We have no assurances that this is the case. For while $\mathsf{P}(\Sigma)$ is the collection of all partitions of $\Sigma$ into chains this is not necessarily true of the relationship between $\mathsf{P}(\mathscr{J}(\Sigma))$ and $\mathscr{J}(\Sigma)$. It is true that every element of $\mathsf{P}(\mathscr{J}(\Sigma))$ is a partition of $\mathscr{J}(\Sigma)$ into chains but we have not shown that every such partition is a member of $\mathsf{P}((\Sigma))$. The conjecture about the maximal chains in $\mathscr{J}(\Sigma)$ is valid and is proven in the next theorem.

*Theorem* I.31: Let $\mathscr{C}^0 = \{C_\lambda \mid \lambda \in \Lambda\}$ be the partition of $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ by its maximal chains and $\mathbb{C}$ a maximal chain of $(\mathscr{J}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. Then $\mathbb{C} = \langle\sigma\rangle_{\mathscr{C}^0}$ for some $\sigma \in \mathscr{J}(\Sigma)$ and $P_{\mathscr{C}^0} \in \mathsf{P}(\mathscr{J}(\Sigma))$ is the partition of $\mathscr{J}(\Sigma)$ into maximal chains.

*Proof*: By Theorem I.26 we know that $\langle\sigma\rangle_{\mathscr{C}^0}$ is a chain and hence a subchain of some maximal chain in $\mathscr{J}(\Sigma)$, that is, $\langle\sigma\rangle_{\mathscr{C}^0} \subset \mathbb{C}$. But $\langle\sigma\rangle_{\mathscr{C}^0}$ is an equivalence class and therefore $\sigma \in \langle\sigma\rangle_{\mathscr{C}^0}$ and therefore $\sigma \in \mathbb{C}$. Now suppose $\bar{\sigma} \in \mathbb{C}$. Then $\sigma, \bar{\sigma} \in \mathbb{C}$ and hence are comparable iff $\sigma \leqslant_{\mathscr{A}} \bar{\sigma}$ or $\bar{\sigma} \leqslant_{\mathscr{A}} \sigma$ iff $\sigma(b) \leqslant_{\mathscr{A}} \bar{\sigma}(b)$ or $\bar{\sigma}(b) \leqslant_{\mathscr{A}} \sigma(b) \forall b \in B$. Thus for each $b \in B$, $\sigma(b)$ and $\bar{\sigma}(b)$ are comparable and thus are elements of the same chain in $\Sigma$ and therefore elements of the same maximal chain in $\Sigma$. Consequently, we see that if an element of $b \in B$ is mapped into a given maximal chain in $\Sigma$ by $\sigma \in \mathbb{C}$ then every other element in $\mathbb{C}$ will do likewise. But then $\forall \bar{\sigma} \in \mathbb{C}$ we see that $\bar{\sigma}^{-1}(C_\lambda) = \sigma^{-1}(C_\lambda) \forall \lambda \in \Lambda$ iff $\bar{\sigma} \equiv_{\mathscr{C}^0} \sigma$ iff $\bar{\sigma} \in \langle\sigma\rangle_{\mathscr{C}^0}$. Thus $\mathbb{C} \subset \langle\sigma\rangle_{\mathscr{C}^0}$ and since we already showed that $\langle\sigma\rangle_{\mathscr{C}^0} \subset \mathbb{C}$ it follows that $\mathbb{C} = \langle\sigma\rangle_{\mathscr{C}^0}$. Since $\langle\sigma\rangle_{\mathscr{C}^0}$ is a maximal chain, we see that $P_{\mathscr{C}^0} = \{\langle\sigma\rangle_{\mathscr{C}^0} \mid \sigma \in \mathscr{J}(\Sigma)\}$, which is the largest member of $\mathsf{P}(\mathscr{J}(\Sigma))$ by Corollary I.30, is a partition of $\mathscr{J}(\Sigma)$ into maximal chains.

In Definition A.I.46 entropy was said to be an order homomorphism from a chain in $(\Sigma, \leqslant_{\mathscr{C}}, =_{\mathscr{C}})$ onto a subset of the reals with the usual order. That is, the entropy was defined to be a real-valued function which reflected the order induced on $\Sigma$ by the adiabatic processes. Does this conception of entropy have a counterpart for the states in $\mathscr{J}(\Sigma)$? Do there exist real-valued functions which mirror the order properties of chains in $\mathscr{J}(\Sigma)$? The answer certainly is yes for the two special cases where $\mathscr{J}(\Sigma)$ and $\Sigma$ become virtually identical. One of these special cases is obtained by requiring the memebers of $\mathscr{J}(\Sigma)$ to be constant functions on $B$ (see the proof of Theorem I.24) and the other arises when $B$ has only one member (see the proof of Theorem I.28). But what about the general case? If such order preserving real-valued functions exist under more general circumstances they, unlike entropy, cannot be intrinsically significant. The reason is simple; a concept can be intrinsically significant only so long as it is independent of the particular body $B$ to which it is applied. But the members of $\mathscr{J}(\Sigma)$ depend upon the choice of body, a fact clearly conveyed by the more complete notation $\mathscr{J}(B, \Sigma)$. Thus $\mathscr{J}(\Sigma)$ itself lacks intrinsic significance and acquires meaning only within the context supplied by a particular body. It follows that any mathematical object which is to mirror the order properties of $\mathscr{J}(\Sigma)$ must itself depend on $B$ and, consequently, must lack intrinsic significance. Despite the lack of intrinsic significance such order preserving real-valued maps would be very useful computationally for they replace chains in $\mathscr{J}(\Sigma)$ with chains of real numbers. While it might be conceptually useful to refer to such a function as an "entropy" for a body $B$ we must keep clearly in mind the distinction between these functions and the intrinsically significant entropies of Definition A.I. 46.

I shall begin a sequence of analysis which will ultimately lead to the construction of "entropy" functions for $\mathscr{A}(\Sigma)$ from the entropy functions for $\Sigma$. I shall first explore the close connection between order homomorphisms for $\mathscr{A}(\Sigma)$ and entropies for chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. This will be followed by taking a look at "entropies" for chains in $\mathscr{A}(\Sigma)$ and their connection with entropies for chains in $\Sigma$.

*Theorem* I.32: Let $\mathbb{C}$ be a chain in $(\mathscr{A}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$, $\mathscr{C}(\mathbb{C})$ the collection of chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ induced by $\mathbb{C}$, and $\mathscr{C} = \{C_\alpha \mid \alpha \in \Delta\}$ a collection of disjoint chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. (1) If each $C_\alpha \in \mathscr{C}$ possesses an entropy $\varphi_\alpha$ and $C(b) \in \mathscr{C}(\mathbb{C}) \Rightarrow C(b) \subset C_\alpha$ for some $\alpha \in \Delta$ then $\mathbb{C}$ is order homomorphic to $\{\Phi \circ \sigma \mid \sigma \in \mathbb{C}\} \subset \mathscr{A}(B, R)$ where $\Phi$ is the real-valued function $\Phi: \cup_{\alpha \in \Delta} C_\alpha \to R$ defined by $\Phi(x) = \varphi_\alpha(x)$ for $x \in C_\alpha$. (2) If $g: \mathbb{C} \to \mathscr{A}(B, R)$ is an order homomorphism then $\exists$ entropies for each chain $C(b) \in \mathscr{C}(\mathbb{C})$.

*Proof*: $\Phi$ is clearly a function because $x_1 = x_2 \Rightarrow \Phi(x_1) = \Phi(x_2)$ is a consequence of the disjoint nature of the members of $\mathscr{C}$ which implies that $x \in \cup_{\alpha \in \Delta} C_\alpha$ can be a member of only one member of $\mathscr{C}$ and, hence, there is no ambiguity in the value of $\Phi(x)$. Both pairs of relations $\leqslant_{\mathscr{A}}$,

$=_{\mathscr{A}}$ and $\leqslant$, $=$ satisfy condition (1) in Theorem A.I.21 and so we need only consider the relationship of $\leqslant_{\mathscr{A}}$ and $\leqslant$. Now suppose $\sigma_1, \sigma_2 \in \mathbb{C}$. Then $\sigma_1 \leqslant_{\mathscr{A}} \sigma_2$ iff $\sigma_1(b) \leqslant_{\mathscr{A}} \sigma_2(b) \forall b \in B$ iff $\varphi_\alpha(\sigma_1(b)) \leqslant \varphi_\alpha(\sigma_2(b)) \forall b \in B$ and some $\alpha \in \Delta$, because $\varphi_\alpha$ are entropies, iff $\Phi(\sigma_1(b)) \leqslant \Phi(\sigma_2(b)) \forall b \in B$ by the definition of the function $\Phi$ and, by definition of the composite function, iff $\Phi \circ \sigma_1(b) \leqslant \Phi \circ \sigma_2(b) \forall b \in B$ iff $\Phi \circ \sigma_1 \leqslant \Phi \circ \sigma_2$. Thus the map $g: \mathbb{C} \to \{\Phi \circ \sigma | \sigma \in \mathbb{C}\}$ where $g(\sigma) = \Phi \circ \sigma$ is an order homomorphism. To prove the second part of the theorem we shall use the notation $g(\sigma) = h_\sigma \in \mathscr{A}(B, R)$. Suppose $\sigma_1, \sigma_2 \in \mathbb{C}$. Then since $g$ is a homomorphism $\sigma_1 \leqslant_{\mathscr{A}} \sigma_2$ iff $g(\sigma_1) \leqslant g(\sigma_2)$ iff $h_{\sigma_1} \leqslant h_{\sigma_2}$ iff $h_{\sigma_1}(b) \leqslant h_{\sigma_2}(b) \forall b \in B$. Therefore, for a given $b \in B$, $\sigma_1(b) \leqslant_{\mathscr{A}} \sigma_2(b)$ iff $h_{\sigma_1}(b) \leqslant h_{\sigma_2}(b)$ and, hence, the map $h_b$: $C(b) \to R$ defined by $h_b(\sigma(b)) = h_\sigma(b)$ is an entropy for the chain $C(b)$.

Theorem I.32 essentially says that chains in $(\mathscr{A}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ are order homomorphic to subsets (chains) of $(\mathscr{A}(B, R), \leqslant, =)$ if and only if entropies exist for appropriate chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. Consequently, it follows that if entropies exist for each maximal chain in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ then each chain in $\mathscr{A}(\Sigma)$, and, hence each maximal chain in $\mathscr{A}(\Sigma)$, will be order homomorphic to some chain in $(\mathscr{A}(B, R), \leqslant, =)$.

We will now use Theorem I.32 to construct "entropies", in the sense of real-valued functions which mimic order properties, for a certain class of chains in $(\mathscr{A}(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. This class is not all inclusive for we will need to impose a requirement of integrability and require the existence of entropies for chains in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. Notwithstanding these conditions, the class is general enough to accommodate all of the usual thermodynamic calculations as we shall see shortly. The next theorem is a generalization of the "entropy maximum" criterion for equilibrium states and, as such, it is the basis for all applications of thermodynamics to the real world.

*Theorem* I.33: Suppose a chain $\mathbb{C}$ in $\mathscr{A}(\Sigma)$ is order homomorphic to a chain $C$ in $\mathscr{A}(B, R)$. If the members of $C$ are integrable over $B$ with respect to a complete measure space $(B, \mathsf{B}, \nu)$ then $\mathbb{C}$ is order homomorphic to a subset of $R$.

*Proof*: Let $F: \mathbb{C} \to C$ be an order homomorphism and $G|C$ be the order isomorphism of Theorem I.8. Then $(G|C) \circ F$ is an order homomorphism from $\mathbb{C}$ to $R$.

A common feature accompanying many thermodynamic discussions is the composite system. It is formed by the assembly of other systems or, equivalently, by partitioning a particular system into subsystems. Such composite systems have not yet been used in my treatment of thermodynamics. If they are to be intrinsically meaningful they cannot be arbitrary but must come from the fundamental thermodynamic structure of $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. Partitions can arise quite naturally from this structure and the details are presented in the next series of theorems and definitions. I shall begin the theoretical treatment by defining such thermodynamically induced partitions and studying some of their properties. This will subsequently be used to impose additional algebraic structure on $\mathscr{A}(\Sigma)$.

*Theorem* I.34: Let $\mathscr{C} = \{C_\alpha | \alpha \in \Delta\} \in \mathsf{P}(\Sigma)$ be a partition of $\Sigma$ into chains and $\sigma \in \mathscr{A}(\Sigma)$ a thermodynamic state for $B$. The collection of non-null preimages of $C_\alpha \in \mathscr{C}$ is a partition of $B$ induced by $\sigma$ and $\mathscr{C}$ and denoted by $P_\sigma(\mathscr{C})$.

*Proof*: Let $\Delta' = \{\alpha | \alpha \in \Delta \text{ and } \sigma^{-1}(C_\alpha) \neq \emptyset\}$ and $P_\sigma(\mathscr{C}) = \{\sigma^{-1}(C_\alpha) | \alpha \in \Delta'\}$. Observe that if $\alpha \in \Delta - \Delta'$ then $\sigma^{-1}(C_\alpha) = \emptyset$. Therefore, it follows that $\cup_{\alpha \in \Delta} \sigma^{-1}(C_\alpha) = \cup_{\alpha \in \Delta} \sigma^{-1}(C_\alpha) = \sigma^{-1}(\cup_{\alpha \in \Delta} C_\alpha) = \sigma^{-1}(\Sigma) = B$ where I used a property of inverse set functions, the fact that $\mathscr{C}$ is a partition of $\Sigma$ and the fact that $\sigma$ is a function with domain $B$. To complete the proof that $P_\sigma(\mathscr{C})$ is a partition we must only show that its members are disjoint. Suppose $\alpha, \beta \in \Delta'$ and $\sigma^{-1}(C_\alpha) \cap \sigma^{-1}(C_\beta) \neq \emptyset$. Then $\exists$ an element $b \in B$ and $b \in \sigma^{-1}(C_\alpha) \cap \sigma^{-1}(C_\beta) = \sigma^{-1}(C_\alpha \cap C_\beta)$ and, therefore, $\sigma(b) \in C_\alpha \cap C_\beta \neq \emptyset$. But since $\mathscr{C}$ is a partition $C_\alpha \cap C_\beta \neq \emptyset \to C_\alpha = C_\beta$ and, hence, $\sigma^{-1}(C_\alpha) = \sigma^{-1}(C_\beta)$. Therefore, $P_\sigma(\mathscr{C})$ is a partition of $B$.

*Definition* I.35: The elements of $P_\sigma(\mathscr{C})$, $\sigma \in \mathscr{A}(\Sigma)$ and $\mathscr{C} \in \mathsf{P}(\Sigma)$, are called the subsystems of $B$ relative to $\sigma$ and $\mathscr{C}$. The thermodynamic body $B$ is said to be a simple system, relative to $\sigma$ and $\mathscr{C}$, iff the cardinality of $P_\sigma(\mathscr{C})$ is one. If $B$ is not a simple system then it is said to be a composite system. The set $\mathsf{P}(B) = \{P_\sigma(\mathscr{C}) | \sigma \in \mathscr{A}(\Sigma) \text{ and } \mathscr{C} \in \mathsf{P}(\Sigma)\}$ is the collection of all partitions of $B$ induced by some $\sigma$ and some $\mathscr{C}$.

The set $\mathsf{P}(B)$ is a collection of partitions of $B$ but it is not necessarily the collection of all partitions of $B$. It is simple to establish the conditions which must be satisfied in order that $\mathsf{P}(B)$ becomes the collection of all partitions of $B$.

*Theorem* I.36: $\mathsf{P}(B)$ is the collection of all partitions of $B$ iff the cardinality of $B$ is less than or equal to the cardinality of $\Sigma$.

*Proof*: Suppose the cardinality of $B$ is less than or equal to the cardinality of $\Sigma$. Then by the definition of cardinality $\exists$ a function $f: B \overset{1\text{-}1}{\to} \Sigma$. Clearly, $f$ is a thermodynamic state of $B$ by Definition I.11 and because it is a 1-1 function we know that $f(b_1) = f(b_2)$ iff $b_1 = b_2$. Let $\mathscr{C} = \{\{x\} | x \in \Sigma\} \in \mathsf{P}(\Sigma)$ and let $\{B_\lambda | \lambda \in \Lambda\}$ be a partition of $B$. By the Axiom of Choice A.I.43 $\exists$ a choice function $\gamma: \Lambda \to B$ such that $\gamma(\lambda) \in B_\lambda$. We can now use the choice function to define a thermodynamic state $\sigma: B \to \Sigma$ be defining its restrictions to $B_\lambda$ to be constant functions with range $\operatorname{Im} \sigma|B_\lambda = \{f(\gamma(\lambda))\}$. But then it follows from the definition of $\sigma$ and $\mathscr{C}$ that $\{B_\lambda | \lambda \in \Lambda\} = P_\sigma(\mathscr{C})$ and, therefore, every partition of $B$ is an element of $\mathsf{P}(B)$. But obviously every element of $\mathsf{P}(B)$ is a member of the collection of all partitions of $B$, so $\mathsf{P}(B)$ is the collection of all partitions of $B$. To establish the converse we suppose that $\mathsf{P}(B)$ is the collection of all partitions of $B$. But this then implies that $\exists$ some $\mathscr{C}\{C_\alpha | \alpha \in \Delta\} \in \mathsf{P}(\Sigma)$ and some $\sigma \in \mathscr{A}(\Sigma)$ such that $P_\sigma(\mathscr{C}) = \{\{b\} | b \in B\}$. but then $\sigma(b) = \sigma(b')$ iff $b = b'$ and $\sigma: B \to \Sigma$ is 1-1 and onto a subset of $\Sigma$ and, therfore, the cardinality of $B$ is less than or equal to the cardinality of $\Sigma$.

The set $\mathsf{P}(B)$ is a collection of partitions of $B$ and can, therfore, be regarded as a partially ordered set with relations $\leqslant_P$ and $=_P$.

*Theorem* I.37: Let $\mathscr{C}, \mathscr{C}' \in \mathsf{P}(\Sigma)$ and consider the partially ordered set $(\mathsf{P}(B), \leqslant_P, =_P)$. Then (1) $\mathscr{C} \leqslant_P \mathscr{C}' \Rightarrow P_\sigma(\mathscr{C}) \leqslant_P P_\sigma(\mathscr{C}') \forall \sigma \in \mathscr{A}(\Sigma)$ and (2) if $B$ has at least two members then $P_\sigma(\mathscr{C}) \leqslant_P P_\sigma(\mathscr{C}') \forall \sigma \in \mathscr{A}(\Sigma) \Rightarrow \mathscr{C} \leqslant_P \mathscr{C}'$.

*Proof*: Suppose $\mathscr{C} = \{C_\alpha | \alpha \in \Delta\}$, $\mathscr{C}' = \{C_\lambda | \lambda \in \Lambda\}$, and $\mathscr{C} \leqslant_P \mathscr{C}'$. Then by the definition of $\leqslant_P$ (Definition I.1) we know that $\forall \alpha \in \Delta$ $\exists$ some $\lambda \in \Lambda$ such that $C_\alpha \subset C_\lambda$, and by the property of inverse set functions $\sigma^{-1}(C_\alpha) \subset \sigma^{-1}(C_\lambda)$

$\forall\sigma\in\mathcal{A}(\Sigma)$. But this then implies $P_\sigma(\mathscr{C})\leqslant_P P_\sigma(\mathscr{C}')\forall\sigma\in\mathcal{A}(\Sigma)$ and establishes (1). To prove (2) suppose $P_\sigma(\mathscr{C})\leqslant_P P_\sigma(\mathscr{C}')$ $\forall\sigma\in\mathcal{A}(\Sigma)$ and $\mathscr{C}\not\leqslant_P\mathscr{C}'$. But $\mathscr{C}\not\leqslant_P\mathscr{C}'$ and $B$ a set with more than two elements permits us to construct the function $\sigma_1$ used in the proof of Theorem I.28 (see Fig. 3) for $\{B\}$ $= P_{\sigma_1}(\mathscr{C})\neq P_{\sigma_1}(\mathscr{C}')=\{B_\lambda, B_{\lambda'}\}$ and which implies that $P_{\sigma_1}(\mathscr{C}')\leqslant_P P_{\sigma_1}(\mathscr{C})$. But $P_{\sigma_1}(\mathscr{C}')\leqslant_P P_{\sigma_1}(\mathscr{C})$ and $P_{\sigma_1}(\mathscr{C})$ $\leqslant_P P_{\sigma_1}(\mathscr{C}')$ iff $P_{\sigma_1}(\mathscr{C})={}_P P_{\sigma_1}(\mathscr{C}')$ which contradicts $P_{\sigma_1}(\mathscr{C})\neq P_{\sigma_1}(\mathscr{C}')$. Hence, $\mathscr{C}\leqslant_P\mathscr{C}'$.

The restriction that $B$ possess at least two members in Theorem I.37 (2) is essential. For if $B=\{b_0\}$ then $P_\sigma(\mathscr{C})$ $=\{B\}\forall\sigma\in\mathcal{A}(\Sigma)$ and $\forall\mathscr{C}\in\mathsf{P}(\Sigma)$ and one cannot then draw any conclusions about $\mathscr{C}$, $\mathscr{C}'\in\mathsf{P}(\Sigma)$ from $\mathcal{A}(\Sigma)$.

*Theorem* I.38: Let $\mathscr{C}\in\mathsf{P}(\Sigma)$ be a partition of $\Sigma$ into chains and define a relation $\equiv_{S(\mathscr{C})}$ on $\mathcal{A}(\Sigma)$, called subsystem equivalence with respect to $\mathscr{C}$, by $\sigma_1\equiv_{S(\mathscr{C})}\sigma_2$ iff $P_{\sigma_1}(\mathscr{C})$ $={}_P P_{\sigma_2}(\mathscr{C})$. Then $\equiv_{S(\mathscr{C})}$ is an equivalence relation on $\mathcal{A}(\Sigma)$ whose equivalence classes are denoted by $\langle\sigma\rangle_{S(\mathscr{C})}$. The equivalence classes of $\equiv_{S(\mathscr{C})}$ contain only complete equivalence classes of $\equiv_{\mathscr{C}}$, that is, $\sigma_1\equiv_{\mathscr{C}}\sigma_2\Rightarrow\sigma_1\equiv_{S(\mathscr{C})}\sigma_2$.

*Proof*: The proof that $\equiv_{S(\mathscr{C})}$ is an equivalence relation follows from its definition and the knowledge that $=_P$ is an equivalence relation. Now $\sigma_1\equiv_{\mathscr{C}}\sigma_2$ iff $\sigma_1^{-1}(C_\alpha)=\sigma_2^{-1}(C_\alpha)$ $\forall\alpha\in\Delta\Rightarrow P_{\sigma_1}(\mathscr{C})=P_{\sigma_2}(\mathscr{C})$ iff $P_{\sigma_1}(\mathscr{C})={}_P P_{\sigma_1}(\mathscr{C})$ and the proof is complete.

From Theorem I.38 we can conclude that each chain $\langle\sigma\rangle_{\mathscr{C}}$ contains only subsystem equivalent states with respect to $\mathscr{C}$ because $\langle\sigma\rangle_{\mathscr{C}}\subset\langle\sigma\rangle_{S(\mathscr{C})}$. This applies even if $\mathscr{C}=\mathscr{C}^0$ in which case $\langle\sigma\rangle_{\mathscr{C}^0}$ is a maximal chain by Theorem I.31. Of course, the equivalence class $\langle\sigma\rangle_{S(\mathscr{C})}$ might contain several chains of the type $\langle\sigma\rangle_{\mathscr{C}}$.

There are still two items which should be mentioned to complete the algebraic analysis of the thermodynamics of an extended thermodynamic system. One concerns coordinate systems for $B$ and the other deals with coordinate representations for thermodynamic states of $B$. Neither topic will be given any comprehensive discussion because, for the most part, it would be similar to discussions already given in another context. The subject of coordinate systems for $B$ is a case in point. Its discussion would be word for word identical to the discussion of coordinate systems for $\Sigma$ (Definition A.I.60 and Theorem A.1.61) with $X$ replaced by the universe $U$ and $\Sigma$ replaced by $B$. But the existence ot these two kinds of coordinate systems, one for $\Sigma$ and another for $B$, compels us to use a more precise terminology to make the necessary distinction between the two. To make the distinction I shall specifically refer either to $\Sigma$-coordinates and $\Sigma$-coordinate systems or to $B$-coordinates and $B$-coordinate systems.

When it comes to coordinate representations of abstract objects we must now contend with two types; one arises from the $B$-coordinates and the other from the $\Sigma$-coordinates. The abstract objects which concern us in extended thermodynamic systems are functions with domain $B$, such as the states $\sigma\in\mathcal{A}(\Sigma)$ and the processes $\mathsf{P}$ on $B$. The $B$-coordinate representations of such quantities are defined in exactly the same manner as the coordinate representations of measurements on $X$ or $\Sigma$ defined in Definition A.I.64. If $e_B$ is an evaluation map induced by a coordinate system for $B$, then the $B$-coordinate representations are composite functions with domain $\mathrm{Im}e_B$ and as typical examples we have the composite functions $\sigma\circ e_B^{-1}$ and $\mathsf{P}\circ e_B^{-1}$. The $\Sigma$-coordinate representations of $\sigma$ and $\mathsf{P}$ deal with their range and so are analogous to the coordinate representation of a process on $\Sigma$ also given in Definition A.I.64. The following definition and theorem deal with the $\Sigma$-coordinate representation of states of $B$.

*Definition* I.39: Let $\mathscr{T}=\{\tau^i|i=1,2,...,n\}$ be a coordinate system for $\Sigma$, $e(\mathscr{T})$ the evaluation map induced by $\mathscr{T}$ and $\pi^i$, $i=1,2,...,n$ the projection maps, that is, $\tau^i=\pi^i\circ e(\mathscr{T})$. A $\Sigma$-coordinate representation of the state $\sigma\in\mathcal{A}(\Sigma)$ is the collection of real-valued functions $\{\sigma^i|\sigma^i: B\to R, \sigma^i\equiv\tau^i\circ\sigma, i=1,2,...,n\}$.

*Theorem* I.40: Let $\sigma_1,\sigma_2\in\mathcal{A}(\Sigma)$. Then $\sigma_1\neq\sigma_2$ iff $\sigma_1^i\neq\sigma_2^i$ for some $i$.

*Proof*: Since $B$ is the domain of all thermodynamic states, two states, $\sigma_1$ and $\sigma_2$, cannot differ because of domain and therefore $\sigma_1\neq\sigma_2$ iff $\sigma_1(b)\neq\sigma_2(b)$ for some $b\in B$. But $\mathscr{T}$ is a coordinate system for $\Sigma$ and separates its points and therefore $\sigma_1(b)\neq\sigma_2(b)$ iff $\sigma_1^i(b)\neq\sigma_2^i(b)$ for some $i$. But then it follows that $\sigma_1\neq\sigma_2$ iff $\sigma_1^i(b)\neq\sigma_2^i(b)$ for some $b\in B$ and some $i$ iff $\sigma_1^i\neq\sigma_2^i$ for some $i$.

The algebraic thermodynamics developed in this paper possesses one conspicuous and, perhaps, surprising feature and that is the behavior of the members of $B$. Their behavior could aptly be anthropomorphized with the observation that one point of $B$ neither knows of, nor seems to care about, the behavior of the other points in $B$. That is, the elements of $B$ seem to exhibit completely independent behavior. But a little reflection should easily dispel the initial surprise. The set $B$ has, as yet, been given no topology and so there is no conception of nearness, neighborhood or continuity in $B$. This situation can be rectified by two actions: (1) The assignment of a topology to $B$, perhaps through the notion of measurements on $B$, as was done for $\Sigma$, or perhaps in some other experimentally significant manner. (2) The imposition of the requirement that the restriction of each state of $B$ to a subsystem of $B$ must be continuous. That is, the state itself need not be continuous, only its restrictions must be. These two actions would establish a communication among the points of $B$ and would thus generate the desired correlation of behavior. This aspect of the problem, although interesting, will not be considered further in this paper.

## II. CONTINUUM CONSIDERATIONS

Three topics related to continuum thermodynamics will be discussed in this section. The first topic will deal with constitutive relations and, for the most part, will merely serve to introduce some notational changes. This will be supplemented by some specifics concerning the expression for free charge and free current which will be required for subsequent calculations. The second item for discussion will be the development of continuum consequences of the algebraic theory, developed in the first part of this paper, and some ramifications of this analogue. The last subject for discussion will be some specific examples of the application of the continuum analogue which demonstrate not only that all of conventional thermodynamics is contained in it but also that a whole new spectrum of problems is amenable to thermody-

namic analysis. These examples will also shed some light on the origin and interpretation of the electrochemical potential and the related thermodynamic functions which are used to take into account the presence of the gravitational potential and centrifugation.

### A. Constitutive equations

In the first paper[1] I made some very nonspecific choices for the constitutive relations which nonetheless were adequate to enable me to obtain a realization of the first law. However, in so doing I made some choices which, in effect, apeared to treat some constitutive equations in a way which was somewhat different from the treatment accorded others. I now wish to make some minor adjustments, little more than notational changes, which will rectify the situation and give a more equitable treatment to all constitutive relations. Much of the detail will be eliminated for the mathematical manipulations are unchanged and, in order to facilitate a simple comparison of the new equations with the old, each new equation will be given not only its own number but also the number of the corresponding equation from the first paper.

The first notational change to be made is in the expression for the internal energy flux which now is written as

$$J_u^k = muv^k + q^k + \hat{\mu}^\lambda d_\lambda^k, \qquad \text{(II.1.1, A.IV,12.3)}$$

where $\hat{\mu}^\lambda$ has the decomposition

$$\hat{\mu}^\lambda = \mu^\lambda + \Delta\mu^\lambda \qquad \text{(II.1.2)}$$

and $\mu^\lambda$ is identified with the chemical potential based on its role in the realization of the first law (A.IV.17.1). This choice slightly alters the appearance but not the content of the expression for the energy flux $J_{\mathscr{E}}^k$ and the evolution equation for internal energy;

$$J_{\mathscr{E}}^l \equiv m\left(u + \frac{v^i v_i}{2} + \Omega\right)v^l + q^l + \hat{\mu}^\lambda d_\lambda^l - \tau^{il}v_i + H^{lk}E_k + \Phi D^l/\epsilon_0, \qquad \text{(II.2.1, A.IV.13.1)}$$

$$m\frac{\delta u}{\delta t} = -\nabla_k(q^k + \hat{\mu}^\lambda d_\lambda^k) + E_k j_f^k - \frac{\Phi\rho_f}{\epsilon_0} - \frac{P^k}{\epsilon_0}\nabla_k\Phi + \frac{\mu_0}{2}\frac{\partial\Phi^2}{\partial t} - m\frac{\partial\Omega}{\partial t} - v^k f_k + \tau^{kj}\nabla_j v_k + E_k\frac{\partial P^k}{\partial t} - \tfrac{1}{2}M^{kl}\frac{\partial B_{kl}}{\partial t}. \qquad \text{(II.2.2, A.IV.13.2)}$$

The expressions formerly used for the polarization and magnetization are replaced by

$$P^k = mp^k + \Delta P^k, \qquad \text{(II.3.1, A.IV.15.1)}$$

$$M^{kl} = mm^{kl} + \Delta M^{kl}, \qquad \text{(II.3.2, A.IV.15.2)}$$

which then lead to

$$E_k\,\partial P^k/\partial t - \tfrac{1}{2}M^{kl}\,\partial B_{kl}/\partial t = m(E_k\,\delta p^k/\delta t - \tfrac{1}{2}m^{kl}\,\delta B_{kl}/\delta t) + E_k[\partial\Delta P^k/\partial t - \nabla_i(mp^k v^i)] - \tfrac{1}{2}\Delta M^{kl}\,\partial B_{kl}/\partial t + \tfrac{1}{2}mm^{kl}v^i\nabla_i B_{kl}. \qquad \text{(II.3.3, A.IV.15.3)}$$

If all of the changes made to this point are combined then we obtain

$$m[\delta u/\delta t - S^{kl}\,\delta e_{kl}/\delta t - E_k\delta p^k/\delta t + \tfrac{1}{2}m^{kl}\,\delta B_{kl}/\delta t - \mu^\lambda\,\delta n_\lambda/\delta t] = -\nabla_k(q^k + \Delta\mu^\lambda d_\lambda^k) + \Delta\tau^{kj}\nabla_j v_k - v^k f_k - m\,\partial\Omega/\partial t - \mu^\lambda R_\lambda - d_\lambda^k\nabla_k\mu^\lambda + E_k j_f^k - \Phi\rho_f/\epsilon_0 - (P^k/\epsilon_0)\nabla_k\Phi + \tfrac{1}{2}\mu_0\,\partial\Phi^2/\partial t + E_k[\partial\Delta P^k/\partial t - \nabla_i(mp^k v^i)] - \tfrac{1}{2}\Delta M^{kl}\frac{\partial B_{kl}}{\partial t} + \tfrac{1}{2}mm^{kl}v^i\nabla_i B_{kl}. \qquad \text{(II.4.1, A.IV.16.1)}$$

The definition of heat (A.IV.17.1) when combined with II.4.1 gives the final result.

$$m\delta Q/\delta t + \nabla_k(q^k + \Delta\mu^\lambda d_\lambda^k) = \Delta\tau^{kj}\nabla_j v_k - v^k f_k - m\,\partial\Omega/\partial t - \mu^\lambda R_\lambda - d_\lambda^k\nabla_k\mu^\lambda + E_k j_f^k - \Phi\rho_f/\epsilon_0 - (P^k/\epsilon_0)\nabla_k\Phi + \tfrac{1}{2}\mu_0\partial\Phi^2/\partial t + E_k[\partial\Delta P^k/\partial t - \nabla_i(mp^k v^i)] - \tfrac{1}{2}\Delta M^{kl}\,\partial B_{kl}/\partial t + \tfrac{1}{2}mm^{kl}v^i\nabla_i B_{kl}. \qquad \text{(II.5.1, A.IV.17.4)}$$

Equations (II.1)–(II.5) have the same content as their counterparts in the previous paper and reduce to them exactly if we set $\Delta\mu^\lambda = \Delta P^k = \Delta M^{kl} = 0$. The chief advantage conferred on the analysis by the new version is not in the form of the temporal evolution equations but in the equivalent treatment shown to all constitutive relations which contribute to the first law and the implication of this treatment for the decomposition of the set of physical states $X$ into thermodynamic states $\Sigma$ and nonthermodynamic states $X$-$\Sigma$. Each constitutive relation ($\hat{\mu}^\lambda$, $P^k$, $M^{kl}$, and $\tau^{ij}$) is decomposed into two parts but only one of these parts appears in the first law. Consequently, it seems reasonable to refer to $\mu^\lambda$, $m^{kl}$, $p^k$, and $S^{kl}$ as the thermodynamic portions of their respective constitutive relations and to refer to the balance of each constitutive relation as the nonthermodynamic portion. It is the function of the nonthermodynamic part of these constitutive relations to account for all phenomena which cannot be described adequately by the thermodynamic part alone. This decomposition of the constitutive relations suggests that perhaps the decomposition could be used as the basis for an indirect definition of the separation of physical states into thermodynamic and nonthermodynamic states. As a part of such a definition we might impose the following stipulations: (1) The thermodynamic portions of the constitutive relations should be independent of the nonthermodynamic coordinates, that is, independent of the elements of $\mathscr{M}$-$\mathscr{T}$. (2) The thermodynamic portions of the constitutive relations should be continuous on the maximal chains of $\Sigma$ and give an integrable first law there. (3) The nonthermodynamic portions of the constitutive relations

should vanish on $\Sigma$ and be nonzero only on $X$-$\Sigma$.

Heretofore I have found it neither necessary nor desirable to say anything of a specific nature about the expressions to be used for the constitutive relations and have instead dealt in broad generalities. But because I shall shortly examine the thermodynamics of systems with free charges I must become just a little more specific about the expressions for free charge and current densities. The free charge density $\rho_f$ is customarily expressed as the superposition of the free charge densitites of each of the charge carriers. Suppose $z^\lambda$ is the free charge per mole of species $\lambda$. Then $z^\lambda$ is an integer multiple of the Faraday constant and

$$\rho_f = mz^\lambda n_\lambda. \tag{II.6.1}$$

By analogy to the expression for the flux of internal energy (II.1.1) we may decompose the free current $j_f^k$ into three parts by the expression

$$j_f^k = \rho_f v^k + \sigma^k + z^\lambda d_\lambda^k, \tag{II.6.2}$$

where $\rho_f v^k$ is the convective flux of free charge, $z^\lambda d_\lambda^k$ is the diffusive flux of free charge and $\sigma^k$ represents the flux that still remains in the absence of convection and diffusion. But $\rho_f$ and $j_f^k$ are not independent since they must satisfy the conservation equation for free charge given as the first equality in (A.IV.7.1). The substitution of (II.6) into the charge conservation equation, coupled with the use of the mass and species conservation equations (A.IV.2.1, A.IV.2.3), and $\delta z^\lambda/\delta t = 0$, produces the equation

$$\Box\Phi = z^\lambda R_\lambda + \nabla_k \sigma^k. \tag{II.6.3}$$

Thus we see that if (II.6) is to be used to represent the free charge and free current densities then the function $\Phi$, which appears in the expressions for the bound charge and bound current densities (A.IV.6.5, A.IV.6.6), cannot be chosen independently but must be regarded as a solution of the inhomogeneous wave equation (II.6.3). Consequently, $\Phi$ must be regarded as an explicit function of time and position and not an independent constitutive relation. The right side of (II.6.3) cannot be expected to be identically zero for that would imply that bound and free charge are separately conserved. This is inconsistent with the existence of insulator to metal transitions which may be viewed as the conversion of bound charge to free charge. If the reactions themselves are to be charge conserving then, of course, the $R_\lambda$ will satisfy the constraint $z^\lambda R_\lambda = 0$ identically.

### B. Consequences of algebraic thermodynamics

The exact algebraic result expressed by Theorem I.33 is fundamental for the application of thermodynamics to actual physical problems for it is a generalization of the "entropy maximum" criterion of equilibrium. It is not, however, a useful computational device because it represents a global exploration for an extremum. While it is important to know the exact result contained in Theorem I.33 it is also important to have a computationally workable scheme for determining the actual equilibrium state in a given situation. This means restricting the exploration to a local exploration in the vicinity of the extremum. With computational utility as my objective I shall now begin a program of specializing the general result of Theorem I.33 until it becomes computationally useful. Since thermodynamics is invariably applied to continua it is essential to translate the algebraic result first into a form directly applicable to continua. The next theorem summarizes the content of Theorems I.32 and I.33 in suitable form for continua.

*Theorem* II.7: Suppose that (1) $\mathbb{C}$ is a chain in $\mathcal{F}(\Sigma)$, (2) $s$ is the $\Sigma$-coordinate representation of a real-valued, extensive function with domain in $\Sigma$ whose restriction to chains in its domain is an entropy, (3) Im $\sigma$ is a subset of the domain of $s\forall\sigma\in\mathbb{C}$, (4) the measure $\nu$ of Theorem I.7 coincides with the mass, $M$, of the body, that is, the function $m$ of Theorem I.7 (d) is the mass density, and (5) $s$ is integrable over $B$ with respect to mass measure $\forall\sigma\in\mathbb{C}$. Then (6) $\mathbb{C}$ is order homomorphic to a chain $C$ of integrable functions in $\mathcal{F}(B, R)$. If $C$ possesses a maximal element, $S \equiv \int_B s\, dM = \int_B sm\, dv$ for each member of $C$, the maps $\delta$ and $\bar{\delta}$ are as defined in Corollary I.9 and the discussion following Corollary I.9, then (7) $\bar{\delta}S = \int_B \delta(ms)\, dv$, (8) $\bar{\delta}S \leqslant 0$, and $\bar{\delta}S = 0$ only for the unique maximal element in $C$ whose preimages in $\mathcal{F}(\Sigma)$ are the equilibrium states of $\mathbb{C}$ iff $\delta(ms) \leqslant 0$ and $\delta(ms) = 0$ only for the unique maximal element in $C$ whose preimages in $\mathcal{F}(\Sigma)$ are the equilibrium states of $\mathbb{C}$.

*Proof*: This theorem is a direct consequence of Theorem I.32(1), Theorem I.33, Corollary I.9, and the discussion following corollary I.9.

Theorem II.7(8) gives two criteria for finding the largest member of $C$, one in terms of $S$ and the other in terms of $ms$, but neither identifies the equilibrium states of $\mathbb{C}$ directly. To actually identify the equilibrium states we must know the order homomorphism from $\mathbb{C}$ to $C$. While both the criterion $\bar{\delta}S = 0$ and the criterion $\delta(ms) = 0$ do locate the largest element of $C$, neither represents a practical computational method. Nevertheless an eminently practical method can be based on the first part of Theorem II.7(8) which identifies the largest member of $C$ with the maximum value of $S$ and is a generalization of the conventional entropy maximum principle. Since $S$ is defined as an integral it immediately suggest the implementation of techniques from the calculus of variations. Indeed, I have already commented on the similarity between the calculus of variations and the results of Theorem I.8 and Corollary I.9 in the duscussion following I.9. All of the computational machinery from the calculus of variations can be made available to thermodynamics merely by imposing the conditions involving normed linear spaces over $R$ mentioned in the discussion following Corollary I.9. This converts the first part of Theorem II.7(8) into a variational statement and, hence, is expressible in terms of the first and second variations. Furthermore, if we require that all variations on the boundary and all boundary variations satisfy the transversality conditions, then the thermodynamic problem of locating the largest element of $C$ is converted into the mathematical problem of solving the Euler–Lagrange equations. This is summarized as a corollary to Theorem II.7.

*Corollary* II.8: Suppose $C$, $s$ and $S$ are as in Theorem II.9. Furthermore, let $C$ be a subset of a normed linear space over $R$ and the space of admissible variations be a normed linear space over $R$. If $\delta S$ and $\delta^2 S$ are the first and second variations of $S$ then $f^0 \in C$ is the largest element of $C$ iff $\delta S = 0$

and $\delta^2 S < 0$ at $f^0$. If members of the space of admissible variations satisfy the transversality conditions then $f^0$ is the solution of the Euler–Lagrange equations implied by $\delta S = 0$.

*Proof*: This corollary is a direct consequence of the calculus of variations except for the sufficiency of the variational criteria for $f^0$. Sufficiency follows from Theorem II.7(8) which says that $S$ decreases monotonically from its value at the unique largest element in $C$.

Corollary II.8 is the variational counterpart of the "entropy maximum" criterion of conventional thermodynamics. The calculus of variations computation is a local exploration for an extremum, that is, an exploration in the vicinity of the extremum. Such a calculation then can only locate relative extrema. In principle, such a local exploration for the largest element represents no loss in generality for the thermodynamic computation because if the chain $C$ possesses a maximal element then, as has been shown [see Theorem I.9(8) and Corollary I.9], that element is unique. In paractice, a lack of uniqueness in the solution of the Euler–Lagrange equations can imply only one of two things. Either $C$ is not a chain or the restriction of $s$ to some chain in its domain is not an entropy for that chain as was required in Theorem II.7(2).

The particular function in $C$ which satisfies the conditions $\delta S = 0$ and $\delta^2 S \leqslant 0$ is determined, in part, by the choice of chain. In particular, we might be interested in subchains of the chain $C$. From the variational point of view, the selection of a subchain can be thought of as the imposition of constraints which limit the set of values of $S$ which must be explored to some subset. These constraints are of two basic types. The first type is the more obvious of the two because it is simply a restriction of the permitted set of variations to a subset of the set of admissible variations. Such constraints may be handled either directly, perhaps by a change of variables, or indirectly by means of Lagrangian multipliers. A more fundamental, but less obvious type of constraint deals with the choice of the Lagrangian itself. That is, how much of the integrand is to be subjected to variation. For thermodynamics this choice amounts to deciding whether to vary the product $sm$ or only $s$. Clearly $dv$ represents geometrical properties and in a nonrelativistic calculation, such as the one being discussed in this section, the geometry is independent of matter. The two choices of Lagrangian will yield the same solution only if the set of variations is the same in both cases and if these variations do not permit a variation in the mass density.

