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Approach to Gravitational Radiation Scattering*

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A method is presented for studying asymptotically flat spaces possessing both incoming and outgoing gravitational radiation at infinity. The method uses multipole expansions and the invariance of general relativity under time reversal; calculations are facilitated by a small-parameter perturbation approach. Some calculations are carried out to second order to show the practicability of the method.

1. INTRODUCTION

SIGNIFICANT progress has been made in recent years in finding and understanding, in an asymptotic approximation, asymptotically flat solutions of the empty-space Einstein field equations. However, this work has been formulated in a way that is suitable primarily for retarded gravitational radiation fields. It is the purpose of this paper to present a method, based on the use of multipole expansions but with a small-parameter perturbation approximation instead of an asymptotic approximation, for treating problems involving both retarded and advanced asymptotic gravitational radiation. We hope the method will facilitate the handling of problems concerning the scattering of gravitational radiation.

The essential first step in the recent progress was taken by Bondi and his co-workers.[1] They expanded the metric in inverse powers of a coordinate r, a luminosity parameter along the null geodesics pointing into the future of the localized source. They substituted their expansion into the empty-space Einstein equations and obtained differential equations for the coefficients in the expansion. They worked out the initial data for their set of equations and found that the principal piece of initial data was an arbitrary function of a timelike coordinate, called the "news function" by Bondi, which described the information radiated to infinity. Bondi's assumption of axial symmetry was dropped by Sachs,[2] and the emphasis was shifted from expanding the metric tensor to expanding the Weyl tensor by Newman and Penrose[3] (which we refer to as NP); the latter also introduced the tetrad formalism used in this paper. In NP it was shown that the assumptions needed to ensure asymptotic flatness of the space could be weakened somewhat from those of Bondi's work.

In a subsequent paper[4] (which we refer to as NU) Newman and Unti analyzed the field equations and solved the initial-value problem in the NP formalism. Their coordinates were built, as were Bondi's, around

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[1] H. Bondi, M. Van der Burg, and A. Metzner, Proc. Roy. Soc. (London) **A269**, 21 (1962).

[2] R. Sachs, Proc. Roy. Soc. (London) **A264**, 309 (1961).

[3] E. Newman and R. Penrose, J. Math. Phys. **3**, 566 (1962).

[4] E. Newman and T. Unti, J. Math. Phys. **3**, 891 (1962).

the families of null hypersurfaces known to exist in any normal hyperbolic Riemannian space. The label u of these hypersurfaces was introduced as a timelike coordinate, and the expansion coordinate r was defined as an affine parameter along the null geodesics lying in these hypersurfaces. Since their data were being given on characteristic hypersurfaces of the space, they were able to give them free of constraints.[5] The initial data consisted essentially of two parts:

(1) an arbitrary function of u (i.e., time) analogous to Bondi's news function, and

(2) a specification of part of the Weyl tensor on a particular null hypersurface labeled by $u = u_0$.

If the null hypersurfaces are taken to be the future null cones, the first piece of data specifies the retarded radiation (asymptotically). The second piece of data gives everything else. In past work it has been interpreted as giving nonradiative information about the space, while we see that it also contains a specification of the advanced radiation.

The formalism and results of NP and NU are outlined in Sec. 2 in sufficient detail for the work that follows. In addition to isolating the initial data NU also derived asymptotic solutions to the field equations on an arbitrary null hypersurface and nonlinear differential equations for the development of the system off the initial hypersurface.

A common method of dealing with the nonlinear calculations of general relativity is to assume the quantities of interest (the Riemann tensor or, equivalently, the departure of the metric tensor from flatness) to be small. One then neglects all second-order products and gets a set of linear differential equations—a linearization of the Einstein field equations. After solving the linearized equations one can go on and attempt to find the second-order corrections to the linear solutions, etc., and discover the nonlinear effects of the theory. This perturbation method has been started on the nonlinear time development equations derived in NU in a paper[6] (which we refer to as JN) by Janis and Newman. They have linearized and found solutions of these equations in the axially symmetric case. In Sec. 3 equations are derived for finding the second-order corrections to any solution of the linearized equations.

The linearized solutions presented in JN were all retarded solutions. Of course, it is a trivial matter to do a time reversal so that we have advanced solutions instead; however, the null hypersurfaces also change from future null cones to past null cones. Thus we end up working in different coordinates as well as with a different solution. In doing a scattering problem we want to be able to express both kinds of radiation in terms of one set of coordinates. In Sec. 4 equations are derived, within the context of the perturbation theory, that enable us to re-express, to second order, given solutions on the "other" cone. This method would enable us to take, for example, the linear advanced solutions in terms of past null cone coordinates, obtained from the retarded JN solutions by a time reversal, and rewrite them in terms of coordinates based on the future cones.

In Sec. 5 the linear theory is investigated in detail. We approach the solution of the linearized equations somewhat differently than did JN. We find it convenient to solve first for the advanced radiation solutions on the future light cones, and then by a time reversal and the transformations of Sec. 4, rederive the retarded solutions of JN. Along with the new advanced solutions we also obtain a simplified form of the JN retarded solutions.

A method of approaching nonlinear scattering calculations is contained in Secs. 3, 4, and 5, in that we have a general method of giving linearized solutions including both retarded and advanced gravitational radiation, and of calculating second-order corrections to those solutions. In Sec. 6 initial data for a particular problem (an imploding–exploding quadrupole wave with a mass at its focus) are given, and incomplete calculations are carried out to second order. In Sec. 7 it is argued that complete second-order corrections could be obtained by lengthy but straightforward manipulations. In addition it is pointed out that even our incomplete results not only include some previously known effects, but suggest some new, physically reasonable characteristics of gravitational radiation.

2. REVIEW OF NEWMAN-PENROSE AND NEWMAN-UNTI

The starting point for the calculations in this paper is a set of nonlinear differential equations, derived in NP and NU, equivalent to the empty-space Einstein equations with certain coordinate conditions imposed. The tetrad l^μ, n^μ, m^μ, and $\bar{m}^\mu$ was introduced, where m^μ is complex and $\bar{m}^\mu$ is the complex conjugate of m^μ. The tetrad is normalized such that $l^\mu n_\mu = -m^\mu \bar{m}_\mu = 1$, and $l^\mu l_\mu = n^\mu n_\mu = m^\mu m_\mu = l^\mu m_\mu = n^\mu m_\mu = 0$, which implies that

$$g^{\mu\nu} = l^\mu n^\nu + l^\nu n^\mu - m^\mu \bar{m}^\nu - m^\nu \bar{m}^\mu. \qquad (2.1)$$

A set of quantities called spin coefficients, closely related to the Ricci rotation coefficients of the tetrad,

[5] R. Penrose, Aeronautical Research Laboratories ARL 63–56 (1963).

[6] A. Janis and E. Newman, J. Math. Phys. 6, 902 (1965).

was then defined as follows[7]:

$$\begin{aligned}
&\kappa = l_{\mu;\nu}m^\mu l^\nu, \quad \pi = -n_{\mu;\nu}\bar{m}^\mu l^\nu,\\
&\epsilon = \tfrac{1}{2}(l_{\mu;\nu}n^\mu l^\nu - m_{\mu;\nu}\bar{m}^\mu l^\nu), \quad \rho = l_{\mu;\nu}m^\mu \bar{m}^\nu,\\
&\lambda = -n_{\mu;\nu}\bar{m}^\mu \bar{m}^\nu, \quad \alpha = \tfrac{1}{2}(l_{\mu;\nu}n^\mu \bar{m}^\nu - m_{\mu;\nu}\bar{m}^\mu \bar{m}^\nu),\\
&\sigma = l_{\mu;\nu}m^\mu m^\nu, \quad \mu = -n_{\mu;\nu}\bar{m}^\mu m^\nu,\\
&\beta = \tfrac{1}{2}(l_{\mu;\nu}n^\mu m^\nu - m_{\mu;\nu}\bar{m}^\mu m^\nu), \quad \nu = -n_{\mu;\nu}\bar{m}^\mu n^\nu,\\
&\gamma = \tfrac{1}{2}(l_{\mu;\nu}n^\mu n^\nu - m_{\mu;\nu}\bar{m}^\mu n^\nu), \quad \tau = l_{\mu;\nu}m^\mu n^\nu.
\end{aligned} \tag{2.2}$$

Using the tetrad one can define physical components of the Weyl tensor (they are called, collectively, ψ_A) by

$$\begin{aligned}
\psi_0 &= -C_{\alpha\beta\gamma\delta}l^\alpha m^\beta l^\gamma m^\delta,\\
\psi_1 &= -C_{\alpha\beta\gamma\delta}l^\alpha n^\beta l^\gamma m^\delta,\\
\psi_2 &= -C_{\alpha\beta\gamma\delta}\bar{m}^\alpha n^\beta l^\gamma m^\delta,\\
\psi_3 &= -C_{\alpha\beta\gamma\delta}\bar{m}^\alpha n^\beta l^\gamma n^\delta,\\
\psi_4 &= -C_{\alpha\beta\gamma\delta}\bar{m}^\alpha n^\beta \bar{m}^\gamma n^\delta.
\end{aligned} \tag{2.3}$$

Without restricting the space one can make several simplifying tetrad and coordinate assumptions. Since there always exists a family of null hypersurfaces, $u(x^\mu) = u_0$ (a constant), in any normal hyperbolic Riemannian space, they could choose $l_\mu = u_{,\mu}$ making l^μ tangent to a congruence of null geodesics. It can be shown[8] that if one chooses $x^0 = u$ and $x^1 = r$, where r is an affine parameter along the null geodesics lying in these null hypersurfaces, then $l^\mu = \delta^\mu_1$ and $l_\mu = \delta^0_\mu$, with x^i labeling the geodesics on each hypersurface. Having l^μ equal to a gradient and tangent to a null geodesic, with r an affine parameter, makes[3] $\kappa = \epsilon + \bar{\epsilon} = 0$, $\rho = \bar{\rho}$, and $\tau = \bar{\alpha} + \beta$, and by parallelly propagating the rest of the tetrad along l^μ they also obtained $\pi = \epsilon - \bar{\epsilon} = 0$. To preserve $l^\mu n_\mu = 1$ and $l^\mu m_\mu = 0$ in the light of $l^\mu = \delta^\mu_1$ and $l_\mu = \delta^0_\mu$, the most general forms m^μ and n^μ can take are

$$n^\mu = \delta^\mu_0 + U\delta^\mu_1 + X^i\delta^\mu_i$$

and $m^\mu = \omega\delta^\mu_1 + \xi^i\delta^\mu_i$, which leads to

$$\begin{aligned}
&g^{00} = g^{0i} = 0, \quad g^{01} = 1, \quad g^{11} = 2(U - \omega\bar{\omega}),\\
&g^{1i} = X^i - (\xi^i\bar{\omega} + \bar{\xi}^i\omega), \quad g^{ij} = -(\xi^i\bar{\xi}^j + \bar{\xi}^i\xi^j).
\end{aligned} \tag{2.4}$$

That subset of the NP form of the Einstein field equations essential for our work is given below, with the simplifying coordinate and tetrad assumptions included. Noting that the differential operators are

$$D \equiv l^\mu\partial/\partial x^\mu = \partial/\partial r,$$

$$\Delta \equiv n^\mu\partial/\partial x^\mu = U\partial/\partial r + \partial/\partial u + X^i\partial/\partial x^i,$$

and

$$\delta \equiv m^\mu\partial/\partial x^\mu = \omega\partial/\partial r + \xi^i\partial/\partial x^i,$$

we call an equation "radial" or "nonradial" depending on whether or not it contains a D derivative. We also call those equations which do not arise from the Bianchi identities "field equations" and group the entire set in the following way. The radial field equations are

$$\begin{aligned}
D\xi^i &= \rho\xi^i + \sigma\bar{\xi}^i,\\
D\omega &= \rho\omega + \sigma\bar{\omega} - (\bar{\alpha} + \beta),\\
DX^i &= \tau\bar{\xi}^i + \bar{\tau}\xi^i,\\
DU &= \tau\bar{\omega} + \bar{\tau}\omega - (\gamma + \bar{\gamma}),\\
D\rho &= \rho^2 + \sigma\bar{\sigma},\\
D\sigma &= 2\rho\sigma + \psi_0,\\
D\tau &= \tau\rho + \bar{\tau}\sigma + \psi_1,\\
D\alpha &= \alpha\rho + \beta\bar{\sigma},\\
D\beta &= \beta\rho + \alpha\sigma + \psi_1,\\
D\gamma &= \tau\alpha + \bar{\tau}\beta + \psi_2,\\
D\lambda &= \lambda\rho + \mu\bar{\sigma},\\
D\mu &= \mu\rho + \lambda\sigma + \psi_2,\\
D\nu &= \tau\lambda + \bar{\tau}\mu + \psi_3.
\end{aligned} \tag{2.5}$$