Before going on to some applications of algebraic thermodynamics, in the form of Corollary II.8, I shall derive alternatives to Corollary II.8 which are suitable for a particular category of constraints which may be imposed without the use of Lagrangian multipliers. Specifically, I shall derive, from Corollary II.8, the variational equivalent of the "internal energy minimum" criterion and the Legendre transforms of these two variational problems. The transforms are the variational analogues of the Massieu function and the thermodynamic potential criteria for equilbrium states in thermodynamics. The thermodynamic Lagrangian, either $ms$ or $s$, is an especially simple one since it is only a function of the thermodynamic coordinates and contains no derivatives. Because of this and the transversality conditions there is a simple relationship between $\delta S$ and the first variation of the Lagrangian, either $\delta(ms)$ or $\delta s$,

$$\delta S = \int_B \delta(ms)\, dv \quad \text{or} \quad \delta S = \int_B \delta s\, dM.$$

Note that $\delta(ms)$ in this context is a variation and does not have the same meaning as the corresponding symbol in Theorem II.7. However, even with the transversality conditions, the second variation $\delta^2 S$ could still contain contributions from the boundary of $B$ in addition to those which arise from second variation of the Lagrangian, either $\delta^2(ms)$ or $\delta^2 s$. But it is always possible to impose sufficient additional conditions so that $\delta^2 S$ is the integral of the second variation of the Lagrangian over the body $B$. Under such circumstances it is clear that $\delta S = 0$ and $\delta^2 S < 0$ iff $\delta(ms) = 0$ and $\delta^2(ms) < 0$ (or $\delta s = 0$ and $\delta^2 s < 0$) for all permitted variations and then one only needs to consider the first and second variations of the Lagrangian. With this in mind let us separately examine the relationship of the first and second variations of functions which are not independent and whose variations are linearly constrained for this is the case of thermodynamic importance. While thermodynamic notation could be used in this analysis, the derivation is more concise and considerably less awkward in a more general notation.

*Theorem* II.9: Suppose that Latin indices $i, j, k \ldots$ use the range $1, 2, \ldots, n, n+1$, Greek indices use the range convention of Definition A.III.13 and no summation convention is used with either Latin or Greek indices. Consider $n+1$ functions $y_k$, $k = 1, 2, \ldots, n+1$ which satisfy the constraint $D(y_k) = 0$, where $D$ is a function, and let $A_k \equiv \partial D / \partial y_k$, $i$ and $l$ be two fixed indices, $(\delta y_i)_{y_l}$ and $(\delta^2 y_i)_{y_l}$ be the first and second variations of $y_i$ subject to the constraint $\delta y_l = 0$, and suppose that $A_i$ and $A_l$ vanish nowhere on $B$. Then (1) $(\delta y_i)_{y_l} = 0$ iff $(\delta y_l)_{y_i} = 0$, (2) if $(\delta y_l)_{y_i} = 0$ then $(\delta^2 y_i)_{y_l} = 0$ iff $(\delta^2 y_l)_{y_i} = 0$, and (3) if $(\delta y_l)_{y_i} = 0$, $(\delta^2 y_l)_{y_i} \neq 0$, then $\operatorname{sgn}(\delta^2 y_i)_{y_l} = [\operatorname{sgn}(A_i A_l)][\operatorname{sgn}(\delta^2 y_l)_{y_i}]$. Suppose $D$ has the form $D = y_{n+1} - E(y_\alpha, y_\mu)$, $f = y_{n+1} + \Sigma_\alpha A_\alpha y_\alpha$ is the Legendre transform of $y_{n+1}$, $(\delta f)_{A_\gamma}$ and $(\delta^2 f)_{A_\gamma}$ are the first and second variations of $f$ subject to the constraints $\delta A_\gamma = 0$, $\gamma = 1, 2, \ldots, \bar{n}$ with $(\delta y_{n+1})_{y_\gamma}$, $(\delta^2 y_{n+1})_{y_\gamma}$ having analogous definitions and $E_{kj} \equiv \partial^2 E / \partial y_k \partial y_j$ for $k, j \neq n+1$. Then (4), $(\delta f)_{A_\gamma} = 0$ iff $(\delta y_{n+1})_{y_\gamma} = 0$; (5), $(\delta^2 y_{n+1})_{y_\gamma} > 0$ ($< 0$) iff $E_{\mu\nu}$ is positive (negative) definite; (6), $(\delta^2 f)_{A_\gamma} > 0$ ($< 0$) iff $E_{\alpha\beta}$ is nonsingular and $E_{\mu\nu} - \Sigma_\alpha \Sigma_\beta E_{\mu\alpha} E^{-1}_{\alpha\beta} E_{\beta\nu}$ is positive (negative) definite; and (7), $E_{kj}$ positive (negative) definite implies $E_{\alpha\beta}$ and $E_{\mu\nu} - \Sigma_\alpha \Sigma_\beta E_{\mu\alpha} E^{-1}_{\alpha\beta} E_{\beta\nu}$ are positive (negative) definite.

*Proof*: From $D = 0$ it follows that we may write $\delta D = 0 = \Sigma_k A_k \delta y_k$ where $A_k \equiv \partial D / \partial y_k = \psi_k(y_j)$ and, hence, $A_l(\delta y_l)_{y_i} = -\Sigma_{k \neq l,i} A_k \delta y_k = A_i(\delta y_i)_{y_l}$ and since $A_i$ and $A_l$ vanish nowhere on $B$, the first part of the thoerem is proved. Solving $\delta D = 0$ for $\delta y_l$ gives $\delta y_l - \Sigma_{k \neq l} A_k \delta y_k / A_l$. From this expression for $\delta y_l$ and the definition $\delta^2 y_l = \delta(\delta y_l)$ it follows that $A_l \delta^2 y_l + \delta y_l \delta A_l = -\Sigma_{k \neq l} \delta A_k \delta y_k$. But $\delta A_k = \Sigma_j A_{kj} \delta y_j$, where

$$A_{kj} \equiv \partial A_k / \partial y_j = \partial \psi_k / \partial y_j = \partial^2 D / \partial y_k \partial y_j = A_{jk}$$

and thus

$$A_l\delta^2 y_l + \delta y_l(\Sigma_{j\neq l} A_{lj}\delta y_j + A_{ll}\delta y_l)$$
$$= -\Sigma_{k\neq l}(\Sigma_{j\neq l} A_{kj}\delta y_j + A_{kl}\delta y_l)\delta y_k.$$

But using the symmetry of $A_{kj}$ in the last term on the right and rearranging terms we find that the second variation can be expressed as $A_l\delta^2 y_l + \delta y_l\,[A_{ll}\delta y_l + 2\Sigma_{k\neq l}A_{lk}\delta y_k\,]$ $= -\Sigma_{k\neq l}\Sigma_{j\neq l} A_{kj}\delta y_k\delta y_l$. From this it follows that if we impose the condition $\delta y_i = 0$, then

$$A_l(\delta^2 y_l)_{y_i} + (\delta y_l)_{y_i}\Big[A_{ll}(\delta y_l)_{y_i} + 2\sum_{k\neq l,i}^{k\neq l,i} A_{lk}\delta y_k\Big]$$
$$= -\sum_{k\neq l,i}\sum_{j\neq l,i} A_{kj}\delta y_k\delta y_j.$$

The right side of this expression is symmetric in $l$ and $i$, thus interchanging $l$ and $i$ to obtain a similar expression for the second variation $(\delta^2 y_i)_{y_l}$ we conclude that

$$A_l(\delta^2 y_l)_{y_i} + (\delta y_l)_{y_i}\Big[A_{ll}(\delta y_l)_{y_i} + 2\sum_{k\neq l,i} A_{lk}\delta y_k\Big]$$
$$= A_i(\delta^2 y_i)_{y_l} + (\delta y_i)_{y_l}\Big[A_{ii}(\delta y_i)_{y_l} + 2\sum_{k\neq l,i} A_{ik}\delta y_k\Big].$$

If $(\delta y_l)_{y_i} = 0$ then this simplifies to $A_l(\delta^2 y_l)_{y_i} = A_i(\delta^2 y_i)_{y_l}$ and the second and third parts of the theorem follow immediately. We now suppose that $D$ takes its special form. Then $A_{n+1} = 1$, $A_\alpha = \psi_\alpha(y_\beta, y_\nu) = -\partial E/\partial y_\alpha$, $A_\mu = \psi_\mu(y_\beta, y_\nu)$ $= -\partial E/\partial y_\mu$ from which we have $\delta y_{n+1} + \Sigma_\alpha A_\alpha\delta y_\alpha$ $+ \Sigma_\mu A_\mu\delta y_\mu = 0$. Now since $A_{n+1} = 1$ we have $A_{n+1,k}$ $= 0 = A_{k,n+1}$ and from the previously derived expression for $\delta^2 y_l$ with $l = n+1$ we can write

$$\delta^2 y_{n+1} = -\sum_{k\neq n+1}\sum_{j\neq n+1} A_{kj}\delta y_k\delta y_l$$
$$= \sum_{k\neq n+1}\sum_{j\neq n+1} E_{kj}\delta y_k\delta y_j.$$

Thus $(\delta y_{n+1})_{y_\gamma} = -\Sigma_\mu A_\mu\delta y_\mu$ and $(\delta^2 y_{n+1})_{y_\gamma}$ $= \Sigma_\mu\Sigma_\nu E_{\mu\nu}\delta y_\mu\delta y_\nu$ and (5) is an immediate consequence of the expression for $(\delta^2 y_{n+1})_{y_\gamma}$. Next we consider the Legendre transform $f$ of $y_{n+1}$ and it follows that

$$\delta f - \sum_\alpha y_\alpha\delta A_\alpha + \sum_\mu A_\mu\delta y_\mu = 0.$$

where now $\partial f/\partial A_\alpha = y_\alpha = \varphi_\alpha(A_\beta, y_\nu)$ and $-\partial f/\partial y_\mu = A_\mu$ $= \varphi_\mu(A_\beta, y_\nu)$. The expression for $\delta f$ gives $(\delta f)_{A_\gamma}$ $= -\Sigma_\mu A_\mu\delta y_\mu$ and comparison with $(\delta y_{n+1})_{y_\gamma}$ establishes (4). The second variation of $f$ satisfies $\delta^2 f - \Sigma_\alpha\delta y_\alpha\delta A_\alpha + \Sigma_\mu$ $\delta A_\mu\delta y_\mu = 0$. But since $\delta A_\mu = \Sigma_\alpha\delta A_\alpha\partial\varphi_\mu/\partial A_\alpha + \Sigma_\nu\delta y_\nu$ $\partial\varphi_\mu/\partial y_\nu$, the expression for $\delta^2 f$ can be rewritten in the form

$$\delta^2 f - \sum_\alpha\delta A_\alpha\Big[\delta y_\alpha - \sum_\mu\delta y_\mu\partial\varphi_\mu/\partial A_\alpha\Big]$$
$$+ \sum_\mu\sum_\nu(\partial\varphi_\mu/\partial y_\nu)\delta y_\mu\delta y_\nu = 0.$$

It is desirable to re-express the derivative $\partial\varphi_\mu/\partial y_\nu$ in terms of derivatives of the functions $\psi_\mu$. First observe that in the transform the variables $A_\alpha$ and $y_\nu$ are independent and, hence, $\partial A_\alpha/\partial y_\nu = 0$. But since we also know that $A_\alpha = \psi_\alpha(y_\beta, y_\nu)$ we can use the chain rule for differentiation to establish the relation $0 = \partial A_\alpha/\partial y_\nu$ $= \Sigma_\beta(\partial\psi_\alpha/\partial y_\beta)(\partial y_\beta/\partial y_\nu) + \partial\psi_\alpha/\partial y_\nu$. If we suppose $A_{\alpha\beta}$ $= \partial\psi_\alpha/\partial y_\beta = -\partial^2 E/\partial y_\alpha\partial y_\beta$ to be nonsingular, then $\partial y_\beta/\partial y_\nu = \Sigma_\alpha E^{-1}_{\beta\alpha}\partial\psi_\alpha/\partial y_\nu$. If we now use this result and $\varphi_\mu(A_\beta, y_\nu) = A_\mu = \psi_\mu(y_\beta, y_\nu)$, then we find by differentiation that

$$\partial\varphi_\mu/\partial y_\nu = \sum_\beta(\partial\psi_\mu/\partial y_\beta)(\partial y_\beta/\partial y_\nu) = \partial\psi_\mu/\partial y_\nu$$
$$= \sum_\alpha\sum_\beta(\partial\psi_\mu/\partial y_\beta)E^{-1}_{\beta\alpha}(\partial\psi_\alpha/\partial y\upsilon) + \partial\psi_\mu/\partial y_\nu$$
$$= \sum_\alpha\sum_\beta E_{\mu\beta}E^{-1}_{\beta\alpha}E_{\alpha\nu} - E_{\mu\nu},$$

where I used $\partial\psi_\mu/\partial y_\beta = -\partial^2 E/\partial y_\beta\partial y_\mu = \partial\psi_\beta/\partial y_\mu$ in the last step. If this is substituted into the expression for $\delta^2 f$ if follows that

$$\delta^2 f - \sum_\alpha\delta A_\alpha\Big[\delta y_\alpha - \sum_\mu\delta y_\mu\partial\varphi_\mu/\partial A_\alpha\Big]$$
$$= -\sum_\mu\sum_\nu(\partial\varphi_\mu/\partial y_\nu)\delta y_\mu\delta y_\nu$$
$$= \sum_\mu\sum_\nu\Big(E_{\mu\nu} - \sum_\alpha\sum_\beta E_{\mu\beta}E^{-1}_{\beta\alpha}E_{\alpha\nu}\Big)\delta y_\mu\delta y_\nu$$

and thus

$$(\delta^2 f)_{A_\gamma} = \sum_\mu\sum_\nu\Big(E_{\mu\nu} - \sum_\alpha\sum_\beta E_{\mu\beta}E^{-1}_{\beta\alpha}E_{\alpha\nu}\Big)\delta y_\mu\delta y_\nu.$$

This immediately establishes (6). To prove (7) it is simpler to use matrix notation rather than subscript notation. A symmetric matrix $E = E^T$ is positive definite iff $y^T E y > 0$ for all vectors $y \neq 0$. Suppose $E$ and $y$ are similarly partitioned, that is,

$$E = \begin{pmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix},$$

where $E_{21} = E^T_{12}$, and $E_{11}$ and $E_{22}$ are square and symmetric. For $y_2 = 0$ we have $y^T E y = y_1^T E_{11} y_1$, for $y_1 = 0$ we have $y^T E y = y_2^T E_{22} y_2$ and for $y_1 = -E^{-1}_{11}E_{12}y_2$ we obtain $y^T E y = y_2^T(E_{22} - E_{21}E^{-1}_{11}E_{12})y_2$. Thus the positive (negative) definiteness of $E$ implies the positive (negative) definiteness of $E_{11}$, $E_{22}$, and $E_{22} - E_{21}E^{-1}_{11}E_{12}$ as well as the existence of $E^{-1}_{11}$ because if $E_{11}$ is positive (negative) definite it is also nonsingular.

To apply this theorem to thermodynamics we only need a translator from the notation used in its proof to thermodynamic notation. When dealing with the variations in $s$ such a translator is supplied by the first law forms for solids and fluids (A.IV.17.1, A.IV.18.1, and A.IV.18.2),

$$T\delta s\begin{cases} = \delta u - S^{kj}\delta e_{kj} - E_k\delta p^k + \tfrac{1}{2}m^{kj}\delta B_{kj} - \mu^\lambda\delta n_\lambda & \text{(solids)} \\ = \delta u + p\delta(1/m) - E_k\delta p^k + \tfrac{1}{2}m^{kj}\delta B_{kj} - \mu^\lambda\delta n_\lambda & \text{(fluids)} \end{cases} \tag{II.10}$$

To write down the translator when dealing with the variations in $ms$ it is convenient to introduce first some notation to denote the product of an extensive variable and the mass density. Such product will be denoted by the same symbol

with a tilde over it,

$$\begin{aligned} &\tilde{s}\equiv ms, \quad \tilde{u}\equiv mu, \quad \tilde{S}^{kj}\equiv mS^{kj}, \\ &\tilde{p}^k\equiv mp^k, \quad \tilde{m}^{kj}\equiv mm^{kj}, \quad \tilde{n}_\lambda\equiv mn_\lambda. \end{aligned} \tag{II.11.1}$$

We can obtain the appropriate translator from the relation $T\delta s = m T\delta s + Ts\delta m$, the expression for the variation $\delta s$ and the Euler relation for $Ts$,

$$T\sigma\tilde{s}\begin{cases} = \delta\tilde{u} - \tilde{S}^{kj}\delta e_{kj} - E_k\delta\tilde{p}^k + \tfrac{1}{2}\tilde{m}^{kj}\delta B_{kj} - \mu^\lambda\delta\tilde{n}_\lambda & \text{(solids)} \\ = \delta\tilde{u} - E_k\delta\tilde{p}^k + \tfrac{1}{2}\tilde{m}^{kj}\delta B_{kj} - \mu^\lambda\delta\tilde{n}_\lambda & \text{(fluids)} \end{cases} \tag{II.11.2}$$

The only difference in form between (II.10) and (II.11) occurs for fluids where the pressure term is present in (II.10) but absent from (II.11). This is really not surprising because if $s$ is extensive then $\tilde{s} = m[s(u, 1/m, p^k, B_{kj}, n_\lambda)] = s(\tilde{u}, 1, \tilde{p}^k, B_{kj}, \tilde{n}_\lambda)$.

Consequently, while we can obtain the variational analogue of the Gibbs free energy criterion for fluids in mass measure, we cannot do so in volume measure.

With the translators (II.10) and (II.11) available, it is now a simple but tedious task to translate the variational form of the "entropy maximum" criterion, Theorem II.8, to other forms. For this reason I shall only deal explicitly with the internal energy and Helmholtz free energy "minimum" criteria in volume measure.

*Theorem* II.12: Suppose $\tilde{f}\equiv\tilde{u} - T\tilde{s} = m(u - Ts)$ and for $\tilde{a}$ equal either $\tilde{s}$, $\tilde{u}$, or $\tilde{f}$ suppose $A = \int_B \tilde{a}\, dv$, $\delta A = \int_B \delta\tilde{a}\, dv$, and $\delta^2 A = \int_B \delta^2\tilde{a}\, dv$. Then (1) $(\delta S)_U = 0$ iff $(\delta U)_S = 0$, (2) if $(\delta S)_U = 0$ and $(\delta^2 S)_U < 0$, then $(\delta U)_S = 0$ and $\operatorname{sgn}(T)(\delta^2 U)_S > 0$, and (3) $(\delta F)_T = 0$ iff $(\delta U)_S = 0$. If $\operatorname{sgn}[(\delta^2\tilde{f})_T] = \operatorname{sgn}[(\delta^2\tilde{u})_{\tilde{s}}]$, then (4), $(\delta U)_S = 0$, $\operatorname{sgn}(T)(\delta^2 U)_S > 0 \Rightarrow (\delta F)_T = 0$, $\operatorname{sgn}(T)(\delta^2 F)_T > 0$.

*Proof*: Since $\delta A = 0$ iff $\delta\tilde{a} = 0$ and $\delta^2 A = 0$ iff $\delta^2\tilde{a} = 0$, we need only identify $y_l$ with $\tilde{s}$ and $y_i$ with $\tilde{u}$ in Theorem II.9(1, 2, 3). This identification together with the identification of $A_i = 1, A_l = -T$ by means of (II.11) proves parts (1) and (2). In Theorem II.9 we identify $\bar{n} = 1, y_{n+1} = \tilde{u}, y_1 = \tilde{s}$, and, hence, $\partial\tilde{u}/\partial\tilde{s} = T = -A_1$. Then part (3) of this corollary is a consequence of Theorem II.11(4). Finally (4) follows from Theorem II.9(5, 6, 7).

The sign conditions on $(\delta^2\tilde{f})_T$ and $(\delta^2\tilde{u})_{\tilde{s}}$ leading to Theorem II.12(4) were not replaced by the definiteness conditions on combinations of submatrices of $E_{kj}$ because the thermodynamic notation for these matrices is too cumbersome. It probably should be mentioned that the notation $(\delta F)_T$ in Theorem II.12 does not imply that $T$ is a constant function on $B$ but merely says that $T$ is not to be varied in the variation of $F$. On the contrary the notation $(\delta S)_U$ does imply that the value of $U$ is fixed. It should also be observed that $U$ [and also $F$ in the context of Theorem II.12(4)] takes on its minimum value for an equilibrium state only if $\operatorname{sgn}(T) > 0$ which does correspond to the usual situation. If $\operatorname{sgn}(T) < 0$, then its value is a maximum. If $y_{n+1}$ had been identified with $\tilde{s}$, and $y_1$ with $\tilde{u}$, then instead of the Helmholtz free energy per unit volume, $\tilde{f}$, we would have encountered the Massieu function $(-\tilde{f}/T)$. Finally if I had chosen to work with mass measure instead of volume measure, then the only change would have been the replacment of $dv$ by $dM$ and the use of the symbol $a$ instead of $\tilde{a}$ in the integrands.

### C. Applications

Theorem II.12 brings us to the conclusion of what I regard as the development of the continuum analogue of the algebraic results given as Theorem I.33 and I shall now look at three examples of the application of this formalism. The purpose of the examples I have selected is to convey some sense of the breadth and versatility of the theory rather than just to serve as computational exercises. My first example is one which will demonstrate that all of conventional thermodynamics, with its partitions and composite systems, falls within the purview of the theory developed here. Thermodynamics is often applied to a composite system with a finite number of sybsystems where the state of each subsystems is constrained to be a constant function. It is easy to show that such states form a chain in $(f(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$. Suppose that $K$ is a finite index set and $\{B_k \subset B \mid k\in K\} \in \mathsf{P}(B)$ is a partition of $B$. Then by the definition of $\mathsf{P}(B)$ given in Definition I.35 there exists a partition of $\Sigma$ into chains. $\mathscr{C} = \{C_\alpha \mid \alpha\in\Delta\} \in \mathsf{P}(\Sigma)$ and a thermodynamic state $\sigma$ such that $P_\sigma(\mathscr{C}) = \{B_k \subset B \mid k\in K\}$ and by Theorem I.38 $\langle\sigma\rangle_{\mathscr{C}}$ is a chain in $(f(\Sigma), \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ containing only subsystem equivalent states. Then for any function $f: K\to\Delta$, where $f(k) = \alpha_k$, we can define a subset $\mathbb{C}$ of $\langle\sigma\rangle_{\mathscr{C}}$ by the prescription $\mathbb{C} = \{\sigma' \mid \sigma'\in\langle\sigma\rangle_{\mathscr{C}}$ and $\forall k\in K$, $\operatorname{Im}\sigma'|B_k \subset C_{\alpha_k}$ and $\sigma'|B_k$ is a constant function$\}$. Then since $\mathbb{C}\subset\langle\sigma\rangle_{\mathscr{C}}$ we know that $\mathbb{C}$ is a chain and is, in fact, the collection of states encountered in conventional thermodynamics. Suppose that $\mathbb{C}$ and $s$ satisfy the conditions of Theorem II.7, then since $\sigma|B_k$ is constant

$$S = \sum_{k\in K} S_k = \sum_{k\in K} \tilde{s}_k V_k = \sum_{k\in K} s_k M_k, \quad \sigma\in\mathbb{C}, \tag{II.13}$$

where $V_k$ is the volume and $M_k$ is the mass of the $k$ th subsystem and $\tilde{s}_k$ and $s_k$ are the functions $\tilde{s}$ and $s$ evaluated for the $k$ th subsystem. The expression for $S$ given in (II.13) is exactly the form ordinarily used in the thermodynamics of composite systems and the direct maximization of $S$ in this form corresponds to the ordinary computations of thermodynamics.

The two examples which will follow differ from this first one in three respects. First, the states of the body are not required to be constant functions when restricted to subsystems. Second, the states cannot be described adequately by thermodynamic variables alone. Third, constraints will be imposed by means of Lagrangian multipliers. Constraint equations used in the calculus of variations can be placed into one of two categories. Either they are functions, whose arguments perhaps may include derivatives and whose values need not be zero, or they are integrals of such functions

over a body. The treatment of both types of constraints is similar for the purposes of generating the Euler–Lagrange equations and the only difference is in the interpretation of the multipliers associated with the constraints. Suppose we have a Lagrangian $L$ and $n$ constraint equations $G_i = 0$, $i = 1,2,...,n$ as constraints. Then the Euler–Lagrange equations are obtained from $\delta \mathscr{L} = 0$, where $\mathscr{L} = L + \lambda\, {}^{i}G_i$ and the $\lambda^{i}$ are functions with domain $B$, subject to the variational procedure and determined by the Euler–Lagrange equations. By contrast, if we wish to impose the constraints $\int_B G_i\, dv = K_i$, where the $K_i$ are constants and $G_i \neq 0$, then the Euler–Lagrange equations are also obtained from $\delta \mathscr{L} = 0$ but now $\mathscr{L} = L + \Lambda\, {}^{i}G_i$, where the $\Lambda^{i}$ are constants, actually constant functions on $B$, which are not to be varied but whose values are determined by the constraints. Thermodynamic systems constrained solely by integrals correspond to closed systems. The thermodynamic systems which are constrained only by functions correspond to open systems. There also can arise hybrid systems which are simultaneously constrained by integrals and by functions. With these preliminaries explained we can now go on to consider two additional examples where the variational technique will be used to derive the equations which describe the system. The first of these two examples will be a closed system whose Euler–Lagrange equations turn out to be a system of nonlinear simultaneous equations for the thermodynamic variables at each point of the body. Of course, these equations can be converted to a system of first order partial differential equations in spatial coordinates by differentiation. The second example will be an open system for which the governing equations are partial differential equations. I will discuss some implications of the closed system equations but I will not go beyond the derivation of the equations for the open system.

Electrolyte solutions have been, and continue to be, a fertile field for the application of thermodynamics. An important source for the thermodynamic data of these solutions have been the measurement of the electromotive force of galvanic cells. The chief advantage of electromotive force measurements as a source for thermodynamic data lies in the relative ease with which one can achieve rather high precision. But the quality of the resultant data is a function not only of the precision of the measurement but also of the validity of the connection between electromotive force and thermodynamics. There are two components to this connection: one the electrochemical potential and the other the cell reaction. The derivations of the electrochemical potential generally seem to be based more on physical arguments coupled with appeals to plausibility[3,4] than rigorous derivation and, at least for me, have not been very convincing. The requirement for a posited cell reaction is contrary to the spirit of thermodynamics. Thermodynamic analysis, presumably, is path independent and therefore should be independent of particular reaction schemes[5] (p. 307). If the connection between electromotive force and thermodynamics is real then it should be possible to deduce it without resorting to *ad hoc* assumptions or cell reactions. I intend to accomplish just this with my closed system example and, since the thermodynamic treatment of the effect of the gravitational field and centrifugation can be similarly faulted, I shall look at all three effects simultaneously. In this example I assume that (1) we are dealing with fluids, (2) volume measure is used for the calculation of $S$, (3) greek indices from the last part of the alphabet are used to label species, and (4) greek indices from the first part of the alphabet are used to label constraints imposed on the composition variables. The specific constraints we wish to impose are all integrals,

$$\begin{aligned} K_{(\pm)} &= \int_B \mathscr{E}_{(\pm)}\, dv, \\ K_1 &= \int_B m\, dv, \\ K_\alpha &= \int_B m b_\alpha\, dv, \end{aligned} \tag{II.14}$$

where

$$\begin{aligned} \mathscr{E}_{(\pm)} &= m(u \pm v^2/2 + \Omega) + \mathscr{U}, \\ b_\alpha &= a_\alpha^\nu n_\nu \end{aligned} \tag{II.15}$$

and $a_\alpha^\nu$ are constants such that the matrix rank of $a_\alpha^\nu$ does not exceed the number of species. The function $\mathscr{E}_{(+)}$ is just the energy density so that $K_{(+)}$ is the energy of the body $B$. Thus the first member of II.14, with positive sign, represents the conservation of energy for the body $B$ and obviously the second member is the conservation of mass. If the constants $a_\alpha^\nu$ represent the number of atoms of element $\alpha$ in species $\nu$ then the last member of II.14 imposes the conservation of elements on the body. If $\mathsf{M}^\nu$ is the molecular weight of species $\nu$ then, if follows that

$$\mathsf{M}^\nu n_\nu = 1, \tag{II.16}$$

and if this is used to rewrite the integrand of the second member of II.14, then the Lagrangian for our problem is

$$\begin{aligned} \mathscr{L} = \tilde{s} &+ \Lambda^{(\pm)}[\tilde{u} + (\Omega \pm v^2/2)\mathsf{M}^\nu \tilde{n}_\nu + \mathscr{U}] \\ &+ \Lambda\, {}^{1}\mathsf{M}^\nu \tilde{n}_\nu + \Lambda\, {}^{\alpha}a_\alpha^\nu \tilde{n}_\nu. \end{aligned} \tag{II.17}$$

In carrying out the variation of $\mathscr{L}$ I shall assume that $\delta\Omega = 0$ and $\delta(v^2/2) = v^k \delta v_k = 0$. This is consistent with the fact that the potential $\Omega$ and the velocity $v^k$ are nonthermodynamic quantities and implies that they are to be determined by nonthermodynamic considerations. Thus they are to be regarded as "external" fields which can affect the thermodynamic state but which cannot be affected by the state directly. On the other hand, the electromagnetic energy $\mathscr{U}$ will be assumed to be at least partly determined by the thermodynamic state and so its variation must be calculated. From the definition of $\mathscr{U}$ (A.IV.9.2) we know that

$$\delta\mathscr{U} = \epsilon_0 E_k \delta E^k + B_{kj} \delta B^{kj}/2\mu_0,$$

but because the electrochemical potential contains the scalar potential we must reexpress $\delta\mathscr{U}$ in terms of the scalar potential $\hat{\phi}$ and the vector potential $A_k$, whose existence is guaranteed by the homogeneous Maxwell equations (A.IV.2.9) and (A.IV.2.10), and which can be used to replace $E_k$ and $B_{kj}$ in $\delta\mathscr{U}$,

$$\begin{aligned} B_{kj} &= \nabla_k A_j - \nabla_j A_k, \\ E_k &= -\nabla_k \hat{\phi} - \partial A_k/\partial t. \end{aligned} \tag{II.18}$$

This substitution, integration by parts and the use of equations (A.IV.6.7), (A.IV.6.8), (A.IV.7.2), and (A.IV.7.3) establish an expression for $\delta\mathscr{U}$ involving $\hat{\phi}$ and $A_k$,

$$\begin{aligned}\delta\mathscr{U} &= \hat{\phi}\delta\rho_f + A_k\delta j_f^k - E_k\delta P^k + B_{kj}\delta M^{kj}/2 \\ &\quad + \nabla_k\left(A_i\delta H^{ki} + A^k\delta\Phi - \hat{\phi}\delta D^k\right) + A_k\partial(\delta D^k)/\partial t \\ &\quad - \delta D^k\left(\partial A_k/\partial t\right) + \mu_0\epsilon_0[\delta\Phi\partial\hat{\phi}/\partial t - \hat{\phi}\partial(\delta\Phi)/\partial t] \\ &\quad - \left(\nabla_k A^k + \mu_0\epsilon_0\partial\hat{\phi}/\partial t\right)\delta\Phi. \qquad \text{(II.19)}\end{aligned}$$

The divergence term in $\delta\mathscr{U}$ will not contribute to the Euler–Lagrange equations because when it is converted to a surface integral it vanishes because of the transversality conditions. The terms involving time derivatives will not contribute in the steady state while the last term can be made to vanish because one can always choose $A^k$ and $\hat{\phi}$ to satisfy the Lorentz condition, $\nabla_k A^k + \mu_0\epsilon_0\partial\hat{\phi}/\partial t = 0$, by choice of a suitable gauge function. Under these circumstances only the first four terms on the right side can contribute to the Euler–Lagrange equations. We shall need only one final bit of information before writing down the expression for $\delta\mathscr{L}$. The function $m^{kj}$ is extensive, that is, $m^{kj}(\lambda u, \lambda/m, \lambda p^i, B_{il}, \lambda n_\nu) = \lambda m^{kj}(u, 1/m, p^i, B_{il}, n_\nu)$ and from this it follows that

$$\partial\tilde{m}^{kj}/\partial\tilde{u} = \partial m^{kj}/\partial u, \quad \partial\tilde{m}^{kj}/\partial\tilde{p}^i = \partial m^{kj}/\partial p^i,$$
$$\partial\tilde{m}^{kj}/\partial B_{il} = m\partial m^{kj}/\partial B_{il}, \quad \partial\tilde{m}^{kj}/\partial\tilde{n}_\nu = \partial m^{kj}/\partial n_\nu$$

and, therefore,

$$\begin{aligned}\delta\tilde{m}^{kj} &= \frac{\partial m^{kj}}{\partial u}\delta\tilde{u} + \frac{\partial m^{kj}}{\partial p^i}\delta\tilde{p}^i \\ &\quad + m\frac{\partial m^{kj}}{\partial B_{il}}\delta B_{il} + \frac{\partial m^{kj}}{\partial n_\sigma}\delta\tilde{n}_\sigma.\end{aligned}$$

If the vector potential $A_k$ and the scalar potential $\hat{\phi}$ satisfy the Lorentz condition and

$$\delta\Omega = 0, \quad \delta v_k = 0, \delta(\Delta P^k) = 0,$$
$$\delta(\Delta M^{kj}) = 0, \quad \delta(\sigma^k + z^\nu d^k_\nu) = 0, \qquad \text{(II.20)}$$

then under steady state conditions and subject to the transversality conditions we have a relatively simple expression for $\delta\mathscr{L}$,

$$\begin{aligned}\delta\mathscr{L} &= \left[T^{-1} + \Lambda^{(\pm)}\left(1 + \tfrac{1}{2}B_{kj}\partial m^{kj}/\partial u\right)\right]\delta\tilde{u} \\ &\quad - \left[\left(T^{-1} + \Lambda^{(\pm)}\right)E_i - \tfrac{1}{2}\Lambda^{(\pm)}B_{kj}\partial m^{kj}/\partial p^i\right]\delta\tilde{p}^i \\ &\quad + \frac{m}{2}\left[T^{-1}m^{kj} + \Lambda^{(\pm)}B_{il}(\partial m^{il}/\partial B_{kj}\right]\delta B_{kj} \\ &\quad - \left\{T^{-1}\mu^\sigma - \Lambda^{(\pm)}\left[\left(\hat{\phi} + A_k v^k\right)z^\sigma\right.\right. \\ &\quad \left.\left. + (\Omega \pm v^2/2)\mathsf{M}^\sigma + \tfrac{1}{2}B_{kj}\partial m^{kj}/\partial n_\sigma\right] \right. \\ &\quad \left. - \Lambda^1\mathsf{M}^\sigma - \Lambda^\alpha a^\sigma_\alpha\right\}\delta\tilde{n}_\sigma.\end{aligned}$$

The conditions (II.20) do not imply that $\Omega$, $v_k$, $\Delta P^k$, $\Delta M^{kj}$, and $(\sigma^k + z^\nu d^k_\nu)$ necessarily vanish nor do they imply that these quantities must be prescribed in advance. But, as my earlier remarks intimated, these conditions do imply that these quantities are determined by nonthermodynamic considerations (equations). Thus the state of the body is only partially determined by the thermodynamic Euler–Lagrange equations. The Euler–Lagrange equations for this problem are obtained from $\delta\mathscr{L} = 0$ and clearly are not a system of differential equations,

$$\begin{aligned}&T^{-1} + \Lambda^{(\pm)}\left(1 + \tfrac{1}{2}B_{kj}\partial m^{kj}/\partial u\right) = 0, \\ &\left(T^{-1} + \Lambda^{(\pm)}\right)E_i - 1/2\Lambda^{(\pm)}B_{kj}(\partial m^{kj}/\partial p^i) = 0, \\ &T^{-1}m^{kj} + \Lambda^{(\pm)}B_{il}(\partial m^{il}/\partial B_{kj}) = 0, \qquad \text{(II.21)} \\ &T^{-1}\mu^\sigma - \Lambda^{(\pm)}\left[\left(\hat{\phi} + A_k v^k\right)z^\sigma + (\Omega \pm v^2/2)\mathsf{M}^\sigma\right. \\ &\left. + \tfrac{1}{2}B_{kj}(\partial m^{kj}/\partial n_\sigma)\right] - \Lambda^1\mathsf{M}^\sigma - \Lambda^\alpha a^\sigma_\alpha = 0.\end{aligned}$$

From this system of equations we can obtain an interesting result for $\Lambda^{(\pm)} \neq 0$,

$$\left(T^{-1} + \Lambda^{(\pm)}\right) = 0$$

$$\text{iff}\begin{cases} B_{kj}\dfrac{\partial M^{kj}}{\partial u} = 0 \\ B_{kj}\dfrac{\partial m^{kj}}{\partial p^i} = 0 \\ m^{kj} - B_{il}\dfrac{\partial m^{il}}{\partial B_{kj}} = 0 \\ \mu^\sigma + \left(\hat{\phi} + A_k v^k\right)z^\sigma + (\Omega \pm v^2/2 + \Lambda^1/\Lambda^{(\pm)})\mathsf{M}^\sigma \\ \quad + \tfrac{1}{2}B_{kj}(\partial m^{kj}/\partial n_\sigma) + (\Lambda^\alpha/\Lambda^{(\pm)})a^\sigma_\alpha = 0 \end{cases} \qquad \text{(II.22)}$$

The multiplier $\Lambda^{(\pm)}$ is a constant and, therefore, $T^{-1} + \Lambda^{(\pm)} = 0$ implies that the equilibrium state for the body is one of constant temperature. Clearly then, the first three equations on the right side of (II.22) may be regarded as a system of first order partial differential equations which might not be satisfied but which the function $m^{kl}$ must satisfy if the equilibrium state of the body is to be one of constant temperature. One class of solutions to these equations is easily written down by inspection,

$$\begin{aligned}&m^{kj} = C^{kjil}B_{il}, \\ &C^{kjil} = C^{kjil}(n_\nu), \\ &C^{kjil}(\lambda n_\nu) = \lambda C^{kjil}(n_\nu), \qquad \text{(II.23)} \\ &C^{kjil} = C^{ilkj}, \\ &C^{kjil} = -C^{jkil} = C^{jkli}.\end{aligned}$$

This includes, as a special case, $m^{kl} = 0$ which comes from (II.23) by choosing the tensor $C^{kjil}$ as the zero tensor. Suppose we ignore the constraint on the total mass by choosing $\Lambda^1 = 0$, and also choose $v^k = 0$, and $C^{kjil}$ independent of composition. Then the last equation on the right side of (II.22) specializes to

$$\mu^\sigma + \hat{\phi}z^\sigma + \Omega\mathsf{M}^\sigma + (\Lambda^\alpha/\Lambda^{(\pm)})a^\sigma_\alpha = 0 \qquad \text{(II.24)}$$

and for $\hat{\phi} = 0 = \Omega$ these equations have exactly the same form as the equations normally used to determine chemical composition for complex chemical equilibria and, consequently, contain all the equilibrium constant relations [Zeleznik and Gordon,[5] Eqs. (9, 16)]. Furthermore, the second term in (II.24) is precisely the modification of the chemical potential which forms the electrochemcial potential while the third term is the modification used in conventional thermodynamics to take into account the gravitational potential. But the manner in which (II.24) was obtained makes it clear that the sources of the second, third, and fourth terms are the constraints, that is, the members of (II.14), and not thermodynamics. This leads me to question the propriety of regard-

ing the electrochemical potential, $\mu^\sigma + \hat{\phi}z^\sigma$, as a thermodynamic function as is the practice in conventional thermodynamics. Certainly I know of no comparable suggestions that the combination $\mu^\sigma + (\Lambda^\alpha/\lambda^{(\pm)})a^\sigma_\alpha$ be regarded as a thermodynamic function. Similar comments apply to the combinations $\mu^\sigma + \Omega\mathsf{M}^\sigma$ and $\mu^\sigma + \hat{\phi}^\sigma + \Omega\mathsf{M}^\sigma$.

We have not yet exhausted the interpretive content of (II.22) and I wish to look at one other special case. That special case is obtained by neglecting all electromagnetic effects ($p^i = 0$, $m^{kj} = 0$, $\hat{\phi} = 0$, $A_k = 0$) and ignoring the mass constraint ($\Lambda^1 = 0$). For these conditions the last member of the right side of (II.22) specializes to

$$\mu^\sigma + (\Omega \pm v^2/2)\mathsf{M}^\sigma + (\Lambda^\alpha/\Lambda^{(\pm)})a^\sigma_\alpha = 0 \qquad \text{(II.25)}$$

and for $\Omega = 0$ and the negative sign for the $v^2$ term this implies

$$\mu^\sigma - (v^2/2)\mathsf{M}^\sigma = \mathsf{C}^\sigma, \qquad \text{(II.26)}$$

where $\mathsf{C}^\sigma$ is a constant function. These equations are the ones normally used to determine chemical compositions during steady state centrifugation [Ref. 3, p. 244, Eq. (15–14)]. If $\mu^\sigma = \mu^\sigma(T, p, n_\nu)$ then

$$n_\sigma \nabla_k \mu^\sigma = -s\nabla_k T + m^{-1}\nabla_k p$$

because by the Gibbs–Duhem relation, $n_\sigma \partial\mu^\sigma/\partial n_\nu = 0$. Therefore (II.26) implies a characteristic property of centrifugation, namely

$$\nabla_k p = m\nabla_k(v^2/2) \qquad \text{(II.27)}$$

because $\nabla_k T = 0$. This result seems to be the basic justification for the use of II.26 in the thermodynamics of centrifugation. The usual derivation of II.26, at least for me, is unsatisfying. Of course the derivation given here is no less *ad hoc* than the usual derivation because the constraint based on $\mathscr{E}_{(-)}$ has no obvious physical interpretation in contrast to the obvious physical interpretation of the constraint based on $\mathscr{E}_{(+)} \equiv \mathscr{E}$.

How does one construct an acceptable thermodynamic treatment of centrifugation? The fundamental objective of such a treatment of centrifugation is the determination of composition by the simpler equations of thermodynamics, rather than the evolution equations (A.IV.2.3), in a manner that is consistent with the fluid dynamics of the problem. But since the fluid dynamical computation must be carried out in any event, there seems to be little point in atempting to incorporate the dynamics, as typified by (II.27), into the thermodynamic equations by what are artificial means, at best. By this reasoning it is clear that only the second and third members of (II.14) would be used as constraints in a thermodynamic variational calculation for centrifugation. If these constraints are used in conjuction with the equilibrium criterion $\delta F = 0$, $\delta T = 0$ of Theorem II.12(3) then the resulting equations which determine the composition are

$$\mu^\sigma + \Lambda^1\mathsf{M}^\sigma + \Lambda^\alpha a^\sigma_\alpha = 0$$

and these must be supplemented by equations to determine $T$, $m$, and $v_k$. These supplementary equations obviously would include the mass continuity equation (A.IV.2.1) and the momentum conservation equation (A.IV.2.4). For fluids the latter takes the form

$$m\frac{\delta v_k}{\delta t} = -\nabla_k(\Omega + p) + f_k + g_{ki}\nabla_j(\Delta\tau^{ij}),$$

where $p = -\partial(u - Ts)/\partial(1/m)$ and this contains (II.27) as a special case. To see this we need only assume that the motion is purely rotational and, hence, that the velocity is described by the skew symmetric vorticity tensor $\omega_{ij} = -\omega_{ji}$. That is, $\nabla_j v_k = \omega_{jk} = -\nabla_k v_j$. Then $\delta v_k/\delta t = \partial v_k/\partial t + v^j\nabla_j v_k = \partial v_k/\partial t - v^j\nabla_k v_j = \partial v_k/\partial t - \nabla_k(v^2/2)$. Hence, momentum conservation becomes

$$\nabla_k(\Omega + p) - m\nabla_k(v^2/2) = -\partial v_k/\partial t + f_k + g_{ki}\nabla_j(\Delta\tau^{ij})$$

which clearly specializes to (II.27).