The radial and nonradial Bianchi identities are

$$\begin{aligned}
&D\psi_1 - \bar{\delta}\psi_0 = 4\rho\psi_1 - 4\alpha\psi_0,\\
&D\psi_2 - \bar{\delta}\psi_1 = 3\rho\psi_2 - 2\alpha\psi_1 - \lambda\psi_0,\\
&D\psi_3 - \bar{\delta}\psi_2 = 2\rho\psi_3 - 2\lambda\psi_1,\\
&D\psi_4 - \bar{\delta}\psi_3 = \rho\psi_4 + 2\alpha\psi_3 - 3\lambda\psi_2,\\
&\Delta\psi_0 - \delta\psi_1 = (4\gamma - \mu)\psi_0 - (4\tau + 2\beta)\psi_1 + 3\sigma\psi_2,\\
&\Delta\psi_1 - \delta\psi_2 = \nu\psi_0 + (2\gamma - 2\mu)\psi_1 - 3\tau\psi_2 + 2\sigma\psi_3,\\
&\Delta\psi_2 - \delta\psi_3 = 2\nu\psi_1 - 3\mu\psi_2 + (-2\tau + 2\beta)\psi_3 + \sigma\psi_4,\\
&\Delta\psi_3 - \delta\psi_4 = 3\nu\psi_2 - (2\gamma + 4\mu)\psi_3 + (-\tau + 4\beta)\psi_4.
\end{aligned} \tag{2.6}$$

There is also a set of 13 nonradial field equations which we do not use directly. The complete set is given in both NP and NU.

The initial data for this set of equations were worked out in NU. They first assumed that $\psi_0(r, u_0, x^i)$ was given; i.e., they assumed they knew ψ_0 on a particular hypersurface $u = u_0$. In NP the assumption $\psi_0 = O(1/r^5)$ was made. In NU the stronger assumption $\psi_0 = \psi_0^\circ(u_0, x^i)/r^5 + O(1/r^6)$ was made in order to specify ψ_0 more explicitly.[9] In integrating the radial equations (including the radial Bianchi identities) the "constants" of integration [there is one for each radial

[7] Greek (values 0, 1, 2, 3) and small Latin (values 2, 3) indices are tensor indices, while capital Latin indices (values 0, 1, 2, 3, 4) number the physical components of the Weyl tensor. Ordinary differentiation is denoted by a comma or by $\partial/\partial x$, while covariant differentiation is indicated by a semicolon. The metric has signature $(1, -1, -1, -1)$.

[8] I. Robinson and A. Trautman, Phys. Rev. Letters 4, 431 (1960).

[9] The precise meaning of the order symbol may be found, for example, in Ref. 3.

equation, and that for the ρ equation is designated as $\rho^\circ(u, x^i)$, that for the ψ_1 equation as $\psi_1^\circ(u, x^i)$, etc.] introduced arbitrariness into the solutions. This arbitrariness included the freedom of specifying additional initial data. Substitution of the radial solutions into the nonradial equations put differential conditions on these arbitrary functions. Between these conditions and further specialization of the coordinates and tetrad vectors[4] the other constants of integration were expressed in terms of $\sigma^\circ(u, x^i)$, $\psi_2^\circ(u_0, x^i) + \bar{\psi}_2^\circ(u_0, x^i)$ and $\psi_1^\circ(u_0, x^i)$, leaving these functions, along with $\psi_0(r, u_0, x^i)$, as the initial data. One other free function, $P(x^i)$, remained but its choice represented further fixing of the coordinates x^i once the topology was known (asymptotically).

We assume the topology to be asymptotically Euclidean. Then the function $P(x^i)$ can be fixed in the following fashion. Choose $P(x^i)$ in NU to be $P(x^i) = \cosh v/\sqrt{2}$, where $x^2 = v$ and $x^3 = \phi$. Then do the coordinate transformation $\cos\theta = \tanh v$. This will put the flat-space specialization of our solutions in null spherical polar coordinates.

The function $\sigma(u, x^i)$ specifies the outgoing radiation at infinity and, through the nonradial Bianchi identities, determines the time development of the solution off the initial hypersurface $u = u_0$. It turns out that asymptotic incoming radiation, which was not considered in NU, is given by $\psi_0(r, u_0, x^i)$, which along with $\psi_1^\circ(u_0, x^i)$ and $\psi_2^\circ(u_0, x^i) + \bar{\psi}_2^\circ(u_0, x^i)$ also gives the necessary nonradiative initial data of the space.

We give the constants of integration in terms of the initial data. These results from NU are needed later:

$$\begin{aligned}
&\gamma^\circ = \rho^\circ = \nu^\circ = X^{i\circ} = \tau^\circ = 0,\\
&U^\circ = \mu^\circ = -1/2,\\
&\alpha^\circ = -\beta^\circ = -\cot\theta/2\sqrt{2},\\
&\xi^2 = -i\sin\theta\xi^3 = 1/\sqrt{2},\\
&\lambda^\circ = \bar{\sigma}^\circ_{,0},\\
&\omega^\circ = (\sigma^\circ_{,2} + 2\cot\theta\sigma^\circ)/\sqrt{2},\\
&\psi_2^\circ - \bar{\psi}_2^\circ = (\sigma^\circ - \bar{\sigma}^\circ)_{,22}/2 + 3\cot\theta(\sigma^\circ - \bar{\sigma}^\circ)_{,2}/2\\
&\qquad\qquad - (\sigma^\circ - \bar{\sigma}^\circ) + \bar{\sigma}^\circ\sigma^\circ_{,0} - \sigma^\circ\bar{\sigma}^\circ_{,0},\\
&\psi_3^\circ = -\bar{\sigma}^\circ_{,20}/\sqrt{2} - \sqrt{2}\cot\theta\bar{\sigma}^\circ_{,0},\\
&\psi_4^\circ = -\bar{\sigma}^\circ_{,00}.
\end{aligned} \tag{2.7}$$

The initial values of ψ_0, ψ_1°, and $\psi_2^\circ + \bar{\psi}_2^\circ$ are initial data and their subsequent values are derived through Eqs. (2.6).

3. SMALL-PARAMETER PERTURBATION METHOD

Our perturbation calculation begins with the flat-space solution of the field equations. To obtain flat space in our formalism one sets[10] $\sigma^\circ(u, \theta)$, $\psi_0(r, u_0, \theta)$, $\psi_1^\circ(u_0, \theta)$, and $\psi_2^\circ(u_0, \theta)$ equal to zero. Since we are interested in solutions with asymptotically Euclidean topology, we make the choice of $P(x^i)$ indicated in Sec. 2. We can then extract the metric, the components of the tetrad vectors, and the spin coefficients for flat space from the asymptotic solutions of NU. They take the following forms:

$$g^{\mu\nu} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1/r^2 & 0 \\ 0 & 0 & 0 & -\csc^2\theta/r^2 \end{pmatrix}, \tag{3.1}$$

$$U = -1/2, \quad \omega = 0, \quad X^i = 0, \quad \xi^i = \begin{pmatrix} 1 \\ i\csc\theta \end{pmatrix} 1/\sqrt{2}\,r, \tag{3.2}$$

and

$$\begin{aligned}
&\rho = -1/r, \quad \alpha = -\beta = -\cot\theta/2\sqrt{2}r,\\
&\mu = -1/2r, \quad \sigma = \nu = \gamma = \lambda = \tau = 0.
\end{aligned} \tag{3.3}$$

The meaning of the coordinates is clear in the flat-space case. The future null cones are labeled by $x^0 = u$. Varying r, numerically equal to $(x^2 + y^2 + z^2)^{\frac{1}{2}}$, and holding the other variables constant defines a straight line lying in a future null cone. Finally one sets u and r equal to constants and coordinatizes the resulting spherical surfaces with spherical polar coordinates θ and ϕ. Flat space in these coordinates is the exact solution to which we seek perturbative corrections.

Consider Eqs. (2.5) and (2.6). [The nonradial field equations have served their purpose in providing us with Eqs. (2.7).] These two sets lend themselves to a perturbation approach. If we assume the ψ_A to be zero, then the set (2.6) is empty, and Eqs. (2.5) can be solved for flat space yielding Eqs. (3.1) through (3.3). If one then thinks of the ψ_A as a field existing in flat space, the Bianchi identities, with the flat space spin coefficients and tetrad components substituted in them, can be looked upon as field equations for that field. Having solved this linearized version of Eqs. (2.6) for particular "first-order" ψ_A, we can then use a linearized form of Eqs. (2.5) to find the corrected spin coefficients and tetrad variables (i.e., metric). At this point the ψ_A display their geometrical significance. We then use the first-order spin coefficients and tetrad vectors in Eqs. (2.6) to obtain the second-order part of these equations. These can then be solved for the second-order ψ_A. This process could, in principle, be iterated.

[10] The ψ_A must vanish in flat space since the Weyl tensor does. One could, however, obtain a nonvanishing news function in flat space by a different choice of coordinates (see Appendix 3 of Ref. 1).

We now derive equations for the first three steps in the perturbation scheme described above. The following notation is introduced: Each quantity is considered to be expandable in a small parameter, e.g., $\rho = \underset{0}{\rho} + \underset{1}{\rho} + \cdots$, where the subscript zero means the flat-space value. (These order indicators are omitted when the context indicates the order of the quantity involved.) Thus the $\underset{0}{\psi_A} = 0$ while the other zero-order quantities are given by Eqs. (3.1)–(3.3). Substituting these expressions into Eqs. (2.6) and collecting first-order terms, we get the following differential equations for the $\underset{1}{\psi_A}$:

$$\begin{aligned}
\partial\psi_1/\partial r + 4\psi_1/r &= -\bar{\eth}\psi_0/\sqrt{2}\,r,\\
\partial\psi_2/\partial r + 3\psi_2/r &= -\bar{\eth}\psi_1/\sqrt{2}\,r,\\
\partial\psi_3/\partial r + 2\psi_3/r &= -\bar{\eth}\psi_2/\sqrt{2}\,r,\\
\partial\psi_4/\partial r + \psi_4/r &= -\bar{\eth}\psi_3/\sqrt{2}\,r,
\end{aligned} \tag{3.4}$$

and

$$\begin{aligned}
(2\partial/\partial u - \partial/\partial r)\psi_0/2 - \psi_0/2r &= -\eth\psi_1/\sqrt{2}\,r,\\
(2\partial/\partial u - \partial/\partial r)\psi_1/2 - \psi_1/r &= -\eth\psi_2/\sqrt{2}\,r,\\
(2\partial/\partial u - \partial/\partial r)\psi_2/2 - 3\psi_2/2r &= -\eth\psi_3/\sqrt{2}\,r,\\
(2\partial/\partial u - \partial/\partial r)\psi_3/2 - 2\psi_3/r &= -\eth\psi_4/\sqrt{2}\,r.
\end{aligned} \tag{3.5}$$

The angular operator $\eth$ ("thop") is defined in the Appendix. If Eqs. (3.4) are integrated and the corresponding (first-order) constants of integration introduced, we get

$$\begin{aligned}
\psi_1 - \psi_1^\circ/r^4 + (1/\sqrt{2}\,r^4)\bar{\eth}\textstyle\int r^3\psi_0\,dr &= 0,\\
\psi_2 - \psi_2^\circ/r^3 + (1/\sqrt{2}\,r^3)\bar{\eth}\textstyle\int r^2\psi_1\,dr &= 0,\\
\psi_3 - \psi_3^\circ/r^2 + (1/\sqrt{2}\,r^2)\bar{\eth}\textstyle\int r\psi_2\,dr &= 0,\\
\psi_4 - \psi_4^\circ/r + (1/\sqrt{2}\,r)\bar{\eth}\textstyle\int \psi_3\,dr &= 0,
\end{aligned} \tag{3.6}$$

which can be substituted into Eqs. (3.5) to give

$$\begin{aligned}
(2\partial/\partial\mu - \partial/\partial r)\psi_0/2 - \psi_0/2r + \eth\psi_1^\circ/\sqrt{2}\,r^5 \\
- (1/2r^5)\eth\bar{\eth}\textstyle\int\psi_0 r^3\,dr = 0,\\
(2\partial/\partial\mu - \partial/\partial r)\psi_1/2 - \psi_1/r + \eth\psi_2^\circ/\sqrt{2}\,r^4 \\
- (1/2r^4)\eth\bar{\eth}\textstyle\int\psi_1 r^2\,dr = 0,\\
(2\partial/\partial\mu - \partial/\partial r)\psi_2/2 - 3\psi_2/2r + \eth\psi_3^\circ/\sqrt{2}\,r^3 \\
- (1/2r^3)\eth\bar{\eth}\textstyle\int\psi_2 r\,dr = 0,\\
(2\partial/\partial\mu - \partial/\partial r)\psi_3/2 - 2\psi_3/r + \eth\psi_4^\circ/\sqrt{2}\,r^2 \\
- (1/2r^2)\eth\bar{\eth}\textstyle\int\psi_3\,dr = 0.
\end{aligned} \tag{3.7}$$