The last example is an open, thermodynamic, fluid system constrained by the differential counterparts of $K_{(+)}$, $K_1$, and $K_2$ in (II.14),

$$\begin{aligned} k_{(+)} &\equiv \nabla_k J^k_{\mathscr{E}} = 0, \\ k_1 &\equiv \nabla_k(mv^k) = \nabla_k(M^\nu \tilde{n}_\nu v^k) = 0, \\ k_\alpha &\equiv \nabla_k(mb_\alpha) = \nabla_k(a^\nu_\alpha \tilde{n}_\nu v^k) = 0. \end{aligned} \qquad \text{(II.28)}$$

The Lagrangian for this problem has the form

$$\mathscr{L} = \tilde{s} + \lambda^{(+)}k_{(+)} + \lambda^1 k_1 + \lambda^\alpha k_\alpha \qquad \text{(II.29)}$$

but I shall make some assumptions about $\tilde{s}$ and $k_{(+)}$ which are not essential but which are made solely to simplify the calculation somewhat. I shall neglect all electromagnetic effects in $\tilde{s}$ and $k_{(+)}$. With this condition $\tilde{s}$ becomes a function of $\tilde{u}$ and $\tilde{n}_\nu$ alone and the energy flux takes the simpler form

$$J^k_{\mathscr{E}} = [\tilde{u} + \mathsf{M}^\nu\tilde{n}_\nu(\Omega + v^2/2)]v^k + (p^{kj} - \Delta\tau^{kj})v_j + q^k + \mu^\nu d^k_\nu,$$

where $-p_{ij} \equiv mS^{kl}B_{klij} = mS_{il}g^{lk}G_{kj}$. Now for a fluid $G_{kj} = Gg_{kj}$ and thus $p^k_k = 3p$ and the energy flux can be written in the form in which I will use it,

$$J^k_{\mathscr{E}} = [\tilde{u} + \mathsf{M}^\nu\tilde{n}_\nu(\Omega + v^2/2) + p]v^k + (p^{kj} - p^i g^{kj}/3 - \Delta\tau^{kj})v_j + q^k + \mu^\nu d^k_\nu. \qquad \text{(II.30)}$$

In this expression for the energy flux $p = T\partial s/\partial(1/m) = p((u, 1/m, n_\nu)$ and since $p$ is intensive $p = p(\tilde{u}, 1, \tilde{n}_\nu)$. Observe that the combination $\tilde{u} + p$ is the enthalpy per unit volume. We can now calculate $\delta\mathscr{L}$ subject to the conditions $\delta\Omega = 0$, $\delta v^k = 0$, $\delta(p^{kj} - g^{kj}p^i/3 - \Delta\tau^{kj}) = 0$, and $\delta(q^k + \mu^\nu d^k_\nu) = 0$,

$$\begin{aligned} \delta\mathscr{L} = {} & k_{(+)}\delta\lambda^{(+)} + k_1\delta\lambda^1 + k_\alpha\delta\lambda^\alpha \\ & + [T^{-1} - (1 + \partial p/\partial\tilde{u})v^k\nabla_k\lambda^{(+)}]\delta\tilde{u} \\ & - \{T^{-1}\mu^\sigma + [\mathsf{M}^\sigma(\Omega + v^2/2) + \partial p/\partial\tilde{n}_\sigma] \\ & \times v^k\nabla_k\lambda^{(+)} + \mathsf{M}^\sigma v^k\nabla_k\lambda^1 + a^\sigma_\alpha v^k\nabla_k\lambda^\alpha\}\delta\tilde{n}_\sigma \\ & + \nabla_k[\lambda^{(+)}\delta J^k_{\mathscr{E}} + (\lambda^1\mathsf{M}^\sigma + \lambda^\alpha a^\sigma_\alpha)\delta\tilde{n}_\sigma v^k]. \end{aligned}$$

To obtain this form for $\delta\mathscr{L}$ I used, for example, relations of the type $\lambda^{(+)}\nabla_k\delta J^k_{\mathscr{E}} = \nabla_k(\lambda^{(+)}\delta J^k_{\mathscr{E}}) - \delta J^k_{\mathscr{E}}\nabla_k\lambda^{(+)}$. The divergence terms in $\delta\mathscr{L}$ will not contribute to the Euler–Lagrange equations for the problem because they vanish by the transversality conditions when converted to integrands on the boundary. Thus these terms can be ignored when we write down the Euler–Lagrange equations implied by $\delta\mathscr{L} = 0$,

$$\nabla_k\{[\tilde{u} + \mathsf{M}^\nu\tilde{n}_\nu(\Omega + v^2/2) + p]v^k + (p^{kj} - g^{kj}p_i^i/3 - \Delta\tau^{kj})v_j + q^k + \mu^\nu d_\nu^k\} = 0,$$
$$\nabla_k(\mathsf{M}^\nu\tilde{n}_\nu v^k) = 0,$$
$$\nabla_k(a_\alpha^\nu\tilde{n}_\nu v^k) = 0,$$
$$T^{-1} - (1 + \partial p/\partial\tilde{u})v^k\nabla_k\lambda^{(+)} = 0,$$
$$T^{-1}\mu^\sigma + [\mathsf{M}^\sigma(\Omega + v^2/2) + \partial p/\partial\tilde{n}_\sigma]v^k\nabla_k\lambda^{(+)} + \mathsf{M}^\sigma v^k\nabla_k\lambda^1 + a_\alpha^\sigma v^k\nabla_k\lambda^\alpha = 0. \quad \text{(II.31)}$$

## CONCLUDING REMARKS

In this paper I have extended the algebraic theory of thermodynamics to include the effect of algebraic sturcture induced by the body itself. The extended theory leads directly to, and justifies, a variational method of thermodynamic calculations which encompasses the traditional thermodynamic calculations as special cases. More importantly it permits the extension of thermodynamic calculations to states which heretofore were considered to be outside the province of thermodynamics. The traditional thermodynamic states, constant functions on a subsystem, are the ones that are important for thermodynamic experiments because they minimize the number of measurements which are necessary to characterize the state of a body. But states with gradients are more common, and technologically more important, so the extension permits thermodynamics to become a more versatile and useful tool.

## APPENDIX

Some typographical errors have been found in the first paper and the corrections are listed below.

1. p. 1586, Definition I.24, line 3 should read "ment of $M$ iff $m \leqslant_M m^0 \forall m \in M$. It is said to be maxi-."

2. p. 1586, Definition I.27, line 6 should read "$m_3 \leqslant_M m_1 \Rightarrow m_2 \leqslant m_3$ or $m_3 \leqslant_M m_2 \forall m_1, m_2, m_3 \in M$."

3. p. 1588, Theorem I.38, line 4 and line 5 should read " a subset of some maximal chain and, $\forall x, x' \in \Sigma, x =_{\mathscr{A}} x'$ iff $x \leqslant_{\mathscr{A}} x'$ and $x' \leqslant_{\mathscr{A}} x$."

4. p. 1589, Theorem I.42, line 2. The statement "$e \in [e]$" should read "$e' \in [e] \cap C$."

5. p. 1599, Corollary III. 5, line 6 of the proof. The symbol "$\partial z^\alpha$" should read "$dz^\alpha$."

6. p. 1600, the first line after Definition III.7. The word "cited" should be deleted.

7. p. 1601, the third line after Theorem III.9. The word "chain" should read "chains."

8. p. 1606, the fifth line after Eq. (IV.2.10), the symbol $\epsilon_{kl}$ should be $e_{kl}$.

9. p. 1608, Eq. (IV.17.3). The symbol $\delta W$ should be $\mathfrak{d}W$.

10. p. 1609, line 9 of the first paragraph. The beginning of the line should read " that is, $\mathfrak{d}q$,."

11. p. 1609, line 22 and line 23. The upper case letter "$P$" should be replaced by a lower case letter "$p$."

The theorem below is an extended version of Theorem A.I.42 obtained by proving the converse of the original theorem.

*Theorem* I.42 (extended): Let $C$ be a chain, not necessarily maximal, in $(\Sigma, \leqslant_{\mathscr{A}}, =_{\mathscr{A}})$ and $e$ an equilibrium state of $C$. Then $e'$ is an equilibrium state of $C$ iff $e' \in [e] \cap C$.

*Proof*: Now $e$ is an equilibrium state and hence $e \in C$. Suppose $e'$ is an equilibrium state of $C$. Then $e' \in C$ and hence $e \leqslant_{\mathscr{A}} e'$ or $e' \leqslant_{\mathscr{A}} e$. But because $e$ is an equilibrium state $e' \leqslant_{\mathscr{A}} e \Rightarrow e =_{\mathscr{A}} e'$ and in either case $e =_{\mathscr{A}} e'$. Thus $e' \in [e]$ and hence $e' \in [e] \cap C$. The converse is established in Theorem A.I.42.


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# Some remarks on the classical vacuum structure of gauge field theories [a)]

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A simple and useful characterization of the global copies of any classical gauge vacuum is given. When the gauge group is abelian we obtain through that characterization a necessary and sufficient condition for the equivalence of the principal fiber bundles on which any two of such copies are defined. We compute by using also that characterization the classical vacuum structures of some nonabelian gauge field theories defined on different space–times.

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## 1. INTRODUCTION

In the last several years, the study of the quantum vacuum structure of the Yang–Mills theory has pointed out important physical properties of such a theory: multiplicity of quantum vacua with different realizations of the quantum Yang–Mills theory for each one of them, resolution of the U(1) problem, appearance of instantons, etc.[1–3] That vacuum structure is built from the classical vacuum of the Yang–Mills theory: the gauge fields whose field strengths are null on the whole of the space–time.

When the space–time is the Minkowski space–time it is clear that all of those gauge fields are trivial, because they are defined on $\mathbb{R}^4$, which is a simply connected manifold, and every flat connection (i.e., with null curvature) defined on a simply connected manifold is trivial.[4] The same result holds for the gauge vacuum of spatially compactified space–times defined over $\mathbb{R}\times S^3$. But if one considers the gauge vacuum on nonsimply connected space–times that result does not hold: nontrivial flat gauge fields may exist. When the gauge group is U(1) and the space–time manifold is $\mathbb{R}\times S^1$ this fact gives rise to the Aharonov–Bohm effect of the electromagnetic gauge field, which points out the physical difference between the global gauge field copies (equivalence classes of connections with equivalent curvatures) of the electromagnetic vacuum.[5,6]

In an early paper,[7] Kostant has shown that the group $\mathrm{Hom}(\pi_1(M),\mathrm{U}(1))$ acts freely over the set of equivalence classes of the connections with gauge group U(1) on an arbitrary manifold $M$ having the same curvature. Hence the global copies of the U(1) classical vacuum on $M$ are in one-to-one correspondence with the elements of the group $\mathrm{Hom}(\pi_1(M),\mathrm{U}(1))$. In particular, for the manifold $\mathbb{R}^3\times S^1$ of the Aharonov–Bohm effect the global copies of the electromagnetic vacuum are in one-to-one correspondence with the elements of $\mathrm{Hom}(\mathbb{Z},\mathrm{U}(1))\approx\mathrm{U}(1)$.

The aim of the present paper is to extend the U(1) analysis of Kostant for any gauge group in order to know the classical degeneracy of the general gauge vacuum. In Sec. 2 we find the extended characterization of the global copies of any gauge vacuum and we give when the gauge group is abelian a criterion through this characterization for the equivalence of the principal fiber bundles in which such copies are defined. General results of Sec. 2 are applied in Sec. 3 to some space–time manifolds and physical gauge groups. Section 4 contains the conclusions and some final remarks about this classical degeneracy of the gauge vacuum.

## 2. GLOBAL COPIES OF THE GAUGE VACUUM

Let $M$ be a connected differentiable manifold and $G$ a Lie group. Let us consider a fixed point $x_0$ of $M$ and the first homotopy group $\pi_1(M)$ of $M$ with base point $x_0$. In the group $\mathrm{Hom}(\pi_1(M),G)$ we have the relation of equivalence such that for any $\xi,\xi'\in\mathrm{Hom}(\pi_1(M),G)$ $\xi\sim\xi'$ ($\xi$ is congruent with $\xi'$) iff there is a $g\in G$ with $\xi'(l)=g^{-1}\xi(l)g$ for every $l\in\pi_1(M)$. Let us denote its quotient space by $\mathrm{Chom}(\pi_1(M),G)$ and the equivalence class of $\xi$ by $[\xi]$. There is also a relation of equivalence in the set of gauge fields on $M$ with gauge group $G$: Two connections $\Gamma$ and $\Gamma'$ defined in two principal fiber bundles $P(M,G)$ and $P'(M,G)$, respectively, are equivalent iff there is an $M$ isomorphism $(\psi,\mathrm{id}_G)$ of $P$ in $P'$ mapping $\Gamma$ in $\Gamma'$ (in such a case the principal fiber bundles $P(M,G)$ and $P'(M,G)$ are said to be also equivalent). We shall denote the equivalence class of $\Gamma$ by $[\Gamma]$.

Each flat connection $\Gamma$ defined on any principal fiber bundle $P(M,G)$ has associated an element of $\mathrm{Chom}(\pi_1(M),G)$ in the following way. If we choose an element $u\in P$ with $\Pi_P(u)=x_0$, each continuous piecewise differentiable closed curve of $M$ beginning and ending at $x_0$ defines an element of the holonomy group of $\Gamma$ at $u$. Since $\Gamma$ is flat this element is the same for all the curves in the same homotopy class, and it is obvious that the mapping $\xi_u:\pi_1(M)\to G$ so defined is a homomorphism of groups. If we choose another point $v\in\Pi_P^{-1}(x_0)$, since there is a $g\in G$ with $v=ug$, we have that $\xi_v(l)=g^{-1}\xi_u(l)g$ for every $l\in\pi_1(M)$. Hence the equivalence class of $\xi_u$ is independent of the $u\in\Pi_P^{-1}(x_0)$ chosen. Moreover, it is trivial to see that this class is the same for all the connections being equivalent to $\Gamma$ and in this way we have built a mapping $\kappa$ of $\mathscr{V}_M^G$ into $\mathrm{Chom}(\pi_1(M),G)$, $\mathscr{V}_M^G$ being the set of equivalence classes of flat connections on $M$ with gauge group $G$ (i.e., the global copies of the gauge vacuum).

*Theorem* 1: For any connected manifold $M$ and any Lie group $G$ the mapping

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$$\kappa: \mathscr{V}_M^G \to \mathrm{Chom}(\pi_1(M), G)$$

is bijective.

*Proof*: In order to see the one-to-one character of $\kappa$ let us assume that $\Gamma$ and $\Gamma'$ are two arbitrary flat connections on $M$ with gauge group $G$ such that

$$\kappa([\Gamma]) = \kappa([\Gamma']). \tag{1}$$

Let $P(M,G)$, $P'(M,G)$ be the principal fiber bundles where $\Gamma$ and $\Gamma'$, respectively, are defined. Since (1) holds there exist two points $u_0 \in P$ and $u_0' \in P'$ with $\Pi_{P'}(u_0') = \Pi_P(u_0) = x_0$ and $\xi_{u_0} = \xi_{u_0'}$ and hence we can define a mapping $\psi$ of $P$ into $P'$ in the following way. Let us consider the holonomy bundle $P_0$ of $\Gamma$ at $u_0$, i.e., the submanifold of $P$ whose points can be joined to $u_0$ by a horizontal curve with respect to $\Gamma$. For every point $u \in P_0$ we can define $\psi(u)$ as the ending point of the horizontal lifting with respect to $\Gamma'$ beginning at $u_0'$ of the projection on $M$ of any horizontal curve of $P_0$ with respect to $\Gamma$ beginning at $u_0$ and ending at $u$, because that end point is independent of the chosen horizontal curve of $P_0$ connecting $u_0$ and $u$. Indeed, if $\gamma_1$ and $\gamma_2$ are two horizontal curves of $P_0$ with $\gamma_1(0) = \gamma_1(0) = u_0$ and $\gamma_1(1) = \gamma_2(1) = u$, the continuous piecewise differentiable curve $\gamma_3$ defined by

$$\begin{aligned} \gamma_3 t &= \gamma_1(2t) \quad \text{if} \quad 0 \leqslant t \leqslant \tfrac{1}{2}, \\ &= \gamma_2(2-2t) \quad \text{if} \quad \tfrac{1}{2} \leqslant t \leqslant 1, \end{aligned}$$

is closed and horizontal in $P_0$ with respect to $\Gamma$. Now, since $\xi_{u_0} = \xi_{u_0'}$, the continuous horizontal lifting at $u_0'$ in $P'$ of the projection on $M$ of $\gamma_3$ is also closed, which implies that $\gamma_1'(1) = \gamma_2'(1)$, $\gamma_1'$ and $\gamma_2'$ being the horizontal liftings at $u_0'$ in $P'$ of the projections on $M$ of $\gamma_1$ and $\gamma_2$, respectively. Since $M$ is a connected manifold, it is arcwise connected. Therefore $P_0$ intersects every fiber of $P$ and we can extend the definition of $\psi$ to the whole of $P$ in such a way that

$$\psi(ug) = \psi(u)g$$

for any $u \in P_0$ and $g \in G$. It is trivial to see that $(\psi, \mathrm{id}_G)$ is a $M$ homomorphism from $P$ into $P'$ which maps $\Gamma$ into $\Gamma'$. In the same way we define a $M$ homomorphism $(\psi', \mathrm{id}_G)$ from $P'$ into $P$ which maps $\Gamma'$ in $\Gamma$. Now from both definitions it follows that $\psi \circ \psi' = \mathrm{id}_{P'}$, $\psi' \circ \psi = \mathrm{id}_P$ and hence that $(\psi, \mathrm{id}_G)$ is a $M$ isomorphism from $P$ into $P'$, which implies that $\Gamma$ and $\Gamma'$ are equivalent, i.e., $[\Gamma] = [\Gamma'] \in \mathscr{V}_M^G$. Thus $\kappa$ is one-to-one.

We shall now prove that $\kappa$ is surjective. Let $\Pi_{\mathscr{M}}: \mathscr{M} \to M$ be a universal covering of $M$ and $x$ a fixed point of $\Pi_{\mathscr{M}}^{-1}(x_0)$. Then there is a differentiable action by the right of $\pi_1(M)$ as discrete group on $\mathscr{M}$ which gives to $\mathscr{M}(M, \Pi_{\mathscr{M}}, \pi_1(M))$ a principal fiber bundle structure and such that for each $l \in \pi_1(M)$, $xl$ is the end point of the differentiable lifting in $\mathscr{M}_M^G$ beginning at $x$ for every closed curve of the homotopy class $l$.[8] Let us now define for each $\xi \in \mathrm{Hom}(\pi_1(M), G)$ the right action of $\pi_1(M)$ on $\mathscr{M} \times G$ given by

$$(y,g)l = (yl, \xi(l)^{-1} g) \tag{2}$$

for every $(y,g) \in \mathscr{M} \times G$ and $l \in \pi_1(M)$. Since the action of $\pi_1(M)$ on $\mathscr{M}$ is properly discontinuous, the action defined by (2) is also properly discontinuous, which implies that the quotient space $P = \mathscr{M} \times G / \pi_1(M)$ is a manifold and that the natural projection $\Pi$ from $\mathscr{M} \times G$ into $P$ is differentiable. On the other hand this action commutes with the canonical action of $G$ on $\mathscr{M} \times G$. Hence we can project the canonical action of $G$ on $\mathscr{M} \times G$ to an action of $G$ on $P$, which corresponding quotient manifold is isomorphic to $M$. It is trivial to see that with this action $P(M,G)$ is a principal fiber bundle and that $(\Pi, \mathrm{id}_G)$ is a homorphism of principal fiber bundles from $\mathscr{M} \times G$ into $P(M,G)$. Let us now consider the trivial connection $\Gamma_0$ in $\mathscr{M} \times G$ defined in each point $(y,g)$ of $\mathscr{M} \times G$ by the subspace of the tangent space of $\mathscr{M} \times G$ at $(y,g)$ which is tangent to the submanifold $\mathscr{M}_g = \{(z,g); z \in \mathscr{M}\}$. Because

$$\mathscr{M}_g l = \mathscr{M}_{\xi(l)^{-1} g}$$

for any $l \in \pi_1(M)$ and $g \in G$, $\Gamma_0$ is invariant by the action of $\pi_1(M)$. Therefore $\Pi$ maps $\Gamma_0$ into a flat connection $\Gamma$ in $P$. On the other hand, since $\mathscr{M}$ is arcwise connected, for every $l \in \pi_1(M)$ there is a curve $\gamma_l: [0,1] \to \mathscr{M}$ with $\gamma_l(0) = x$ and $\gamma_l(1) = xl$. The projection through $\Pi_{\mathscr{M}}$ on $M$ of such a curve $\Pi_{\mathscr{M}} \circ \gamma_l$ is a closed curve beginning and ending at $\Pi_{\mathscr{M}}(x) = \Pi_{\mathscr{M}}(xl) = x_0$ which belongs to the homotopy class $l$ of $\pi_1(M)$. From the construction of $\Gamma$ it follows that the horizontal lifting of $\Pi_{\mathscr{M}} \circ \gamma_l$ with respect to $\Gamma$ at $u = \Pi(x,e)$ is the projection through $\Pi$ of the horizontal lifting $\bar{\gamma}_l$ of $\gamma_l$ with respect to $\Gamma_0$ at $u_0 = (x,e)$. Since $\bar{\gamma}_l(t) = (\gamma_l(t), e)$ for every $t \in [0,1]$ we have that $\Pi \circ \bar{\gamma}_l(1) = \Pi(\bar{\gamma}_l(0)) \xi(l)$ and therefore that

$$\xi_u(l) = \xi(l). \tag{3}$$

Finally, because (3) holds for every $l \in \pi_1(M)$ we have proved that $\kappa([\Gamma]) = [\xi]$, which points out the surjective character of the map $\kappa$. Q.E.D.

The above theorem gives us a faithful characterization of the classical gauge vacuum structure through the set $\mathrm{Chom}(\pi_1(H), G)$ which obviously depends on the gauge group and on the topological structure of the space–time.

Note that this simple characterization of the global copies with null curvature is a consequence of the unicity of the local copy with null curvature. When the curvature of a non–abelian gauge field is not null it may have many local copies[9,10] and therefore in this case the characterization of the global ones is more complex.

Whenever $\pi_1(M) = 0$ we have that $\mathrm{Chom}(\pi_1(M), G) = 0$ and in this case Theorem 1 shows us again that all flat gauge fields on a connected and simply connected manifold $M$ are trivial, i.e., all the classical gauge vacuum structures on $M$ are trivial.

If $G$ is abelian, for any connected manifold $M$

$$\mathrm{Chom}(\pi_1(M), G) = \mathrm{Hom}(\pi_1(M), G).$$

Therefore in this case the global copies of the gauge vacuum are in one-to-one correspondence with the elements of the abelian group $\mathrm{Hom}(\pi_1(M), G)$, which agrees with the Kostant result when $G = \mathrm{U}(1)$. We shall now see by using this correspondence which of those global copies of the abelian gauge vacuum are defined in the same equivalence class of principal fiber bundles. Let $\mathfrak{g}$ be the abelian Lie algebra of $G$. The exponential map

$$\exp: \mathfrak{g} \to G$$

is in this case a homomorphism of abelian groups, and hence the mapping

$$\mathrm{EXP}: \mathrm{Hom}(\pi_1(M), \mathfrak{g}) \to \mathrm{Hom}(\pi_1(M), G)$$

defined by

$$\mathrm{EXP}\xi(l) = \exp(\xi(l))$$

for any $\xi \in \mathrm{Hom}(\pi_1(H),\mathfrak{g})$ and $l \in \pi_1(M)$ is also a homomorphism of abelian groups.

*Theorem* 2: Two flat connections $\Gamma$ and $\Gamma'$ on a connected manifold $M$ with abelian gauge group $G$ are defined in equivalent principal fiber bundles iff there exists a homomorphism $\eta \in \mathrm{Hom}(\pi_1(M),\mathfrak{g})$ such that

$$\kappa([\Gamma']) = \kappa([\Gamma])\mathrm{EXP}\eta. \tag{4}$$

*Proof*: Suppose that $\Gamma$ and $\Gamma'$ are defined in equivalent principal fiber bundles. Then there is a principal fiber bundle $P(M,G)$ where the connection $\Gamma$ and a connection equivalent to $\Gamma'$ which we shall also denote by $\Gamma'$ are simultaneously defined.

If $\omega$ and $\omega'$ are the connections 1-forms in $P$ of $\Gamma$ and $\Gamma'$, respectively, we have that $\tau = \omega' - \omega$ is a $\mathfrak{g}$-valued tensorial 1-form of type ad$G$ of $P$. Since $\mathfrak{g}$ is abelian there is a $\mathfrak{g}$-valued 1-form $\alpha$ of $M$ such that $\tau = \Pi_P^* \alpha$, $\Pi_P$ being the projection from $P$ on $M$.

$$\{e^i,\ i = 1,\ldots,n\}$$

be a basis of $\mathfrak{g}$, where $n = \dim G$. The $\mathfrak{g}$-valued 1-form $\alpha$ splits into $n$ real 1-forms $\alpha_i$ in such a way that

$$\alpha = \sum_{i=1}^{n} \alpha_i e_i.$$

Since $\Gamma$ and $\Gamma'$ are flat we have $d\alpha = 0$, which implies that $d\alpha_i = 0$, $i = 1,\ldots,n$, i.e., each real 1-form $\alpha_i$ is closed. Accordingly the mapping associating

$$\sum_{i=1}^{n} \left( - \int_\gamma \alpha_i \right) e^i \in \mathfrak{g}$$

to each closed curve $\gamma$ in $M$ beginning and ending at $x_0$, which obviously is independent of the basis of $\mathfrak{g}$ chosen, only depends on the homotopy class of $\gamma$, because

$$\int_\gamma \alpha_i = \int_{\gamma'} \alpha_i \quad i = 1,\ldots,n,$$

for every closed curve $\gamma'$ in $M$ of the same homotopy class of $\gamma$. Let $\eta$ be the homomorphism of $\pi_1(M)$ into $\mathfrak{g}$ defined by that mapping. In order to prove that $\eta$ satisfies the equality (4) it is sufficient to see that for each horizontal lift $\bar{\gamma}$ in $P$ with respect to $\Gamma$ of any closed curve $\gamma$ in $M$ the curve $\bar{\gamma}'$ defined by

$$\bar{\gamma}'(t) = \gamma(t) \exp\left\{ \sum_{i=1}^{n} \left( - \int_0^t \alpha_i(\dot{\gamma}_t)\, dt \right) e^i \right\}$$

is an horizontal lift of $\gamma$ in $P$ with respect to $\Gamma'$, $\dot{\gamma}_t$ being the tangent vector to $\gamma$ at $\gamma(t)$. Now by Leibniz's formula

$$\dot{\bar{\gamma}}'_t = \dot{\bar{\gamma}}_t \exp\left\{ \sum_{i=1}^{n} \left( - \int_0^t \alpha_i(\dot{\gamma}_t)\, dt \right) e^i \right\} - \sum_{i=1}^{n} \alpha_i(\dot{\gamma}_t) \chi^i_{\bar{\gamma}(t)}$$

for every $t \in [0,1]$, $\chi^i$ being the vector field of $P$ defined by the corresponding element $e^i$ of $\mathfrak{g}$ through the action of $G$ on $P$ and $\dot{\bar{\gamma}}_t \exp\{\Sigma_{i=1}^n (-\int_0^t \alpha_i(\dot{\gamma}_t)\, dt) e^i\}$ being the transformed tangent vector of $\dot{\bar{\gamma}}_t$ through the action of $\exp\{\Sigma_{i=1}^n (-\int_0^t \alpha_i(\dot{\gamma}_t)\, dt) e^i\} \in G$ on $P$. Thus, since $\omega(\dot{\bar{\gamma}}_t) = 0$ and $\omega(\chi^i_{\bar{\gamma}(t)}) = e^i$, we have

$$\omega'(\dot{\bar{\gamma}}'_t) = 0$$

for every $t \in [0,1]$, which shows that $\bar{\gamma}'$ is a horizontal lift of $\gamma$ in $P$ with respect to $\Gamma'$.

Conversely, suppose that equality (4) holds for some $\eta \in \mathrm{hom}(\pi_1(M),\mathfrak{g})$. In the basis $\{e^i, i = 1,\ldots,n\}$ of $\mathfrak{g}$ the homomorphism $\eta$ splits into $\eta$ homomorphisms $\eta_i$, $i = 1,\ldots,n$, of $\pi_1(M)$ into $\mathbb{R}$ in such a way that

$$\eta = \sum_{i=1}^{n} \eta_i e^i.$$

By Rham's theorem[11] there are in $M$ $n$ closed real 1-forms $\alpha_i$, $i = 1,\ldots,n$, such that for any $l \in \pi_1(M)$

$$\eta_i(l) = \int_\gamma \alpha_i,$$

$\gamma$ being any closed curve in $M$ of the homotopy class $l$. Let $\alpha$ be the closed $\mathfrak{g}$-valued 1-form of $M$ defined by

$$\alpha = \sum_{i=1}^{n} \alpha_i e^i,$$

which obviously is independent of the basis of $\mathfrak{g}$ chosen. It is easy to see that the $\mathfrak{g}$-valued 1-form

$$\bar{\omega} = \omega + \Pi_P^* \alpha$$

defines a flat connection $\bar{\Gamma}$ in the principal fiber bundle $P(M,G)$ where $\Gamma$ is defined. Then we have

$$\kappa([\bar{\Gamma}]) = \kappa([\Gamma])\ \mathrm{EXP}\eta = \kappa([\Gamma']),$$

which implies by Theorem 1 that $\Gamma'$ and $\bar{\Gamma}$ are equivalent. Thus the principal fiber bundle where $\Gamma'$ is defined is equivalent to $P$. Q.E.D.

The preceding theorem enables us to know that the global copies of any abelian gauge vacuum on a connected space–time manifold $M$ which are defined in trivial principal fiber bundles are given by the elements of

$$\kappa^{-1} \circ \mathrm{EXP}(\mathrm{Hom}(\pi_1(M),\mathfrak{g})) \subset \mathscr{V}_M^G.$$

Another important consequence of Theorem 2 is that the equivalence classes of principal fiber bundles on a connected manifold $M$ with abelian structure group $G$ where flat connections are defined are in one-to-one correspondence with the elements of the group

$$\mathrm{Hom}(\pi_1(M),G)/\mathrm{Hom}(\pi_1(M),\mathfrak{g}),$$

where $\mathrm{Hom}(\pi,(M),\mathfrak{g})$ and its image in $\mathrm{Hom}(\pi_1(M),G)$ through the mapping EXP are identified. In particular, the existence of space–time manifolds with

$$\mathrm{Hom}(\pi_1(M),\mathrm{U}(1))/\mathrm{Hom}(\pi_1(M),\mathbb{R}) \neq \{0\}$$

was used by Boya and myself[12] in order to point out the existence of electromagnetic gauge fields without monopoles defined in nontrivial fiber bundles.

Accordingly, the two preceding theorems give us a simple and complete description of the classical vacuum structure of any abelian gauge field theory. Nevertheless most of the fundamental gauge field theories appearing in physics are non-abelian and their vacuum structure is more complex, because in general

$$\mathrm{Chom}(\pi_1(M),G) \neq \mathrm{Hom}(\pi_1(M),G)$$

and, theorem 2 does not hold for them. We shall analyze some simple cases of such vacua in the next section.

## 3. SOME VACUUM STRUCTURES OF NONABELIAN GAUGE FIELD THEORIES

For the sake of simplicity we shall only consider special orthogonal gauge groups SO($N$) and special unitary gauge groups SU($N$) with $N \geqslant 2$.

### A. $\pi_1(M) = \mathbb{Z}$

First, let us analyze the nonabelian gauge vacua of the space–time manifold of the Aharonov–Bohm effect $\mathbb{R}^3 \times S^1$. Since $\pi_1(\mathbb{R}^3 \times S^1) = \mathbb{Z}$ every $\xi \in \mathrm{Hom}(\pi_1(M),G)$ is completely given by $\xi(1) \in G$. When $G = \mathrm{SU}(N)$ every $A \in \mathrm{SU}(N)$ can be diagonalized by means of a unitary transformation, i.e., there exists $U \in \mathrm{U}(N)$ such that $U^{-1}AU$ is diagonal. Therefore, $U_1 = (\det U)^{-1/N} U \in \mathrm{SU}(N)$ verifies that $U_1^{-1}AU_1$ is also diagonal, which implies that $A$ is congruent with a diagonal element of SU($N$). In the same way, since the matrices of the invertible linear transformations interchanging the vectors of the natural basis of $\mathbb{C}^N$ are unitary, $A$ is always congruent with a diagonal matrix of the form

$$\begin{pmatrix} \exp i\lambda_1 & 0 & \cdots & 0 & 0 \\ 0 & \exp i\lambda_2 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \exp i\lambda_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \exp\left(-i\sum_{i=1}^{N-1}\lambda_i\right) \end{pmatrix} \in \mathrm{SU}(N), \tag{5}$$

with $\lambda_1,\ldots,\lambda_{N-1} \in [0,2\pi)$ and $\lambda_1 \leqslant \cdots \leqslant \lambda_{N-1}$. Accordingly,

$$\mathscr{Y}^{\mathrm{SU}(N)}_{\mathbb{R}^3\times S^1} \approx \mathrm{Chom}(\mathbb{Z},\mathrm{SU}(N)) \approx \mathcal{A}_1^N U(1),$$

where

$$\mathcal{A}_1^N \mathrm{U}(1) = \{(\exp i\lambda_1,\ldots,\exp i\lambda_N) \in \mathrm{U}(1)^N : \lambda_i \in [0,2\pi), \lambda_1 \leqslant \cdots \leqslant \lambda_{N-1}, (1/2\pi)\sum_{i=1}^{N}\lambda_i \in \mathbb{N}\}.$$

In a similar way we obtain for $G = \mathrm{SO}(N)$

$$\mathscr{Y}^{\mathrm{SO}(N)}_{\mathbb{R}^3\times S^1} \approx \mathrm{Chom}(\mathbb{Z},\mathrm{SO}(N)) \approx \mathcal{A}^{[N/2]}\mathrm{SO}(2),$$

where $[N/2]$ is the highest integer $z$ with $z \leqslant N/2$ and where

$$\mathcal{A}^{[N/2]}\mathrm{SO}(2) = \left\{ (\exp i\lambda_1\sigma,\ldots,\exp i\lambda_{[N/2]}\sigma) \in \mathrm{SO}(2)^{[N/2]} : \sigma = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ \lambda_i \in [0,2\pi),\ \lambda_1 \leqslant \cdots \leqslant \lambda_{[N/2]} \right\}.$$

On the other hand, since the classes of principal fiber bundles on $\mathbb{R}^3 \times S^1$ with gauge group $G$ are in one-to-one correspondence with homotopy classes of mappings of $S^0 = \{1,-1\}$ into $G$,[8] when $G$ is connected all principal fiber bundles on $\mathbb{R}^3 \times S^1$ with gauge group $G$ are trivial. Thus the global copies of $\mathscr{Y}^{\mathrm{SO}(N)}_{\mathbb{R}^3\times S^1}$ and $\mathscr{Y}^{\mathrm{SU}(N)}_{\mathbb{R}^3\times S^1}$ are defined in trivial principal fiber bundles.

Note that the SU(2) and SO(3) gauge vacuum structures on $\mathbb{R}^3 \times S^1$ are similar to the electromagentic ones giving rise to the Aharonov–Bohm effect. Indeed

$$\mathscr{Y}^{\mathrm{SU}(2)}_{\mathbb{R}^3\times S^1} \approx \mathrm{U}(1) \approx \mathscr{Y}^{\mathrm{SO}(3)}_{\mathbb{R}^3\times S^1} \approx \mathrm{SO}(2) \approx \mathscr{Y}^{\mathrm{U}(1)}_{\mathbb{R}^3\times S^1} \approx \mathrm{U}(1),$$

and all the copies of these vacuum structures are defined in trivial principal fiber bundles on $\mathbb{R}^3 \times S^1$ with gauge group SU(2), SO(3), and U(1), respectively.

### B. $\pi_1(M) = \mathbb{Z}_p$ $(p > 1)$

Let $L(p,1)$ be the quotient manifold (lens space) of the action of $\mathbb{Z}_p = \{a,a^2,\ldots,a^p = e\}$ in the sphere $S^3$ given by

$$(x^1,x^2,x^3,x^4)a^r = (x^1\cos 2\pi r/p - x^2\sin 2\pi r/p, x^1\sin 2\pi r/p + x^2\cos 2\pi r/p, x^3\cos 2\pi r/p - x^4\sin 2\pi r/p, x^3\sin 2\pi r/p + x^4\cos 2\pi r/p),$$

for $r = 1,2,\ldots,p$ and for all $(x^1,x^2,x^3,x^4) \in S^3 \subset \mathbb{R}^4$. The manifold $\mathbb{R} \times L(p,1)$ supports some admissible space–time structures.[12] How are the gauge vacuum structures defined on those space–times? Since $\pi_1(L(p,1)) = \mathbb{Z}_p$, $\pi_1(\mathbb{R}\times L(p,1)) = \mathbb{Z}_p$. Thus every $\xi \in \mathrm{Hom}(\pi_1(\mathbb{R}\times L(p,1)),G)$ is completely determined by $\xi(a)$. Now since every $A \in \mathrm{SU}(N)$ is congruent to a diagonal matrix of the form (5), we have

$$\mathscr{Y}^{\mathrm{SU}(N)}_{\mathbb{R}\times L(p,1)} \approx \mathrm{Chom}(\mathbb{R}\times L(p,1),\mathrm{SU}(N)) \approx \mathcal{A}_1^N \mathbb{Z}_p,$$

where

$$\mathcal{A}_1^N \mathbb{Z}_p = \{(a^{r_1},a^{r_2},\ldots,a^{r_N}) \in \mathbb{Z}^N : r_1 \leqslant r_2 \leqslant \cdots \leqslant r_N,\ (1/p)\sum_{i=1}^{N} r_i \in \mathbb{N}\},$$

and that each global copy of the vacuum $\mathscr{Y}^{\mathrm{SU}(N)}_{\mathbb{R}\times L(p,1)}$ is reducible to a global copy of the abelian vacuum $\mathscr{Y}^{\mathrm{U}(1)^N}_{\mathbb{R}\times L(p,1)}$. Nevertheless, though the copies of $\mathscr{Y}^{\mathrm{U}(1)^N}_{\mathbb{R}\times L(p,1)}$ are defined in nonequivalent principal fiber bundles because $\mathrm{Hom}(\mathbb{Z}_p,\mathbb{R}^N) = 0$, two copies of $\mathscr{Y}^{\mathrm{SU}(N)}_{\mathbb{R}\times L(p,1)}$ may be defined in equivalent principal fiber bundles because theorem 2 does not hold for the SU($N$) groups when $N \geqslant 2$.

In the same way, we prove that

$$\mathscr{Y}^{\mathrm{SO}(N)}_{\mathbb{R}\times L(p,1)} \approx \mathrm{Chom}(\pi_1(M),\mathrm{SO}(N)) = \mathcal{A}^{[N/2]}\mathbb{Z}_p,$$

and that each global copy of the vacuum $\mathscr{Y}^{\mathrm{SO}(N)}_{\mathbb{R}\times L(p,1)}$ is reducible to a global copy of the abelian vacuum $\mathscr{Y}^{\mathrm{SO}(2)^{[N/2]}}_{\mathbb{R}\times L(p,1)}$. In spite of this, two copies of $\mathscr{Y}^{\mathrm{SO}(N)}_{\mathbb{R}\times L(p,1)}$ may also be defined in equivalent principal fiber bundles when $N \geqslant 3$.

Up to now all the space–time manifolds considered had abelian first homotopy groups and hence the holonomy groups of the global copies of the gauge vacua on them were also abelian, which simplified the computation of the corresponding gauge vacuum structures. We shall now analyze a more complex case: the vacuum structures on a space–time manifold whose first homotopy group is not abelian.

### C. $\pi_1(M) = Q$

Let us consider the quaternion subgroup $Q$ of SU(2)

$$Q = \{\mathrm{I}, -\mathrm{I}, i\sigma_x, i\sigma_y, i\sigma_z, -i\sigma_x, -i\sigma_y, -i\sigma_z\},$$

where I is the identity of SU(2) and $\sigma_x$, $\sigma_y$, and $\sigma_z$ are the standard Pauli matrices. The action of $Q$ in SU(2) defined by the right product in SU(2) is free and properly discontinuous. Thus the corresponding quotient manifold $S_Q$ is paracompact and satisfies the exact homotopy sequence

$$\cdots\to\pi_1(\mathrm{SU}(2))\to\pi_1(S_Q)\to\pi_0(Q)+\pi_0(\mathrm{SU}(2))\to\cdots.$$

Then $\pi_1(M)\approx\pi_0(Q)\approx Q$ because $\pi_1(\mathrm{SU}(2))=\pi_0(\mathrm{SU}(2))=0$. $Q$ is the lowest non-abelian group which can be realized as the first homotopy group of the quotient manifold of a free action of a group over $\mathrm{SU}(2)\approx S^3$ (diffeomorphically). Indeed, the lowest non-abelian finite groups are the dihedra groups $D_3$ (order 6) and $D_4$ (order 8), and the quaternion group $Q$ (order 8). But there are no free actions of $D_3$ and $D_4$ on $S^3$ because in $D_3$ and $D_4$ there are involutive elements which do not lie in their corresponding group centers.[13]

On the other hand, since SU(2) is a Lie group it admits a right invariant orientation, which implies that $S_Q$ is also orientable. If we consider in $S_Q$ a Riemannian metric $g$ (there always exists such a metric because $S_Q$ is paracompact), we may define in $\mathbf{R}\times S_Q$ a Lorentzian metric $\bar{g}$ in such a way that for every $(t,x)\in\mathbf{R}\times S_Q$ we have

$$\bar{g}(v,v')=g(y,y')-ss'$$

for any two vectors $v=(s,y)$ and $v'=(s',y')$ of

$$T_{(t,x)}(\mathbf{R}\times S_Q)\approx T_t(\mathbf{R})\times T_x(S_Q)\approx\mathbf{R}\times T_x(S_Q).$$

Since $\mathbf{R}\times S_Q$ is orientable and $\mathbf{R}\times S_Q$ is time orientable with respect to $\bar{g}$, $(\mathbf{R}\times S_Q,\bar{g})$ is an admissible space–time which satisfies the causality condition. We shall now study the gauge vacuum structures of such kinds of space–times.

There are only five classes of inequivalent irreducible unitary representations of $Q$: the classes described by

(1) a two dimensional representation $\xi_0$ defined by the inclusion of $Q$ in SU(2);

(2) four unidimensional representations defined by

$$\xi_1(i\sigma_x)=\xi_1(i\sigma_y)=-1,\quad \xi_1(i\sigma_z)=\xi_1(-I)=1,$$
$$\xi_2(i\sigma_y)=\xi_2(i\sigma_z)=-1,\quad \xi_2(i\sigma_x)=\xi_2(-I)=1,$$
$$\xi_3(i\sigma_x)=\xi_3(i\sigma_z)=-1,\quad \xi_3(i\sigma_y)=\xi_3(-I)=1,$$
$$\xi_4(i\sigma_x)=\xi_4(i\sigma_y)=\xi_4(i\sigma_z)=\xi_4(-I)=1.$$

Consequently, since for any $i,j=1,2,3,4$ the representations $\xi_i\oplus\xi_j$ and $\xi_j\oplus\xi_i$ of $Q$ are equivalent, there are only eleven classes of nonequivalent two - dimensional unitary representations of $Q$: the classes described by the representations

$$\xi_0,\quad \xi_{ij}=\xi_i\oplus\xi_j\quad i<j,\quad i,j=1,2,3,4.$$

Now, if two $N$-dimensional special unitary representations $\xi,\xi'$ of $Q$ are equivalent they are unitary equivalent. Then there exists a matrix $U\in\mathrm{U}(N)$ with

$$U^{-1}\xi(A)U=\xi'(A),$$

for any $A\in Q$. Hence we have for $U_1=(\det U)^{-1/N}U\in\mathrm{SU}(N)$ also

$$U_1^{-1}\xi(A)U_1=\xi'(A),$$

for every $A\in Q$, which implies that $\xi$ and $\xi'$ are two congruent homomorphisms of $Q$ in SU($N$). Accordingly.

$$\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}\times S_Q}\approx\mathrm{Chom}(Q,\mathrm{SU}(2))\approx\{[\xi_0],[\xi_{ii}],\quad i=1,2,3,4\},$$

i.e., there are five global copies of the SU(2) gauge vacuum on $\mathbf{R}\times S_Q$. The copy corresponding to $[\xi_0]$ is the only copy of $\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}\times S_Q}$ having non-abelian holonomy groups. Note that $\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}\times S_Q}$ does not have a natural group structure.

In the same way, for any special unitary gauge group SU($N$) we find that

$$\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}\times S_Q}\approx\mathrm{Chom}(Q,\mathrm{SU}(N))\approx\bigcup_{i=0}^{[N/2]}\boldsymbol{A}_1^{N-2i}D_2,$$

where

$$\boldsymbol{A}_1^K D_2=\{(a_{i_1},\ldots,a_{i_k})\in D_2^K;i_1\leqslant\cdots\leqslant i_K,a_{i_1}\cdots a_{i_k}=e\}\ \text{ for } K>0,$$
$$\boldsymbol{A}_1^0 D_2=\{1\},$$
$$D_2=\{a_1,a_2,a_3,a_4=e\}\text{ being the second dihedral group.}$$

Similarly, we obtain

$$\mathscr{V}^{\mathrm{SO}(N)}_{\mathbf{R}\times LS_Q}\mathrm{Chom}(Q,\mathrm{SO}(N))\approx\{[\xi_{i_1\cdots i_N}]=[\xi_{i_1}\oplus\cdots\oplus\xi_{i_n}];i_1\leqslant\cdots\leqslant i_N,i_1,\ldots,i_N=1,2,3,4,\ \det\xi_{i_1\cdots i_N}(a)=1,a\in Q\}$$

i.e., there are $\mathrm{Card}\,\boldsymbol{A}_1^N D_2$ global copies of the SO($N$) gauge vacuum on $\mathbf{R}\times S_Q$. It is obvious that in this case all of these global copies have abelian holonomy groups.