That set of solutions to essentially these integro-differential equations given in JN corresponds to a particular choice of the first-order constants of integration ψ_1°, ψ_2°, ψ_3°, ψ_4°. In Sec. 5, we find a broad class of solutions including those of JN.

Assuming we now know the first-order ψ_A we can calculate the other quantities to first order. Equations (2.5) can be linearized to give

$$\begin{aligned}
\underset{1}{\rho} &= 0,\\
\underset{1}{\sigma} &= \frac{\sigma^\circ}{r^2} + \frac{1}{r^2}\int r^2\psi_0\,dr,\\
\underset{1}{\alpha} &= \frac{\cot\theta}{2\sqrt{2}\,r}\int\bar{\sigma}\,dr,\\
\underset{1}{\beta} &= -\bar{\alpha} + \frac{1}{r}\int r\psi_1\,dr,\\
\underset{1}{\tau} &= \bar{\alpha} + \beta,\\
\underset{1}{\gamma} &= \frac{\cot\theta}{2\sqrt{2}}\int\frac{\bar{\tau}-\tau}{r}\,dr + \int\psi_2\,dr,\\
\underset{1}{\mu} &= \frac{1}{r}\int r\psi_2\,dr,\\
\underset{1}{\lambda} &= -\frac{1}{2r}\int\bar{\sigma}\,dr + \frac{1}{r}\bar{\sigma}^\circ_{,0},
\end{aligned} \tag{3.8}$$

$$\begin{aligned}
\underset{1}{\nu} &= -\int\frac{\bar{\tau}}{2r}\,dr + \int\psi_3\,dr,\\
\underset{1}{U} &= -\int(\gamma + \bar{\gamma})\,dr,\\
\underset{1}{\omega} &= -\frac{1}{r}\int r\bar{\tau}\,dr + \frac{\csc^2\theta}{\sqrt{2}\,r}(\sin^2\theta\sigma^\circ)_{,2},\\
\underset{1}{X^i} &= \left(\frac{1}{\sqrt{2}}\right)\begin{pmatrix}1\\ -i\csc\theta\end{pmatrix}\int\frac{\tau}{r}\,dr \\
&\qquad + \left(\frac{1}{\sqrt{2}}\right)\begin{pmatrix}1\\ i\csc\theta\end{pmatrix}\int\frac{\bar{\tau}}{r}\,dr,\\
\underset{1}{\xi^i} &= \left(\frac{1}{\sqrt{2}\,r}\right)\begin{pmatrix}1\\ -i\csc\theta\end{pmatrix}\int\sigma\,dr.
\end{aligned}$$

This completes the derivation of the equations necessary to find a full, first-order solution.

If we now go back to the Bianchi identities and collect all the second-order terms, we find that we obtain, for $\underset{2}{\psi_A}$, differential equations like Eqs. (3.4), (3.5), and (3.6), but with driving terms constructed from the first-order solutions. If the same integrations and substitutions are done as before, the resulting equations for the $\underset{2}{\psi_A}$ are identical to Eqs. (3.6) and (3.7) except that the right-hand sides are now R_1, R_2,

R_3, and R_4, and D_0, D_1, D_2, and D_3, respectively, where

$$\begin{aligned}
R_{1\,2} &= (1/r^4)\int r^4\Big(\bar{\omega}\partial/\partial r + \bar{\xi}^i\partial/\partial x^i - 4\alpha_1\Big)\psi_{0\,1}\,dr,\\
R_{2\,2} &= (1/r^3)\int\Big[r^3\Big(\bar{\omega}\partial/\partial r + \bar{\xi}^i\partial/\partial x^i - 2\alpha_1\Big)\psi_{1\,1}\\
&\qquad - r^3\lambda_{11}\psi_0\Big]dr,\\
R_{3\,2} &= (1/r^2)\int\Big[r^2\Big(\bar{\omega}\partial/\partial r + \bar{\xi}^i\partial/\partial x^i\Big)\psi_{2\,1} \qquad (3.9)\\
&\qquad - 2r^2\lambda_{11}\psi_2\Big]\,dr,\\
R_{4\,2} &= (1/r)\int\Big[r\Big(\bar{\omega}\partial/\partial r + \bar{\xi}^i\partial/\partial x^i + 2\alpha_1\Big)\psi_{3\,1}\\
&\qquad - 3r\lambda_{11}\psi_2\Big]\,dr,
\end{aligned}$$

$$\begin{aligned}
D_{0\,2} &= \Big(-U\partial/\partial r - X^i\partial/\partial x^i + 4\gamma_1 - \mu_1\Big)\psi_{0\,1}\\
&\quad + \Big(\xi^i\partial/\partial x^i + \omega\partial/\partial r - 4\tau_1 - 2\beta_1\Big)\psi_{1\,1}\\
&\quad + 3\sigma_{11}\psi_2 + (1/\sqrt{2}\,r)\eth R_{1\,2}, \qquad (3.10)
\end{aligned}$$

etc.

(We do not need D_1, D_2, or D_3.) We call Eqs. (3.6) and (3.7) the "undriven equations," and their driven form the "driven equations." Solutions of the driven equations can be varied by adding to them any linear combination of solutions of the undriven equations. There are, of course, driven forms of Eqs. (3.8) as well; however, we do not need them here.

4. TRANSFORMATIONS BETWEEN THE NULL CONES

The coordinate and tetrad systems introduced in NP and NU were built around the null hypersurfaces always present in a normal hyperbolic Riemannian space. These hypersurfaces were assumed to be defined by $u(x^\mu) = u_0$, and $x^0 = u$ introduced a timelike coordinate labeling the hypersurfaces. There is, however, an ambiguity in that the coordinate u could label either the future or the past null cones. Let us take it to label the future cones. Then there must exist a coordinate transformation preserving all the coordinate conditions, but re-expressing everything in terms of coordinates built around the past null cones. There must also exist a tetrad transformation, preserving Eq. (2.1), but giving us a new tetrad bearing the same relationship to the past null cones as the old one did to the future null cones. These transformations can, of course, also be interpreted as taking us from the past null cones to the future null cones. We realize that the new u will increase into the past if the original u increased into the future. The relationship between the direction of increasing u and the direction in which the null cones open is built into the coordinate conditions. In this section we present a method of finding these transformations for approximate solutions found by the perturbation method outlined in the last section.

The starting point is to find the transformation re-expressing flat space on the "other" cone. Working with the flat-space metric given by Eq. (3.1), we see that if u labels the future null cones, then $u' = -u - 2r$ labels the past null cones. The full coordinate transformation is

$$\begin{aligned}
u' &= -u - 2r,\\
r' &= r,\\
\theta' &= \theta,\\
\phi' &= \phi.
\end{aligned} \qquad (4.1)$$

(This transformation is also an isometry for this metric, but this is not true in general.) We also wish to preserve the form of the relations $l^\mu = \delta^\mu_1$, $n^\mu = \delta^\mu_0 + U\delta^\mu_1 + X^i\delta^\mu_i$ and $m^\mu = \omega\delta^\mu_1 + \xi^i\delta^\mu_i$, and find it necessary to take

$$\begin{aligned}
\underset{0}{\tilde{l}}^{\mu'} &= -2\underset{0}{n}^{\mu'},\\
\underset{0}{\tilde{n}}^{\mu'} &= -(\tfrac{1}{2})\underset{0}{l}^{\mu'},\\
\underset{0}{\tilde{m}}^{\mu'} &= \underset{0}{m}^{\mu'}.
\end{aligned} \qquad (4.2)$$

The components of the new tetrad vectors in the primed coordinates (ω', etc.) can be determined by examining Eqs. (4.2) (the components are unchanged to this order), and the new spin coefficients can be found by working out the spin coefficient transformations induced by Eqs. (4.2). For example,

$$\underset{0}{\tilde{\rho}} \equiv \underset{0\ 0\ 0}{\tilde{l}_{\mu;\nu}}\tilde{m}^\mu\bar{\tilde{m}}^\nu = -2\underset{0\ 0\ 0}{n_{\mu;\nu}}m^\mu\bar{m}^\mu \equiv 2\underset{0}{\bar{\mu}} = -1/r = -1/r'.$$

Likewise all the other spin coefficients are unchanged. The remaining variables, the ψ_A, are zero and remain so since the space is flat. ^{0}

Suppose we have a solution ψ_A of the linearized Bianchi identities. It is important to note that these ψ_A can be transformed knowing only the zero-order coordinate and tetrad transformations derived above. As an example, we have

$$\underset{1}{\tilde{\psi}_0} = -\underset{1\ 0\ 0\ 0\ 0}{C_{\alpha\beta\gamma\delta}\tilde{l}^\alpha\tilde{m}^\beta\tilde{l}^\gamma\tilde{m}^\delta} = -4\underset{1\ 0\ 0\ 0\ 0}{C_{\alpha\beta\gamma\delta}n^\alpha m^\beta n^\gamma m^\delta} \equiv 4\underset{1}{\bar{\psi}_4},$$

where the first-order corrections to Eqs. (4.1) and (4.2) lead to (negligible) second-order corrections here.

Thus we can derive the full set of transformed ψ_A:

$$\begin{aligned}
\tilde{\psi}_0 &= 4\bar{\psi}_4, \\
\tilde{\psi}_1 &= -2\bar{\psi}_3, \\
\tilde{\psi}_2 &= \bar{\psi}_2, \\
\tilde{\psi}_3 &= -\tfrac{1}{2}\bar{\psi}_1, \\
\tilde{\psi}_4 &= \tfrac{1}{4}\bar{\psi}_0,
\end{aligned} \tag{4.3}$$

where the ψ_A can be expressed in terms of the primed variables by taking the inverses of Eqs. (4.1).

Now that we know the ψ_A in the primed coordinates, we can go on and calculate the corresponding first-order spin coefficients and components of the tetrad vectors via Eqs. (3.8). Since we have preserved every coordinate and tetrad condition used in deriving Eqs. (3.8), they take the same form in the new language as they did in the old. Thus we can find all the variables to first order in terms of either coordinate and tetrad frame.

We can now find the coordinate and tetrad transformations to first order for a given solution, since we know that solution to first order in both the old and the new frames. We know that the coordinate transformation must be the flat-space transformation plus a first-order correction, so we write

$$\begin{aligned}
u' &= -u - 2r + \epsilon^0, \\
r' &= r + \epsilon^1, \\
\theta' &= \theta + \epsilon^2, \\
\phi' &= \phi + \epsilon^3,
\end{aligned} \tag{4.4}$$

where we now assume axial symmetry for simplicity, which implies that $\epsilon^\mu_{,3} = 0$.

We begin by demanding that

$$g^{00'} = (\partial\mu'/\partial x^\alpha)(\partial\mu'/\partial x^\beta)\, g^{\alpha\beta} = 0,$$

$g^{01'} = 1$, and $g^{0i'} = 0$. From these we get, to first order,

$$\begin{aligned}
\epsilon^0_{,0} &= \underset{1}{g}^{11} + \tfrac{1}{2}\epsilon^0_{,1}, \\
\epsilon^1_{,0} &= \frac{1}{2}\left(-\underset{1}{g}^{11} + \epsilon^1_{,1} - \tfrac{1}{2}\epsilon^0_{,1}\right), \\
\epsilon^2_{,0} &= -\underset{1}{g}^{12} + \tfrac{1}{2}(\epsilon^2_{,1} - r^{-2}\epsilon^0_{,2}), \\
\epsilon^3_{,0} &= -\underset{1}{g}^{13} + \tfrac{1}{2}\epsilon^3_{,1}.
\end{aligned} \tag{4.5}$$