Accordingly, the structure of nonabelian gauge vacua is more complex than the structure of the abelian ones. [For instance for the abelian groups U(1) and $\mathbf{R}$ we have

$$\mathscr{V}^{\mathrm{U}(1)}_{\mathbf{R}\times S_Q}\approx\mathrm{Hom}(Q,\mathrm{U}(1))\approx\{\xi_1,\xi_2,\xi_3,\xi_4\}=D_2,$$

and

$$\mathscr{V}^{\mathbf{R}}_{\mathbf{R}\times S_Q}\approx\mathrm{Hom}(Q,\mathbf{R})=0,$$

respectively.] In spite of that, Theorem 1 provides us with a powerful and useful tool for the study of both kinds of gauge vacua.

TABLE I. The vacuum structure $\mathscr{V}^G_M\approx\mathrm{Chom}(\pi_1(M),G)$ for some space–time manifolds $M$ and some elementary gauge groups $G$. Note that $\mathscr{V}^{\mathrm{SO}(3)}_{\mathbf{R}^3\times S^1}\approx\mathrm{SO}(2)$, $\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}^3\times S^1}\approx\mathrm{U}(1)$, $\mathscr{V}^{\mathrm{SO}(3)}_{\mathbf{R}\times L(p,1)}=\mathbf{Z}_p$, and $\mathscr{V}^{\mathrm{SU}(2)}_{\mathbf{R}\times L(p,1)}=\mathbf{Z}_p$, are the only nontrivial and nonabelian vacuum structures in this table having a natural group structure.

| Space–time Manifold $M$ | Gauge Group $G$: U(1) | R | SU($N$) | SO($N$) |
|---|---|---|---|---|
| $\mathbf{R}^4$ | 0 | 0 | 0 | 0 |
| $S^4$ | 0 | 0 | 0 | 0 |
| $\mathbf{R}^3\times S^1$ | U(1) | R | $\boldsymbol{A}_1^N\mathrm{U}(1)$ | $\boldsymbol{A}^{[N/2]}\mathrm{SO}(2)$ |
| $\mathbf{R}\times L(p,1)$ | $\mathbf{Z}_p$ | 0 | $\boldsymbol{A}_1^N\mathbf{Z}_p$ | $\boldsymbol{A}^{[N/2]}\mathbf{Z}_p$ |
| $\mathbf{R}\times S_Q$ | $D_2$ | 0 | $\bigcup_{i=0}^{[N/2]}\boldsymbol{A}_1^{N-2i}D_2$ | $\boldsymbol{A}_1^N D_2$ |

Most of the results of this section are summarized in Table I.

## 4. CONCLUSIONS

The main physical consequence of Theorem 1 is that in general the classical gauge field vacuum is degenerate and that the degree of this degeneracy is given by the cardinality of the set

$$\mathrm{Chom}(\pi_1(M),G,)$$

$M$ being the space–time manifold and $G$ being the corresponding gauge group.

In the electromagnetic case this degeneracy was known from the discovery of the Aharonov–Bohm effect, which shows us that such a degeneracy is broken by the presence of charged material particles in the space–time manifold $\mathbb{R}^3\times S^1$. In the same way one may expect that for all gauge field theories vacuum degeneracy is broken by the presence of material particles feeling the corresponding gauge interactions.

In a recent paper[14] Mayer and Wiswanathan discuss the quantum structure of the gauge vacua for non-one-point compactifications of the spacelike subspace $\mathbb{R}^3$ of the Minkowski space–time. In particular, they consider the quantum vacua arising from the trivial SU(2)(SO(3)) gauge field copy on $\mathbb{R}P^3$. Since $\pi_1(\mathbb{R}P^3)=\mathbb{Z}_2$, Theorem 1 says that there is another SU(2)(SO(3)) gauge vacuum copy on $\mathbb{R}P^3$. Therefore, another quantum vacua sector may be derived from this classical vacuum copy. This new sector must also be studied for the complete understanding of the quantum vacuum structure in that compactification.

Finally, vacua sectors of this kind may also appear in the construction of the quantum gauge vacua on space–time whose manifolds are not simply connected when the corresponding classical vacua are degenerate. But in general the quantum structure of the gauge vacuum on such space–times is not well known yet.

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# Hilbert space approach to the three- and four-nucleon systems

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A Hilbert space formulation is proposed for the three-nucleon scattering problem. Scattering integral equations are given derived from Alt–Grassberger–Sandhas equations. Using the momentum representation, the kernel of the iterated integral equation is shown to be compact in an adjusted Hilbert space. The extension to four nucleons is given.

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## I. INTRODUCTION

In his famous work Faddeev[1] established three-body scattering integral equations and showed the iterated kernels to be compact in a given Banach space. Compactness would be a strong tool for powerful approximation techniques for practical solutions if the space were a Hilbert space. Much work has been done since on the investigation of few-body scattering equations.[2–11] It is a common feature of these equations that their kernels are built up from transition amplitudes or Green's functions corresponding to a lower particle number. By probability conservation, one is forced to take into account all the subsystems particle breakup poles and corresponding cuts. These singularities give rise to the difficulty that the kernels are not compact on the ordinary $L_2$ Hilbert space. For three particles in coordinate representation Ginibre and Moulin[12] showed compactness of kernels in a Hilbert space. For three particles nonsingular scattering equations in momentum space have also been proposed.[13] In momentum representation, widely used in practical few-body calculations, this work gives a Hilbert space approach. It allows one to calculate the scattering amplitudes from integral equations in Hilbert space with compact kernels. It is shown in detail for three particles, and for four particles the basic equations are given. The main point is the application of the substraction technique which splits a Cauchy type singularity into a nonsingular part and a singular part which is analytically solvable. This idea has been used by Noyes and Kowalski,[14] in order to extract from a two-body scattering equation a nonsingular equation. Here it is used to construct a scalar product from a function and the subtracted function, thus giving an appropriate Hilbert space. This method already has been shown to work in the two-body case and a special low energy three-body case.[15] It is briefly reviewed in Sec. 2. For the three-body case, it is generalized to more variables.

It is well known[1] that the original Faddeev kernel is not compact, as it is not connected. The same is true for the equations given here, so that iterations are needed which will, firstly, make the kernels connected and secondly, will make the singularities less severe. In Sec. 3 the notation and the equations are given for the three-body case. The next section defines the basic Hilbert space. In Sec. 4 a condition is formulated which is shown to be sufficient for compactness of the kernels. In Sec. 5 we show that it applies to the class of Hölder continuous potentials defined by Faddeev[1] in a certain approximation. In the final section, for the four-body case, the basic set of equations is given in analogy to the three-body case.

## 2. TWO-BODY CASE

Let us briefly review our method given for the two-body case.[15] In the case of a rotationally symmetric two-body potential, the angular momentum decomposed scattering equation (Lippmann–Schwinger equation) is of the type

$$f(q') = g(q') + \lim_{\epsilon \to +0} \int_0^\infty dq \, \frac{k(q',q)}{q_0 + i\epsilon - q} f(q) , \tag{2.1}$$

$$f = g + Kf .$$

Let us introduce for technical simplicity a momentum cutoff $a > 0$, although rotational invariance and momentum cutoff are not needed. We define

$$\mathscr{H}^0 = \left\{ \psi | \psi(q) \in \mathscr{L}_2(0,a), \phi^{\psi}(q) = \frac{\psi(q) - \psi(q_0)}{q - q_0} \in \mathscr{L}_2(0,a) \right\} , \tag{2.2}$$

and on $\mathscr{H}^0$ a scalar product

$$(\psi,\chi)_{\mathscr{H}^0} = (\psi,\chi)_{\mathscr{L}_2} + (\phi^{\psi},\phi^{\chi})_{\mathscr{L}_2} . \tag{2.3}$$

It turns out that $\mathscr{H}^0$ is a Hilbert space. The following conditions on $k$ turn out to be sufficient for $K$ to be compact on $\mathscr{H}^0$:

$$k(q',q) \in \mathscr{L}_2(0,a) \times (0,a) ,$$

$$\phi^{k}_{,q_0}(q',q) = \frac{k(q',q) - k(q',q_0)}{q - q_0} \in \mathscr{L}_2(0,a) \times (0,a) ,$$

$$\phi^{k}_{q_0}(q',q) = \frac{k(q',q) - k(q_0,q)}{q' - q_0} \in \mathscr{L}_2(0,a) \times (0,a) ,$$

$$\phi^{k}_{q_0,q_0}(q',q) = \frac{k(q',q) - k(q',q_0) - k(q_0,q) + k(q_0,q_0)}{(q' - q_0)(q - q_0)} \in \mathscr{L}_2(0,a) \times (0,a) . \tag{2.4}$$

The compactness is made transparent by the following steps:

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$$\lim_{\epsilon\to 0+}\int_0^a dq\,\frac{k(q',q)}{q_0+i\epsilon-q}f(q)$$
$$=\int_0^a dq\,\frac{k(q',q)-k(q',q_0)}{q_0-q}f(q)+k(q',q_0)$$
$$\times\int_0^a dq\,\frac{f(q)-f(q_0)}{q_0-q}$$
$$+k(q',q_0)f(q_0)\lim_{\epsilon\to+0}\int_0^a dq\,\frac{1}{q_0+i\epsilon-q}$$
$$=-\int_0^a dq\,\phi^{k}_{,q_0}(q',q)f(q)-k(q',q_0)\int_0^a dq\,\phi^{f}(q)$$
$$+k(q',q_0)f(q_0)\left[\ln\frac{q_0}{a-q_0}-i\pi\right]$$
$$=-\int_0^a dq\,\phi^{k}_{,q_0}(q',q)f(q)$$
$$-\int_0^a dq\,[k(q',q)+\phi^{k}_{,q_0}(q',q)(q_0-q)]\phi^{f}(q)$$
$$+\int_0^a dq\,[k(q',q)+\phi^{k}_{,q_0}(q',q)(q_0-q)]$$
$$\times[f(q)+\phi^{f}(q)(q_0-q)]\frac{1}{a}\left[\ln\frac{q_0}{a-q_0}-i\pi\right]. \tag{2.5}$$

## 3. THREE-NUCLEON CASE: NOTATION AND EQUATIONS

Let us consider three particles of identical mass $m$. Throughout this paper we use the convention $\hbar=m=1$. The index $\alpha$ denotes the particle, also the subsystem of two particles in which particle $\alpha$ is not contained, and the channel index of three particles containing this subsystem. Let $\mathbf{q}$ be the relative momentum between two particles and $\mathbf{p}$ the relative momentum between the third particle and the center of mass of the two-particle subsystem. Thus, a plane-wave state in the channel $\alpha$, e.g., is expressed as $|\mathbf{p},\mathbf{q}\rangle_\alpha$. In the following an operator $O$ defined in the two-body space is denoted without index or as $O$.[2] Let $V$ be the two-body interaction, $G_0^{(2)}(Z)$ the two-body free Green's function and $T(Z)$ the two-body transition amplitude. Let $V_\alpha$ be a two-body potential read in the three-body space as

$$_\alpha\langle\mathbf{p}',\mathbf{q}'|V_\alpha|\mathbf{p},\mathbf{q}\rangle_\alpha=\delta(\mathbf{p}'-\mathbf{p})\langle\mathbf{q}'|V|\mathbf{q}\rangle. \tag{3.1}$$

Let $G_0(Z)$ be the free Green's function in the three-body space, $T_\alpha(Z)$ be the two-body transition amplitude read in the three-body space obeying

$$T_\alpha(Z)=V_\alpha+V_\alpha G_0(Z)T_\alpha(Z). \tag{3.2}$$

Let $U_{\beta\alpha}(Z)$ be the three-body transition amplitude, which fulfills the Alt–Grassberger–Sandhas equations,[16] with $\delta_{\beta\alpha}=1-\delta_{\beta\alpha}$

$$U_{\beta\alpha}=\delta_{\beta\alpha}G_0^{-1}+\sum_\gamma\delta_{\beta\gamma}T_\gamma G_0U_{\gamma\alpha}, \tag{3.3}$$

where $\alpha,\beta,\gamma$ run over all particles. Defining

$$\bar{U}_{\beta\alpha}=T_\beta G_0U_{\beta\alpha}, \tag{3.4}$$

one obtains from Eq. (3.3)

$$\bar{U}_{\beta\alpha}=T_\beta\delta_{\beta\alpha}+\sum_\gamma\delta_{\beta\gamma}T_\beta G_0\bar{U}_{\gamma\alpha}. \tag{3.5}$$

In the following, the energy is constrained by $E$ = Real $(Z)>0$, which means we are dealing with the most complicated case. The singular behavior of Eq. (3.5) arises from poles of the kernel. $_\beta\langle\mathbf{p}',\mathbf{q}'|G_0(Z)|\mathbf{p},\mathbf{q}\rangle_\beta$ has a pole at $Z=\frac{3}{4}p^2+q^2$, while $_\beta\langle\mathbf{p}',\mathbf{q}'|T_\beta(Z)|\mathbf{p},\mathbf{q}\rangle_\beta$ has a pole at $Z=\frac{3}{4}p^2+E_d$. Here the technically simplifying (but not crucial) assumption is made that there is only one two-body bound state at $E_d<0$. We make a variable transformation $\tilde{\mathbf{p}}=(\sqrt{3/4})\mathbf{p}$ but omit the tilde in the following. Now let us split $G_0$ and $T_\alpha$ into singular parts and nonsingular parts defining

$$_\alpha\langle\mathbf{p}',\mathbf{q}'|S_\alpha(Z)|\mathbf{p},\mathbf{q}\rangle_\alpha$$
$$=\delta(\mathbf{p}'-\mathbf{p})\delta(\mathbf{q}'-\mathbf{q})(-|Z|-p^2-|E_d|)$$
$$/(Z-p^2-E_d),$$
$$_\alpha\langle\mathbf{p}',\mathbf{q}'|S_0(Z)|\mathbf{p},\mathbf{q}\rangle_\alpha \tag{3.6}$$
$$=\delta(\mathbf{p}'-\mathbf{p})\delta(\mathbf{q}'-\mathbf{q})(-|Z|-p^2-q^2)/(Z-p^2-q^2),$$

and $B_\alpha(Z)$ and $B_0(Z)$ via

$$G_0=S_0B_0, \tag{3.7}$$
$$T_\alpha=S_\alpha B_\alpha.$$

It is valid that $[S_\alpha,B_\alpha]=[S_\alpha,G_0]=[S_\alpha,S_0]$ $=[S_\alpha,B_0]=[S_0,B_0]=0$. Let us introduce $\tilde{U}_{\beta\alpha}$ via

$$\bar{U}_{\beta\alpha}=S_\beta\tilde{U}_{\beta\alpha}. \tag{3.8}$$

From Eq. (3.5) one obtains

$$\tilde{U}_{\beta\alpha}=B_\beta\delta_{\beta\alpha}+\sum_\gamma\delta_{\beta\gamma}B_\beta G_0S_\gamma\tilde{U}_{\gamma\alpha}. \tag{3.9}$$

For physical relevance, it is sufficient to investigate this equation multiplied from the right by a state $|\phi\rangle_\alpha$, with the definition $|\tilde{f}\rangle_\beta=\tilde{U}_{\beta\alpha}|\phi\rangle_\alpha$, $|\tilde{g}\rangle_\beta=B_\beta\delta_{\beta\alpha}|\phi\rangle_\alpha$, thus giving

$$|\tilde{f}\rangle_\beta=|\tilde{g}\rangle_\beta+\sum_\gamma\delta_{\beta\gamma}B_\beta G_0S_\gamma|\tilde{f}\rangle_\gamma. \tag{3.10}$$

Our aim is a Hilbert space $\mathscr{H}$ with $g$ and $f$ belonging to $\mathscr{H}$ and a compact integral operator $K$ mapping $\mathscr{H}$ into $\mathscr{H}$ with

$$f=g+Kf, \tag{3.11}$$

such that the solution $f$ is closely related to the solution $\tilde{f}$ of (3.10). A step toward this goal is the iteration of Eq. (3.10). The reason is that our kernel is similar to that of Faddeev's equation for which iteration was shown[1] to make the kernel smoother. After three-fold iteration Eq. (3.10) reads

$$|\tilde{f}\rangle_{\beta_1}=|\tilde{g}\rangle_{\beta_1}+\sum_{\beta_2}\delta_{\beta_1\beta_2}B_{\beta_1}G_0S_{\beta_2}|\tilde{g}\rangle_{\beta_2}$$
$$+\sum_{\beta_2\beta_3}\delta_{\beta_1\beta_2}\delta_{\beta_2\beta_3}B_{\beta_1}G_0S_{\beta_2}B_{\beta_2}G_0S_{\beta_3}|\tilde{g}\rangle_{\beta_3}$$
$$+\sum_{\beta_2\beta_3\beta_4}\delta_{\beta_1\beta_2}\delta_{\beta_2\beta_3}\delta_{\beta_3\beta_4}B_{\beta_1}G_0S_{\beta_2}B_{\beta_2}G_0S_{\beta_3}B_{\beta_3}G_0S_{\beta_4}|\tilde{g}\rangle_{\beta_4}$$
$$+\sum_{\beta_2\beta_3\beta_4\beta_5}\delta_{\beta_1\beta_2}\delta_{\beta_2\beta_3}\delta_{\beta_3\beta_4}\delta_{\beta_4\beta_5}B_{\beta_1}G_0S_{\beta_2}B_{\beta_2}G_0S_{\beta_3}B_{\beta_3}$$
$$\times G_0S_{\beta_4}B_{\beta_4}G_0S_{\beta_5}|\tilde{f}\rangle_{\beta_5}, \tag{3.12}$$

which is our basic three-body equation. The inhomogeneous term is called $|g\rangle_{\beta_1}$ and

$$K_{\beta_1\beta_2\beta_3\beta_4\beta_5} = B_{\beta_1} G_0 T_{\beta_2} G_0 T_{\beta_3} G_0 B_{\beta_4} B_0 S_0 S_{\beta_4} S_{\beta_5} , \tag{3.13}$$

$$H_{\beta_1\beta_2\beta_3\beta_4} = B_{\beta_1} G_0 T_{\beta_2} G_0 T_{\beta_3} G_0 B_{\beta_4} B_0 .$$

Thus (3.12) reads

$$|\tilde{f}\rangle_{\beta_1} = |g\rangle_{\beta_1} + \sum_{\beta_2\beta_3\beta_4\beta_5} \delta_{\beta_1\beta_2}\delta_{\beta_2\beta_3}\delta_{\beta_3\beta_4}\delta_{\beta_4\beta_5} K_{\beta_1\beta_2\beta_3\beta_4\beta_5} |\tilde{f}\rangle_{\beta_5} \tag{3.14}$$

and the kernel $K_{\beta_1\beta_2\beta_3\beta_4\beta_5}$ is factored into

$$K_{\beta_1\beta_2\beta_3\beta_4\beta_5} = H_{\beta_1\beta_2\beta_3\beta_4} S_0 S_{\beta_4} S_{\beta_5} , \tag{3.15}$$

$H_{\beta_1\beta_2\beta_3\beta_4}$ will turn out to be the nonsingular part, while the singularities are contained in $S_0 S_{\beta_4} S_{\beta_5}$. That is, $S_0$ contains the free pole, $S_{\beta_4}$ the deuteron pole in the channel $\beta_4$, $S_{\beta_5}$ the deuteron pole in the channel $\beta_5$. Remember only channels $\beta_4 \neq \beta_5$ contribute in (3.14). As poles emerge in different channels, let us define some channel and variable transformations. For each $\beta_1 \neq \beta_2$

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}_{\beta_1} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}_{\beta_2} \tag{3.16}$$

$A = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ with real coefficients $a, b, c, d$,

$$\begin{aligned} {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle_{\beta_1} &= {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|A\,|\mathbf{p},\mathbf{q}\rangle_{\beta_2} \\ &= {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|a\mathbf{p}+b\mathbf{q}, c\mathbf{p}+d\mathbf{q}\rangle_{\beta_2} . \end{aligned} \tag{3.17}$$

Instead of characterizing a Hilbert state by the momenta $\mathbf{p}_\beta, \mathbf{q}_\beta$, one could also use $\mathbf{p}_\beta, \mathbf{p}_\gamma = \mathbf{k}_\gamma$ with $\beta \neq \gamma$,

$$\begin{pmatrix} \mathbf{p}_{\beta_2} \\ \mathbf{k}_{\beta_1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ a & b \end{pmatrix} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}_{\beta_2} , \tag{3.18}$$

$B = \left(\begin{smallmatrix} 1 & 0 \\ a & b \end{smallmatrix}\right)$ with real coefficients $a, b$,

$$\begin{aligned} {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{k}\rangle_{\beta_2\beta_1} &= {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|B\,|\mathbf{p},\mathbf{q}\rangle_{\beta_2} \\ &= {}_{\beta_2}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p}, a\mathbf{p}+b\mathbf{q}\rangle_{\beta_2} . \end{aligned} \tag{3.19}$$

Let us use the Hilbert states in the $|\mathbf{p},\mathbf{q}\rangle_{\beta_5}$ representation in order to describe the singularities of $S_0, S_{\beta_4}, S_{\beta_5}$. The pole of $S_0$ emerges for $E - p^2 - q^2 = 0$, the pole of $S_{\beta_4}$ emerges for $E - (a\mathbf{p}+b\mathbf{q})^2 - E_d = 0$, while that of $S_{\beta_5}$ emerges for $E - p^2 - E_d = 0$.

One can define a hypersphere of singular points. Let $G = \mathbb{R}^3 \times \mathbb{R}^3$ and

$$\begin{aligned} G_E &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G,\ E - p^2 - q^2 = 0\} , \\ G_{E-E_d,B} &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G,\ E - E_d - (a\mathbf{p}+b\mathbf{q})^2 = 0\} \\ &= \{(\mathbf{p},\mathbf{k})|(\mathbf{p},\mathbf{k})\in G,\ E - E_d - k^2 = 0\} , \end{aligned} \tag{3.20}$$

$$\begin{aligned} G_{E-E_d,1} &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G,\ E - E_d - p^2 = 0\} \\ &= \{(\mathbf{p},\mathbf{k})|(\mathbf{p},\mathbf{k})\in G,\ E - E_d - p^2 = 0\} , \end{aligned}$$

with $\mathbf{p},\mathbf{k}$ defined by (3.18). Note the following properties:

$$\begin{aligned} G_E \cap G_{E-E_d,B} &= \emptyset , \\ G_E \cap G_{E-E_d,1} &= \emptyset , \end{aligned} \tag{3.21}$$

which can be verified easily. Assume on the contrary $(\mathbf{p},\mathbf{q})\in G_E \cap G_{E-E_d,B}$. That means $0 = E - p^2 - q^2 = E - E_d - (a\mathbf{p}+b\mathbf{q})^2$. Calculating the coefficients of $A$, (3.16), one finds $A$ to be an orthogonal matrix. Thus, $p^2 + q^2 = (a\mathbf{p}+b\mathbf{q})^2 + (c\mathbf{p}+d\mathbf{q})^2$. Combining this with the foregoing equation means $0 > -(c\mathbf{p}+d\mathbf{q})^2 = -E_d > 0$, which is a contradiction. Similarly, assuming $(\mathbf{p},\mathbf{q})\in G_E \cap G_{E-E_d,1}$ means $0 = E - p^2 - q^2 = E - E_d - p^2$, and thus $0 > -q^2 = -E_d > 0$, which is also a contradiction. Moreover, one can define corresponding domains

$$\begin{aligned} U_E &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G, 0 \leqslant p^2 + q^2 < E + \tfrac{1}{2}|E_d|\} , \\ U_{E-E_d,B} &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G, |E - E_d - (a\mathbf{p}+b\mathbf{q})^2| < \tfrac{1}{2}|E_d|\} \\ &= \{(\mathbf{p},\mathbf{k})|(\mathbf{p},\mathbf{k})|\in G, |E - E_d - k^2| < \tfrac{1}{2}|E_d|\} , \\ U_{E-E_d,1} &= \{(\mathbf{p},\mathbf{q})|(\mathbf{p},\mathbf{q})\in G, |E - E_d - p^2| < \tfrac{1}{2}|E_d|\} \\ &= \{(\mathbf{p},\mathbf{k})|(\mathbf{p},\mathbf{k})\in G, |E - E_d - k^2| < \tfrac{1}{2}|E_d|\} , \end{aligned} \tag{3.22}$$

with

$$G_E \subset U_E , \quad G_{E-E_d,B} \subset U_{E-E_d,B} , \quad G_{E-E_d,1} \subset U_{E-E_d,1}$$

and

$$\begin{aligned} U_E \cap U_{E-E_d,B} &= \emptyset , \\ U_E \cap U_{E-E_d,1} &= \emptyset , \end{aligned} \tag{3.23}$$

where the boundary of each $U$ has a finite distance to the corresponding $G$. Defining

$$\begin{aligned} U_{E-E_d} &= U_{E-E_d,B} \cup U_{E-E_d,1} , \\ U_R &= G \setminus U_{E-E_d} . \end{aligned} \tag{3.24}$$

One has a disjoint decomposition of $G$

$$G = U_E \cup U_{E-E_d} \cup U_R . \tag{3.25}$$

Now we are able to split a matrix element of the kernel $K_{\beta_1\beta_2\beta_3\beta_4\beta_5}$:

$$\begin{aligned} &\lim_{\epsilon\to+0} {}_{\beta_1}\langle \mathbf{p}',\mathbf{q}'|K_{\beta_1\beta_2\beta_3\beta_4\beta_5}(E+i\epsilon)|\psi\rangle_{\beta_5} \\ &= \lim_{\epsilon\to+0} {}_{\beta_1}\langle \mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon) S_0(E+i\epsilon) S_{\beta_4}(E+i\epsilon) S_{\beta_5}(E+i\epsilon)|\psi\rangle_{\beta_5} \\ &= \lim_{\epsilon\to+0} \int_{U_R} d\mathbf{p}\, d\mathbf{q}\ {}_{\beta_1}\langle \mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4} \\ &\quad \times \frac{(-|E| - p^2 - q^2)(-|E| - |E_d| - p^2)(-|E| - |E_d| - (a\mathbf{p}+b\mathbf{q})^2)}{(E - p^2 - q^2)(E - E_d - p^2)(E - E_d - (a\mathbf{p}+b\mathbf{q})^2)} {}_{\beta_4}\langle \mathbf{p},\mathbf{q}|\psi\rangle_{\beta_5} \\ &\quad + \lim_{\epsilon\to+0} \int_{U_E} d\mathbf{p}\, d\mathbf{q}\ {}_{\beta_1}\langle \mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4} \end{aligned}$$

$$\times \frac{(-|E|-p^2-q^2)(-|E|-|E_d|-p^2)(-|E|-|E_d|-(a\mathbf{p}+b\mathbf{q})^2)}{(E+i\epsilon-p^2-q^2)(E-E_d-p^2)(E-E_d-(a\mathbf{p}+b\mathbf{q})^2)}\,{}_{\beta_4}\langle \mathbf{p},\mathbf{q}|\psi\rangle_{\beta_5}$$

$$+\lim_{\epsilon\to+0}\int_{U_E-U_{E_d}} d\mathbf{p}\,d\mathbf{k}\;{}_{\beta_1}\langle \mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{k}\rangle_{\beta_4\beta_5}$$

$$\times \frac{(-|E|-\frac{4}{3}(p^2+k^2+\mathbf{p}\cdot\mathbf{k}))(-|E|-|E_d|-p^2)(-|E|-|E_d|-k^2)}{(E-\frac{4}{3}(p^2+k^2+\mathbf{p}\cdot\mathbf{k}))(E+i\epsilon-E_d-p^2)(E+i\epsilon-E_d-k^2)}\,{}_{\beta_4\beta_5}\langle \mathbf{p},\mathbf{k}|\psi\rangle_{\beta_5}\,. \tag{3.26}$$

In the domain $U_R$, no pole contributes from $S_0, S_{\beta_4}, S_{\beta_5}$; in $U_E$ only the pole from $S_0$ contributes, and in $U_{E-E_d}$ only the poles from $S_{\beta_4}, S_{\beta_5}$ contribute; thus the $i\epsilon$ can be omitted in the denominator terms which give no pole contribution.

## 4. HILBERT SPACE

In this section a scalar product space is introduced appropriate to handle the above discussed singularities, guided by the same idea as in the two-body case. It is shown that the space is complete; i.e., a Hilbert space. Let us start with some definitions. Let

$$\mathscr{L}_2(G)=\{\psi|\int d\mathbf{p}\,d\mathbf{q}\,|\psi(\mathbf{p},\mathbf{q})|^2 \text{exists in the sense of Lebesgue}\} \tag{4.1}$$

and similarly $\mathscr{L}_2(U_E)$, $\mathscr{L}_2(U_{E-E_d})$, and $\mathscr{L}_2(U_R)$. Let

$$\mathscr{H}(U_E)=\left\{\psi|\psi\in\mathscr{L}_2(U_E),\phi^{\psi}_E(\mathbf{p},\mathbf{q})=(\psi(\mathbf{p},\mathbf{q})-\psi(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)})(E-p^2-q^2)^{-1}\in\mathscr{L}_2(U_E)\right\},$$

where $\psi(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)}=\psi\left(\frac{\mathbf{p}}{[(p^2+q^2)/E]^{1/2}},\frac{\mathbf{q}}{[(p^2+q^2)/E)]^{1/2}}\right)$,

$$\mathscr{H}(U_{E-E_d})=\left\{\psi|\psi\in\mathscr{L}_2(U_{E-E_d}),\phi^{\psi}_{E-E_d},(\mathbf{p},\mathbf{k})=(\psi(\mathbf{p},\mathbf{k})-\psi(\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)})(E-E_d-p^2)^{-1}\Pi_{E-E_d}(\mathbf{p})\in\mathscr{L}_2(U_{E-E_d})\right.,$$

$$\phi^{\psi}_{,E-E_d}(\mathbf{p},\mathbf{k})=(\psi(\mathbf{p},\mathbf{k})-\psi(\mathbf{p},\mathbf{k})|_{(k^2=E-E_d)})(E-E_d-k^2)^{-1}\Pi_{E-E_d}(\mathbf{k})\in\mathscr{L}_2(U_{E-E_d}),$$

$$\phi^{\psi}_{E-E_d,E-E_d}(\mathbf{p},\mathbf{k})=(\psi(\mathbf{p},\mathbf{k})-\psi(\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)}-\psi(\mathbf{p},\mathbf{k})|_{(k^2=E-E_d)}+\psi(\mathbf{p},\mathbf{k})|_{(p^2=k^2=E-E_d)})$$

$$\left.\times[(E-E_d-p^2)(E-E_d-k^2)]^{-1}\Pi_{E-E_d}(\mathbf{p})\Pi_{E-E_d}(\mathbf{k})\in\mathscr{L}_2(U_{E-E_d})\right\},$$

where $\Pi_{E-E_d}(\mathbf{x})=1$ if $|E-E_d-x^2|<\frac{1}{2}|E_d|$ and 0 elsewhere,

$$\mathscr{H}(U_R)=\mathscr{L}_2(U_R),$$

$$\mathscr{H}(G)=\mathscr{H}(U_E)+\mathscr{H}(U_{E-E_d})+\mathscr{H}(U_R).$$

From the ordinary scalar products in $\mathscr{L}_2$, we construct new scalar products. We define

$$(\psi,\theta)_{\mathscr{H}(U_E)}=(\psi,\theta)_{\mathscr{L}_2(U_E)}+(\phi^{\psi}_E,\phi^{\theta}_E)_{\mathscr{L}_2(U_E)},$$

$$\begin{aligned}(\psi,\theta)_{\mathscr{H}(U_E-U_{E_d})}&=(\psi,\theta)_{\mathscr{L}_2(U_E-U_{E_d})}+(\phi^{\psi}_{E-E_d},\phi^{\theta}_{E-E_d})_{\mathscr{L}_2(U_E-U_{E_d})}\\&+(\phi^{\psi}_{,E-E_d},\phi^{\theta}_{,E-E_d})_{\mathscr{L}_2(U_E-U_{E_d})}\\&+(\phi^{\psi}_{E-E_d,E-E_d},\phi^{\theta}_{E-E_d,E-E_d})_{\mathscr{L}_2(U_E-U_{E_d})},\end{aligned} \tag{4.2}$$

$$(\psi,\theta)_{\mathscr{H}(U_R)}=(\psi,\theta)_{\mathscr{L}_2(U_R)},$$

$$(\psi,\theta)_{\mathscr{H}(G)}=(\psi,\theta)_{\mathscr{H}(U_E)}+(\psi,\theta)_{\mathscr{H}(U_E-U_{E_d})}+(\psi,\theta)_{\mathscr{H}(U_R)}.$$

*Theorem* 1: $\mathscr{H}(G)$ is a Hilbert space

*Proof*: From the properties of the scalar product $(.,.)_{\mathscr{L}_2}$, it is clear that $(.,.)_{\mathscr{H}}$ is a scalar product. It remains to establish the completeness.

(i) Let us begin with $\mathscr{H}(U_E)$. Let $f_n$ be a Cauchy sequence in $\mathscr{H}(U_E)$. From that it follows that $f_n$ and $\phi^{f_n}_E$ are Cauchy sequences in $\mathscr{L}_2(U_E)$. As $\mathscr{L}_2(U_E)$ is complete, limiting elements $f,g\in\mathscr{L}_2(U_E)$ exist, such that

$$f_{n_n}\to f,\quad \phi^{f_n}_E\underset{n}{\to}g \text{ in the } L_2(U_E) \text{ norm}. \tag{4.3}$$

One has to show that $\phi^f_E(\mathbf{p},\mathbf{q})=g(\mathbf{p},\mathbf{q})$ almost everywhere in $U_E$. Now the following variable transformation will be useful.

$$\mathbf{p}=\hat{p}\rho\sin\xi,\quad \mathbf{q}=\hat{q}\rho\cos\xi, \tag{4.4}$$

with $\hat{p}$ and $\hat{q}$ unit vectors of $\mathbf{p}$ and $\mathbf{q}$, respectively, which fulfills $p^2+q^2=\rho^2$. It is claimed that $f_n(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)}$ is a Cauchy sequence in the space $\mathscr{L}_2(\hat{p},\hat{q},\xi)$ defined as

$$\mathscr{L}_2(\hat{p},\hat{q},\xi)=\{\psi|\int d\hat{p}\,d\hat{q}\int_0^{\pi/2}d\xi\,|\psi(\hat{p},\hat{q},\xi)|^2$$

exists in the sense of Lebesgue.$\}$ (4.5)

It can be seen this way:

$$\begin{aligned}&\left(\int d\hat{p}d\hat{q}\int_0^{\pi/2}d\xi\,|f_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}\right.\\&\qquad\left.-f_m(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}|^2\right)^{1/2}\\&=\left(\int d\hat{p}d\hat{q}\int_0^{\pi/2}d\xi\,|f_n(\hat{p},\hat{q},\rho=\sqrt{E},\xi)\right.\\&\qquad\left.-f_m(\hat{p},\hat{q},\rho=\sqrt{E},\xi)|^2\right)^{1/2}\\&=\left(6E^{-3}\int_0^{\sqrt{E}}d\rho\,\rho^5\int d\hat{p}d\hat{q}\int_0^{\pi/2}d\xi\,|f_n(\hat{p},\hat{q},\rho\right.\\&\qquad\left.=\sqrt{E},\xi)-f_m(\hat{p},\hat{q},\rho=\sqrt{E},\xi)|^2\right)^{1/2}\end{aligned}$$

$$= \left(6E^{-3}\int_{U_E} d\mathbf{p}d\mathbf{q}\,|f_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} - f_m(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}|^2\right)^{1/2}. \tag{4.6}$$

Using $f_n(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)} = f_n(\mathbf{p},\mathbf{q}) - \phi_E^{f_n}(\mathbf{p},\mathbf{q})(E-p^2-q^2)$, an upper bound for the last expression is

$$\left(6E^{-3}\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,|f_n(\mathbf{p},\mathbf{q}) - f_m(\mathbf{p},\mathbf{q})|^2\right)^{1/2} + \left(6E^{-3}\right.$$

$$\left.\times \int_{U_E} d\mathbf{p}d\mathbf{q}|\,(\phi_E^{f_n}(\mathbf{p},\mathbf{q}) - \phi_E^{f_m}(\mathbf{p},\mathbf{q}))(E-p^2-q^2)|^2\right)^{1/2}.$$

In $U_E$ $|E-p^2-q^2| < E + \frac{1}{2}|E_d|$ holds, such that we obtain the estimate

$$(6/E^3)^{1/2}\|f_n - f_m\|_{\mathscr{L}^2(U_E)} + (6/E^3)(E+\tfrac{1}{2}|E_d|)$$
$$\times \|\phi_E^{f_n} - \phi_E^{f_m}\|_{\mathscr{L}_2(U_E)},$$

which is a Cauchy sequence. From the completeness of $\mathscr{L}_2(\hat{p},\hat{q},\xi)$ we conclude the existence of a limiting element $h(\hat{p},\hat{q},\xi)$, such that

$$f_n(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)} \xrightarrow[n]{} h(\hat{p},\hat{q},\xi) \text{ in } \mathscr{L}_2(\hat{p},\hat{q},\xi).$$

As $G_E$ is a subset of measure 0 in $U_E$, one is free to set

$$f(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)} = f(\hat{p},\hat{q},\rho=\sqrt{E},\xi) = h(\hat{p},\hat{q},\xi), \tag{4.7}$$

which does not modify $f \in \mathscr{L}_2(U_E)$. Thus, one has

$$\int d\hat{p}\,d\hat{q}\int_0^{\pi/2} d\xi\,|f_n(\mathbf{p},\mathbf{q})_{(p^2+q^2=E)} - f(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}|^2 \xrightarrow[n]{} 0 \tag{4.8}$$

which implies

$$\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,|f_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} - f(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}|^2 \xrightarrow[n]{} 0. \tag{4.9}$$

Then one concludes

$$\int_{U_E} d\mathbf{p}\,d\mathbf{q}|\,f(\mathbf{p},\mathbf{q}) - f(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}$$
$$\left. - g(\mathbf{p},\mathbf{q})(E-p^2-q^2)|^2\right)^{1/2}$$
$$\leqslant \left(\int_{U_E} dp\,dq|\,f(\mathbf{p},\mathbf{q}) - f_n(\mathbf{p},\mathbf{q})|^2\right)^{1/2}$$
$$+\left(\int_{U_E} d\mathbf{p}\,d\mathbf{q}|\,f(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} - f_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}|^2\right)^{1/2}$$
$$+\left(\int_{U_E} d\mathbf{p}\,d\mathbf{q}|\,(\phi_E^{f_n}(\mathbf{p},\mathbf{q}) - g(\mathbf{p},\mathbf{q}))(E-p^2-q^2)|^2\right)^{1/2} \xrightarrow[n]{} 0. \tag{4.10}$$

The first and the third term tend to zero because of (4.3) and the second because of (4.9). That means

$$f(\mathbf{p},\mathbf{q}) - f(\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)} = g(\mathbf{p},\mathbf{q})(E-p^2-q^2) \text{a.e. in } U_E.$$

As $g \in \mathscr{L}_2(U_E)$,

$$\phi_E^f(\mathbf{p},\mathbf{q}) = (f(\mathbf{p},\mathbf{q}) - f(\mathbf{p},\mathbf{q})_{|(p^2q^2=E)})/(E-p^2-q^2)$$
$$= g(\mathbf{p},\mathbf{q}) \text{a.e. in } U_E \text{ and } \phi_E^f \in \mathscr{L}_2(U_E),$$

which establishes the existence of a limit element $f \in \mathscr{H}(U_E)$, which means completeness of $\mathscr{H}(U_E)$.

(ii) Guided by the same idea (but technically a little different) goes the proof for $\mathscr{H}(U_{E-E_d})$. Assume $f_n$ is a Cauchy sequence in $\mathscr{H}(U_{E-E_d})$. Thus, $f_n$, $\phi_{E-E_d}^{f_n}$, $\phi_{,E-E_d}^{f_n}$, and $\phi_{E-E_d,E-E_d}^{f_n}$ are Cauchy sequences in $\mathscr{L}_2(U_{E-E_d})$, having limit elements

$$f_n \xrightarrow[n]{} f, \phi_{E-E_d}^{f_n} \xrightarrow[n]{} g, \phi_{,E-E_d}^{f_n} \xrightarrow[n]{} h, \phi_{E-E_d,E-E_d}^{f_n} \xrightarrow[n]{} i$$
$$\text{in the } \mathscr{L}_2(U_E - E_d) \text{ norm.} \tag{4.11}$$

It is claimed that $f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}$ is a Cauchy sequence in

$$\mathscr{L}_2(\hat{p},\mathbf{k}) = \{\psi|\int d\hat{p}\int d\mathbf{k}\,|\psi(\hat{p},\mathbf{k})|^2$$
$$\text{exists in the sense of Lebesgue}\}. \tag{4.12}$$

It turns out as follows:

$$\left(\int d\hat{p}\int d\mathbf{k}\,|f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} - f_m(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}|^2\right)^{1/2}$$
$$= \left(\frac{3}{(E+\frac{3}{2}|E_d|)^3 - (E+\frac{1}{2}|E_d|)^3}\int_{E+(1/2)|E_d|}^{E+(3/2)|E_d|} dp\,p^2 d\hat{p}\right.$$
$$\left.\times\int d\mathbf{k}\,|f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} - f_m(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}|^2\right)^{1/2}$$
$$= \left(N\int_{U_{E-E_d,1}} d\mathbf{p}d\mathbf{k}\,|f_n(\mathbf{p},\mathbf{k}) - f_m(\mathbf{p},\mathbf{k})\right.$$
$$\left. - [\phi_{E-E_d}^{f_n}(\mathbf{p},\mathbf{k}) - \phi_{E-E_d}^{f_m}(\mathbf{p},\mathbf{k})](E-E_d-p^2)|^2\right)^{1/2}, \tag{4.13}$$

where $N$, is the integral preceding constant $(3/|(E+\frac{3}{2}|E_d|)^3 - (E+\frac{1}{2}|E_d|)^3|)$. Making use of $|E-E_d-p^2| < \frac{1}{2}|E_d|$, one obtains an upper bound

$$N^{1/2}\|f_n - f_n\|_{\mathscr{L}^2(U_{E-E_d})} + \tfrac{1}{2}|E_d|\sqrt{N}$$
$$\times \|\phi_{E-E_d}^{f_n} - \phi_{E-E_d}^{f_m}\|_{\mathscr{L}_2(U_{E-E_d})},$$

which is a Cauchy sequence. From the completeness of $\mathscr{L}_2(\hat{p},\mathbf{k})$, one infers the existence of a limit element $s(\hat{p},\mathbf{k})$ such that $f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} \xrightarrow[n]{} s(\hat{p},\mathbf{k})$ in $\mathscr{L}_2(\hat{p},\mathbf{k})$. As $G_{E-E_d,1}$ is a subset of $U_{E-E_d,1}$ of measure 0, one can put $f(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} = s(\hat{p},\mathbf{k})$. Without modification $f \in \mathscr{L}_2(U_{E-E_d,1})$; that implies

$$\int d\hat{p}\int d\mathbf{k}\,|f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} - f(\mathbf{p},\mathbf{k})_{|(p^2-E-E_d)}|^2 \xrightarrow[n]{} 0, \tag{4.14}$$

and thus

$$\int_{U_{E-E_d,1}} d\mathbf{p}\,d\mathbf{k}\,|f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)} - f(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}|^2 \xrightarrow[n]{} 0. \tag{4.15}$$

Then the following estimate holds:

$$\left(\int_{U_{E-E_d,1}} d\mathbf{p}\,d\mathbf{k}|\,f(\mathbf{p},\mathbf{k}) - f(\mathbf{p},\mathbf{k})_{(p^2=E-E_d)}\right.$$
$$\left. - g(\mathbf{p},\mathbf{k})(E-E_d-p^2)|^2\right)^{1/2}$$

$$\leq\Big(\int_{U_{E-E_d,1}} d\mathbf{p}\,d\mathbf{k}\,|f(\mathbf{p},\mathbf{k})-f_n(\mathbf{p},\mathbf{k})|^2\Big)^{1/2}$$
$$+\Big(\int_{U_{E-E_d,1}} d\mathbf{p}\,d\mathbf{k}\,|f(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}$$
$$-f_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}|^2\Big)^{1/2}$$
$$+\Big(\int_{U_{E-E_d,1}} d\mathbf{p}\,d\mathbf{k}\,|(\phi^{f_n}_{E-E_d}(\mathbf{p},\mathbf{k})$$
$$-g(\mathbf{p},\mathbf{k}))(E-E_d-p^2)|^2\Big)^{1/2}\underset{n}{\to}0\,. \tag{4.16}$$

The first term and the third one tend to zero because of (4.11), the second term because of (4.15). This means

$$f(\mathbf{p},\mathbf{k})-f(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}=g(\mathbf{p},\mathbf{k})(E-E_d-p^2)\text{a.e.} \tag{4.17}$$

in $U_{E-E_d,1}$, as $g\in\mathcal{L}_2U_{E-E_d,1}$), this reads

$$\phi^{f}_{E-E_d}(\mathbf{p},\mathbf{k})$$
$$=\big[\,(f(\mathbf{p},\mathbf{k})-f(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)})/(E-E_d-p^2)\big]\,\Pi_{E-E_d}(\mathbf{p})$$
$$=g(\mathbf{p},\mathbf{k})\text{a.e. in } U_{E-E_d,1}\,. \tag{4.18}$$

From this it easily follows that

$$\phi^{f}_{E-E_d}(\mathbf{p},\mathbf{k})=g(\mathbf{p},\mathbf{k})\text{a.e. in } U_{E-E_d}\,. \tag{4.19}$$

Analogously, one shows

$$\phi^{f}_{,E-E_d}(\mathbf{p},\mathbf{k})=h(\mathbf{p},\mathbf{k})\text{a.e. in } U_{E-E_d} \tag{4.20}$$

and

$$\phi^{f}_{E-E_d,E-E_d}(\mathbf{p},\mathbf{k})=i(\mathbf{p},\mathbf{k})\text{a.e. in } U_{E-E_d}\,. \tag{4.21}$$

Equations (4.19), 4.20), and (4.21) together mean completeness of $\mathcal{H}(U_{E-E_d})$.