From

$$g^{11'} = (\partial r'/\partial x^\alpha)(\partial r'/\partial x^\beta) g^{\alpha\beta}$$

and

$$g^{12'} = (\partial r'/\partial x^\alpha)(\partial x^{i'}/\partial x^\beta) g^{\alpha\beta}$$

combined with Eqs. (4.5) we get, to first order,

$$\begin{aligned}
\epsilon^1 + \tfrac{1}{2}\epsilon^0 &= -\int \underset{1}{g}^{11'}\, dr + C_1(u, \theta), \\
\epsilon^2 &= -2\int \underset{1}{g}^{12'}\, dr + 2\int\left[r^{-2}\left(\int \underset{1}{g}^{11'}\, dr\right)_{,2}\right] dr \\
&\quad + 2r^{-1}C_1(u, \theta)_{,2} + C_2(u, \theta), \\
\epsilon^3 &= -2\int \underset{1}{g}^{13'}\, dr + C_3(u, \theta).
\end{aligned} \tag{4.6}$$

From

$$g^{22'} = (\partial\theta'/\partial x^\alpha)(\partial\theta'/\partial x^\beta) g^{\alpha\beta},$$

we get

$$\begin{aligned}
\epsilon^1 = -r\epsilon^2_{,2} + \tfrac{1}{2}r^3[(g^{22} + 1/r^2) - (g^{22'} + 1/r'^2)] \\
- 2C_1(u, \theta)_{,22} - rC_2(u, \theta)_{,2}.
\end{aligned}$$

Putting these ϵ^μ into the transformations for $g^{23'}$ and $g^{33'}$ gives only differential conditions on C_1, C_2, and C_3 which can be integrated to give

$$C_3 = f(u), \quad C_1 = g(u)\cos\theta + h(u), \quad C_2 = j(u)\sin\theta.$$

Substituting back into Eqs. (4.5), we obtain further differential conditions on f, g, h, and j, whose solutions tells us that the only freedom in the coordinate transformation is given by

$$\begin{aligned}
u' &= -u - 2r + (u + 2r)A\cos\theta + B\cos\theta + C, \\
r' &= r - [A(u + r) + B]\cos\theta, \\
\theta' &= \theta + (Au + B)\sin\theta/r + A\sin\theta, \\
\varphi' &= \varphi + D,
\end{aligned}$$

where A, B, C, and D are first-order constants. However, the transformation with only $C \neq 0$ is simply a time translation, and the one with only $D \neq 0$ is simply a rotation about the axis of symmetry. Finally, the A and B freedom is a linearization of the BMS group[1] with $\alpha(\theta) = B\cos\theta$ and A identified with ν. Thus B and A correspond to a translation and a Lorentz transformation, each along the axis of symmetry, respectively. Therefore the constants of integration contain nothing of interest and can be set equal to zero leaving

$$\begin{aligned}
\epsilon^0 &= -2\int \underset{1}{g}^{11'}\, dr - 2\epsilon^1, \\
\epsilon^1 &= -r\epsilon^2_{,2} + \tfrac{1}{2}r^3[(g^{22} + 1/r^2) - (g^{22'} + 1/r'^2)], \\
\epsilon^2 &= -2\int \underset{1}{g}^{12'}\, dr + 2\int r^{-2}\left(\int \underset{1}{g}^{11'}\, dr\right)_{,2} dr, \\
\epsilon^3 &= -2\int \underset{1}{g}^{13'}\, dr.
\end{aligned} \tag{4.7}$$

Now that we know the coordinate transformation,

i.e., the ϵ^μ, we must find the associated tetrad transformation. We define

$$\begin{aligned} \tilde{l}^\mu &\equiv L_1 l^\mu + (L_2 - 2)n^\mu + L_3 m^\mu + \bar{L}_3 \bar{m}^\mu, \\ \tilde{n}^\mu &\equiv (N_1 - \tfrac{1}{2})l^\mu + N_2 n^\mu + N_3 m^\mu + \bar{N}_3 \bar{m}^\mu, \\ \tilde{m}^\mu &\equiv M_1 l^\mu + M_2 n^\mu + (1 + M_3)m^\mu + M_4 \bar{m}^\mu, \end{aligned} \tag{4.8}$$

where we wish to know the L's, N's, and M's to first order. Transforming to the primed coordinates, we demand that $\tilde{l}^{\mu'} = \delta_1^\mu$, $\tilde{n}^{\mu'} = \delta_0^\mu + \tilde{U}'\delta_1^\mu + \tilde{X}^{i'}\delta_2^\mu$, and $\tilde{m}^{\mu'} = \tilde{\omega}'\delta_i^\mu + \tilde{\xi}^{i'}\delta_i^\mu$, and we find, after some manipulation, that

$$\underset{1}{L_1} = 0, \quad \underset{1}{L_2} = \epsilon^0_{,1},$$

$$\underset{1}{L_3} = \left(\underset{1}{X^2} + \epsilon^2_{,0} - \tfrac{1}{2}\epsilon^2_{,1}\right)\Big/\underset{0}{\xi^2} + \left(\underset{1}{g^{13'}} + \underset{1}{X^3}\right)\Big/\underset{0}{\xi^3}, \tag{4.9}$$

$$\underset{1}{N_1} = -\tfrac{1}{4}\epsilon^0_{,1}, \quad \underset{1}{N_2} = 0, \tag{4.10}$$

$$\underset{1}{N_3} = \left(\underset{1}{\tilde{X}^{2'}} + \tfrac{1}{2}\epsilon^2_{,1}\right)\Big/2\underset{0}{\xi^2} + \left(\underset{1}{\tilde{X}^{3'}} + \tfrac{1}{2}\epsilon^3_{,1}\right)\Big/2\underset{0}{\xi^3};$$

and

$$\begin{aligned} \underset{1}{M_1} &= \tfrac{1}{2}\left(\underset{1}{\xi^2}\epsilon^0_{,2} - 2\underset{1}{\omega}\right), \\ \underset{1}{M_2} &= \underset{1}{\xi^2}(\epsilon^0 + 2\epsilon^1)_{,2} - 2\underset{1}{\tilde{\omega}'}, \\ \underset{1}{M_3} &= \frac{\underset{1}{\xi^{2\prime}} - \underset{1}{\xi^2}}{2\underset{0}{\xi^2}} + \frac{\underset{1}{\xi^{3\prime}} - \underset{1}{\xi^3}}{2\underset{0}{\xi^3}} - \tfrac{1}{2}\epsilon^2_{,2} - \frac{\underset{1}{\xi^2}\epsilon^3_{,2}}{2\underset{0}{\xi^3}}, \\ \underset{1}{M_4} &= \frac{\underset{1}{\xi^{2\prime}} - \underset{1}{\xi^2}}{2\underset{0}{\xi^2}} - \frac{\underset{1}{\xi^{3\prime}} - \underset{1}{\xi^3}}{2\underset{0}{\xi^3}} - \tfrac{1}{2}\epsilon^2_{,2} + \frac{\underset{1}{\xi^2}\epsilon^3_{,2}}{2\underset{0}{\xi^3}}. \end{aligned} \tag{4.11}$$