(iii) Obviously $\mathcal{H}(U_R)=\mathcal{L}_2(U_R)$ is complete. Thus (i), (ii), and (iii) imply completeness of $\mathcal{H}(G)$.

## 5. COMPACT KERNEL

Let us define

$$\mathcal{L}_2(U_E\times U_E)=\{\psi|\int_{U_E\times U_E} d\mathbf{p}'\,d\mathbf{q}'\,d\mathbf{p}\,d\mathbf{q}\,|\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})|^2$$
exists in the sense of Lebesgue$\}$. (5.1)

$\mathcal{L}_2(U_i\times U_j), U_i,U_j\in U_E, U_{E-E_d}, U_R$ are analogously defined. In the following, one needs not only functions in $\mathcal{L}_2(U_i\times U_j)$ but also all possible combinations of its subtractions, which is a generalization of the definition of subtractions given in (4.1) in $\mathcal{L}_2(U_i)$. Let us give some notation. $\phi^{\psi}$ means subtractions of $\psi$. A semiconlon separates substraction on $U_i$ from that on $U_j$. A colon separates between the subtractions corresponding to the $\mathbf{p}$ and $\mathbf{k}$ variable in the case of $U_{E-E_d}$. Note that in the case of substractions on $U_{E-E_d}$ the $\Pi_{E-E_d}$ function is included. Here are some sample cases:

$\psi\in\mathcal{L}_2(U_E\times U_E)$:

$$\phi^{\psi}_{;E}(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})=(\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})-\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})_{|p^2+q^2=E)})$$
$$/(E-p^2-q^2)\,,$$

where

$$\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}=\psi\Big(\mathbf{p}',\mathbf{q}',\frac{\mathbf{p}}{[(p^2+q^2)/E]^{1/2}},\frac{\mathbf{q}}{[(p^2+q^2)/E]^{1/2}}\Big),$$

$$\phi^{\psi}_{E;E}(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})=\{\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})-\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})|_{(p'^2+q'^2=E)}$$
$$-\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})|_{(p^2+q^2=E)}$$
$$+\psi(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})|_{(p'^2+q'^2=p^2+q^2=E)}\}$$
$$\times(E-p'^2-q'^2)^{-1}(E-p^2-q^2)^{-1};$$

$\psi\in\mathcal{L}_2(U_{E-E_d}\times U_{E-E_d})$:

$$\phi^{\psi}_{;;E-E_d}(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})$$
$$=[(\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})-\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})_{|(k^2=E-E_d)})/$$
$$(E-E_d-k^2)]\Pi_{E-E_d}(\mathbf{k})\,,$$
$$\phi^{\psi}_{E-E_d;;E-E_d}(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})=\{\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})$$
$$-\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})|_{(p'^2=E-E_d)}-\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})|_{(k^2=E-E_d)}$$
$$+\psi(\mathbf{p}',\mathbf{k}',\mathbf{p},\mathbf{k})|_{(p'^2=k^2=E-E_d)}\}(E-E_d-p'^2)^{-1}$$
$$\times(E-E_d-k^2)^{-1}\Pi_{E-E_d}(\mathbf{p}')\Pi_{E-E_d}(\mathbf{k})\,.$$

*Assumption* (5.2): Every space $\mathcal{L}_2(U_i\times U_j)$ is assumed to contain the functions listed in Table 1.

*Definition* (5.3): Let the condition (5.2) be fulfilled for $k$. Then one defines mappings $K(U_i,U_j)$ on $\mathcal{H}(U_j)$, where $U_i,U_j$ run over $U_E,U_{E-E_d},U_R$, via: for each $\psi\in\mathcal{H}(U_E)$, $(\mathbf{s}',\mathbf{t}')\in U_i$

$$(K(U_i,U_E)\psi)(\mathbf{s}',\mathbf{t}')$$
$$=\lim_{\epsilon\to+0}\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,\frac{k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})}{E+i\epsilon-p^2-q^2}\,\psi(\mathbf{p},\mathbf{q})\,.$$

Analogously, for each

$$\psi\in\mathcal{H}(U_{E-E_d}),(\mathbf{s}',\mathbf{t}')\in U_i\,;(K(U_i,U_{E-E_d})\psi)(\mathbf{s}',\mathbf{t}')$$
$$=\lim_{\epsilon\to+0}\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi(\mathbf{p},\mathbf{k})$$
$$\times(E+i\epsilon-E_d-p^2)^{-1}(E+i\epsilon-E_d-k^2)^{-1},$$

and for each $\psi\in\mathcal{H}(U_R)$, $(\mathbf{s}',\mathbf{t}')\in U_i$,

$$(K(U_i,U_R\psi)(\mathbf{s}',\mathbf{t}')=\int_{U_R} d\mathbf{p}\,d\mathbf{q}\,k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})\psi(\mathbf{p},\mathbf{q})\,.$$

*Theorem* 2: The mapping $K(U_i,U_j)$ is a linear compact mapping from $\mathcal{H}(U_j)$ into $\mathcal{H}(U_i)$. Thus $K=\Sigma_{ij}K(U_i,U_j)$ is a linear compact mapping from $\mathcal{H}(G)$ into $\mathcal{H}(G)$.

*Proof*: Clearly $K(U_i,U_j)$ and thus $K$ is linear. The proof of compactness is given in several steps:

(i) Firstly, we want to show that $K(U_i,E_E)$ maps a bounded $\mathcal{H}(U_E)$ sequence to a $\mathcal{L}_2(U_i)$ sequence, containing a convergent subsequence in $\mathcal{L}_2(U_i)$. Let $\psi_n$ be bound in $\mathcal{H}(U_E)$,

TABLE I. List of functions.

| $\mathcal{L}_2(U_E \times U_E)$ | $\mathcal{L}_2(U_E \times U_{E-E_d})$ | $\mathcal{L}_2(U_E \times U_R)$ |
|---|---|---|
| $k$<br>$\phi^k_{;E}$<br>$\phi^k_{E;}$<br>$\phi^k_{E;E}$ | $k$<br>$\phi^k_{;,E-E_d}$<br>$\phi^k_{;E-E_d,}$<br>$\phi^k_{E;,}$<br>$\phi^k_{;E-E_d,E-E_d}$<br>$\phi^k_{E;,E-E_d}$<br>$\phi^k_{E;E-E_d,}$<br>$\phi^k_{E;E-E_d,E-E_d}$ | $k$<br>$\phi^k_{E;}$ |
| $\mathcal{L}_2(U_{E-E_d} \times U_E)$ | $\mathcal{L}_2(U_{E-E_d} \times U_{E-E_d})$ | $\mathcal{L}_2(U_{E-E_d} \times U_R)$ |
| $k$<br>$\phi^k_{,;E}$<br>$\phi^k_{,E-E_d;}$<br>$\phi^k_{E-E_d;}$<br>$\phi^k_{,E-E_d;E}$<br>$\phi^k_{E-E_d;E}$<br>$\phi^k_{E-E_d,E-E_d;}$<br>$\phi^k_{E-E_d,E-E_d;E}$ | $k$<br>$\phi^k_{,;,E-E_d}$<br>$\phi^k_{,;E-E_d,}$<br>$\phi^k_{,E-E_d;,}$<br>$\phi^k_{E-E_d;,}$<br>$\phi^k_{,;E-E_d,E-E_d}$<br>$\phi^k_{,E-E_d;,E-E_d}$<br>$\phi^k_{E-E_d;,E-E_d}$<br>$\phi^k_{,E-E_d;E-E_d,}$<br>$\phi^k_{E-E_d;E-E_d,}$<br>$\phi^k_{E-E_d,E-E_d;}$<br>$\phi^k_{,E-E_d;E-E_d,E-E_d}$<br>$\phi^k_{E-E_d;E-E_d,E-E_d}$<br>$\phi^k_{E-E_d,E-E_d;,E-E_d}$<br>$\phi^k_{E-E_d,E-E_d;E-E_d,}$<br>$\phi^k_{E-E_d,E-E_d;E-E_d,E-E_d}$ | $k$<br>$\phi^k_{,E-E_d;}$<br>$\phi^k_{E-E_d;}$<br>$\phi^k_{E-E_d,E-E_d;}$ |
| $\mathcal{L}_2(U_R \times U_E)$ | $\mathcal{L}_2(U_R \times U_{E-E_d})$ | $\mathcal{L}_2(U_R \times U_R)$ |
| $k$<br>$\phi^k_{;E}$ | $k$<br>$\phi^k_{;,E-E_d}$<br>$\phi^k_{;E-E_d,}$<br>$\phi^k_{;E-E_d,E-E_d}$ | $k$ |

$$\lim_{\epsilon \to +0} \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, [k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})/(E+i\epsilon-p^2-q^2)]\psi_n(\mathbf{p},\mathbf{q})$$

$$= \lim_{\epsilon \to +0} \Bigg\{ \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, [(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q}) - k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)})/(E-p^2-q^2)]\psi_n(\mathbf{p},\mathbf{q})$$

$$+ \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, \frac{k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q}) - k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)}}{(E-p^2-q^2)} \frac{i\epsilon}{(E+i\epsilon-p^2-q^2)} \psi_n(\mathbf{p},\mathbf{q})$$

$$+ \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} (\psi_n(\mathbf{p},\mathbf{q}) - \psi_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)})/(E-p^2-q^2)$$

$$+ \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} [i\epsilon/(E+i\epsilon-p^2-q^2)](\psi_n(\mathbf{p},\mathbf{q}) - \psi_n(\mathbf{p},\mathbf{q})_{|(p^2q^2=E)}) /(E-p^2-q^2)$$

$$+ \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} \psi_n(\mathbf{p},\mathbf{q})_{|(p^2+q^2=E)} [1/(E+i\epsilon-p^2-q^2)] \Bigg\}$$

$$= \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, \phi^k_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})\psi_n(\mathbf{p},\mathbf{q}) + \lim_{\epsilon \to +0} \int_{U_E} d\mathbf{p}\, d\mathbf{q}\, \phi^k_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})[i\epsilon/(E+i\epsilon-p^2-q^2)]\psi_n(\mathbf{p},\mathbf{q})$$

$$+\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})-\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})(E-p^2-q^2))\phi^{\psi_n}_{E}(\mathbf{p},\mathbf{q})$$

$$+\lim_{\epsilon\to+0}\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})-\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})(E-p^2-q^2))[i\epsilon/(E+i\epsilon-p^2-q^2)]\phi^{\psi_n}_{E}(\mathbf{p},\mathbf{q})$$

$$+\int d\hat{p}\,d\hat{q}\int_0^{\pi/2} d\xi\,\sin^2\xi\cos^2\xi\,k(\mathbf{s}',\mathbf{t}',\hat{p},\hat{q},\rho=\sqrt{E},\xi)\psi_n(\hat{p},\hat{q},\rho=\sqrt{E},\xi)$$

$$\times\lim_{\epsilon\to+0}\int_0^{E+\frac{1}{2}|E_d|} d\rho\,\rho^5/(E+i\epsilon-\rho^2)\,. \tag{5.4}$$

From $\psi_n$ being bounded in $\mathscr{H}(U_E)$ follows $\psi_n$ and $\phi^{\psi_n}_{E}$ are bounded sequences in $\mathscr{L}_2(U_E)$. Assumption (5.2) assures $k$ and $\phi^{k}_{;E}$ to be elements of $\mathscr{L}_2(U_i\times U_E)$ as $E-p^2-q^2$ is bounded on $U_E$ also $\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})(E-p^2-q^2)$ is an element of $\mathscr{L}_2(U_i\times U_E)$. Thus, from a standard theorem it follows that the first and the third terms contain convergent subsequences in $\mathscr{L}_2(U_i)$. The second and the fourth terms tend to 0 with $\epsilon\to+0$ uniformly in $n$ as $k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})\times[i\epsilon/(E+i\epsilon-p^2-q^2)]$, $\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})\times[i\epsilon/(E+i\epsilon-p^2-q^2)]$ and $\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})(E-p^2-q^2)[i\epsilon/(E+i\epsilon-p^2-q^2)]$ tend to 0 with $\epsilon\to0$ in $\mathscr{L}_2(U_i\times U_E)$ by an argument given explicitly in Ref. 15. In the fifth term the $\rho$ integration and later $\epsilon$-limitation can be performed explicitly, giving a complex number $c_0$. Thus, the fifth term reads

$$\frac{{c_0}^6}{(E+(1/2)|E_d|)^6}\int_0^{E+\frac{1}{2}|E_d|} d\rho\,\rho^5 d\hat{p}\,d\hat{q}\int_0^{\pi/2} d\xi\,\sin^2\xi\,\cos^2\xi\;k(\mathbf{s}',\mathbf{t}',\hat{p},\hat{q},\rho=\sqrt{E},\xi)\psi_n(\hat{p},\hat{q},\rho=\sqrt{E},\xi)$$

$$=\frac{{c_0}^6}{(E+(1/2)|E_d|)^6}\int_{U_E} d\mathbf{p}\,d\mathbf{q}\,(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})-\phi^{k}_{;E}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})(E-p^2-q^2))$$
$$\times(\psi_n(\mathbf{p},\mathbf{q})-\phi^{\psi_n}_{E}(\mathbf{p},\mathbf{q})(E-p^2-q^2)) \tag{5.5}$$

which also contains a convergent subsequence in $\mathscr{L}_2(U_i)$.

(ii) Next we want to show that $k(U_i,U_{E-E_d})$ maps a bounded sequence $\psi_n$ from $\mathscr{H}(U_{E-E_d})$ into a sequence in $\mathscr{L}_2(U_i)$, which contains a convergent subsequence. Splitting into disjoint components

$$U_{E-E_d}=(U_{E-E_d,1}\setminus U_{E-E_d,B})\cup(U_{E-E_d,B}\setminus U_{E-E_d,1})\cup(U_{E-E_d,1}\cap U_{E-E_d,B}) \tag{5.6}$$

(see Fig. 1) and also decomposing the 1 function on $U_{E-E_d}$

$$1|_{U_{E-E_d}}=\Pi_{E-E_d}(\mathbf{p})(1-\Pi_{E-E_d}(\mathbf{k}))+\Pi_{E-E_d}(\mathbf{k})(1-\Pi_{E-E_d}(\mathbf{p}))+\Pi_{E-E_d}(\mathbf{p})\Pi_{E-E_d}(\mathbf{k})\,, \tag{5.7}$$

one arrives at

$$\lim_{\epsilon\to+0}\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})(E+i\epsilon-E_d-p^2)^{-1}(E+i\epsilon-E_d-k^2)^{-1}$$

$$=\lim_{\epsilon\to+0}\Bigg\{\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,\Pi_{E-E_d}(\mathbf{p})(1-\Pi_{E-E_d}(\mathbf{k}))k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})(E+i\epsilon-E_d-p^2)^{-1}(E+i\epsilon-E_d-k^2)^{-1}$$
$$+\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,\Pi_{E-E_d}(\mathbf{k})(1-\Pi_{E-E_d}(\mathbf{p}))k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})(E+i\epsilon-E_d-p^2)^{-1}(E+i\epsilon-E_d-k^2)^{-1}$$
$$+\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,\Pi_{E-E_d}(\mathbf{p})\Pi_{E-E_d}(\mathbf{k})k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})(E+i\epsilon-E_d-p^2)^{-1}(E+i\epsilon-E_d-k^2)^{-1}\Bigg\}. \tag{5.8}$$

Note that in the first term the "dangerous points" at $E-E_d=k^2$ are excluded, while in the second term those points at $E-E_d=p^2$ are excluded. Now let us look upon the first term and proceed as in (1). Using the abbreviations $\Pi(\mathbf{x})=\Pi_{E-E_d}(\mathbf{x})$ and $D(\mathbf{x},\epsilon)=1/(E+i\epsilon-E_d-x^2)$, one obtains

$$\lim_{\epsilon\to+0}\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,\Pi(\mathbf{p})(1-\Pi(\mathbf{k}))D(\mathbf{k},\epsilon)[k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})/(E+i\epsilon-E_d-p^2)]\psi_n(\mathbf{p},\mathbf{k})$$

$$=\lim_{\epsilon\to+0}\int_{U_{E-E_d}} d\mathbf{p}\,d\mathbf{k}\,\Pi(\mathbf{p})(1-\Pi(\mathbf{k}))D(\mathbf{k},\epsilon)\Big\{[(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})-k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)})/(E-E_d-p^2)]\psi_n(\mathbf{p},\mathbf{k})$$
$$+[(k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})-k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})_{|(p^2=E=E_d)})/(E-E_d-p^2)][i\epsilon/(E+i\epsilon-E_d-p^2)]\psi_n(\mathbf{p},\mathbf{k})$$
$$+k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}\,[(\psi_n(\mathbf{p},\mathbf{k})-\psi_n(\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)})/(E-E_d-p^2)]$$
$$+k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)}[i\epsilon/(E+i\epsilon-E_d-p^2)][(\psi_n(\mathbf{p},\mathbf{k})-\psi_n(\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)})/(E-E_d-p^2)]$$
$$+k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)}\psi_n(\mathbf{p},\mathbf{k})|_{(p^2=E-E_d)}[1/(E+i\epsilon-E_d-p^2)]\Big\}$$

$$= \lim_{\epsilon \to +0} \int_{U_{E-E_d}} d\mathbf{p}\, d\mathbf{k}\, \Pi(\mathbf{p})(1-\Pi(\mathbf{k}))D(\mathbf{k},\epsilon)\Big\{\phi^{k}_{;E-E_{d'}}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})$$
$$+ \phi^{k}_{;E-E_{d'}}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})[i\epsilon/(E+i\epsilon-E_d-p^2)]\psi_n(\mathbf{p},\mathbf{k})$$
$$+ (k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k}) - \phi^{k}_{;E-E_{d'}}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})(E-E_d-p^2))\phi^{\psi_n}_{E-E_{d'}}(\mathbf{p},\mathbf{k})$$
$$+ (k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k}) - \phi^{k}_{;E-E_{d'}}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})(E-E_d-p^2))[i\epsilon/(E+i\epsilon-E_d-p^2)]\phi^{\psi_n}_{E-E_{d'}}(\mathbf{p},\mathbf{k})\Big\}$$
$$+ \lim_{\epsilon \to +0} \int d\hat{p}\, d\mathbf{k}\, (1-\Pi(\mathbf{k})D(\mathbf{k},\epsilon)k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}\psi_n(\mathbf{p},\mathbf{k})_{|(p^2=E-E_d)}$$
$$\times \int_{E+(1/2)|E_d|}^{E+(3/2)|E_d|} dp\, p^2/(E+i\epsilon-E_d-p^2)\,. \tag{5.9}$$

$|\Pi(\mathbf{p})(1-\Pi(\mathbf{k}))D(\mathbf{k},\epsilon)|$ is bounded in $U_E$. Arguing as in (i), one gets the first and third term in the curly bracket contribute to a sequence with a convergent subsequence in $\mathscr{L}_2(U_i)$, while the second and fourth term contributions tend to 0 in $\mathscr{L}_2(U_i)$. In the last term the $\int dp$ integration gives a complex number $C_0(\epsilon)$ and the $\lim_{\epsilon \to +0} C_0(\epsilon)$ exists. Thus the last term can be written

$$\lim_{\epsilon \to +0} \frac{3C_0(\epsilon)}{(E+(3/2)|E_d|)^3-(E+(1/2)|E_d|)^3}$$
$$\times \int_{U_E} d\mathbf{p}\, d\mathbf{k}\, \Pi(\mathbf{p})(1-\Pi(\mathbf{k}))D(\mathbf{k},\epsilon)$$
$$\times (k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k}) - \phi^{k}_{;E-E_{d'}}(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})(E-E_d-p^2))$$
$$\times (\psi_n(\mathbf{p},\mathbf{k}) - \phi^{\psi_n}_{E-E_{d'}}(\mathbf{p},\mathbf{k})(E-E_d-p^2))\,,$$

which also gives a convergent subsequence in $\mathscr{L}_2(U_i)$. Completely analogously

$$\lim_{\epsilon \to +0} \int_{U_{E-E_d}} d\mathbf{p}\, d\mathbf{k}\, \Pi(\mathbf{k})(1-\Pi(\mathbf{p}))$$
$$\times \frac{k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})}{(E+i\epsilon-E_d-p^2)(E+i\epsilon-E_d-k^2)}$$

and

$$\lim_{\epsilon \to +0} \int_{U_{E-E_d}} d\mathbf{p}\, d\mathbf{k}\, \Pi(\mathbf{p})\Pi(\mathbf{k})$$
$$\times \frac{k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})\psi_n(\mathbf{p},\mathbf{k})}{(E+i\epsilon-E_d-p^2)(E+i\epsilon-E_d-k^2)}$$

contain convergent subsequences in $\mathscr{L}_2(U_i)$.

(3) Finally, consider $K(U_i,U_R)$. From $\mathscr{H}(U_R) = \mathscr{L}_2(U_R)$ and the property 5.2 of the kernels it follows that a bounded sequence is mapped on a sequence with a convergent subsequence.

Up to now it has been shown that $K(U_i,U_j)$ is a linear compact mapping form $\mathscr{H}(U_j)$ on $\mathscr{L}_2(U_i)$. In order to show that it is a compact mapping from $\mathscr{H}(U_j)$ on $\mathscr{H}(U_i)$, it is necessary that all the subtractions on $\mathscr{L}_2(U_i)$ defined in 4.1 also have convergent subsequences. But that is fulfilled as all occurring subtractions of the kernel corresponding to the variables of $U_i$ have by definition 5.3 and Assumption 5.2 all the properties of being square integrable; the proof runs the same as in (i), (ii), and (iii), but instead of using the kernel $k$, now using the kernel $k$ subtracted corresponding to the variables of $U_i$. That completes the proof that a bounded sequence on $\mathscr{H}(U_j)$ is mapped by $K(U_i,U_j)$ on $\mathscr{H}(U_i)$ containing a convergent subsequence which means compactness.

## 6. APPLICATION ON TWO-BODY POTENTIALS

As we want to make use of Faddeev's famous work in Banach space,[1] we use the class of potentials introduced therein.

The two-body potential (3.1) has the properties

$$\langle \mathbf{q}'|V|\mathbf{q}\rangle = v(\mathbf{q}'-\mathbf{q})\,. \tag{6.1}$$

On the function $v$ several conditions are imposed which are assumed to hold throughout this section:

(1) Boundedness and sufficiently fast falling off:

$$|v(\mathbf{q})| \leqslant C(1+|\mathbf{q}|)^{-1-\theta_0}; \tag{6.2}$$

(2) Smoothness:

$$|v(\mathbf{q})-v(\mathbf{q}+\mathbf{h})| \leqslant C(1+|\mathbf{q}|)^{-1-\theta_0}|\mathbf{h}|^{\mu_0};$$
$$|\mathbf{h}| \leqslant 1, \quad \mu_0 > 0; \tag{6.3}$$

(3) Real valuedness:

$$v(-\mathbf{q}) = \overline{v(\mathbf{q})}\,. \tag{6.4}$$

As we need square integrability, we impose the constraint $\theta_0 \geqslant 1$. We need some further definitions:

$$N(\mathbf{p},\mathbf{q},\theta) = \sum_{\alpha,\beta} \delta_{\alpha\beta}(1+|\mathbf{p}_\alpha|)^{-1-\theta}(1+|\mathbf{p}_\beta|)^{-1-\theta} \tag{6.5}$$

where $\alpha, \beta$ run over all channels, and $\mathbf{p}_\alpha, \mathbf{p}_\beta$ are expressed by $\mathbf{p},\mathbf{q}$ via the transformation (3.18).

$\chi_{E_d}(\mathbf{q})$ is defined as a solution of

$$VG_0(E_d)\chi_{E_d} = \chi_{E_d}\,. \tag{6.6}$$

Faddeev[1] shows that $\chi_{E_d}(\mathbf{q})$ has the properties

$$|\chi_{E_d}(\mathbf{q})| \leqslant C(1+|\mathbf{q}|)^{-1-\theta_0},$$
$$|\chi_{E_d}(\mathbf{q}+\mathbf{h})-\chi_{E_d}(\mathbf{q})| \leqslant C(1+|\mathbf{q}|)^{-1-\theta_0}|\mathbf{h}|^{\mu_0}; \quad |\mathbf{h}| \leqslant 1\,. \tag{6.7}$$

An integral kernel $Q(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z)$ is said to be of the type $\mathcal{Q}$ if it may be expressed in the form

$$Q(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z) = F(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z) + G(\mathbf{p}',\mathbf{q}',\mathbf{p},z)$$
$$\times \left[\overline{\chi_{E_d}(\mathbf{q})}/(z-p^2-E_d^2)\right]$$
$$+ \left[\chi_{E_d}(\mathbf{q}')/(z-p^2-E_d^2)\right]\tilde{G}(\mathbf{p}',\mathbf{p},\mathbf{q},z) \tag{6.8}$$

$$+\left[\chi_{E_d}(\mathbf{q}')/(z-p^2-E_d^2)\right]\cdot$$
$$\times H(\mathbf{p}',\mathbf{p},z)\left[\overline{\chi_{E_d}(\mathbf{q})}/(z-p^2-E_d^2)\right].$$

An integral kernel $Q(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z)$ of type $\mathcal{Q}$ is said to belong to the class $\mathcal{Q}(\theta,\mu)$ if $F(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z)$ satisfies the following estimates:

$$|F(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z)|\leqslant CN(\mathbf{p}',\mathbf{q}',\theta)(1+p^2)^{-1},$$
$$|F(\mathbf{p}'+\mathbf{h}',\mathbf{q}'+\mathbf{l}',\mathbf{p}+\mathbf{h},\mathbf{q}+\mathbf{l},z+\Delta z)-F(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},z)| \quad (6.9)$$
$$\leqslant CN(\mathbf{p}',\mathbf{q}',\theta)(1+p^2)^{-1}$$
$$\times(|\mathbf{h}'|^{\mu}+|\mathbf{l}'|^{\mu}+|\mathbf{h}|^{\mu}+|\mathbf{l}|^{\mu}+|\Delta z|^{\mu}),$$

and if the kernels $G(\mathbf{p}',\mathbf{q}',\mathbf{p},z)$, $\tilde{G}(\mathbf{p}',\mathbf{p},\mathbf{q},z)$ and $H(\mathbf{p}',\mathbf{p},z)$ satisfy the estimates from (6.8) and (6.9) on setting, respectively, $\mathbf{q}'=0$, $\mathbf{q}=0$, and set simultaneously $\mathbf{q}'=0$ and $\mathbf{q}=0$, while $N$ is given by (6.5). Then Faddeev proves the following result:

Faddeev's theorem. The integral kernels

$${}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|T_{\beta_1}(Z)G_0(Z)T_{\beta_2}(Z)G_0(Z)T_{\beta_3}(Z)G_0(Z)T_{\beta_4}(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4},$$

belong for $\beta_i\neq\beta_{i+1}$ to the class $\mathcal{Q}(\tilde{\theta},\tilde{\mu})$ with certain indices $\tilde{\theta},\tilde{\mu},\tilde{\theta}>\frac{1}{2}$, uniformly over any finite region of the complex $Z$-plane, denoted by $\pi_{E_d}$ to indicate that it is slit along the real axis from the point $E_d$ to $+\infty$. Let us investigate the matrix element of $H_{\beta_1\beta_2\beta_3\beta_4}$ (3.13),

$$\begin{aligned}
&{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&={}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|B_{\beta_1}(Z)G_0(Z)T_{\beta_2}(Z)G_0(Z)T_{\beta_3}(Z)G_0(Z)\\
&\quad\times B_{\beta_4}(Z)B_0(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&=\frac{Z-p'^2-E_d}{-|Z|-p'^2-|E_d|}\\
&\quad\times{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|T_{\beta_1}(Z)G_0(Z)T_{\beta_2}(Z)G_0(Z)T_{\beta_3}(Z)\\
&\quad\times G_0(Z)T_{\beta_4}(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&\quad\times\frac{(Z-p^2-E_d)}{(-|Z|-p^2-|E_d|)(-|Z|-p^2-q^2)}. \qquad (6.10)
\end{aligned}$$

Using Faddeev's theorem, this reads

$$\begin{aligned}
&{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&=\frac{(Z-p'^2-E_d)}{(-|Z|-p'^2-|E_d|)}Q(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},Z)\\
&\quad\times\frac{(Z-p^2-E_d)}{(-|Z|-p^2-|E_d|)(-|Z|-p^2-q^2)}\\
&=\frac{(Z-p'^2-E_d)}{(-|Z|-p'^2-|E_d|)}F(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q},Z)\\
&\quad\times\frac{(Z-p^2-E_d)}{(-|Z|-p^2-|E_d|)(-|Z|-p^2-q^2)}\\
&+G(\mathbf{p}',\mathbf{q}',\mathbf{p},Z)\frac{\overline{\chi_{E_d}(\mathbf{q})}}{(-|Z|-p^2-|E_d|)(-|Z|-p^2-q^2)}\\
&\quad+\frac{\chi_{E_d}(\mathbf{q}')}{-|Z|-p'^2-|E_d|}\tilde{G}(\mathbf{p}',\mathbf{p},\mathbf{q},Z)\frac{1}{-|Z|-p^2-q^2}\\
&\quad+\frac{\chi_{E_d}(\mathbf{q}')}{-|Z|-p'^2-|E_d|}H(\mathbf{p}',\mathbf{p},Z)\\
&\quad\times\frac{\overline{\chi_{E_d}(\mathbf{q})}}{(-|Z|-p^2-|E_d|)(-|Z|-p^2-q^2)}. \qquad (6.11)
\end{aligned}$$

Our aim is $k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{q})=\lim_{\epsilon\to+0}\langle\mathbf{s}',\mathbf{t}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}$, respectively, $k(\mathbf{s}',\mathbf{t}',\mathbf{p},\mathbf{k})=\lim_{\epsilon\to+0}\langle\mathbf{s}',\mathbf{t}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{k}\rangle_{\beta_4\beta_5}$ defined by (5.3) and (3.26) to fulfill condition (5.2) which would yield, with the help of Theorem 2, the desired result. Let us switch for the moment from the class of local two-body potentials defined by (6.1)–(6.4) to the wide class of separable two-body potentials. It was shown by Kröger and Fenske[15] that below the three-body breakup threshold even the noniterated kernel of the scattering equations is compact. It is shown in the Appendix that for a separable potential $\lim_{\epsilon\to+0}\langle\mathbf{s}',\mathbf{t}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}$, respectively, $\lim_{\epsilon\to+0}\langle\mathbf{s}',\mathbf{t}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{k}\rangle_{\beta_4\beta_5}$ fulfills the conditions (5.2) and yields the desired result. Returning now to the local potential given by (6.1)–(6.4), one reads from (6.11), (6.9), (6.5), and (6.7) that $\lim_{\epsilon\to+0}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}$ is bounded, continuous and square integrable in $\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q}\in G\times G$. That is close to, but not quite, sufficient to guarantee the requirements (5.2) because the index $\tilde{\mu}<1$. Thus, we make an approximation,

$$\lim_{\epsilon\to+0}H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)\to\tilde{H}_{\beta_1\beta_2\beta_3\beta_4}\ \text{ in }\ L_2(G\times G) \qquad (6.12)$$

and require also that ${}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|\tilde{H}_{\beta_1\beta_2\beta_3\beta_4}|\mathbf{p},\mathbf{q}\rangle_{\beta_4}$ be once continuously differentiable with respect to $\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q}\in G\times G$. Then $\tilde{H}_{\beta_1\beta_2\beta_3\beta_4}$ fulfills the condition (5.2). We remark that this approximation is not continuous going over to $\mathcal{H}(G)$. But it definitely makes sense, as it is closely related to the separable approximation of the two-body potential, which gives the desired result as mentioned above and turned out to be quite successful in many practical calculations. Thus Theorem 2 can be applied and yields:

*Theorem* 3: For the class of separable two-body potentials defined in the Appendix, the kernel $K_{\beta_1\beta_2\beta_3\beta_4\beta_5}=H_{\beta_1\beta_2\beta_3\beta_4}S_0S_{\beta_4}S_{\beta_5}$ given by (3.13), (3.15), and (3.16) and for the class of Hölder–type two-body potentials given by (6.1)–(6.4), the kernel $\tilde{K}_{\beta_1\beta_2\beta_3\beta_4\beta_5}=\tilde{H}_{\beta_1\beta_2\beta_3\beta_4}S_0S_{\beta_4}S_{\beta_5}$ given by (3.13), (3.15), (3.16), and (6.12) is a compact kernel for the scattering equations (3.12) in the physical limit $Z=E+i\epsilon$, $\epsilon\to+0$ in the Hilbert space $\mathcal{H}(G)$ given by (4.1) and (4.2).

## 7. FOUR-NUCLEON CASE

In this section the treatment for the three-nucleon case is extended to four bodies. Let us recall two important features concerning the structure of the three-body operator equation and the sphere of singular points. The splitting of $T_\alpha$, $G_0$ into a "harmless" and a "singular" part allows an operator equation with a kernel of the structure "harmless" operator times a "singular" operator and the solution being a "harmless" operator. The other property is that the sphere of singular points given by (3.20) due to the free propagator and that of the deuteron propagator do not intersect. In the following, we want to show that analogues of these properties also hold in the four-nucleon case. To derive operator equations, we start from the four-body Alt–Grassberger–Sandhas equations.[16] They read

$$U^{\sigma\rho}_{\beta\alpha} = \bar{\delta}^{\sigma\rho}\delta_{\beta\alpha}G_0^{-1}T_\beta^{-1}G_0^{-1} + \sum_{\tau,\gamma}\bar{\delta}^{\sigma\tau}U^{\tau}_{\beta\gamma}G_0T_\gamma G_0U^{\tau\rho}_{\gamma\alpha}\,,$$

$$U^{\tau}_{\beta\alpha} = \bar{\delta}^{\tau}_{\beta\alpha}G_0^{-1} + \sum_{\gamma}\bar{\delta}^{\tau}_{\beta\gamma}T_\gamma G_0U^{\tau}_{\gamma\alpha}\,. \tag{7.1}$$

We define

$$\bar{U}^{\tau}_{\beta\alpha} = T_\beta G_0U^{\tau}_{\beta\alpha}\,,$$

$$\bar{U}^{\sigma\rho}_{\beta\alpha} = T_\beta G_0\sum_{\mu}U^{\sigma}_{\beta\mu}G_0T_\mu G_0U^{\sigma\rho}_{\mu\alpha} \tag{7.2}$$

which fulfills

$$\bar{U}^{\tau}_{\beta\alpha} = \bar{\delta}_{\beta\alpha}T_\beta + \sum_{\gamma}T_\beta G_0\bar{\delta}^{\tau}_{\beta\gamma}\bar{U}^{\tau}_{\gamma\alpha}\,,$$

$$\bar{U}^{\sigma\rho}_{\beta\alpha} = \bar{\delta}^{\sigma\rho}\bar{U}^{\sigma}_{\beta\alpha} + \sum_{\tau,\mu}\bar{U}^{\sigma}_{\beta\mu}\bar{\delta}^{\sigma\tau}G_0\bar{U}^{\tau\rho}_{\mu\alpha}\,. \tag{7.3}$$

The operator $\bar{U}^{\sigma}_{\beta\alpha}$ contains the deuteron pole, the triton pole in the $\sigma = (i,kjl)$ channels, and the double deuteron pole in the $\sigma = (ij,kl)$ channels. For explicit details on the structure of equations we refer to Ref. 17.

In order to split the kernel into "harmless" and "singular" parts, we introduce $S_\beta$, containing the deuteron pole in those channels $\sigma$ where the two-body subsystem is contained, via

$$\begin{aligned}{}_\sigma\langle \mathbf{k}',\mathbf{p}',\mathbf{q}'|S_\beta(Z)|\mathbf{k},\mathbf{p},\mathbf{q}\rangle_\sigma &= \delta(\mathbf{uk}-\mathbf{k})\delta(\mathbf{p}'-\mathbf{p})\delta(\mathbf{q}'-\mathbf{q}) \\ &\times \frac{-|Z| - (2/3)k^2 - (3/4)p^2 - |E_d|}{Z - (2/3)k^2 - (3/4)p^2 - E_d}\,,\end{aligned} \tag{7.4}$$

$S^\sigma$, containing the triton pole in the $\sigma = (i,jkl)$ channel via

$$\begin{aligned}{}_\sigma\langle \mathbf{k}',\mathbf{p}',\mathbf{q}'|S^\sigma(Z)|\mathbf{k},\mathbf{p},\mathbf{q}\rangle_\sigma &= \delta(\mathbf{k}'-\mathbf{k})\delta(\mathbf{p}'-\mathbf{p})\delta(\mathbf{q}'-\mathbf{q})\frac{-|Z| - (2/3)k^2 - |E_d|}{Z - (2/3)k^2 - E_d}\,,\end{aligned} \tag{7.5}$$

and $S^\sigma$, containing the double deuteron pole in the $\sigma = (ij,kl)$ channel via

$$\begin{aligned}{}_\sigma\langle \mathbf{k}',\tilde{\mathbf{q}}',\mathbf{q}'|S^\sigma(Z)|\mathbf{k},\tilde{\mathbf{q}},\mathbf{q}\rangle_\sigma &= \delta(\mathbf{k}'-\mathbf{k})\delta(\tilde{\mathbf{q}}'-\tilde{\mathbf{q}})\delta(\mathbf{q}'-\mathbf{q})\frac{-|Z| - \frac{1}{2}k^2 - |E_{dd}|}{Z - \frac{1}{2}k^2 - E_{dd}}\,.\end{aligned} \tag{7.6}$$

We assume for technical simplicity that the four-body system has only the triton and deuteron as subsystem bound states.

Now we define

$$T_\beta = S_\beta\tilde{T}_\beta\,,$$
$$\bar{U}^{\tau}_{\beta\alpha} = S_\beta S^\tau\tilde{U}^{\tau}_{\beta\alpha}\,, \tag{7.7}$$
$$\bar{U}^{\sigma\rho}_{\beta\alpha} = S_\beta S^\sigma\tilde{U}^{\sigma\rho}_{\beta\alpha}\,.$$

From (7.3) we imply

$$\tilde{U}^{\sigma\rho}_{\beta\alpha} = \tilde{U}^{\sigma}_{\beta\alpha}\bar{\delta}^{\sigma\rho} + \sum_{\tau,\mu}\bar{\delta}^{\sigma\tau}\tilde{U}^{\sigma}_{\beta\mu}G_0S_\mu S^\tau\tilde{U}^{\tau\rho}_{\mu\alpha}\,. \tag{7.8}$$

The operator $\tilde{U}^{\sigma}_{\beta\alpha}$ does not contain either the deuteron pole or the triton pole or the double deuteron pole. The poles are contained in $G_0$, $S_\mu$ and $S^\tau$. Equation (7.8) is the four-body analogue to Eq. (3.9). It has a kernel of the desired structure "harmless" times "singular" operator. But the kernel $\tilde{U}^{\sigma}_{\beta\mu}G_0S_\mu S^\tau$ is not compact. That requires further iterations.

Let us finally demonstrate the four-body analogue property of nonintersection of spheres of singular points. In the channels of the type $(i,jkl)$ one has the following singular points:

(i) $E - \frac{2}{3}k^2 - \frac{3}{4}p^2 - q^2 = 0$ due to the free pole in $G_0$,

(ii) $E - \frac{2}{3}k^2 - \frac{3}{4}p^2 - E_d = 0$ due to the deuteron pole in $S_\beta$,

(iii) $E - \frac{2}{3}k^2 - E_t = 0$ due to the triton pole in $S^\tau$.

It is valid $E_t < E_d < 0$. If one assumes on the contrary that (i) intersects (ii), then

$$E - \tfrac{2}{3}k^2 - \tfrac{3}{4}p^2 - q^2 = E - \tfrac{2}{3}k^2 - \tfrac{3}{4}p^2 - E_d\,,$$

thus $0 > -q^2 = -E_d > 0$ gives a contradiction. If (ii) were to intersect (iii), then

$$E - \tfrac{2}{3}k^2 - \tfrac{3}{4}p^2 - E_d = E - \tfrac{2}{3}k^2 - E_t\,,$$

and $0 < (3/4)p^2 = E_t - E_d < 0$ would give a contradiction. If (iii) were to intersect (i), then

$$E - \tfrac{2}{3}k^2 - E_t = E - \tfrac{2}{3}k^2 - \tfrac{3}{4}p^2 - q^2\,,$$

and $0 < -E_t = -\frac{3}{4}p^2 - q^2 < 0$ would be a contradiction. In the channels of the type $(ij,kl)$ one has the singular points:

(i) $E - \frac{1}{2}k^2 - \tilde{q}^2 - q^2 = 0$ due to the free pole in $G_0$,

(ii) $E - \frac{1}{2}k^2 - \tilde{q}^2 - E_d = 0$ due to the deuteron pole in $S_\beta$,

(iii) $E - \frac{1}{2}k^2 - E_{dd} = 0$ due to the double deuteron pole in $S^\tau$.

The energies are $E_{dd} < E_d < 0$. The spheres (i, ii, iii) do not intersect each other, as one verifies similarly. Thus, in the four-nucleon system two important features of the three-body case also hold: the "harmless" times "singular" structure of the kernel of equations and the separation property of the singular spheres. The four-nucleon case is open to proceeding in detail with the same technique applied as in the three-body case.


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## APPENDIX

In this section we want to show that for the widely used class of separable two-body potentials $\lim_{\epsilon\to+0}H_{\beta,\beta,\beta,\beta}(E+i\epsilon)$ fulfills condition (5.2), such that Theorem 3 holds without approximation (6.12). A separable two-body interaction is defined as

$$V = \lambda\,|\chi\rangle\langle\chi|\,, \tag{A1}$$

where we restrict ourselves for simplicity to the rank-one case. Additionally, a fall-off condition and a smoothness condition is required,

$$\chi\in\mathscr{L}_2(\mathbb{R}^3),\quad \chi(\mathbf{q}) \text{ analytic for } \mathbf{q}\in\mathbb{R}^3\,. \tag{A2}$$

The two-body transition operator $T$ reads

$$T(Z)=t(Z)|\chi\rangle\langle\chi|,\quad t(Z)=\frac{\lambda}{\lambda-\langle\chi|G_0(Z)|\chi\rangle}, \tag{A3}$$

which leads to

$$T_\alpha(Z)=\int d\mathbf{p}\,|\mathbf{p},\chi\rangle_\alpha t(Z-p^2)_\alpha\langle\mathbf{p},\chi|, \tag{A4}$$

$$B_\alpha(Z)=\int d\mathbf{p}\,|\mathbf{p},\chi\rangle_\alpha b(Z-p^2)_\alpha\langle\mathbf{p},\chi|,$$

$$b(Z-p^2)=\frac{Z-p^2-E^d}{-|Z|-p^2-|E^d|}t(Z-p^2) \tag{A5}$$

$$\begin{aligned}H_{\beta_1\beta_2\beta_3\beta_4}(Z)=&\int d\mathbf{p}\,d\mathbf{p}'d\mathbf{p}''d\mathbf{p}'''|\mathbf{p},\chi\rangle_{\beta_1}b(Z-p^2)\\&\times_{\beta_1}\langle\mathbf{p},\chi|G_0(Z)|\mathbf{p}',\chi\rangle_{\beta_2}t(Z-p'^2)\\&\times_{\beta_2}\langle\mathbf{p}',\chi|G_0(Z)|\mathbf{p}'',\chi\rangle_{\beta_3}t(Z-p''^2)\\&\times_{\beta_3}\langle\mathbf{p}'',\chi|G_0(Z)|\mathbf{p}''',\chi\rangle_{\beta_4}b(Z-p'''^2)_{\beta_4}\langle\mathbf{p}''',\chi|B_0(Z).\end{aligned} \tag{A6}$$

With the following definition for $I$

$$\begin{aligned}I(\mathbf{p}',\mathbf{p},z)=&\int d\mathbf{p}''d\mathbf{p}'''\,{}_{\beta_1}\langle\mathbf{p}',\chi|G_0(Z)|\mathbf{p}'',\chi\rangle_{\beta_2}t(Z-p''^2)\\&\times_{\beta_2}\langle\mathbf{p}'',\chi|G_0(Z)|\mathbf{p}''',\chi\rangle_{\beta_3}t(Z-p'''^2)\\&\times_{\beta_3}\langle\mathbf{p}''',\chi|G_0(Z)|\mathbf{p},\chi\rangle_{\beta_4},\end{aligned} \tag{A7}$$

one has

$$\begin{aligned}&{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(Z)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\&\quad=b(Z-p'^2)\overline{\chi(\mathbf{q}')}I(\mathbf{p}',\mathbf{p},z)\frac{b(Z-p^2)\chi(\mathbf{q})}{-|Z|-p^2-q^2}.\end{aligned} \tag{A8}$$

The function $\lim_{\epsilon\to+0}t(E+i\epsilon-p^2)$ has the properties:

(i) It tends asymptotically to a constant as $p$ tends to infinity;

(ii) It is analytical in $\mathbf{p}$ except at $E-p^2-E^d=0$, the deuteron pole, and at $E-p^2=0$, where it behaves like $b_1+b_2(Z-p^2)^{1/2}$.

The same holds for $\lim_{\epsilon\to+0}b(E+i\epsilon-p^2)$, except having the deuteron pole. It remains to investigate $\lim_{\epsilon\to+0}I(\mathbf{p}',\mathbf{p},E+i\epsilon)$. Defining the function $\xi(\mathbf{p}',\mathbf{p})$ via

$$\begin{aligned}&{}_\beta\langle\mathbf{p}',\chi|G_0(Z)|\mathbf{p},\chi\rangle_\alpha\\&=\frac{\overline{\chi(a\mathbf{p}'+b\mathbf{p})}\,\chi(c\mathbf{p}'+d\mathbf{p})}{Z-\frac{4}{3}(p'^2+p^2+\mathbf{p}'\cdot\mathbf{p})}=\frac{\xi(\mathbf{p}',\mathbf{p})}{Z-\frac{4}{3}(p'^2+p^2+\mathbf{p}'\cdot\mathbf{p})},\end{aligned} \tag{A9}$$

where the constants $a, b, c, d$ result from channel recoupling. $I$ reads

$$I(\mathbf{p}',\mathbf{p},Z)=\int d\mathbf{p}''\,d\mathbf{p}'''\frac{\xi(\mathbf{p}',\mathbf{p}'')t(Z-p''^2)\xi(\mathbf{p}'',\mathbf{p}''')t(Z-p'''^2)\xi(\mathbf{p}''',\mathbf{p})}{(Z-\frac{4}{3}(p'^2+p''^2+\mathbf{p}'\cdot\mathbf{p}''))(Z-\frac{4}{3}(p''^2+p'''^2+\mathbf{p}''\cdot\mathbf{p}'''))(Z-\frac{4}{3}(p'''^2+p^2+\mathbf{p}'''\cdot\mathbf{p}))}. \tag{A10}$$

Because of $\chi\in\mathcal{L}_2(\mathbb{R}^3)$, one has $\xi\in\mathcal{L}_2(\mathbb{R}^3\times\mathbb{R}^3)$ and thus for $\mathrm{Im}(Z)\neq0$ $I\in\mathcal{L}_2(\mathbb{R}^3\times\mathbb{R}^3)$. This would hold also in the limit $Z=E+i\epsilon$, $\epsilon\to+0$, if there were no singularities. First of all, one notes that the deuteron pole of $t(Z-p^2)$ cannot coincide with any singularities arising from the denominator, similar to property (3.21). Performing the integration in the neighborhood of the deuteron pole gives a contribution, which is square integrable and analytic in $\mathbf{p}',\mathbf{p}$ also in the limit $\epsilon\to+0$. In order to investigate the analytic structure of the remaining part, one can also look at

$$\begin{aligned}I_0(\mathbf{p}',\mathbf{p},Z)=&\int_D d\mathbf{p}''\,d\mathbf{p}'''\,(N(\mathbf{p}',\mathbf{p}'',Z)N(\mathbf{p}'',\mathbf{p}''',Z)\\&\times N(\mathbf{p}''',\mathbf{p},Z))^{-1},\\N(\mathbf{p}',\mathbf{p},Z)=&Z-\tfrac{4}{3}(p'^2+p^2+\mathbf{p}'\cdot\mathbf{p}).\end{aligned} \tag{A11}$$

The integration domain $D$ can be chosen large enough to include the singularities of the integrand, but must be smaller than $\mathbb{R}^3\times\mathbb{R}^3$, in order that $I_0$ exist. The integration of $\mathbf{p}''$ can be performed following Lewis,[18] which yields

$$\begin{aligned}J_0(\mathbf{p}',\mathbf{p},Z)=&\int d\mathbf{p}''\,(N(\mathbf{p}',\mathbf{p}'',Z)N(\mathbf{p}'',\mathbf{p},Z))^{-1}\\=&\frac{8\pi i}{9|\mathbf{p}'-\mathbf{p}|}\ln\frac{\mu'+\mu-i|\mathbf{p}'-\mathbf{p}|}{\mu'+\mu+i|\mathbf{p}'-\mathbf{p}|},\\\mu'=&[3(p'^2-Z)]^{1/2},\quad\mu=[3(p^2-Z)]^{1/2}.\end{aligned} \tag{A12}$$

The result is that $\lim_{\epsilon\to+0}I_0(\mathbf{p}',\mathbf{p},E+i\epsilon)$ exists for all $\mathbf{p}',\mathbf{p}\in\mathbb{R}^3\times\mathbb{R}^3$ and is a continuous and square integrable function. Excluding once the behavior in the neighborhood of the critical points $p'^2-E=0$ and $p^2-E=0$, $\lim_{\epsilon\to+0}I_0(\mathbf{p}',\mathbf{p},E+i\epsilon)$ is even a smooth function in the sense of being locally subtractable and square integrable. The same holds for $\lim_{\epsilon\to+0}I(\mathbf{p}',\mathbf{p},E+i\epsilon)$ because $\xi(\mathbf{p}',\mathbf{p})$ is an analytic function. $\lim_{\epsilon\to+0}I_0(\mathbf{p}',\mathbf{p},E+i\epsilon)$ and thus $\lim_{\epsilon\to+0}I(\mathbf{p}',\mathbf{p},E+i\epsilon)$ behave in the neighborhood of $p'^2-E=0$ and $p^2-E=0$ like

$$\begin{aligned}&\lim_{\epsilon\to+0}I(\mathbf{p}',\mathbf{p},E+i\epsilon)|_{p'^2\simeq p^2\simeq E}\\&=C_1+\lim_{\epsilon\to+0}[C_2(E+i\epsilon-p'^2)^{1/2}+C_3(E+i\epsilon-p^2)^{1/2}\\&\quad+C_4((E+i\epsilon-p'^2)(E+i\epsilon-p^2))^{1/2}].\end{aligned} \tag{A13}$$

That can be seen from (A12). Integrating the term $1/N(\mathbf{p}'',\mathbf{p},Z)$ in the neighborhood of $\mathbf{p}''=-\frac{1}{2}\mathbf{p}$, where it becomes singular, yields

$$\begin{aligned}&\int_{U(\mathbf{p}''=\frac{1}{2}\mathbf{p})}d\mathbf{p}''\frac{1}{Z-\frac{4}{3}(p''^2+p^2+\mathbf{p}''\cdot\mathbf{p})}\\&\quad=\int_{U(\mathbf{q}=0)}d\mathbf{q}\frac{1}{Z-p^2-\frac{1}{3}q^2}=C_1+C_2(Z-p^2)^{1/2}\end{aligned} \tag{A14}$$

If $U$ is a ball. Because of the symmetry of $I$ under $\mathbf{p}',\mathbf{p}$ exchange (A13) is evident. From the properties of $b(Z-p^2)$ and $I(\mathbf{p}',\mathbf{p},Z)$ found so far one can conclude

$$\begin{aligned}k(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})=&\lim_{\epsilon\to+0}{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\=&\lim_{\epsilon\to+0}(b(E+i\epsilon-p'^3)\overline{\chi(\mathbf{q}')}I(\mathbf{p}',\mathbf{p},E+i\epsilon)\end{aligned}$$

$$\times\frac{b(E+i\epsilon-p^2)\chi(\mathbf{q})}{-|E|-p^2-q^2}\Big)\in\mathscr{S}_2(G\times G)\,, \tag{A15}$$

which means that $k$ is contained in the table (5.2). Next, we want to show that for such a $k$ also $\phi^{\,k}_{E;E}$ is contained in table (5.2)

$$\begin{aligned}
&\int_{U_2\times U_2} d\mathbf{p}'d\mathbf{q}'d\mathbf{p}\,d\mathbf{q}|\phi^{\,k}_{E;E}(\mathbf{p}',\mathbf{q}',\mathbf{p},\mathbf{q})|^2\\
&=\int d\mathbf{p}'d\mathbf{q}'d\mathbf{p}d\mathbf{q}|\lim_{\epsilon\to+0}\Big({}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&\quad-{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\big|_{p'^2+q'^2=E}\\
&\quad-{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\big|_{p^2+q^2=E}\\
&\quad+{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\big|_{\substack{p'^2+q'^2=E\\ p^2+q^2=E}}\Big)|^2\\
&\quad/((E-p'^2-q'^2)(E-p^2-q^2))^2\,.
\end{aligned}\tag{A16}$$

Because $\lim_{\epsilon\to+0}\, b(E+i\epsilon-p^2)$ and $\lim_{\epsilon\to+0}\, I(\mathbf{p}',\mathbf{p},E+i\epsilon)$ are smooth functions except at the points $E-p'^2=0$ and $E-p^2=0$, we insert for $\lim_{\epsilon\to+0}{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}$ the asymptotic expression for $b$ and $I$ (A13) in the neighborhood of $E-p'^2=0$ and $E-p^2=0$

$$\begin{aligned}
&\lim_{\epsilon\to+0}{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&=\lim_{\epsilon\to+0}(b_1+b_2(E+i\epsilon-p'^2)^{1/2})\,\overline{\chi(\mathbf{q}')}\\
&\quad\times[C_1+C_2(E+i\epsilon-p'^2)^{1/2}+C_3(E+i\epsilon-p^2)^{1/2}\\
&\quad+C_4((E+i\epsilon-p'^2)(E+i\epsilon-p^2))^{1/2}]\\
&\quad\times\frac{((b_1+b_2(E+i\epsilon-p^2)^{1/2})\chi(\mathbf{q})}{-|E|-p^2-q^2}
\end{aligned}\tag{A17}$$

$$\begin{aligned}
&=\lim_{\epsilon\to+0}\overline{\chi(\mathbf{q}')}\,[d_1+d_2(E+i\epsilon-p'^2)^{1/2}\\
&\quad+d_3(E+i\epsilon-p^2)^{1/2}\\
&\quad+d_4((E+i\epsilon-p'^2)(E+i\epsilon-p^2))^{1/2}]\\
&\quad\times\frac{\chi(\mathbf{q})}{-|E|-p^2-q^2}\,.
\end{aligned}$$

Because $\overline{\chi(\mathbf{q}')}\chi(\mathbf{q})/(-|E|-p^2-q^2)$ is an analytic function in the integration domain, it is sufficient to substitute in Eq. (A17)

$$\begin{aligned}
&\lim_{\epsilon\to+0}{}_{\beta_1}\langle\mathbf{p}',\mathbf{q}'|H_{\beta_1\beta_2\beta_3\beta_4}(E+i\epsilon)|\mathbf{p},\mathbf{q}\rangle_{\beta_4}\\
&\quad\to\lim_{\epsilon\to+0}[d_1+d_2(E+i\epsilon-p'^2)^{1/2}+d_3(E+i\epsilon-p^2)^{1/2}\\
&\qquad+d_4((E+i\epsilon-p'^2)(E+i\epsilon-p^2))^{1/2}]\,.
\end{aligned}\tag{A18}$$

Abbreviating

$$\begin{aligned}
W'&=\lim_{\epsilon\to+0}(E+i\epsilon-p'^2)^{1/2},\\
\underline{W}'&=\lim_{\epsilon\to+0}(E+i\epsilon-p'^2)^{1/2}\big|_{p'^2+q'^2=E}\,,\\
W&=\lim_{\epsilon\to+0}(E+i\epsilon-p^2)^{1/2},
\end{aligned}\tag{A19}$$

$$\underline{W}=\lim_{\epsilon\to+0}(E+i\epsilon-p^2)^{1/2}\big|_{p^2+q^2=E}\,,$$

and inserting (A18) in (A16), one has

$$\begin{aligned}
&\int_{U_2\times U_2}d\mathbf{p}'d\mathbf{q}'d\mathbf{p}\,d\mathbf{q}|d_1+d_2W'+d_3W+d_4W'W\\
&\quad-(d_1+d_2\underline{W}'+d_3W+d_4\underline{W}'W)\\
&\quad-(d_1+d_2W'+d_3\underline{W}+d_4W'\underline{W})\\
&\quad+d_1+d_2\underline{W}'+d_3\underline{W}+d_4\underline{W}'\underline{W}|^2/\\
&\quad((E-p'^2-q'^2)(E-p^2-q^2))^2\\
&=\int_{U_2\times U_2}d\mathbf{p}'d\mathbf{q}'d\mathbf{p}\,d\mathbf{q}\,|d_4|^2\\
&\quad\times\left|\frac{(W'-\underline{W}')(W-\underline{W})}{(E-p'^2-q'^2)(E-p^2-q^2)}\right|^2\\
&=\left(|d_4|\int_{U_2}d\mathbf{p}\,d\mathbf{q}\left|\frac{W-\underline{W}}{E-p^2-q^2}\right|^2\right)^2.
\end{aligned}\tag{A20}$$

Equation (A19) gives

$$W=\lim_{\epsilon\to+0}(E+i\epsilon-p^2)^{1/2}=\begin{cases}(|E-p^2|)^{1/2}, & E>p^2\\ i(|E-p^2|)^{1/2}, & E<p^2\end{cases}\tag{A21}$$

$$\underline{W}=\lim_{\epsilon\to+0}\left(E+i\epsilon-\frac{p^2E}{p^2+q^2}\right)^{1/2}=\frac{E^{1/2}}{(p^2+q^2)^{1/2}}q\,.$$

Thus, one has to estimate the following integral

$$\begin{aligned}
&\int_{U_2}d\mathbf{p}\,d\mathbf{q}\left|\frac{W-\underline{W}}{E-p^2-q^2}\right|^2=(4\pi)^2\\
&\times\Bigg[\int_0^{E^{1/2}}dp\,p^2\int_0^{(E+\frac{1}{2}|E_d|-p^2)^{1/2}}dq\,q^2\\
&\times\left|\frac{(|E-p^2|)^{1/2}-(E)^{1/2}q^2/(p^2+q^2)^{1/2}}{E-p^2-q^2}\right|\\
&+\int_{(E)^{1/2}}^{(E+\frac{1}{2}|E_d|)^{1/2}}dp\,p^2\int_0^{(E+\frac{1}{2}|E_d|-p^2)^{1/2}}dq\,q^2\,\frac{p^2-E}{(E-p^2-q^2)^2}\\
&+\int_{(E)^{1/2}}^{(E+\frac{1}{2}|E_d|)^{1/2}}dp\,p^2\int_0^{(E+\frac{1}{2}|E_d|-p^2)^{1/2}}dq\,q^2\\
&\times\frac{Eq^2}{(p^2+q^2)(E-p^2-q^2)^2}\Bigg].
\end{aligned}\tag{A22}$$

The first term, with the substitution $E-p^2=s^2$, reads

$$\begin{aligned}
&\int_0^{(E)^{1/2}}ds\times\int_0^{[s^2+\frac{1}{2}|E_d|]^{1/2}}dq\,q^2\left(\frac{s(E-s^2+q^2)^{\frac{1}{2}}-(E)^{\frac{1}{2}}q}{s-q}\right)^2\\
&\quad\times\frac{q(E-s^2)^{\frac{1}{2}}}{E-s^2+q^2}\,\frac{sq}{(s+q)^2}\,.
\end{aligned}$$

In the integration domain all factors are bounded and the integral exists. The second term, with the substitution $p^2-E=s^2$, reads

$$\int_0^{[(1/2)|E_d|]^{1/2}}ds\,s(s^2+E)^{1/2}\int_0^{[(1/2)|E_d|-s^2\}^{1/2}}dq\,q^2$$

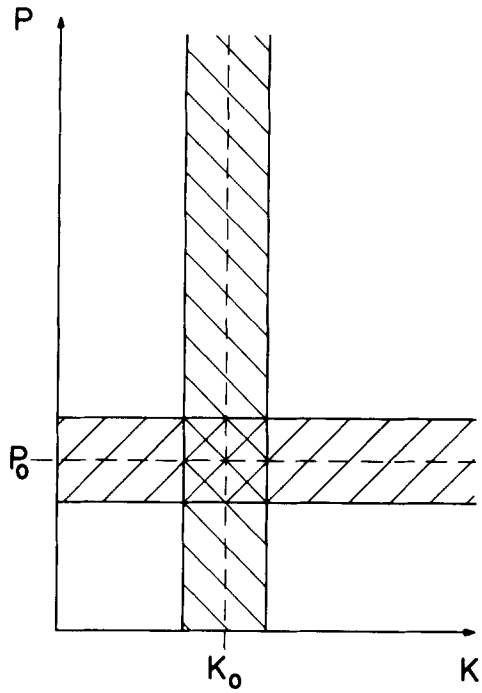


FIG. 1. Schematic plot of $U_{E-E_{\alpha 1}}$ (///) and $U_{E-E_{\alpha B}}$ (\\\); $U_{E-E_d} = U_{E-E_{\alpha 1}} \cup U_{E-E_{\alpha B}}$, the lines of singular points are $p_0^2 = E - E_d$ $k_0^2 = E - E_d$.

$$\times\left(\frac{s^2}{(-s^2-q^2)^2} \leqslant M \int_0^{[(1/2)|E_d|]^{1/2}} ds \right.$$
$$\times \int_0^{[(1/2)|E_d|-s^2]^{1/2}} dq \, \frac{s^2 q^2}{(s^2+q^2)^2}$$

and exists also. The third term, with the same substitution, reads

$$\int_0^{[(1/2)|E_d|]^{1/2}} ds\, s(s^2+E)^{1/2}$$
$$\times \int_0^{[(1/2)|E_d|-s^2]^{1/2}} dq \, \frac{E}{s^2+E} \frac{q^4}{(s^2+q^2)^2}$$

and exists because $q^4/(s^2+q^2)^2 \leqslant 1$. Thus, from the existence of the expression given by (A22), we conclude the existence of the expression given by (A16) and thus $\phi^k_{E;E}$ is contained in Assumption (5.2). Finally, let us consider if for the function $k$ defined by (A15) $\phi^k_{E-E_d,E-E_d;E-E_d,E-E_d}$ is contained in (5.2). Using (A15) and (3.18), one has

$$\begin{aligned} &{}_{\beta_0\beta_1}\langle \mathbf{p}',\mathbf{k}'|H_{\beta_1\beta_2\beta_3\beta_4}(Z)|\mathbf{p},\mathbf{k}\rangle_{\beta_4\beta_0} \\ &= {}_{\beta_1}\langle \mathbf{k}', e\mathbf{p}' + f\mathbf{k}'|H_{\beta_1\beta_2\beta_3\beta_4}(Z)|\mathbf{p}, a\mathbf{p}+b\mathbf{k}\rangle_{\beta_4} \qquad \text{(A23)} \\ &= b(Z-k'^2)\,\overline{\chi(e\mathbf{p}+f\mathbf{k}')}\, I(\mathbf{k},\mathbf{p},Z) \\ &\quad \times \frac{b(Z-p^2)\chi(a\mathbf{p}+b\mathbf{k})}{-|E|-p^2-(a\mathbf{p}+b\mathbf{k})^2}, \end{aligned}$$

with some channel recoupling coefficients e,f. $\phi^k_{E-E_d,E-E_d;E-E_d,E-E_d}$ requires subtractions at the points $E-E_d = p'^2$, $E-E_d = k'^2$, $E-E_d = p^2$, $E-E_d = k^2$. But in a neighborhood of those points $\lim_{\epsilon \to +0} b(E+i\epsilon - k'^2) I(\mathbf{k}',\mathbf{p},E+i\epsilon) b(E+i\epsilon - p^2)$ is a smooth, i.e., locally subtractable and square integrable, function. Because $\overline{\chi(e\mathbf{p}'+f\mathbf{k}')}\chi(a\mathbf{p}+b\mathbf{k})/(-|E|-p^2-(a\mathbf{p}+b\mathbf{k})^2)$ is an analytic function one concludes that $\phi^k_{E-E_d,E-E_d;E-E_d,E-E_d}$ is contained in (5.2). Combining all the arguments given above, one finds also all terms of mixed subtractions to be contained in (5.2) which was the claim of this Appendix.


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# Inverse problem transport calculations for anisotropic scattering coefficients

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One-speed transport anisotropic scattering coefficients are calculated by an inverse transport model which requires only emerging angular distributions from a homogeneous slab uniformly irradiated by a monodirectionally incident beam. The solution of the direct problem used to test the inverse calculations is obtained with the $F_N$ method of Siewert. New numerical schemes are developed which are applicable for the $F_N$ solution of other one-speed problems. The inverse transport method shows promise for characterizing media by only measurements of reflected and transmitted laser light from a slab.

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## I. INTRODUCTION

Recently a method has been proposed for obtaining the one-speed transport anisotropic scattering coefficients from reflection and transmission measurements for a homogeneous slab target uniformly illuminated by an azimuthally dependent incident beam.[1] If such an inverse transport method can be shown to provide relatively accurate predictions for the angular expansion coefficients of the scattering kernel, then the method should have application for identification of materials using noninvasive measurements.

It is the purpose of this investigation to test the conjecture that the anisotropic scattering coefficients can be determined accurately from appropriately selected angular moments of the emerging distributions. To accomplish this test, the reflected and transmitted angular distributions are assumed to be the solutions of the direct transport problem for a slab illuminated by a monodirectionally incident beam. This direct problem is solved using a slight generalization of the slab geometry azimuthally independent solution of Siewert[2] which was obtained with the $F_N$ method.[3–5] This generalization also has been carried out concurrently with our analysis by Devaux and Siewert.[6]

The equations required to calculate the scattering coefficients using the inverse problem solution are summarized in Sec. II, and the $F_N$ solution of the direct transport problem is developed in Sec. III. Additional equations for implementing the $F_N$ method are presented in Sec. IV, while Sec. V contains a description of the different numerical schemes used to solve the $F_N$ equations. Numerical tests of the direct problem solution are in Sec. VI. Finally, results of test calculations in Sec. VII substantiate agreement of the scattering coefficients obtained by the inverse solution with the assumed scattering coefficients. Conclusions and possible implications for use of the method with experimental data are presented in Sec. VIII.

## II. INVERSE PROBLEM SOLUTION

The equation of transfer for monochromatic radiation in plane geometry is

$$\mu \frac{\partial I(\tau,\mu,\phi)}{\partial \tau} + I(\tau,\mu,\phi) = \frac{1}{4\pi}\int_{-1}^{1} d\mu' \int_{0}^{2\pi} d\phi'\, p(\cos\delta) I(\tau,\mu',\phi'), \quad 0 \leqslant \tau \leqslant \tau_o, \tag{1}$$

where anisotropic scattering of finite order $K$ is assumed, distances are in mean free paths,

$$p(\cos\delta) = \sum_{k=0}^{K} \omega_k P_k(\cos\delta), \tag{2}$$

and where $0 < \omega_0 < 1$. Here the $P_k$ are Legendre polynomials and $\delta$ is the angle between the direction defined by $\mu'$ and $\phi'$ and that defined by $\mu$ and $\phi$. It will be assume that

$$I(0,\mu,\phi) = \delta(\mu-\mu_o)\delta(\phi), \quad 0 < \mu \leqslant 1, \tag{3}$$

$$I(\tau_o,-\mu,\phi) = 0, \quad 0 < \mu \leqslant 1. \tag{4}$$

The equations for calculating $\omega_k$, $k = 0$ to $K$, require the use of moments of the radiation angular intensity $I(\tau,\mu,\phi)$, defined as[1]

$$i_{lk}^{m}(\tau) = (2\pi)^{-1}\int_{0}^{2\pi} d\phi \cos m\phi \times \int_{-1}^{1} d\mu\, \mu^{l} P_k^m(\mu) I(\tau,\mu,\phi), \tag{5}$$

and evaluated on the surfaces $\tau = 0$ and $\tau = \tau_o$. Here the $P_k^m(\mu)$ are the associated Legendre functions. Use of Eqs. (3) and (4) reduces the equations for $i_{lk}^m(0)$ and $i_{lk}^m(\tau_o)$ to integrals over the angular intensities emerging from the slab surfaces. Also required is a second set of moments, involving products of the angular intensity, which are defined as[1]

$$S_l^m = 4\int_0^1 d\mu\, \mu^{2l}\left((2\pi)^{-1}\int_0^{2\pi} d\phi\, I(0,-\mu,\phi)\cos m\phi\right) \times \left((2\pi)^{-1}\int_0^{2\pi} d\phi\, I(0,\mu,\phi)\cos m\phi\right). \tag{6}$$

The $\omega_k$ values may be evaluated by either of two schemes. The first approach, which may be called the "angular intensity method," uses moments of $I(\tau,\mu,\phi)$ in the equations[1]

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$$
\begin{aligned}
S_0^0 &= \omega_0 s_{00}^0 + \omega_1 s_{01}^0 + \cdots + \omega_K s_{0K}^0,\\
S_0^1 &= \omega_1 s_{01}^1 + \cdots + \omega_K s_{0K}^1,\\
&\vdots\\
S_0^K &= \omega_K s_{0K}^K,
\end{aligned}
\tag{7}
$$

where the $s$ values are defined in terms of the integrals in Eq. (5) as

$$
s_{0k}^m = (-1)^{k-m}[(k-m)!/(k+m)!]\{[i_{0k}^m(0)]^2 - [i_{0k}^m(\tau_o)]^2\}. \tag{8}
$$

The second scheme, which provides an independent means of determining the $\omega_k$, may be termed the "angular heat flux method" since it uses moments of $\mu I(\tau,\mu,\phi)$, and is based on the equations[1]

$$
\begin{aligned}
S_1^0 &= (\omega_0/h_0) s_{10}^0 + (\omega_1/h_1) s_{11}^0 + \cdots + (\omega_K/h_K) s_{1K}^0,\\
S_1^1 &= (\omega_1/h_1) s_{11}^1 + \cdots + (\omega_K/h_K) s_{1K}^1,\\
&\vdots\\
S_1^K &= (\omega_K/h_K) s_{1K}^K.
\end{aligned}
\tag{9}
$$

In Eq. (9) the $s$ values are defined as

$$
\begin{aligned}
s_{1k}^m &= (-1)^{k-m}(2k+1)[(k-m)!/(k+m)!]\\
&\quad\times\{[i_{1k}^m(0)]^2 - [i_{1k}^m(\tau_o)]^2\},
\end{aligned}
\tag{10}
$$

and the $h_k$ values are

$$
h_k = 2k + 1 - \omega_k. \tag{11}
$$

## III. DIRECT PROBLEM SOLUTION

The direct transport problem defined by Eqs. (1) through (4) has been solved, for the azimuthally symmetric case, by Siewert who used his $F_N$ method.[2] The extension to the azimuthally dependent case, as done here, follows straight forwardly.

In order to separate the azimuthally dependent problem into a set of $(K+1)$ azimuthally independent problems, we expand $I(\tau,\mu,\phi)$ in a finite Fourier expansion[1,7]

$$
\begin{aligned}
I(\tau,\mu,\phi) &= \sum_{m=0}^{K}(2-\delta_{m0})I^m(\tau,\mu)(1-\mu^2)^{m/2}\cos m\phi\\
&\quad + I_u(\tau,\mu,\phi),
\end{aligned}
\tag{12}
$$

where $I_u(\tau,\mu,\phi)$ is part of the uncollided intensity,

$$
\begin{aligned}
I_u(\tau,\mu,\phi) &= \delta(\mu-\mu_o)e^{-\tau/\mu}\Big(\delta(\phi) - (2\pi)^{-1}\\
&\quad\times\sum_{m=0}^{K}(2-\delta_{m0})\cos m\phi\Big).
\end{aligned}
\tag{13}
$$

The $F_N$ method is based upon a set of equations derived by expanding $I^m(\tau,\mu)$ in its singular eigenfunction expansion[8] and using the full-range orthogonality relations to eliminate the expansion coefficients in terms of the intensities at the boundaries. The resulting equations for the unknown outgoing surface angular distributions, $I^m(0,-\mu)$ and $I^m(\tau_o,\mu)$, $0\leqslant m\leqslant K$, are expressed for the positive eigenvalues $\nu\in\sigma+$, as

$$
\begin{aligned}
&\int_0^1 \mu\phi^m(\nu,\mu)I^m(0,-\mu)\,dm(\mu)\\
&\quad + e^{-\tau_o/\nu}\int_0^1 \mu\phi^m(-\nu,\mu)I^m(\tau_o,\mu)dm(\mu)\\
&\quad = L_1^m(\nu),
\end{aligned}
\tag{14a}
$$

$$
\begin{aligned}
&\int_0^1 \mu\phi^m(\nu,\mu)I^m(\tau_o,\mu)\,dm(\mu)\\
&\quad + e^{-\tau_o/\nu}\int_0^1 \mu\phi^m(-\nu,\mu)I^m(0,-\mu)dm(\mu)\\
&\quad = L_2^m(\nu),
\end{aligned}
\tag{14b}
$$

where

$$
\begin{aligned}
L_1(\nu) &= \int_0^1 \mu\phi(-\nu,\mu)I(0,\mu)\,dm(\mu) + e^{-\tau_o/\nu}\\
&\quad\times\int_0^1 \mu\phi(\nu,\mu)I(\tau_o,-\mu)\,dm(\mu),
\end{aligned}
\tag{15a}
$$

$$
\begin{aligned}
L_2(\nu) &= \int_0^1 \mu\phi(-\nu,\mu)I(\tau_o,-\mu)\,dm(\mu) + e^{-\tau_o/\nu}\\
&\quad\times\int_0^1 \mu\phi(\nu,\mu)I(0,\mu)\,dm(\mu).
\end{aligned}
\tag{15b}
$$

For convenience in Eq. (15) and in the following, the superscript $m$ with $I^m(\tau,\mu)$ and other functions is suppressed if no confusion is possible; in such cases all relevant quantities in any of the equations must be understood as referring to the particular azimuthal component under consideration.

The positive spectrum $\sigma+$ consists of the continuum (0, 1) and of the set of discrete positive eigenvalues $\{\nu_j, j=1 \text{ to } J\}$ which are zeros of[8]

$$
\Lambda(z) = 1 - \tfrac{1}{2}z\int_{-1}^{1}(z-\mu)^{-1}g(\mu,\mu)\,dm(\mu). \tag{16}
$$

It is known that[8] $J\leqslant K-m+1$, although for $m$ exceeding 2, $J$ typically has been found to equal zero.[9]

The eigenfunctions $\phi(\nu,\mu)$ in Eqs. (14) and (15) are defined by the equation

$$
\phi(\nu,\mu) = \tfrac{1}{2}\nu\mathcal{P}g(\nu,\mu)/(\nu-\mu) + \lambda(\nu)(1-\nu^2)^{-m}\delta(\nu-\mu),
$$

$$0<\nu<1,$$
$$= \tfrac{1}{2}\nu_j g(\nu_j,\mu)/(\nu_j-\mu), \quad \nu=\nu_j,\ j=1 \text{ to } J, \tag{17}$$

where $\mathscr{P}$ stands for principal value, and

$$\lambda(\nu) = 1 - \tfrac{1}{2}\nu\mathscr{P}\int_{-1}^{1}(\nu-\mu)^{-1}g(\mu,\mu)\,dm(\mu). \tag{18}$$

Here $g(\nu,\mu)$ is defined as

$$g(\nu,\mu) = \sum_{k=m}^{K} c_k g_k(\nu) p_k(\mu), \tag{19}$$

and

$$p_k^m(\mu) = (d^m/d\mu^m)P_k(\mu) = (1-\mu^2)^{-m/2}P_k^m(\mu),$$
$$c_k = \omega_k(k-m)!/(k+m)!$$
$$dm(\mu) = (1-\mu^2)^m\,d\mu. \tag{20}$$

The $g_k(\nu)$ in Eq. (19) are polynomials of order $(k-m)$, alternatively even and odd, defined by the recursion relation

$$(k+1-m)g_{k+1}(\nu) - h_k\nu g_k(\nu) + (k+m)g_{k-1}(\nu) = 0, \quad k\geqslant m, \tag{21}$$

with the starting conditions $g_{m-1}(\nu)=0$ and[10]

$$g_m(\nu) = p_m(\nu) = \prod_{k=0}^{m-1}(2k+1) = (2m-1)!! \tag{22}$$

The $g_k(\nu)$ polynomials reduce to the $p_k(\nu)$ polynomials in the limit that $\omega_k = 0$, $k\geqslant m$.

To solve Eq. (14) with boundary conditions (3) and (4) by the $F_N$ method, $I(0,-\mu)$ and $I(\tau_o,\mu)$ are expanded as[2,11]

$$I(0,-\mu) = \sum_{n=0}^{N} a_n\mu^n, \quad 0<\mu\leqslant 1, \tag{23a}$$

$$I(\tau_o,\mu) = \sum_{n=0}^{N} b_n\mu^n + \frac{e^{-\tau_o/\mu_o}\delta(\mu-\mu_o)}{2\pi(1-\mu_o^2)^{m/2}}, \quad 0<\mu\leqslant 1. \tag{23b}$$

The second term in Eq. (23b) completely eliminates the singular nature of $I(\tau_o,\mu)$ and is necessary for good convergence with increasing $N$, especially when $\tau_o$ is small.

Use of Eqs. (3), (4), and (23) in Eqs. (14) and (15) gives the set of equations

$$\sum_{n=0}^{N}\left[a_nB_n(\nu) + e^{-\tau_o/\nu}b_nA_n(\nu)\right] = (2/\nu)L_1(\nu), \quad \nu\in\sigma+, \tag{24a}$$

$$\sum_{n=0}^{N}\left[b_nB_n(\nu) + e^{-\tau_o/\nu}a_nA_n(\nu)\right] = (2/\nu)L_2(\nu), \quad \nu\in\sigma+, \tag{24b}$$

where

$$L_1(\nu) = (\mu_o/2\pi)\phi(-\nu,\mu_o)(1-\mu_o^2)^{m/2} \times[1-\exp\tau_o(-1/\nu-1/\mu_o)], \tag{25a}$$

$$L_2(\nu) = e^{-\tau_o/\nu}(\mu_o/2\pi)\phi(\nu,\mu_o)(1-\mu_o^2)^{m/2} \times[1-\exp\tau_o(1/\nu-1/\mu_o)], \quad \nu\neq\mu_o,$$
$$= e^{-\tau_o/\mu_o}(\tau_o/4\pi)g(\mu_o,\mu_o)(1-\mu_o^2)^{m/2}, \quad \nu=\mu_o, \tag{25b}$$

and where the coefficients $B_n(\nu)$ and $A_n(\nu)$ are defined as

$$B_n(\nu) = \frac{2}{\nu}\int_0^1 \mu^{n+1}\phi(\nu,\mu)\,dm(\mu), \tag{26a}$$

$$A_n(\nu) = \frac{2}{\nu}\int_0^1 \mu^{n+1}\phi(-\nu,\mu)\,dm(\mu) = -B_n(-\nu). \tag{26b}$$

The expansion coefficients $a_n$ and $b_n$ are calculated by specializing the $F_N$ equations (24) to $(N+1)$ $\nu$ values in $\sigma+$. The moments needed for the inverse problem solution are calculated using the intensities in Eq. (23). Use of Eqs. (3), (4), (12), and (20) leads to the results

$$i_{lk}(0) = (2\pi)^{-1}\mu_o^l P_k^m(\mu_o) + (-1)^{k-m+l}\sum_{n=0}^{N} a_n\Delta_{l+n,k}, \tag{27a}$$

$$i_{lk}(\tau_o) = (2\pi)^{-1}\mu_o^l P_k^m(\mu_o)e^{-\tau_o/\mu_o} + \sum_{n=0}^{N} b_n\Delta_{l+n,k}, \tag{27b}$$

$$S_l = \frac{2}{\pi}(1-\mu_o^2)^{m/2}\mu_o^{2l}\sum_{n=0}^{N} a_n\mu_o^n, \tag{28}$$

where

$$\Delta_{n,l} = \int_0^1 \mu^n p_l(\mu)\,dm(\mu), \quad n\geqslant 0,\ l\geqslant m. \tag{29}$$

## IV. ADDITIONAL EQUATIONS FOR DIRECT PROBLEM SOLUTION

The $B_n(\nu)$ and $A_n(\nu)$ may be evaluated, in terms of the numbers $\Delta_{n,l}$, using the recursion relations

$$B_{n+1}(\nu) = \nu B_n(\nu) - \sum_{k=m}^{K} c_k g_k(\nu)\Delta_{n+1,k}, \tag{30a}$$

$$A_{n+1}(\nu) = -\nu A_n(\nu) + \sum_{k=m}^{K}(-1)^{k-m}c_k g_k(\nu)\Delta_{n+1,k}. \tag{30b}$$

In turn, the $\Delta$'s themselves satisfy

$$(l+1-m)\Delta_{n,l+1} - (2l+1)\Delta_{n+1,l} + (l+m)\Delta_{n,l-1} = 0, \tag{31}$$

with the first few values given by

$$\Delta_{n,m-1} = 0,$$
$$\Delta_{n,m} = (2m)!(n-1)!!/(2m+n+1)!!,$$
$$\Delta_{n,m+1} = (2m+1)!n!!/(2m+n+2)!!, \tag{32}$$

for $l\geqslant m$ and $n\geqslant 0$. It also may be shown that

$$\Delta_{n,m+n+2j} = 0, \quad j=1,2,\cdots. \tag{33}$$

It should be mentioned that a two-term recursion relation for $\Delta_{n,l}$ also exists.[6]

The starting conditions for the recursion relations (30) are related by the identity

$$B_0(\nu) - A_0(\nu) = \frac{2}{\nu}\int_{-1}^{1}\mu\phi(\nu,\mu)\,dm(\mu) = 2h_m/(2m+1), \tag{34}$$

so only $A_0(\nu)$ need be calculated using Eq. (26b). The result is

$$A_0(\nu) = \sum_{k=m}^{K} c_k g_k(\nu)T_k(\nu), \tag{35}$$

where

$$T_k(\nu) = (-1)^{k-m}\int_0^1 \frac{\mu p_k(\mu)\, dm(\mu)}{\nu+\mu}, \quad k \geqslant m. \tag{36}$$

The $T_k(\nu)$ satisfy the recursion relation

$$\begin{aligned}(k+1-m)T_{k+1}(\nu) &- (2k+1)\nu T_k(\nu) + (k+m)T_{k-1}(\nu) \\ &= (-1)^{k-m-1}(2k+1)\Delta_{1,k},\end{aligned} \tag{37}$$

with $T_{m-1}(\nu) = 0$. The other starting condition is

$$T_m(\nu) = \Delta_{0,m} - (2m-1)!!\nu R^m(\nu), \tag{38}$$

where $R^m(\nu)$ is defined as

$$R^m(\nu) = \int_0^1 \frac{dm(\mu)}{\nu+\mu}, \tag{39}$$

and obeys the recursion relation

$$\begin{aligned}R^m(\nu) = (1-\nu^2)R^{m-1}(\nu) &+ (2m-2)!! \\ &\times [\nu/(2m-1)!! - 1/(2m)!!],\end{aligned} \tag{40}$$

with the starting condition

$$R^0(\nu) = \ln(1+1/\nu). \tag{41}$$

For $\nu \gtrsim 2$, the recursion relations (30) do not work well because differences of large, nearly identical numbers must be calculated. In such cases, Siewert[11] has suggested the use of series expansions derived from Eq. (26),

$$B_n(\nu) = \sum_{l=0}^{\infty}\sum_{k=m}^{K} c_k \Delta_{n+l+1,k}\nu^{-(l+1)}g_k(\nu), \tag{42a}$$

$$\begin{aligned}A_n(\nu) = \sum_{l=0}^{\infty}\sum_{k=m}^{K} &(-1)^{k-m+l}c_k\Delta_{n+l+1,k} \\ &\times \nu^{-(l+1)}g_k(\nu).\end{aligned} \tag{42b}$$

Also for $\nu \gtrsim 2$ the calculation of $g_k(\nu)$ from recursion relation (21) may give trouble, in which case a continued fraction expansion works better.[12] Such an expansion can be derived by rewriting Eq. (21) as

$$\begin{aligned}\frac{g_{k+1}(\nu)}{g_k(\nu)} &= \frac{h_k\nu}{(k+1-m)}\left\{1 - \frac{(k+m)}{h_k\nu}\left[\frac{g_k(\nu)}{g_{k-1}(\nu)}\right]^{-1}\right\} \\ &= \frac{h_k\nu}{(k+1-m)(\mathrm{CF})_k}\end{aligned} \tag{43}$$

where the terminating continued fraction $(\mathrm{CF})_k$ implicitly defined in Eq. (43) is obtained from the recursion relation

$$(\mathrm{CF})_k = \left[1 - \frac{(k+m)(k-m)}{h_k h_{k-1}\nu^2}(\mathrm{CF})_{k-1}\right]^{-1} \tag{44}$$

and the starting condition $(\mathrm{CF})_m = 1$.

We turn now to the numerical evaluation of $\Lambda(z)$ which is required when calculating the eigenvalues $\nu_j$. Equation (16) may be expressed as

$$\Lambda(z) = 1 + z\sum_{k=m}^{K} c_k g_k(z) q_k(z), \tag{45}$$

where

$$q_k(z) = \frac{1}{2}\int_{-1}^{1} \frac{p_k(\mu)\, dm(\mu)}{\mu - z}. \tag{46}$$

Use of Eq. (21) in Eq. (46) gives the recursion relation

$$\begin{aligned}(k+1-m)q_{k+1}(z) &- (2k+1)zq_k(z) + (k+m)q_{k-1}(z) \\ &= (2m)!!\delta_{km},\end{aligned} \tag{47}$$

where $q_{m-1}(z) = 0$. To calculate the starting condition $q_m(z)$, another recursion relation is used,

$$\begin{aligned}q_m^m(z) = (2m-1)(1-z^2)q_{m-1}^{m-1}(z) &\\ - z(2m-2)!!,&\end{aligned} \tag{48}$$

where

$$q_0^0(z) = \tfrac{1}{2}\ln\left(\frac{z-1}{z+1}\right). \tag{49}$$

Equations (45) through (49) remain valid for the calculation of $\lambda(\nu)$ provided the principal value integral is taken in Eq. (46) and the sign of the argument of the logarithm in Eq. (49) is reversed. Also, for $z \gtrsim 2$, Eq. (47) may be replaced by the rapidly converging power series

$$q_k(z) = -\sum_{l=k-m}^{\infty} \Delta_{2l-(k-m),k} z^{k-m-1-2l}. \tag{50}$$

A better form than Eq. (45) for evaluation of $\Lambda(z)$ and $\lambda(\nu)$ can be derived by multiplying the equivalent of Eq. (21) for $p_k(z)$ by $q_k(z)$ and Eq. (47) by $p_k(z)$ and subtracting. After multiplying the result by $(k-m)!/(k+m)!$ and summing over $k$, the Christoffel–Darboux formula[9,13]

$$\begin{aligned}\Lambda(z) = [(K+1-m)!/(K+m)!]\,&[g_K(z)q_{K+1}(z) \\ &- g_{K+1}(z)q_K(z)]\end{aligned} \tag{51}$$

is obtained.

To calculate the zeros of $\Lambda(z)$, i.e., the values of $\nu_j$, Siewert[14] has developed a formally exact method which requires that complicated integrals be performed. Such a scheme has been used to provide a very accurate first guess for each $\nu_j$, which was then utilized with a Newton–Raphson iteration method to obtain even more accurate values.[6] For highly anisotropic scattering, for which $(K+1)$ separate calculations must be performed (one for each $m$), direct use of Eq. (51) with a Newton–Raphson iteration is more expedient. A criterion for limiting the $z$ value in the iterative search of the discrete eigenvalues follows from [8]

$$\Lambda(z) = \prod_{k=m}^{K}\frac{h_k}{2k+1} - \sum_{n=1}^{\infty}\frac{\eta_{2n}}{z^{2n}}, \quad |z| > 1, \tag{52}$$

where $\eta_{2n}$ is calculated in terms of $g(\mu,\mu)$ of Eq. (19) using the definition

$$\eta_{2n} = \frac{1}{2}\int_{-1}^{1}\mu^{2n}g(\mu,\mu)\, dm(\mu). \tag{53}$$

A procedure similar to that used to derive Eq. (51) leads to the single integral

$$\begin{aligned}\eta_{2n} = \frac{(K-m+1)!}{(K+m)!}\int_0^1 \mu^{2n-1}&[g_K(\mu)p_{K+1}(\mu) \\ &- g_{K+1}(\mu)p_K(\mu)]\, dm(\mu).\end{aligned} \tag{54}$$

Certainly the simplest method for calculating the eigen-

values is to use the positive roots $\nu \in (0, 1)$ of the polynomial

$$g_{L+m}(\nu) = 0, \quad L \text{ large.} \tag{55}$$

These roots converge to the $\nu_j$ values as $L \to \infty$ [13]; in practice, surprisingly high-accurate estimations are obtained from small $L$ values ($L \sim 10$).

## V. NUMERICAL SCHEMES FOR DIRECT PROBLEM SOLUTION

Two fundamentally different approaches were used to solve the $F_N$ equations (24): the collocation or nodal method and the projection or modal method. The collocation method is the approach used by Siewert and co-workers and requires that the equations be evaluated at $(N+1)$ collocation points. The scheme used by Siewert[2,4] is to select all the exact values $\nu_j$ and to space the remaining values $\nu_l$, $l = (J+1)$ to $(N+1)$, equally distant in [0, 1]. The collocation points are selected by dividing [0, 1] into equally spaced intervals. In our calculations a first set of collocation points (set C1) is defined by the endpoints of every interval, including 0 and 1,[2] a second set C2 follows by using all endpoints except 0 and 1, and a third set C3 is obtained by using the midpoints of the intervals. Still a different scheme would be to use the values of $\nu_j, j = 1$ to $J$, and select the remaining values $\nu_l$ as the positive roots of the polynomial

$$p_{2(N-J+1)+m}(\nu) = 0. \tag{56}$$

Thus the remaining values would be selected as nodes from a Gauss–Legendre quadrature set.

In the preceding collocation schemes, the points in [0, 1] do not depend upon the properties of the medium. One way of introducing such a dependence is to select all nodes as the positive roots of the polynomial

$$g_{2(N+1)+m}(\nu) = 0. \tag{57}$$

The nodes from Eq. (57) will be called collocation set C4.

For the projection technique, equations (24) are projected onto a set of linearly independent functions $X_i^m(\nu)$, $i = 0$ to $N$, by multiplying Eqs. (24) by each of the functions and integrating over the entire positive spectrum $\sigma+$. This results in

$$\sum_{n=0}^{N} [a_n B_{n,i} + b_n A_{n,i}] = L_{1,i}, \tag{58a}$$

$$\sum_{n=0}^{N} [b_n B_{n,i} + a_n A_{n,i}] = L_{2,i}, \tag{58b}$$

where

$$B_{n,i} = \int_{\sigma+} B_n(\nu) X_i(\nu)\, d\nu = \sum_{j=1}^{J} B_n(\nu_j) X_i(\nu_j) + \int_0^1 B_n(\nu) X_i(\nu)\, d\nu, \tag{59a}$$

$$A_{n,i} = \int_{\sigma+} e^{-\tau_0/\nu} A_n(\nu) X_i(\nu)\, d\nu, \tag{59b}$$

and where

$$L_{r,i} = 2\int_{\sigma+} \nu^{-1} L_r(\nu) X_i(\nu)\, d\nu, \quad r = 1, 2. \tag{60}$$

We have used two projection schemes. The first, P1, is defined by the set of functions

$$X_i^m(\nu) = g_{i+m}^m(\nu), \tag{61a}$$

and the second, P2, by

$$X_i(\nu) = \delta(\nu - \nu_j), \quad i = 1 \text{ to } J$$
$$= \nu^{i-J-1}, \quad i = J+1 \text{ to } N. \tag{61b}$$

The last scheme gives a hybrid method consisting of a collocation for the $\nu_j$ values and a projection for $0 < \nu < 1$.

Instead of analytically evaluating the integrals over $0 < \nu < 1$ in Eqs. (59) and (60), we have opted to carry them out using a numerical quadrature technique. In our evaluation we divide the interval $0 < \nu < 1$ into $\alpha$ equal subintervals, and use a $\beta$-point Gauss–Legendre formula in each subinterval.

TABLE I. Accuracy test for $F_5$ calculations for isotropic scattering with $\omega_0 = 0.999$ and $\tau_o = 2$ and $\mu_o = 0.5$.

| $\tau_o$ | Method | $i_{00}(0)$ | $i_{10}(0)$ | $i_{00}(\tau_o)$ | $i_{10}(\tau_o)$ |
|---|---|---|---|---|---|
| 2 | C1 | 2.7243 − 1 | − 2.7470 − 2 | 4.9104 − 2 | 2.7141 − 2 |
| | C2 | 2.7276 − 1 | − 2.7469 − 2 | 4.9279 − 2 | 2.7140 − 2 |
| | C3 | 2.7271 − 1 | − 2.7469 − 2 | 4.9213 − 2 | 2.7140 − 2 |
| | C4 | 2.7276 − 1 | − 2.7469 − 2 | 4.9242 − 2 | 2.7140 − 2 |
| | P1 | 2.7262 − 1 | − 2.7469 − 2 | 4.9167 − 2 | 2.7140 − 2 |
| | P2 | 2.7262 − 1 | − 2.7469 − 2 | 4.9167 − 2 | 2.7140 − 2 |
| | Exact | 2.7262 − 1 | − 2.7469 − 2 | 4.9165 − 2 | 2.7140 − 2 |
| 20 | C1 | 3.0967 − 1 | − 6.0029 − 3 | 6.0028 − 3 | 3.4691 − 3 |
| | C2 | 3.1004 − 1 | − 6.0023 − 3 | 6.0082 − 3 | 3.4688 − 3 |
| | C3 | 3.0997 − 1 | − 6.0025 − 3 | 6.0074 − 3 | 3.4689 − 3 |
| | C4 | 3.1004 − 1 | − 6.0024 − 3 | 6.0084 − 3 | 3.4688 − 3 |
| | P1 | 3.0988 − 1 | − 6.0025 − 3 | 6.0059 − 3 | 3.4689 − 3 |
| | P2 | 3.0988 − 1 | − 6.0025 − 3 | 6.0059 − 3 | 3.4689 − 3 |
| | Exact | 3.0987 − 1 | − 6.0025 − 3 | 6.0057 − 3 | 3.4689 − 3 |

TABLE II. Selected coefficients $a_n$ and $b_n$ for the $F_N$ method calculated using the C1 method with the binomial scattering model of $\omega_0 = 0.95$ and $\alpha = 4$ for $\tau_o = 2$ and $\mu_o = 0.5$.

| | $N=5$ | | | | $N=10$ | | | | $N=15$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $m=0$ | | $m=1$ | | $m=0$ | | $m=1$ | | $m=0$ | | $m=1$ | |
| $n$ | $a_n$ | $b_n$ | $a_n$ | $b_n$ | $a_n$ | $b_n$ | $a_n$ | $b_n$ | $a_n$ | $b_n$ | $a_n$ | $b_n$ |
| 0 | 1.2075 − 1 | 2.8919 − 2 | 7.9649 − 2 | 6.5388 − 3 | 1.2086 − 1 | 2.8963 − 2 | 7.9705 − 2 | 6.5552 − 3 | 1.2088 − 1 | 2.8967 − 2 | 7.9712 − 2 | 6.5562 − 3 |
| 1 | − 2.1267 − 2 | 8.4812 − 2 | − 9.1287 − 2 | 1.6087 − 2 | 6.2261 − 2 | 1.1018 − 1 | − 4.5715 − 2 | 2.4234 − 2 | 1.0573 − 1 | 1.2213 − 1 | − 2.1641 − 2 | 2.8206 − 2 |
| 2 | − 4.0347 − 1 | 2.4403 − 2 | − 6.8727 − 2 | 5.6262 − 2 | − 1.7150 | − 2.8360 − 1 | − 7.7173 − 1 | − 2.6558 − 3 | − 3.1866 | − 7.1394 − 1 | − 1.5737 | − 1.5050 − 1 |
| 3 | 7.4038 − 1 | − 9.5808 − 2 | 2.5471 − 1 | − 5.3475 − 2 | 9.4754 | 1.2646 | 4.8852 | − 1.4979 − 1 | 3.1066 + 1 | 8.0002 | 1.6476 + 1 | 2.2329 |
| 4 | − 5.8757 − 1 | 2.4588 − 2 | − 2.3734 − 1 | − 1.2524 − 3 | − 3.4047 + 1 | − 2.5433 | − 1.7841 + 1 | 2.1126 | − 2.1973 + 2 | − 6.4143 + 1 | − 1.1610 + 2 | − 2.0172 + 1 |
| 5 | 1.8001 − 1 | 7.7896 − 3 | 7.7347 − 2 | 1.0708 − 2 | 8.2445 + 1 | 5.8320 − 1 | 4.3104 + 1 | − 8.7119 | 1.1409 + 3 | 3.7132 + 2 | 5.9555 + 2 | 1.2740 + 2 |
| 6 | | | | | − 1.3486 + 2 | 6.5598 | − 7.0143 + 1 | 1.8556 + 1 | − 4.3992 + 3 | − 1.5558 + 3 | − 2.2671 + 3 | − 5.5927 + 2 |
| 7 | | | | | 1.4687 + 2 | − 1.3222 + 1 | 7.5946 + 1 | − 2.3357 + 1 | 1.2737 + 4 | 4.7629 + 3 | 6.4833 + 3 | 1.7448 + 3 |
| 8 | | | | | − 1.0199 + 2 | 1.2213 + 1 | − 5.2410 + 1 | 1.7633 + 1 | − 2.7865 + 4 | − 1.0788 + 4 | − 1.4021 + 4 | − 3.9641 + 3 |
| 9 | | | | | 4.0834 + 1 | − 5.7564 | 2.0846 + 1 | − 7.4163 | 4.6079 + 4 | 1.8205 + 4 | 2.2940 + 4 | 6.6521 + 3 |
| 10 | | | | | − 7.1689 | 1.1198 | − 3.6346 | 1.3404 | − 5.7198 + 4 | − 2.2845 + 4 | − 2.8194 + 4 | − 8.2626 + 3 |
| 11 | | | | | | | | | 5.2415 + 4 | 2.1038 + 4 | 2.5597 + 4 | 7.5140 + 3 |
| 12 | | | | | | | | | − 3.4377 + 4 | − 1.3816 + 4 | − 1.6642 + 4 | − 4.8675 + 3 |
| 13 | | | | | | | | | 1.5257 + 4 | 6.1254 + 3 | 7.3245 + 3 | 2.1281 + 3 |
| 14 | | | | | | | | | − 4.1024 + 3 | − 1.6433 + 3 | − 1.9540 + 3 | − 5.6304 + 2 |
| 15 | | | | | | | | | 5.0448 + 2 | 2.0146 + 2 | 2.3846 + 2 | 6.8098 + 1 |

## VI. CALCULATIONS FOR DIRECT PROBLEM SOLUTION

The $F_N$ calculations performed by Devaux and Siewert[6] were reproduced with the calculational methods developed in Secs. III–V. Thus, the emphasis of the direct problem calculations discussed here will be on comparing the accuracy and rate of convergence with increasing $N$ of the numerical schemes presented in the last section.

Three scattering models were used for the numerical tests. The binomial model with predominantly forward ( + ) or backward ( − ) scattering is defined by[9,15]

$$p(\cos\delta) = \omega_0(\alpha+1)2^{-\alpha}(1 \pm \cos\delta)^{\alpha}, \quad \alpha \geqslant 0, \tag{62}$$

where the coefficients $\omega_k(\alpha \pm)$ of Eq. (2) may be evaluated with the (apparently new) recursion relation

$$\omega_k(\alpha \pm) = \pm \left(\frac{2k+1}{2k-1}\right)\left(\frac{\alpha+1-k}{\alpha+1+k}\right)\omega_{k-1}(\alpha \pm), \quad k \geqslant 1, \tag{63}$$

once $\omega_0$ is specified. If $\alpha$ is a positive integer, $K = \alpha$.

A second scattering model, due to Henyey and Greenstein,[16] is

$$p(\cos\delta) = (1-g^2)(1+g^2-2g\cos\delta)^{-3/2}, \quad -1 < g < 1, \tag{64}$$

for which the expansion coefficients $\omega_k(g)$ are

$$\omega_k(g) = (2k+1)g^k\omega_0. \tag{65}$$

The third model represents the scattering of visible light in fog,[17] approximated with the coefficients[18]

$$\begin{aligned} &\omega_0 = 1, && \omega_5 = 1.0716, \\ &\omega_1 = 2.1053, && \omega_6 = 0.4803, \\ &\omega_2 = 2.7424, && \omega_7 = 0.3615, \\ &\omega_3 = 2.1929, && \omega_8 = 0.1587, \\ &\omega_4 = 1.5578, && \omega_9 = 0.0075. \end{aligned} \tag{66}$$

To avoid modifying our computer program for cases when the largest $\nu_j \to \infty$ as $\omega_0 \to 1$, we have replaced the value of $\omega_0$ in Eq. (66) by 0.999 in our calculations.

To test the accuracy of the $F_N$ calculations, the moments $i_{lm}(0)$ and $i_{lm}(\tau_o)$ for $l = 0$ and 1, given in Eq. (27), were examined. (These moments are proportional to the angle-integrated intensity and heat flux in the $m$th Fourier component, respectively.) We first performed $F_N$ calculations from $N = 2$ to 15 for isotropic scattering with $\omega_0 = 0.999$ and 0.2 for $\mu_o = 0.5$ and slab thicknesses of $\tau_o = 2$ and 20. All six methods proposed in Sec. V converged for $N \leqslant 15$, but the projection methods converged faster. The $F_5$ results for $\omega_0 = 0.999$ in Table I illustrate that there is only a very small difference in accuracy between the six schemes.

For anisotropic scattering the convergence is more rapid for Fourier components with larger $m$; the convergence is not appreciably affected by the value of $\mu_o$, $0.5 \leqslant \mu_o \leqslant 0.9$. It also was generally observed that the $i_{1m}$ converged more rapidly than $i_{0m}$, a fact that has implications for the inverse problem calculations in Sec. VII.

TABLE III. Selected coefficients $\omega_k$ calculated for an assumed $\tilde{K}$ by angular intensity (AI) and angular heat flux (AHF) methods for the binomial scattering model with $\omega_0 = 0.95$ and $\alpha = 19$.

| $\tilde{K}$ | Method | $\omega_0$ | $\omega_3$ | $\omega_7$ | $\omega_{11}$ | $\omega_{15}$ | $\omega_{19}$ |
|---|---|---|---|---|---|---|---|
| | AI | 8.205 − 1 | | | | | |
| 0 | AHF | 7.925 − 1 | | | | | |
| | AI | 9.422 − 1 | 7.092 − 1 | | | | |
| 3 | AHF | 9.029 − 1 | 7.777 − 1 | | | | |
| | AI | 9.923 − 1 | 2.316 | 4.155 − 2 | | | |
| 7 | AHF | 9.370 − 1 | 2.447 | 4.219 − 2 | | | |
| | AI | 9.715 − 1 | 3.347 | 5.104 − 1 | 2.020 − 3 | | |
| 11 | AHF | 9.515 − 1 | 3.384 | 5.159 − 1 | 2.021 − 3 | | |
| | AI | 9.599 − 1 | 3.631 | 7.974 − 1 | 1.792 − 2 | 1.117 − 5 | |
| 15 | AHF | 9.550 − 1 | 3.632 | 7.976 − 1 | 1.792 − 2 | 1.117 − 5 | |
| | AI | 9.595 − 1 | 3.638 | 8.086 − 1 | 1.950 − 2 | 3.514 − 5 | 5.376 − 10 |
| 19 | AHF | 9.551 − 1 | 3.639 | 8.086 − 1 | 1.950 − 2 | 3.514 − 5 | 5.376 − 10 |
| Exact | | 9.500 − 1 | 3.639 | 8.086 − 1 | 1.950 − 2 | 3.514 − 5 | 5.376 − 10 |

TABLE IV. Selected coefficients $\omega_k$ calculated by angular intensity (AI) and angular heat flux (AHF) methods using $F_N$ results with C4 for Henyey–Greenstein model with $\omega_0 = 0.99$, $g = 0.9$, and $K = 10$ for $\tau_o = 2$ and $\mu_o = 0.5$.

| $N$ | Method | $\omega_0$ | $\omega_3$ | $\omega_6$ | $\omega_{10}$ |
|---|---|---|---|---|---|
| | AI | 8.531 − 1 | − 4.909 | 4.393 | 7.241 |
| 4 | AHF | 9.901 − 1 | 5.004 | 6.861 | 7.249 |
| | AI | 1.035 | 3.249 | 6.007 | 7.246 |
| 8 | AHF | 9.899 − 1 | 5.078 | 6.844 | 7.249 |
| | AI | 1.015 | 4.289 | 6.476 | 7.248 |
| 12 | AHF | 9.900 − 1 | 5.077 | 6.844 | 7.249 |
| Exact | | 9.900 − 1 | 5.052 | 6.840 | 7.249 |

TABLE V. Selected coefficients $\omega_k$ calculated for an assumed $\tilde{K}$ by the angular heat flux method for binomial scattering model with $\omega_0 = 0.95$, $\alpha = 4.1$, and $K = 15$.

| $\tilde{K}$ | $\omega_0$ | $\omega_1$ | $\omega_2$ | $\omega_3$ | $\omega_4$ | $\omega_5$ | $\omega_6$ |
|---|---|---|---|---|---|---|---|
| 3 | 9.484 − 1 | 1.881 | 1.295 | 3.807 − 1 | | | |
| 4 | 9.500 − 1 | 1.915 | 1.392 | 5.030 − 1 | 7.639 − 2 | | |
| 5 | 9.500 − 1 | 1.916 | 1.394 | 5.066 − 1 | 7.915 − 2 | 1.243 − 3 | |
| 6 | 9.500 − 1 | 1.915 | 1.394 | 5.057 − 1 | 7.839 − 2 | 8.001 − 4 | − 1.611 − 4 |
| 7 | 9.500 − 1 | 1.916 | 1.394 | 5.061 − 1 | 7.880 − 2 | 1.062 − 3 | − 3.246 − 5 |
| 8 | 9.500 − 1 | 1.916 | 1.394 | 5.058 − 1 | 7.850 − 2 | 8.539 − 4 | − 1.495 − 4 |
| Exact | 9.500 − 1 | 1.916 | 1.394 | 5.060 − 1 | 7.863 − 2 | 9.515 − 4 | − 9.118 − 5 |

TABLE VI. Coefficients $\omega_k$ calculated for $D$-digit accuracy by angular heat flux method using $F_N$ results of Table II.

| $N$ | $D$ | $\omega_0$ | $\omega_1$ | $\omega_2$ | $\omega_3$ | $\omega_4$ |
|---|---|---|---|---|---|---|
| 5 | 1 | 8.3284 − 1 | 2.0467 | 1.0530 | 4.1545 − 1 | 4.5817 − 2 |
| | 2 | 9.4965 − 1 | 1.8757 | 1.3264 | 4.5189 − 1 | 6.9900 − 2 |
| | 3 | 9.5048 − 1 | 1.9014 | 1.3605 | 4.7506 − 1 | 6.7563 − 2 |
| | 4 | 9.4982 − 1 | 1.8995 | 1.3567 | 4.7499 − 1 | 6.7873 − 2 |
| | 15 | 9.5000 − 1 | 1.8996 | 1.3570 | 4.7513 − 1 | 6.7878 − 2 |
| 10 | 1 | 1.6973 | 7.1351 | − 2.4011 | − 3.8097 − 1 | 3.6796 − 2 |
| | 2 | 8.9261 − 1 | 2.3052 | 1.7939 | 4.8876 − 1 | 7.0452 − 2 |
| | 3 | 9.2205 − 1 | 1.9929 | 1.3770 | 4.8009 − 1 | 6.8307 − 2 |
| | 4 | 9.3477 − 1 | 1.9024 | 1.3487 | 4.7503 − 1 | 6.7864 − 2 |
| | 15 | 9.5003 − 1 | 1.9000 | 1.3571 | 4.7500 − 1 | 6.7857 − 2 |
| 15 | 1 | 1.0286 | 3.0368 | 5.0768 | 7.7390 | 9.3345 − 1 |
| | 2 | 5.5381 − 1 | 8.0394 − 1 | − 1.9459 | − 1.7712 | 1.1308 − 1 |
| | 3 | 1.2255 | 4.9620 | − 7.6316 − 1 | 3.6121 − 1 | 6.9353 − 2 |
| | 4 | 1.0236 | 2.7431 | 1.0036 | 4.5880 − 1 | 6.8727 − 2 |
| | 15 | 9.5003 − 1 | 1.9000 | 1.3571 | 4.7500 − 1 | 6.7857 − 2 |
| Exact | | 9.5000 − 1 | 1.9000 | 1.3571 | 4.7500 − 1 | 6.7857 − 2 |

TABLE VII. Selected moments $i_{0m}(0)$, $i_{1m}(0)$, $i_{0m}(\tau_o)$, and $i_{1m}(\tau_o)$ obtained by rounding to $D$ digits the $F_N$ results of Table II.

| | | | $N=5$ | | | $N=10$ | | | $N=15$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D$ | $m$ | $i_{0m}(0)$ | $i_{1m}(0)$ | $i_{0m}(\tau_o)$ | $i_{1m}(\tau_o)$ | $i_{0m}(0)$ | $i_{1m}(0)$ | $i_{0m}(\tau_o)$ | $i_{1m}(\tau_o)$ | $i_{0m}(0)$ | $i_{1m}(0)$ | $i_{0m}(\tau_o)$ | $i_{1m}(\tau_o)$ |
| 2 | 0 | 2.3232 − 1 | − 5.1197 − 2 | 6.4715 − 2 | 3.6372 − 2 | 1.4981 | 1.0677 | 8.6439 − 2 | 5.3764 − 2 | − 2.8559 | − 3.2538 | − 7.6356 + 1 | − 6.9485 + 1 |
| 2 | 3 | 1.5830 | − 7.6855 − 1 | 3.1295 − 2 | 1.5336 − 2 | 1.5848 | − 7.6719 − 1 | 2.6187 − 2 | 1.1854 − 2 | 1.5465 | − 7.8731 − 1 | 8.5295 − 2 | 6.1686 − 2 |
| 4 | 0 | 2.3230 − 1 | − 5.1332 − 2 | 6.4637 − 2 | 3.6337 − 2 | 2.2895 − 1 | − 5.4429 − 2 | 6.4819 − 2 | 3.6424 − 2 | 7.2981 − 1 | 3.8047 − 1 | − 4.3611 − 1 | − 4.1718 − 1 |
| 4 | 3 | 1.5839 | − 7.6817 − 1 | 3.1318 − 2 | 1.5339 − 2 | 1.5839 | − 7.6816 − 1 | 3.1337 − 2 | 1.5348 − 2 | 1.5824 | − 7.6929 − 1 | 3.3631 − 2 | 1.7076 − 2 |
| 6 | 0 | 2.3236 − 1 | − 5.1295 − 2 | 6.4639 − 2 | 3.6338 − 2 | 2.3259 − 1 | − 5.1252 − 2 | 6.4705 − 2 | 3.6338 − 2 | 2.4159 − 1 | − 4.3236 − 2 | 6.0312 − 2 | 3.2350 − 2 |
| 6 | 3 | 1.5839 | − 7.6817 − 1 | 3.1317 − 2 | 1.5339 − 2 | 1.5839 | − 7.6817 − 1 | 3.1328 − 2 | 1.5340 − 2 | 1.5839 | − 7.6816 − 1 | 3.1320 − 2 | 1.5331 − 2 |
| 15 | 0 | 2.3236 − 1 | − 5.1295 − 2 | 6.4638 − 2 | 3.6338 − 2 | 2.3254 − 1 | − 5.1294 − 2 | 6.4704 − 2 | 3.6337 − 2 | 2.3256 − 1 | − 5.1293 − 2 | 6.4709 − 2 | 3.6337 − 2 |
| 15 | 3 | 1.5839 | − 7.6817 − 1 | 3.1317 − 2 | 1.5339 − 2 | 1.5839 | − 7.6817 − 1 | 3.1328 − 2 | 1.5339 − 2 | 1.5839 | − 7.6817 − 1 | 3.1339 − 2 | 1.5340 − 2 |

Two important observations follow from our numerical tests:

(i) The finite accuracy available for digital calculations sets an upper limit for $N$, denoted as $N_{\max}$, beyond which the $F_N$ system of equations becomes ill conditioned. This limit depends upon the scattering model and the numerical scheme used for the calculation. Generally, for calculations with 15-digit precision, $N_{\max} \lesssim 10$ for projection techniques P1 and P2, whereas for collocation methods C1 through C3, $N_{\max} \gtrsim 15$. The $F_N$ solutions with collocation method C4 tended to be the best for $N \gtrsim 15$.

For the fog of Eq. (66) and for strongly anisotropic scattering with $\omega_0$ close to unity, such as the Henyey–Greenstein model with $g$ large or the binomial model with $\alpha$ large, the C4 model works better than any other. All methods other than C4 require the exact values of $\nu_j$, which are difficult to calculate for a weakly absorbing medium because the functions $\Lambda(z)$ and $\Lambda'(z)$ become very small for $z$ large. On the other hand, the estimated $\nu_j$ values used in C4 calculations are easily obtained because $g'(\nu_j)$ is enormous.

(ii) The coefficients $a_n$ and $b_n$ oscillate with the value of $n$, and the magnitude of these oscillations increases monotonically with increasing values of $N$, as illustrated in Table II for a binomial scattering model. This is due to the fact that the $F_N$ calculation gives polynomial approximations of degree $N$ for the intensities, and that the coefficients of finite polynomial approximations of strongly nonuniform functions have oscillations that increase with the order $N$ of the approximation. This phenomenon has implications for the inverse problem calculations.

## VII. CALCULATIONS FOR INVERSE PROBLEM SOLUTION

Inverse problem calculations were performed using $F_N$ results for the direct problem. The case of isotropic scattering was considered first. With $\omega_0 = 0.999$ and 0.2, and with $\tau_o = 2$ and 20 and $\mu_o = 0.5$, results for $\omega_0$ accurate to three decimal places were obtained using $F_3$ calculations based on collocation methods C1 through C4 and $F_4$ calculations using projection methods P1 and P2.

For the anisotropic scattering of fog, the angular heat flux method reproduced all $\omega_k$ values to four-digit accuracy, while the angular intensity method gave the same results except for $\omega_0$, which was 1.0012 instead of 0.9990. These inverse computations were done using $F_{15}$ calculations with collocation method C4 for a slab with $\tau_o = 2$ and $\mu_o = 0.5$.

One of the requirements of the inverse problem is that the $K$ value has to be estimated; this assumed $K$ value will be denoted by $\tilde{K}$. It is obvious from Eqs. (7) and (9) that $\tilde{K}$ must equal or exceed $K$, or the higher-order coefficients cannot be calculated. Table III shows different sets of $\omega_k$ obtained for different $\tilde{K}$ for the binomial model with $\omega_0 = 0.95$ and $\alpha = 19$. These calculations were based upon $F_{13}$ results using C4 for a slab with $\tau_o = 2$ and $\mu_o = 0.5$. A comparison of the calculated $\omega_k$'s with the exact ones used in the $F_N$ calculations shows that the lower-$k$ coefficients are considerably in error for $\tilde{K} < K$. The errors in the $\omega_k$'s were smaller for the binomial scattering law with $\omega_0 = 0.2$.

For $\tilde{K} = 19$, the angular heat flux algorithm provided slightly better $\omega_k$ values for the inverse problem calculations than the angular intensity algorithm. This difference is possibly because the $i_{1k}$ values converge faster with $N$ than the $i_{0k}$ values. The "upper triangular" structure of Eqs. (7) and (9) aggravates this difference for small $k$ values because of error propagation.

Inverse computations based upon an $F_6$ direct calculation for the case in Table III give nearly identical results to those obtained from the $F_{13}$ calculation. This suggests that the inverse problem results could be relatively insensitive to the $N$ of the direct problem calculations provided, of course, that $N$ is not too small.

To test this hypothesis, the Henyey–Greenstein scattering model with $\omega_0 = 0.99$, $g = 0.9$, and $K = 10$ was considered. Such a scattering model represents a severe test of the $F_N$ method because the scattering coefficients $\omega_k$ monotonically increase for $k \leqslant 9$. Table IV shows results for the inverse problem based upon $F_N$ calculations using the C4 technique for $N = 4$, 8, and 12. In this case, accurate results were obtained for the small $N$ values; also, the angular heat flux method was markedly superior to the angular intensity method.

When the assumed $\tilde{K}$ exceeds the value $K$ used in the $F_N$ calculations, all $\omega_k$, $k > K$, obtained from the inverse calculations are identically zero. If experimental data were used to perform the inverse problem calculations, no sharp cutoff would exist. Such a case has been simulated by using the binomial scattering model for $\alpha = 4.1$ and $\omega_0 = 0.95$ in an $F_{10}$ calculation with $K = 15$ for $\tau_o = 2$ and $\mu_o = 0.5$. The corresponding $\omega_k$ values are distributed in two groups: one group for $0 \leqslant k \leqslant 4$ is nearly the same for the scattering model with $\alpha = K = 4$ and much larger than the second group, for $5 \leqslant k \leqslant 15$, which acts as a "perturbation." The results in Table V show that accurate values for $\omega_k$, $k \leqslant 4$, are obtained for $\tilde{K} = 4$ and do not change appreciably for $\tilde{K} > 4$, while the values of $\omega_k$, $k > 4$, stabilize only when $\tilde{K} \approx 15$.

Perhaps the most important test of the inverse method is to examine the $\omega_k$ values predicted when the precision of the angular intensities is limited. To assess this, inverse problem calculations were done by rounding to $D$ digits the $I^m(\tau, \mu)$, i.e., the $a_n$ and $b_n$ values of the $F_N$ calculations. The $F_5$, $F_{10}$, and $F_{15}$ calculations of Table II for the binomial model with $\omega_0 = 0.95$ and $\alpha = 4$ were used in this test. The results for $D \leqslant 4$ in Table VI show than an inverse calculation based on the $F_5$ data is better than the corresponding one based on the $F_{15}$ data.

The rounding off of the coefficients $a_n$ and $b_n$ leads to a loss of precision because of the oscillation of these coefficients shown in Table II. Since the magnitude of the oscillations increases with $N$, the loss of precision is greater with larger $N$. This explains the poorer results of the inverse calculations in Table VI based on $F_{10}$ and $F_{15}$ data. Also the relatively good results obtained for small $N$ are due to the fact that the inverse calculations depend only upon the moments of the intensity, and not on the detailed shape of the angular intensity. As shown in Table VII, these moments are calculated with enough precision for small $N$.

## VIII. CONCLUSIONS

The direct slab albedo problem with azimuthal dependence has been solved with the $F_N$ method and been found to converge for $N \simeq 10$–15. The $F_N$ system of equations becomes ill conditioned for $N$ too large because of the finite precision available in the digital calculations. The convergence depends upon the degree of anisotropy of the scattering and the value of $\omega_0$ and, to a lesser extent, upon the slab thickness and the angle of incident radiation (provided $\mu_o \lesssim 0.9$ so that there is sufficient azimuthal dependence).

The recursion relations and series expansions in Sec. IV were found to be helpful (and sometimes necessary) to obtain good numerical accuracy with the $F_N$ method. Of the six numerical schemes proposed in Sec. V, the four collocation methods gave good results, although the collocation approach C4 was best for strongly anisotropic scattering. The projection techniques P1 and P2 were less satisfactory for many cases of anisotropic scattering.

The inverse problem for a homogeneous slab has been numerically evaluated with the results from the direct problem calculations. Generally the angular heat flux method provided slightly better accuracy, but the differences were small. Consequently, the method of determining the $\omega_k$ coefficients should depend upon whether the intensity or heat flux is easier to measure experimentally.

When using experimental data, a series of calculations should be performed with increasing assumed values $\tilde{K}$ of the anisotropy of the scattering. If the actual $\omega_k$ coefficients diminish rather gradually with increasing $k$ beyond some value $k_m$, then the first $(k_m + 1)$ coefficients will converge with increasing $\tilde{K}$ for $\tilde{K} > k_m$, as seen in Table III. If the $\omega_k$ values exhibit a rather sharp drop in magnitude for $k > k_m$, the larger coefficients are accurately obtained with inverse calculations even for $\tilde{K} = k_m$, as shown in Table V.

The precision test in Sec. VII is moderately encouraging for the use of the inverse problem algorithms. It was observed that for small $N$, two-digit accuracy in the angular intensities at the slab surfaces gave two-digit precision in the $\omega_k$ values, and that four-digit accuracy gave three-digit precision, as shown in Table VI. Because of the upper triangular form of the inverse method equations, the calculated $\omega_k$ values are generally worse for small $k$.


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# On the scattering of plane electromagnetic waves off spherically confined cold plasmas with overdense and steep densities

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In this paper we study the scattering of a plane electromagnetic wave off a spherical plasma pellet. The plasma density is taken to be overdense and very steep. This causes the cut off radius, $r_0$, to be within a fraction of a wavelength from the spherical boundary. The problem is studied in the asymptotic limit $(a\omega/c)\to\infty$ with $0<1-r_0=O(c/a\omega)$. Here $a$ is the radius of the sphere, $\omega$ is the frequency of the incident radiation, and $c$ is the velocity of light in free space. We develop an asymptotic technique which reduces Maxwell's equations to three ordinary differential equations within the plasma. Our method is a blend of geometrical optics and boundary layer techniques. Straightforward geometrical optics is used to describe the scattered field.

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## I. INTRODUCTION

The conversion of electromagnetic energy into kinetic energy is a major factor in the laser fusion concept.[1] As a first step to understanding this process, one linearizes the pertinent equations, neglects ionic motion, and assumes a cold plasma. The ensuing equations give rise to a linear scattering problem. This problem has been extensively studied when the plasma is planar.[2,3] Recently, the case of a spherical plasma target has received considerable attention.[1,4,5] The interest in this geometrical configuration arises from the fact that the plasma pellet, used in the fusion process, is initially spherical in shape.

The scattering of a plane electromagnetic wave off a perfectly conducting sphere coated with an inhomogeneous dielectric was studied by Alexopoulos.[5] The metal sphere was used to model the cut–off surface. In this paper the author performs a modal analysis using a specific index of refraction $(r/a)^m$ (where $r$ is the radial variable and $a$ is the radius of the sphere). He computes the asymptotic approximation to the backscattered field in the limit $a\omega/c\to\infty$ (here $\omega$ is the frequency of the incident plane wave and $c$ is the speed of light in free space). His analysis is made amenable by his particular choice of refractive index which, for $m>0$, is a reasonable model for a plasma medium.

Thomson, Max, and Erkkila[4] have studied certain aspects of the scattering problem for an overdense cold spherical pellet. They allowed the index of refraction to vanish on the surface $r=r_0<1$ (both the variable $r$ and $r_0$ are now scaled with respect to $a$). Thus, their model is more realistic than the one studied by Alexopoulos. It also gives rise to interesting cutoff and resonant phenomenon. However, they assumed that $1-r_0\gg c/a\omega$. This restriction allowed them to asymptotically approximate the radial eigenfunctions (as $\omega a/c\to\infty$) which occur in the full wave expansion of the Debye potentials. From these approximate potentials they deduce the scattered field, the field within the plasma, and the energy absorbed by the pellet. Their results become invalid when $1-r_0=O(c/a\omega)$.

In this paper we assume that the profile is steep enough to give $1-r_0=O(c/a\omega)$. Moreover, we fix $\omega$ and seek an asymptotic approximation of the electric field as $a\omega/c\to\infty$. In this work we modify a technique reported elsewhere[6] which exploits the smallness of $1-r_0$ and the largeness of $a\omega/c$. This method reduces the vector partial differential equation, describing the electric field within the plasma, into three uncoupled ordinary differential equations. It is basically a blend of geometrical optics[7] and boundary layer techniques.[8] Outside the plasma pellet the scattered wave is approximated by using straight geometrical optics.

We shall now give a brief outline of this paper and a summary of the main results. The statement of the scattering problem and the hypotheses regarding the plasma are given in Sec. 2. The asymptotic technique is presented in Sec. 3. The case of a lossless plasma is studied in Sec. 4. There it is analytically shown that the amplitude of the vector cross section equals one-half. This far field result is identical to the cross section of a metal sphere which is irradiated by a scalar plane wave. Section 5 is concerned with the effect of damping on the electric field. Of the three ordinary differential equations which describe the electric field within the plasma, only one can be solved in terms of tabulated functions. The other two equations must be solved numerically. However, the determination of the vector cross section's amplitude requires the numerical solution of only one. This information is used to define a "scattered" energy density, $\rho$, which is computed numerically. The function $\rho$ is found to possess a minimum at an angle which depends upon certain physical parameters. In the case of slab geometry, Freidberg, Mitchell, Morse, and Rudinski[9] report that the absorption coefficient has a minimum for a certain angle of incidence. This is the resonant absorption phenomenon. Their angle and ours is found to differ by only two degrees. Finally, $\rho$ is used to obtain a crude approximation of the energy absorbed by the plasma.

## 2. FORMULATION

A high frequency plane electromagnetic wave impinges upon a spherically confined "cold" plasma of radius $a$ and scatters from it. The time harmonic electric field $\mathbf{E}\exp(-i\omega t)$ satisfies[10]

$$\nabla\times\nabla\times\mathbf{E}=k^2n\mathbf{E}, \tag{2.1}$$

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where $k = k'a$ and the index of refraction $n$ is given by

$$n = (1 - i\delta)n_0 + i\delta,\ \delta > 0. \tag{2.2}$$

In (2.2) the parameter $\delta$ is the damping coefficient and $n_0$ is given by

$$n_0 = 1 - 4\pi e^2 N(ar)/m\omega^2, \tag{2.3}$$

where $\omega$ is the frequency of the incident plane wave, $e$ is the radial variable, and $N(ar)$ is the charge density. Implicit in (2.3) are the assumptions that $\omega$ is large enough to neglect ionic motion and the density is dependent only upon $r$.

We now assume that the plasma is overdense, is confined to the region $0 \leqslant r \leqslant 1$, and is very steep. These assumptions lead us to make the following hypotheses about $n_0(r)$:

(H1) $n_0(r) = 1,\ r \geqslant 1$,

(H2) $n_0(r_0) = 0,\ 0 < 1 - r_0 = O(1/k)$,

(H3) $n_0'(r_0) = mk,\ m = O(1)$,

and

(H4) $n_0^{(l)}(r_0) = o(k^l)$.

These conditions are met when an infrared laser initially irradiates an overdense plasma target.[1]

To complete the mathematical statement of this problem, we must impose further conditions. First, we demand that **E** and its first partial derivatives are continuous everywhere. Secondly, the scattered field must satisfy the radiation condition. Finally, we choose the $z$ axis to be parallel to the incident wave vector $\mathbf{k}'$ and the $y$ axis to be parallel to the incident electric field.

We shall now suppose that $k \gg 1$ which corresponds to the physical situation mentioned above. Thus we seek an asymptotic approximation of **E** as $k \to \infty$. At first this seems to be a natural setting for the method of geometrical optics. However, the cutoff radius is a fraction of a wavelength away from the boundary of the plasma (H2). Thus, geometrical optics cannot be used directly to determine an asymptotic approximation of $u$ within the plasma.

## 3. THE ASYMPTOTIC METHOD

The largeness of $k$ and the smallness of $1 - r_0$ will now be exploited to change (2.1) into a system of ordinary differential equations. The field within the plasma is assumed to be of the form

$$\begin{aligned}\mathbf{E}(r, \theta, \phi; k) &= e^{ik\cos\theta}[\sin\phi u(\bar{r}, \theta)\hat{r} \\ &\quad + \sin\phi v(\bar{r}, \theta)\hat{\theta} + \cos\phi w(\bar{r}, \theta)\hat{\phi} + O(1/k)]\end{aligned} \tag{3.1}$$

as $k \to \infty$ where the boundary layer variable $\bar{r}$ is defined by[8]

$$\bar{r} = km(r - r_0). \tag{3.2}$$

The variables $r$, $\theta$, and $\phi$ are the spherical coordinates of a point in the plasma and $\hat{r}$, $\hat{\theta}$, and $\hat{\phi}$ are unit vectors.

The index of refraction within the plasma is expressed in terms of $\bar{r}$ as

$$n(r) = b(\bar{r}) = (1 - i\delta)\bar{r} + i\delta + o(1) \tag{3.3}$$

as $k \to \infty$. This follows from (H2)–(H4), (2.2), and from expanding $n_0$ in a Taylor series about $r = r_0$.

Upon inserting (3.1)–(3.3) into (2.1) it is found that $u$, $v$, and $w$ satisfy

$$\sin\theta v' = i\gamma(b - \sin^2\theta)u, \tag{3.4}$$

$$v'' + \gamma^2 b v = -i\gamma\sin\theta u', \tag{3.5}$$

$$L_\phi w = w'' + \gamma^2(b - \sin^2\theta)w = 0, \tag{3.6}$$

where $\gamma = 1/m$ and the prime denotes differentiation with respect to $\bar{r}$. Equations (3.4) and (3.5) are easily decoupled to give

$$L_r u = u'' + \frac{b'u'}{b} + \left[\gamma^2(b - \sin^2\theta) - \left(\frac{b'}{b}\right)^2\right]u = 0, \tag{3.7}$$

$$L_\theta v = v'' - \frac{b'\sin^2\theta v'}{b(b - \sin^2\theta)} + \gamma^2(b - \sin^2\theta)v = 0. \tag{3.8}$$

Outside the plasma target ($r > 1$) the electric field is assumed to be of the form

$$\mathbf{E} = e^{ikz}\hat{y} + e^{ik\psi(x,y,z)}[\mathbf{A}(x,y,z) + O(1/k)] \tag{3.9}$$

as $k \to \infty$. The first term is the incident plane wave and the second is the scattered field. Upon inserting (3.9) into (2.1) and equating the coefficients of like powers of $k$ to zero, it is found that $\psi$ and **A** to zero, satisfy

$$\nabla\psi\cdot\nabla\psi = 1 \text{ (eiconal equation)}, \tag{3.10}$$

$$2\nabla\mathbf{A}\cdot\nabla\psi + \mathbf{A}\nabla^2\psi = 0 \text{ (vector transport equation)}. \tag{3.11}$$

Thus, the scattered electric field will be approximated by the method of geometrical optics.[7]

Now to compute **E**, boundary conditions must be specified for (3.6)–(3.8) and initial data must be given for (3.10)–(3.11). For a fixed $r < r_0$ it follows from (3.2) that $\bar{r} \to -\infty$ as $k \to \infty$. Thus, the limits of $u$, $v$, and $w$ must be specified as $\bar{r} \to -\infty$. By applying the WKB method[11] to (3.6)–(3.8) it is found that each equation has one solution which grows exponentially and another which decays exponentially in this limit. The modest assumption that the field remains bounded in the plasma implies

$$\lim_{\bar{r}\to-\infty}(u, v, w) = (0, 0, 0). \tag{3.12}$$

From (3.1), (3.9), and the assumptions that **E** and its first partial derivatives are continuous at $r = 1$, it follows that

$$\psi_0(\theta) = \psi(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) = \cos\theta, \tag{3.13}$$

$$\sin\phi u(1, \theta) = \sin\phi\sin\theta + A_r(1, \theta, \phi), \tag{3.14}$$

$$\sin\phi v(1, \theta) = \sin\phi\cos\theta + A_\theta(1, \theta, \phi), \tag{3.15}$$

$$\cos\phi w(1, \theta) = \cos\phi + A_\phi(1, \theta, \phi), \tag{3.16}$$

$$\sin\phi u'(1, \theta) = i\gamma\sin\theta\cos\theta\sin\phi + i\gamma\psi_r A_r(1, \theta, \phi), \tag{3.17}$$

$$\sin\phi v'(1, \theta) = i\gamma\cos^2\theta\sin\phi + i\gamma\psi_r A_\theta(1, \theta, \phi), \tag{3.18}$$

$$\cos\phi w'(1, \theta) = i\gamma\cos\theta\cos\phi + i\gamma\psi_r A_\phi(1, \theta, \phi), \tag{3.19}$$

where $A_r$, $A_\theta$, and $A_\phi$ are the components of **A** in spherical coordinates. In deriving (3.17)–(3.19) a term of order $O(1/k)$ was neglected and $\bar{r}$ was set equal to one at the plasma boundary. The later approximation follows from (2.2), (H1), and (3.2). It introduces an error of order $O(1/k)$; we have consistently neglected terms of this order.

From (3.10) and (3.13), it follows that

$$\psi_r(1,\theta,\phi)=\frac{\partial\psi}{\partial r}(1,\theta,\phi)=|\cos\theta|. \tag{3.20}$$

When this result is inserted into (3.17)–(3.19), we find from (3.14)–(3.19) that

$$\begin{pmatrix}u'(1,\theta)\\ v'(1,\theta)\\ w'(1,\theta)\end{pmatrix}-i\gamma|\cos\theta|\begin{pmatrix}u(1,\theta)\\ v(1,\theta)\\ w(1,\theta)\end{pmatrix}=i\gamma\Delta\begin{pmatrix}\sin\theta\\ \cos\theta\\ 1\end{pmatrix}, \tag{3.21}$$

where $\Delta=\cos\theta-|\cos\theta|$. Thus, to find the electric field within the plasma we must solve (3.6)–(3.8) subject to the boundary conditions (3.12) and (3.21).

Once $u$, $v$, and $w$ are computed it follows from (3.14)–(3.16) that

$$\begin{aligned}A_r(1,\theta,\phi)&=\sin\phi\,[u(1,\theta)-\sin\theta\,],\\ A_\theta(1,\theta,\phi)&=\sin\phi\,[v(1,\theta)-\cos\theta\,].\\ A_\phi(1,\theta,\phi)&=\cos\phi\,[w(1,\theta)-1\,].\end{aligned} \tag{3.22}$$

This information and (3.13) are the initial data needed to solve (3.10)–(3.11). The eiconal and vector transport equation are easily solved by making the following observation: The initial phase given in (3.13) is the same phase that would occur if a scalar plane wave impinged upon a "metal" sphere (the total scalar wave vanishes there) of unit radius. Thus the reflected rays and phase of the present problem are identical to those of the irradiated metal sphere. Since each Cartesian component of **A** satisfies the transport equation and the ray pattern determines the expansion ratio[6] we find that

$$\mathbf{A}=-\mathbf{A}_0A_s(x,y,z), \tag{3.23}$$

where $A_s$ is the amplitude for the "metal" sphere problem and $\mathbf{A}_0$ is the value of **A** on $r=1$ given by (3.22). The rays, $\psi$, and $A_s$ are computed in Appendix A for completeness.

The far field result is given by

$$\mathbf{E}\sim e^{ikz}\hat{y}+\mathbf{S}(\Theta,\phi)\frac{e^{ikR}}{R} \tag{3.24}$$

as $R\to\infty$ where $\mathbf{S}(\Theta,\phi)$ is defined by

$$\mathbf{S}(\Theta,\phi)=0.5\exp\left[-2ik\sin\frac{\Theta}{2}\right]\mathbf{A}_0\left(\frac{\pi}{2}+\frac{\Theta}{2},\phi\right). \tag{3.25}$$

The variables $R$, $\Theta$, and $\phi$ are the spherical coordinates of the far field point. This result becomes inaccurate as $\Theta$ approaches zero; the observation point then lies in the shadow region which is devoid of scattered rays.

## 4. THE LOSSLESS PLASMA

In this section we shall study the differential equations (3.6)–(3.8) and boundary conditions (3.12) and (3.21) when $\delta=0$. If these equations could be solved exactly, then (3.1) would give the electric field within the plasma. Moreover, Eqs. (3.22), (3.24), and (3.25) would determine **E** in the far field. Unfortunately, only (3.6) can be solved exactly to give

$$w=\begin{cases}0, & |\theta|\leqslant\pi/2,\\ \dfrac{-2i\gamma\cos\theta}{Z_0}A_i(-\xi), & \pi/2<\theta<3\pi/2,\end{cases} \tag{4.1}$$

where $\xi=\gamma^{2/3}(\bar{r}-\sin^2\theta)$, $\xi_1=\gamma^{2/3}\cos^2\theta$,

$A_i(-\xi)$ is the Airy function,

and

$$Z_0=\gamma^{2/3}A_i'(-\xi_1)-i\gamma\cos\theta\,A_i(-\xi_1). \tag{4.2}$$

From (3.22) and (4.1) it follows that

$$A_\phi(1,\theta,\phi)=\begin{cases}-\cos\phi, & |\theta|\leqslant\pi/2,\\ (Z_0/Z_0^*)\cos\phi, & \pi/2<\theta<3\pi/2.\end{cases} \tag{4.3}$$

Now to the best of our knowledge neither $u$ nor $v$ can be expressed in terms of tabulated functions. They must be computed numerically from (3.7)–(3.8). However certain qualitative information can be gleaned from the differential equations and boundary conditions.

Let $u(\bar{r},\theta)$ satisfy (3.7) with (3.12) and (3.21). Then $u^*(\bar{r},\theta)$ satisfies

$$\begin{aligned}&L_ru^*=0,\quad\lim_{\bar{r}\to-\infty}u^*=0,\\ &\frac{du^*}{d\bar{r}}(1,\theta)+i\gamma|\cos\theta\,|u^*(1,\theta)=-i\gamma\Delta\sin\theta.\end{aligned} \tag{4.4}$$

Integrating the difference

$$\bar{r}[u^*L_ru-u\,L_ru^*]=0 \tag{4.5}$$

by parts from $-\infty$ to 1 gives

$$\bar{r}(u^*u'-uu^{*\prime})\big|_{-\infty}^{1}=0. \tag{4.6}$$

Since $u$ approaches zero exponentially as $\bar{r}\to-\infty$, it follows from (3.21), (4.4), and (4.6) that

$$|\cos\theta\,|\,|u|^2+\Delta\sin\theta\,(u+u^*)=0. \tag{4.7}$$

When $|\theta|\leqslant\pi/2$, $\Delta=0$ and (3.21) with (4.7) give $u(1,\theta)=u'(1,\theta)=0$.

This result implies $u(\bar{r},\theta)=0$ for $\theta$ in this range. When $\theta$ lies in the interval $[\pi/2,3\pi/2]$, $\Delta=2\cos\theta$ and (4.7) gives

$$|u(1,\theta)-\sin\theta\,|^2=\sin^2\theta. \tag{4.8}$$

A similar argument works for $v$ and gives $v(\bar{r},\theta)=0$ when $|\theta|\leqslant\pi/2$ and

$$|v(1,\theta)-\cos\theta\,|^2=\cos^2\theta \tag{4.9}$$

when $\theta$ lies in $[\pi/2,3\pi/2]$. It is apparent from (3.22), (4.8), and (4.9) that

$$|A_r(1,\theta,\phi)|^2=\sin^2\phi\sin^2\theta,\quad|A_\theta(1,\theta,\phi)|^2=\sin^2\phi\cos^2\theta, \tag{4.10}$$

$$|A_\phi(1,\theta,\phi)|^2=\cos^2\phi. \tag{4.11}$$

These results hold for all $\theta$ and $\phi$ and imply that $|\mathbf{A}_0|=1$. From (3.25) we deduce

$$|\mathbf{S}(\Theta,\phi)|=0.5. \tag{4.12}$$

Thus the magnitude of the vector cross section is the same as the amplitude of the scalar cross section for the "metal" sphere problem. (This agrees with the result of Alexopoulos[5] when the thickness of the dielectric coating approaches zero.)

Any additional information about $A_r$, $A_\theta$, and $A_\phi$ necessitates a numerical integration of the differential equations (3.6)–(3.8). We do not pursue this here.

## 5 THE EFFECT OF DAMPING: ENERGY ABSORPTION

We begin this section by computing the amplitude of the vector cross section, **S**. This quantity will be used later to

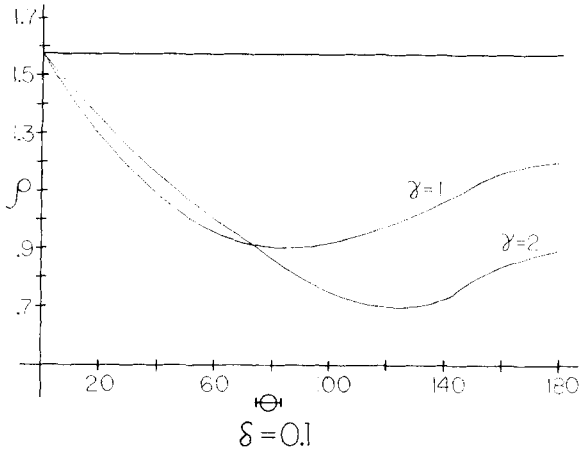


FIG. 1. The scattered energy density, $\rho(\Theta)$, for $\delta = 0.1$ with $\gamma = 1$ and 2.

approximate the energy absorbed by the plasma. From (3.22) and (3.25) it follows that

$$|\mathbf{S}(\Theta,\phi)|^2 = \tfrac{1}{4}\sin^2\phi\,[|u(1,\Theta/2+\pi/2)-\cos(\Theta/2)|^2 + |v(1,\Theta/2+\pi/2)+\sin(\Theta/2)|^2] + \tfrac{1}{4}\cos^2\phi\,|w(1,\Theta/2+\pi/2)-1|^2. \quad (5.1)$$

By using (3.4) and (3.21) this result simplifies to

$$|\mathbf{S}(\Theta,\phi)|^2 = \tfrac{1}{4}\sin^2\phi\,\sec^2(\Theta/2) \times|u(1,\Theta/2+\pi/2)-\cos(\Theta/2)|^2 + \tfrac{1}{4}\cos^2\phi\,|w(1,\Theta/2+\pi/2)-1|^2 \quad (5.2)$$

when $\Theta \neq \pi$. When $\Theta$ equals $\pi$, Eq. (3.4) gives $u = 0$ while (3.6), (3.8), (3.12), and (3.21) yield $v = -w$. Thus (5.1) becomes

$$|\mathbf{S}(\pi,\phi)|^2 = \tfrac{1}{4}|w(1,\pi)-1|^2 \quad (5.3)$$

in the backscattered direction.

The scattered energy density, $\rho(\Theta)$, is defined to be the integral of $|\mathbf{S}|^2$, with respect to $\phi$, from 0 to $2\pi$. It is given by

$$\rho(\Theta) = (\pi/4)\sec^2(\Theta/2)|u(1,\Theta/2+\pi/2)-\cos(\Theta/2)|^2 + (\pi/4)|w(1,\Theta/2+\pi/2)-1|^2 \quad (5.4)$$

when $\Theta \neq \pi$ and

$$\rho(\pi) = (\pi/2)|w(1,\pi)-1|^2 \quad (5.5)$$

when $\Theta = \pi$.

To determine the functional dependence of $\rho$ on $\Theta$ necessitates the computation of $u$ and $w$. The later function can be obtained directly from (3.6), (3.12), and (3.21). It is given by

$$w(\bar{r},\Theta) = \begin{cases} 0, & |\Theta| \leqslant \pi/2, \\ \dfrac{-2\,i\gamma\cos\Theta}{Z} A_i(-\xi), & \pi/2 \leqslant \Theta \leqslant 3\pi/2, \end{cases} \quad (5.6)$$

where

$$\xi = [\gamma/(1-i\delta)]^{2/3}[(1-i\delta)\bar{r} + i\delta - \sin^2\Theta],$$

$$\xi_1 = [\gamma/(1-i\delta)]^{2/3}\cos^2\Theta,$$

and

$$Z(\Theta) = \gamma^{2/3}(1-i\delta)^{1/3}A_i'(-\xi_1) - i\gamma\cos\Theta A_i(-\xi_1). \quad (5.7)$$

Thus, the second term in (5.4) is given by

$$\frac{\pi}{4}\left|w\left(1,\frac{\pi}{2}+\frac{\Theta}{2}\right)-1\right|^2 = \frac{\pi}{4}\left|\frac{Z(\pi/2-\Theta/2)}{Z(\pi/2+\Theta/2)}\right|^2. \quad (5.8)$$

Unfortunately, the function $u(\bar{r},\Theta)$ cannot be determined in terms of tabulated functions. Equations (3.7), (3.12), and (3.21) must be solved numerically to deduce $u(1,\Theta/2+\pi/2)$. The problem is simplified somewhat by substituting

$$u(\bar{r},\Theta) = q(\bar{r},\Theta)/b(\bar{r},\delta) \quad (5.9)$$

into these equations. It is evident that $q$ must satisfy

$$q'' - (b'/b)q' + (\gamma^2 b - \sin^2\Theta)q = 0, \quad (5.10)$$

$$\lim_{\bar{r}\to-\infty} q = 0, \quad (5.11)$$

$$q'(1,\Theta) + (1 - i\delta + i\gamma|\cos\Theta|)q(1,\Theta) = i\gamma\Delta\sin\Theta. \quad (5.12)$$

Equation (5.10) with $b = (1-i\delta)\bar{r}$, has been the object of considerable interest (see Ref. 6 for a modest bibliography).

We have numerically solved (5.10) using the finite difference method.[12] To perform the calculations, a step size of 0.1 was used and the boundary condition (5.11) was replaced by $q(-10,\Theta) = 0$. To test the sensitivity of the results to this approximate boundary condition, we replaced $-10$ by $-15$, kept the step size fixed, and reran the program. The numerical values were found to change insignificantly.

We obtain from this calculation and (5.9) the value of $u(1,\Theta)$. The functional dependence of $\rho$ on $\Theta$ is obtained by introducing this information and (5.8) into (5.4). This dependence is shown in Fig. 1 for $\delta = 0.1$ ($\gamma = 1, 2$) and in Fig. 2 for $\delta = 0.05$ ($\gamma = 1, 2$). The line $\rho = \pi/2$ is plotted in both figures; this is the value of $\rho$ when damping is neglected [see Eq. (4.12)].

It is interesting to note that $\rho$ possesses a minimum at an angle which depends upon $\gamma$ and $\delta$. This angle corresponds to a small portion of the sphere where a maximum amount of energy is absorbed. In the case of a plasma slab, Freidberg *et al.*[9] report that their absorption coefficient possesses a maximum at a particular angle of incidence. This coefficient is defined to be proportional to

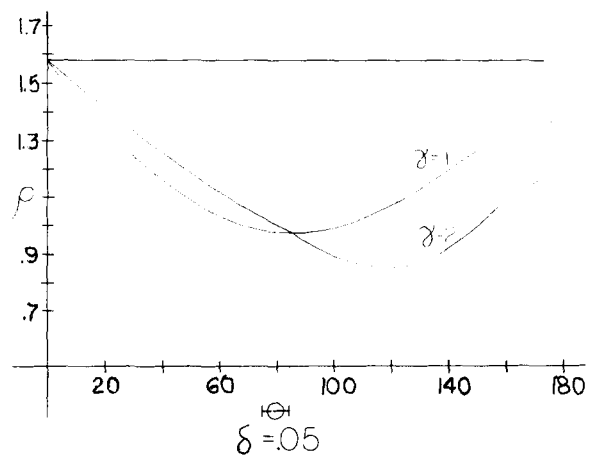


FIG. 2. The scattered energy density, $\rho(\Theta)$, for $\delta = 0.05$ with $\gamma = 1$ and 2.

TABLE I. The absorbed energy for $\delta = 0.1, 0.2$ and $\gamma = 1, 2$.

| $\gamma$ \ $\delta$ | .05 | 0.1 |
|---|---|---|
| 1 | .96 | 1.13 |
| 2 | 1.08 | 1.36 |

$$\tilde{A}(\Theta) = \lim_{\delta \to 0} [\sin\Theta\, |E(0,\delta)|],$$

where $\Theta$ is the angle of incidence and $E(0, \delta)$ is the component of the electric field along the slab's normal, evaluated at the cutoff. It is remarkable that our angle of minimum $\rho$ differs from their angle of maximum absorption by only two degrees when $\gamma = 1, \delta = 0.05$. This error is due to numerical inaccuracies and the fact that $\delta \neq 0$. Unfortunately, here is where the direct comparison of $\tilde{A}(\Theta)$ and $\rho(\Theta)$ ends. Our problem is inherently three dimensional whereas theirs is two. The function $\tilde{A}(\Theta)$ represents the absorption coefficient only in the latter case. However, we did compute $\tilde{A}(\Theta)$ using $u|_{r=0}$ in place of $E(0, \delta)$. Upon inserting the proper proportionality constant we found that our numerical results agreed with theirs to within 5% when $\gamma = 1$ and $\delta = 0.05$.

The function $\rho(\Theta)$ will now be used to obtain a crude approximation of the energy absorbed by the plasma pellet. In Appendix B we have derived the result

$$T = -\int_0^{\pi} \sin\Theta\, \rho(\Theta)\, d\Theta - (1/k)\,\mathrm{Im}\int_0^{2\pi} A_{0y}(\pi/2, \phi)\, d\phi. \tag{5.13}$$

where $T$ is the energy absorbed and $A_{0y}$ is the $y$ component of $\mathbf{A}_0$. The second term in this equation comes from a stationary phase analysis[11] of an integral involving the scattered field. The main contribution to this integral comes from a small neighborhood about $\Theta = 0$. Unfortunately, this corresponds to the shadow region where our results are inaccurate. Thus, we do not have a handle on $A_{0y}(\pi/2, \phi)$ when $\delta \neq 0$.

If no damping were present, then $T$ would be zero. Equation (4.12), the definition of $\rho$, and (5.13) would then give

$$\frac{1}{k}\,\mathrm{Im}\int_0^{\pi} A_{0y}(\pi/2, \phi)\, d\phi = -\pi. \tag{5.14}$$

A crude approximation to $T$ is obtained by inserting this result into (5.13). It gives

$$T \sim \pi - \int_0^{\pi} \sin\Theta\, \rho(\Theta)\, d\Theta. \tag{5.15}$$

The results of this approximation are given in Table I. These results make good qualitative sense. For a fixed $\gamma$, $T$ is seen to increase as $\delta$ becomes larger.

To explain the dependence of $T$ on $\gamma$, recall that $\gamma$ equals $1/m$ where $m$ is defined in (H3). As $m$ increases, the density gradient becomes steeper and reflects more of the incident radiation. Thus as $m$ increases ($\gamma$ decreases), less energy is absorbed by the plasma for a fixed $\delta$. This feature is also born out in Table I.

## APPENDIX A

Consider a scalar plane wave impinging upon a metal sphere and scattering from it. The geometrical optics approximation to the scattered wave is given by

$$u(x,y,z,k) = [A_s(x,y,z) + O(1/k)]e^{ik\psi(x,y,z)} \tag{A1}$$

where the amplitude satisfies

$$2\nabla A_s \cdot \nabla\psi + A_s \nabla^2\psi = 0, \tag{A2}$$

and the phase $\psi$ satisfies (3.10). Since the total field vanishes on the unit sphere,

$$A_s(\sin\Theta\cos\phi, \sin\Theta\sin\phi, \cos\Theta) = -1$$

and

$$\psi(\sin\Theta\cos\phi, \sin\Theta\sin\phi, \cos\Theta) = \cos\Theta.$$

The argument of $A_s$ (and $\psi$) is the intersection point of an incident ray with the sphere. From (3.10) and the initial data it follows that the scattered rays satisfy the law of reflection. Thus they are given

$$\begin{aligned} X &= \sin\Theta\cos\phi - \sigma\cos\phi\sin 2\Theta, \\ Y &= \sin\Theta\sin\phi - \sigma\sin\phi\sin 2\Theta, \\ Z &= \cos\Theta - \sigma\cos 2\Theta, \end{aligned} \tag{A3}$$

where $\sigma$ is the arclength. These rays form a two-parameter family of straight lines.

Equations (3.10) and (A2) are readily solved to give

$$\psi = \sigma + \cos\Theta, \tag{A4}$$

$$A_s = -\left(\frac{J(0,\Theta,\phi)}{J(\sigma,\Theta,\phi)}\right)^{1/2}, \tag{A5}$$

where $J(\sigma, \Theta, \phi)$ is the Jacobian of the ray map $(\sigma, \Theta, \phi) \to (x,y,z)$ given by (A 13). It is easily found to be

$$J = (2\sigma - \cos\Theta)(\sin\Theta - \sigma\sin 2\Theta). \tag{A6}$$

Now in the far field $\sigma \gg 1$. From (A3)–(A5) we deduce that

$$\begin{aligned} &\sigma \simeq R + \cos\Theta, \quad J \simeq 2R^2\sin 2\Theta, \quad \psi \simeq R + 2\cos\Theta, \\ &A \simeq 1/2R, \quad \Phi \simeq \phi, \quad \Theta = \Theta - \pi, \end{aligned} \tag{A7}$$

where $R$, $\Phi$, and $\Theta$ are the spherical coordinates of the far field point. When (A7) is inserted into (A1) we obtain

$$u \simeq \tfrac{1}{2} e^{-2ik\sin(\theta/2)} \frac{e^{ikR}}{R}, \text{ as } R \to \infty. \tag{A8}$$

Now each Cartesian component of the scattered field vector $\mathbf{A}$ satisfies (A2). Let $A_x$ be the $x$ component of $\mathbf{A}$ and let $A_{0x}$ be the value of $A_x$ on $r = 1$. The $A_x$ is given by $-uA_{0x}$ for $r > 1$. This proves (3.23).

## APPENDIX B

It follows from Maxwell's equations,[13] the incident wave form, and the hypotheses on $n(r)$ that

$$\begin{aligned} -R^2\mathrm{Re}\int_0^{2\pi}\int_0^{\pi} (\mathbf{E}\times\mathbf{H}^*)\cdot\hat{R}\sin\Theta\, d\Theta\, d\phi = k\delta \\ \times\int\int_{V_P}\int (1 - n_0)|\mathbf{E}|^2\, dv, \end{aligned} \tag{B1}$$

where $\mathbf{E}$ is the total electric field, $\mathbf{H}^*$ is the conjugate of the total magnetic field, $\hat{R}$ is a unit vector in the direction of the far field point, and $V_P$ is the region occupied by the pellet.

The right-hand side of (B1) is the energy absorbed by the plasma which will be denoted by $T$.

From the far field result (3.24) and the relation

$$\nabla \times \mathbf{E} = ik\,\mathbf{H} \tag{B2}$$

it follows that

$$\mathbf{H}^* = -e^{ikz}\hat{\mathbf{x}} + (\hat{R} \times \mathbf{A}_0)e^{ikR}/R \text{ as } R \to \infty. \tag{B3}$$

When (3.24) and (B3) are inserted into the left-hand side of (B1) we find that

$$T = -\int_0^{\pi} \rho(\Theta)\sin\Theta\, d\Theta + \frac{R}{2} \times \mathrm{Re}\int_0^{2\pi}\int_0^{\pi} K(\Theta,\phi)e^{ikR\psi}\, d\Theta\, d\phi, \tag{B4}$$

where

$$\psi = 1 - \cos\Theta - 1/R\,\sin(\Theta/2),$$

$$K = \sin\Theta I(1 + \cos\Theta)A_{oy}(\pi/2 + \Theta/2,\phi) - \sin\Theta\,\sin\phi A_{0z}(\pi/2 + \Theta/2,\phi)].$$

The functions $A_{0y}$ and $A_{0z}$ are the $y$ and $z$ components of $\mathbf{A}_0$ respectively. Since $R \to \infty$, the method of stationary[11] phase can be applied to the second integral in (B4). The energy absorbed in then approximated by

$$T = -\int_0^{\pi} \rho(\Theta)\sin\Theta\, d\Theta - \frac{1}{k}\,\mathrm{Im}\int_0^{2\pi} A_{0y}(\pi/2, \phi)\, d\phi. \tag{B5}$$

This is just a statement of the optical theorem.[13]


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# On the topology of charged spherical collapse [a)]

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It is shown that in the gravitational collapse of a charged fluid sphere only one of the two Reissner–Nordström curvature singularities is present, under the assumption that the charge density evaluated at the surface of the sphere and the total charge on the sphere do not have opposite sign. Arguments are presented to show that this assumption is physically reasonable. Ignoring possible naked singularities formed within the collapsing matter, this implies that the only Cauchy horizon in the interior of a charged black hole is the future inner event horizon ($r = r_-$, $t = +\infty$), which is known to be both classically and quantum mechanically unstable.

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## I. INTRODUCTION

Determining the validity of the cosmic censorship hypothesis is widely regarded as one of the most important problems in classical general relativity today. The cosmic censorship hypothesis[1] basically says that any naked singularity which is created by the evolution of "regular" initial conditions will always be hidden behind an absolute event horizon. Such a naked singularity is visible (or "naked") only to observers who fall through the absolute event horizon into the black hole containing the singularity. The local (or "strong") version of the cosmic censorship hypothesis[2] simply states that naked singularities are never produced. A singularity is considered naked only if there exists some observer for whom the singularity lies initially to his future, and, some subsequent proper time later, the singularity lies to his past. This definition is local in that it makes no reference to a special set of observers at asymptotic infinity. Note also that the big bang is not naked according to this definition.

If the local cosmic censorship hypothesis is true, then the geometry of a black hole interior may be completely determined by solving the Cauchy problem for the space-time. Ignoring perturbations occuring at late times, this amounts to determining the time-dependent metric and matter fields in the gravitational collapse which forms the black hole.

Conversely, by studying classical gravitational collapse, we can to some extent study the validity of the local cosmic censorship hypothesis. Several different approaches can be taken. First, one might study the formation of curvature singularities within the collapsing matter and determine whether they are locally naked. This is likely to be a very difficult problem, as the nature of the singularities is likely to depend on the specific details of the collapse, and may not be amenable to a general analysis. In Sec. II. I review the progress made on this problem to date. Second, one might study the possible trajectories the surface of the collapsing body can follow, in order to determine which regions of the interior are likely to be vacuum. In particular, if the geometry is spherically symmetric, we can determine which portions of the Reissner–Nordström interior are relevant to realistic gravitational collapse. In Sec. III of this paper, I prove that in the collapse of a charged spherical star the left hand $r = 0$ curvature singularity in Fig. 1 will *never* be exposed (unless nature contains an additional attractive force which diverges faster than $r^{-3}$). Thus, ignoring possible naked singularities formed, within the matter, only the right hand Reissner–Nordström singularity is naked, and only the future inner horizon (labeled $\mathcal{H}^+$) is a Cauchy horizon.

It is now well established that the future inner event horizon ($\mathcal{H}^+$) is both classically[3,4,5,6] and quantum mechanically[7,8,9] unstable. Thus, it appears that the only possible

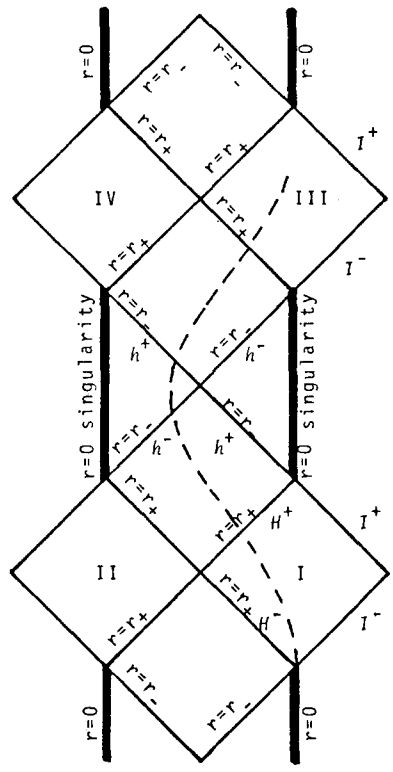


FIG. 1. Penrose diagram of the Reissner–Nordström space-time with $Q^2 < M^2$. The region denoted I represents our exterior universe. Note the existence of multiple asymptotically flat exteriors, such as regions II, III, and IV. The Penrose diagram repeats endlessly off the top and bottom of the page. The dashed curve indicates a typical timelike geodesic.

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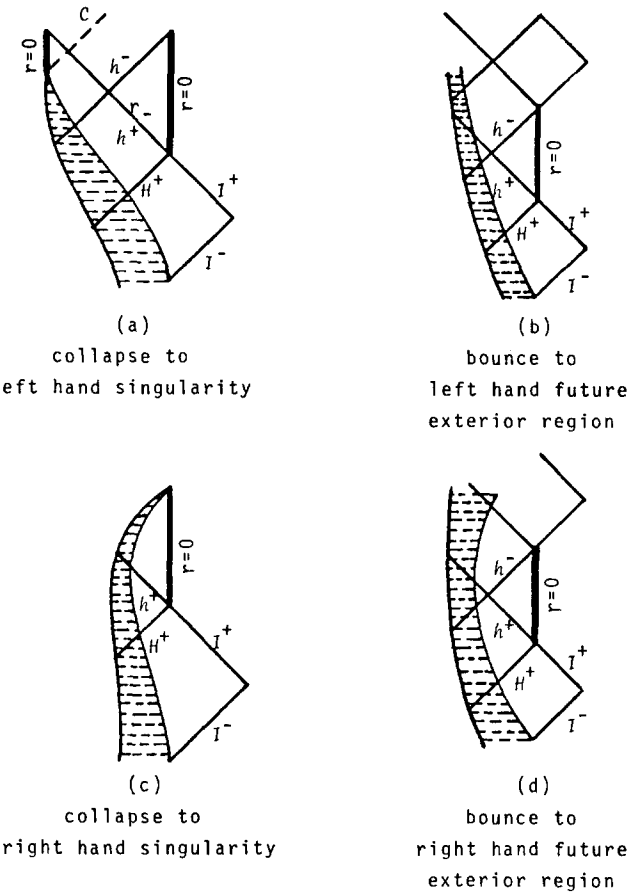


FIG. 2. Possible topologies for charged spherical collapse. The shaded region represents the collapsing matter, and is bounded on the left by $r = 0$ (origin of coordinates). The heavy lines labeled $r = 0$ are the Reissner–Nordström curvature singularities.

naked singularities formed in spherical collapse are singularities formed *within* the collapsing matter. The instability of $\mathcal{H}^+$, combined with the result obtained in this paper, guarantees that the timelike, locally naked character of the singularities in the analytically extended Reissner–Nordström metric will not be important in any physically realistic situation.

## II. REVIEW OF SPHERICAL COLLAPSE RESULTS

The general gravitational collapse problem is incredibly difficult. There is no reason to assume any *a priori* symmetry for the collapsing body. Thus the metric and matter fields may depend on all four space-time coordinates. Even with today's computer power the problem appears intractable. If we assume axisymmetry (a physically reasonable assumption—stars seem likely to be almost axisymmetric, even when highly time-dependent—e.g., a supernova) the situation does not improve much. Axisymmetric collapse calculations should be within the range of today's numerical techniques, but have not yet been completed. Only when we specialize to *spherical symmetry* does the gravitational collapse problem become relatively easy. To a large extent this is because spherical collapse is not complicated by the presence of gravitational radiation.

The first detailed study of the gravitational collapse of a spherically symmetric perfect fluid was the work of May and White.[10] They found that the singularities formed were always within an event horizon (supporting the cosmic censorship hypothesis, which had not yet been formally proposed). The singularity was formed at $r = 0$, and is necessarily spacelike since it is formed inside $r = 2M(\mu)$ ($M$ defined in terms of the proper mass $\mu$, of all spherical shells interior to that value of $r$), where $g_{rr} < 0$, making $r =$ const a spacelike surface.

The collapse of charged spherical dust (pressure $= 0$) has been thoroughly studied. The collapse of charged spherical shells of dust has been treated by De La Cruz and Israel,[11] by Kuchař,[12] By Chase,[13] and by Boulware.[14] The anlaysis of De La Cruz and Israel is the most general (they match two Reissner–Nordström geometries on the shell: most other authors only consider the case of matching Minkowski space to Reissner–Nordström on the shell). Unfortunately, as Boulware points out, De La Cruz and Israel usually worked with the *square* of the equations of motion for the shell. Because of this, they fail to distinguish between positive and negative proper mass shells. Boulware points out that the negative proper mass shell can collapse to a naked singularity, violating cosmic censorship (and the weak energy condition). The collapse of charged balls of dust has been considered by Novikov[15] and Bardeen.[16]

The hydrodynamic equations for spherically symmetric charged fluid collapse were set up by Bekenstein,[17] but he did not go on to numerically integrate them.

More recently, Mashhoon and Partovi[18] have studied a class of exact solutions of Einstein's equations which represent the collapse of a charged perfect fluid ball of matter. They discovered several interesting generic features of the singularities formed in collapse. First, if a singularity is formed, it is either a spacelike or null hypersurface, never timelike. Second, any singularity which forms does so between the inner and outer event horizons ($r_- < r_{\text{singularity}} < r_+$). These conclusions could lead one to believe that no locally naked singularities are produced within the matter in spherical charged fluid collapse, but the case cannot yet be regarded as closed. The singularity in the Mashhoon–Partovi solutions is a pressure singularity ($p = +\infty$). Exactly how the singularity ($p = \infty$) approaches the surface of the collapsing ball (defined to be $p = 0$) is unclear. In the uncharged case it was clear that the surface of the collapsing matter must run into the Schwarzschild singularity at $r = 0$. Here, however, the space-time exterior to the collapsing matter must be a portion of the Reissner–Nordström space-time (by the electrovacuum generalization of Birkhoff's theorem), and thus the surface of the collapsing matter need not run into a singularity of the exterior geometry.

In the face of this uncertainty and lack of knowledge concerning the nature of the singularities formed with the matter during charged spherical collapse, it behooves us to determine which portions of the analytically extended Reissner–Nordström interior are relevant to physically realistic collapse.

## III. ON THE TOPOLOGY OF CHARGED FLUID SPHERICAL COLLAPSE

In this section I study the possible paths the surface of a spherically symmetric charged star might follow during its gravitational collapse. Within one physically reasonable assumption, I prove that the possible trajectories fall into two categories, neither of which ever exposes the left-hand curvature singularity in the Reissner–Nordström-Penrose diagram (Fig. 1). Thus, ignoring possible locally naked singularities formed within the collapsing matter, only the inner horizon labeled $\mathcal{H}^+$ in Fig. 1 is a Cauchy horizon. The other segment of the inner horizon, $\mathcal{H}^-$, is an event horizon, but not a Cauchy horizon in this case.

We consider the gravitational collapse of a spherically symmetric star with nonzero net electromagnetic charge. Since the space-time exterior to the star is spherically symmetric and its stress-energy tensor is that of a pure electromagnetic field, it must be a portion of the Reissner–Nordström solution, by the generalization of Birkhoff's theorem.

There are four conceivable Penrose diagrams of the collapse, illustrated in Fig. 2. Figure 2 (a) illustrates collapse into the left-hand Reissner–Nordström singularity. The inner event horizon $\mathcal{H}^-$ is no longer a Cauchy horizon. The dashed null line (marked $\mathscr{C}$) and the other inner event horizon ($\mathcal{H}^+$) are now the Cauchy horizons. Possibility (b) is for the star to bounce into the left-hand future exterior region. Figure 2 (c) represents collapse into the right-hand Reissner–Nordström singularity, and (d) represents a bounce into the right-hand future exterior region. Note that the paths (b) and (d) are open-ended: the star, re-expanded into an exterior region, could expand to infinity, recollapse to form another black hole, etc. In possibilities (b), (c), and (d), the Cauchy horizon is the inner event horizon $\mathcal{H}^+$.

I will now prove that no realistic star can collapse into the left-hand singularity, along path (a). The different paths which the surface of the collapsing star may follow can be characterized by the number and type of their *turning points*. A *turning point* is defined to be any point along the trajectory of the surface where a component at the four-velocity of the surface is zero ($u^\alpha = dx^\alpha/d\tau = 0$), while at the same point the corresponding coordinate acceleration is nonzero ($d^2x^\alpha/d\tau^2 \neq 0$). The second criterion excludes points of inflection from our definition, and thus insures that $x^\alpha$ (the coordinates of the world-tube defining the surface of the star) reaches a maximum or minimum value at the turning point. Path (a) contains *no* turning points. The radial component of the four-velocity, $dr/d\tau$, is negative all the way down to $r = 0$. Path (c) is distinguished from path (a) by its one turning point. In order for the surface to reach the right-hand singularity, there must be a point where $dt/d\tau = 0$ on the path (c). This is because near the right-hand singularity (for all $r < r_-$) any future directed particle will have $dt/d\tau < 0$. In contrast, any future directed particle near the left-hand singularity (for all $r < r_-$) must have $dt/d\tau > 0$. Because the Reissner–Nordström manifold is time-orientable, the $t$-turning point on path (c) must lie between $r_+$ and $r_-$, where the $t$ coordinate is spacelike.

Since the space-time is spherically symmetric, the only nonzero component of the four-velocity of the fluid are $u^t = dt/d\tau$ and $u^r = dr/d\tau$. If a typical fluid element within the star has charge $q$ and proper mass $m$, then the equations of motion for that element are

$$a^\mu = Du^\mu/D\tau = u^\mu{}_{;\nu}u^\nu = (q/m)F^\mu{}_\nu u^\nu + f^\mu/m, \tag{1}$$

where $F^\mu{}_\nu$ is the Maxwell electromagnetic field tensor, and $f^\mu$ represents all additional forces generated within the fluid (e.g., a pressure gradient).

Care must be taken in evaluating Eq. (1) at the surface of the star, as the surface is a surface of discontinuity where the interior coordinate system joins onto the static external Reissner–Nordström coordinates. Since $f^\mu$ represents forces generated within the matter, its components must be evaluated in the interior coordinate system. If we contract Eq. (1) with the normal vector to the surface of the star, $n^\mu$, we obtain

$$u^\mu{}_{;\nu}u^\nu n_\mu = (q/m)F^\mu{}_\nu u^\nu n_\mu + f^\mu n_\mu/m. \tag{2}$$

The left-hand side of Eq. (2) is simply $K_{uu}$, a component of the extrinsic curvature tensor, as may be seen by using the elementary identity

$$0 = u^\nu(n_\mu u^\mu)_{;\nu} = u^\mu u^\nu n_{\mu;\nu} + u^\nu n_\mu u^\mu{}_{;\nu} \tag{3}$$

along with the definition of the extrinsic curvature tensor (specialized to the $K_{uu}$ component)

$$K_{uu} = -u^\mu u^\nu n_{\mu;\nu}. \tag{4}$$

Since I will assume that there is no delta functional shell of matter at the surface, $K_{uu}$ will be continuous across the surface, and the left-hand side of Eq. (3) may be evaluated in either coordinate system.

The electromagnetic term in Eq. (3), $F^\mu{}_\nu u^\nu n_\mu$, represents the electric field perpendicular to the surface. Since I assume there is no delta-functional surface charge layer, the field is continuous and this term may also be evaluated in either coordinate system.

As noted previously, the vector $f^\mu$ must be evaluated in the interior coordinate system. The radial coordinate, $r$, is specified geometrically, and must agree at the surface, so $r_{\text{in}} = r_{\text{out}}$ and $dr_{\text{in}}/d\tau = dr_{\text{out}}/d\tau$. Inside the star there is no exceptionally preferred time coordinate (in the sense that the exterior Killing time coordinate is preferred), however, the interior time coordinate may be chosen such that at the surface $\langle dt, dr\rangle = 0$ and the interior and exterior coordinates match, $t_{\text{in}} = t_{\text{out}}$. We can now evaluate $f^\mu n_\mu$ by noting that

$$f^\mu u_\mu = 0 = -\frac{\Delta}{r^2}\frac{dt}{d\tau}f^t + \frac{r^2}{\Delta}\frac{dr}{d\tau}f^r, \tag{5}$$

which implies

$$f^\mu n_\mu = \frac{r^2}{\Delta}\left(\frac{dt}{d\tau}\right)^{-1} f^r, \tag{6}$$

where $\Delta = r^2 - 2Mr + Q^2$.

If we now put the Reissner–Nordström values for the connection and Maxwell tensor into Eq. (3) (as was justified above), we can reduce it to an ordinary differential equation for the radius of the surface as a function of proper time:

$$\frac{d^2r}{d\tau^2} = -\frac{M}{r^2} + \frac{Q^2}{r^3} + \frac{qQ\Delta}{mr^4}\frac{dt}{d\tau} + \frac{f^r}{m}. \tag{7}$$

Note that the most obvious force $f^\mu$, namely the pressure gradient in a perfect fluid star ($f_\mu = -p_{,\mu}$), will always be positive at the surface of the star. The star's surface is, for a perfect fluid, defined to be the radius at which $p = 0$. Since any reasonable fluid has $p > 0$ (inside the star), $n^\mu p_{,\mu} < 0$ at the surface. This implies that $f^\mu n_\mu$ will always be positive. Since $(r^2/\Delta)(dt/d\tau)^{-1}$ will always be positive, $f^r$ will always be positive in Eq. (7). The important point is that any standard pressure-gradient sort of force contained in $f^r$ will necessarily be positive as $r \to 0$.

We next note that the charge density evaluated at the surface of the collapsing star would, in any physically reasonable collapse, have the same sign as the net charge on the star ($Q$). Since the matter is in motion, $u^r \neq 0$, and also quite likely acting as a conductor to some extent, it seems likely that the electrostatic repulsion of the excess charge on the star should drive the excess charge to the surface. Even if the charge $Q$ were concentrated at the core of the star, surface particles would not have an opposite charge ($q'$; such that $q'Q < 0$), as the $q'$ charge would be electrostatically attracted toward the center during collapse, leaving the surface particles with charge $q$ such that $qQ \geqslant 0$.

Of course the validity of these simple arguments hinges crucially on the assumption of spherical symmetry. It is spherical symmetry that makes the magnetohydrodynamics trivial. There can be no magnetic fields or rotational currents within this assumption. The only electromagnetic field present is the simple $Q(r)/r^2$ Coulomb field. On this basis, we will now assume that $qQ \geqslant 0$.

Let us then suppose that the stellar surface is approaching the left-hand singularity, apparently following path (a). As $r \to 0$, Eq. (7) becomes

$$\frac{d^2r}{d\tau^2} \to \frac{Q^2}{r^3} + \frac{qQ^3}{mr^4}\frac{dt}{d\tau} + \frac{f^r}{m}. \tag{8}$$

Recall that near the left-hand singularity, $dt/d\tau$ is necessarily positive. Since we assumed $qQ \geqslant 0$, the first two terms are necessarily positive.

If we consider the motion of a charged test particle ($f^r = 0$), we see that the coordinate acceleration diverges at least as fast as $r^{-3}$ as $r \to 0$. This immediately implies that no charged test particle (with $qQ \geqslant 0$) can even reach the left-hand singularity, as it is infinitely repulsive as $r \to 0$.

Now, if $f^r$ is nonzero, it is obvious that it must, in order to collapse the star into the left-hand singularity [path (a)], be *negative* (attractive) and diverge as $r \to 0$ faster than $Q^2/r^3$. There is no known macroscopic force in nature with this behavior, so we would conclude that no physically reasonable collapse will have a Penrose diagram like Fig. 2(a). As I noted earlier, the most obvious force $f^r$, a pressure gradient, is repulsive [positive sign in Eq. (8)] rather than attractive.

Collapse to the right-hand singularity [along path (c)] *is* possible, because $dt/d\tau$ is *negative* near the singularity, and the second term in Eq. (8) can overcome the other two to make $d^2r/d\tau^2 < 0$ all the way down to $r = 0$.

The result may now be summarized:

Given a collapsing charged spherical body of matter whose exterior is described by the Reissner–Nordström metric. If:

(1) the product of the charge on a surface particle, $q$, and the total charge, $Q$, is non-negative ($qQ \geqslant 0$); and

(2) there is no additional (i.e., not electromagnetic or gravitational) attractive force within the matter which diverges at least as fast as $r^{-3}$ as $r \to 0$; then collapse to the left-hand Reissner–Nordström singularity [Fig. 2(a)] is impossible.

Thus, if no locally naked singularities are produced within collapsing charged spherical matter, then the only Cauchy horizon in the black hole interior is the future inner event horizon, $\mathcal{H}^+$, which is both classically and quantum mechanically unstable.

## ACKNOWLEDGMENT

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# Erratum: Solutions of the nonlinear 3-wave equations in three spatial dimensions [J. Math. Phys. 20, 1653 (1979)]

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p. 1654:

$y_\nu = \sum_1^4 \eta_{\nu\mu} x_\mu$ instead of $\sum_1^4 \eta_{\nu\mu}$

should read

$K_j^i(y;x_1,...,x_4) = (1 - \rho_{j\mu}^i)F_{j\mu}^i(y;x_1,...) + .....$

p. 1661: The first line of the last integral equation

# Erratum: A concept of spin 1/2 approximation in the quantum theory of lattice Bose systems [J. Math. Phys. 21, 2670 (1980)]

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The Editorial Board apologizes for the inadvertent transposition, through no fault of the author, of the contents of pp. 2673 and 2674.

  