Now that we know the transformations to first order, we assume we have solved the driven integro-differential equations corresponding to (3.7) for the second-order ψ_A and do a transformation to find the second-order $\tilde{\psi}_A$. Using Eqs. (2.3), (4.8), and (4.9)–(4.11) we can derive

$$\begin{aligned} \underset{2}{\tilde{\psi}_0} &= 4\underset{2}{\bar{\psi}_4} + \left(2\underset{1}{M_3} - \underset{1}{L_2}\right)4\underset{1}{\bar{\psi}_4} + \left(2\underset{1}{M_1} - \underset{1}{\bar{L}_3}\right)4\underset{1}{\bar{\psi}_3}, \\ \underset{2}{\tilde{\psi}_1} &= -2\underset{2}{\bar{\psi}_3} + 4\underset{1}{N_3}\underset{1}{\bar{\psi}_4} + \left(2\underset{1}{L_2} - 2\underset{1}{M_3} + 4\underset{1}{N_1}\right)\underset{1}{\bar{\psi}_3} \\ &\quad - 2\underset{1}{M_4}\underset{1}{\psi_3} + \left(2\underset{1}{\bar{L}_3} - 2\underset{1}{M_1}\right)\underset{1}{\bar{\psi}_2} - \left(\underset{1}{\bar{L}_3} + 2\underset{1}{M_1}\right)\underset{1}{\psi_2}, \\ \underset{2}{\tilde{\psi}_2} &= \underset{2}{\bar{\psi}_2} + \left(\underset{1}{\bar{M}_2} - 2\underset{1}{N_3}\right)\underset{1}{\bar{\psi}_3} \\ &\quad + \left(\underset{1}{M_3} - \tfrac{1}{2}\underset{1}{L_2} - 2\underset{1}{N_1} + \underset{1}{\bar{M}_3}\right)\underset{1}{\bar{\psi}_2} + \left(\underset{1}{M_1} - \tfrac{1}{2}\underset{1}{\bar{L}_3}\right)\underset{1}{\bar{\psi}_1}, \\ \underset{2}{\tilde{\psi}_3} &= -\tfrac{1}{2}\underset{2}{\bar{\psi}_1} + \left(2\underset{1}{N_3} - \tfrac{1}{2}\underset{1}{\bar{M}_2}\right)\underset{1}{\bar{\psi}_2} + \left(-\underset{1}{N_3} - \tfrac{1}{2}\underset{1}{\bar{M}_2}\right)\underset{1}{\psi_2} \\ &\quad + \left(2\underset{1}{N_1} + \tfrac{1}{4}\underset{1}{L_2} - \tfrac{1}{2}\underset{1}{\bar{M}_3}\right)\underset{1}{\bar{\psi}_1} - \tfrac{1}{2}\underset{1}{\bar{M}_4}\underset{1}{\psi_1} + \tfrac{1}{4}\underset{1}{\bar{L}_3}\underset{1}{\psi_0}, \\ \underset{2}{\tilde{\psi}_4} &= \tfrac{1}{4}\underset{2}{\bar{\psi}_0} + \left(\tfrac{1}{2}\underset{1}{\bar{M}_3} - \underset{1}{N_1}\right)\underset{1}{\bar{\psi}_0} + \left(\tfrac{1}{2}\underset{1}{\bar{M}_2} - \underset{1}{N_3}\right)\underset{1}{\bar{\psi}_1}. \end{aligned} \tag{4.12}$$

5. THE LINEAR THEORY

A. Advanced Solutions

Because of their physical significance one generally studies retarded solutions rather than advanced solutions, and in our case we have an incentive to look at the retarded solutions first in that they have already been worked out in JN. However, it turns out to be simpler to start with the advanced solutions, and we then obtain an improved form of the retarded solutions by doing a time reversal.

Suppose we look for solutions of Eqs. (3.7) with the simplifying property $\psi_1^\circ = \psi_2^\circ = \psi_3^\circ = \psi_4^\circ = 0$ (which excludes the JN solutions). We look for separable solutions of the form

$$\begin{aligned} &\psi_0 = \Theta_0(\theta, \varphi)f_0(u, r), \quad \psi_1 = \Theta_1(\theta, \varphi)f_1(u, r), \\ &\psi_2 = \Theta_2(\theta, \varphi)f_2(u, r), \quad \psi_3 = \Theta_3(\theta, \varphi)f_3(u, r), \\ &\psi_4 = \Theta_4(\theta, \varphi)f_4(u, r). \end{aligned} \tag{5.1}$$

Substituting these assumptions into Eqs. (3.7), using the last of Eqs. (3.6), and using $\eth\bar{\eth}_s Y_{lm} = -(l + s) \times (l - s + 1)_s Y_{lm}$ (see Appendix), we find that

$$\begin{aligned} \psi_0 &= \sum_{lm} f_{0lm}\,{}_2Y_{lm}, \\ \psi_1 &= \sum_{lm} f_{1lm}\,{}_1Y_{lm}, \\ \psi_2 &= \sum_{lm} f_{2lm}\,{}_0Y_{lm}, \\ \psi_3 &= \sum_{lm} f_{3lm}\,{}_{-1}Y_{lm}, \\ \psi_4 &= \sum_{lm} f_{4lm}\,{}_{-2}Y_{lm}, \end{aligned} \qquad \begin{aligned} &2 \le l, \\ &-l \le m \le +l, \end{aligned} \tag{5.2}$$

are solutions if

$$\begin{aligned} &\partial f_{0lm}/\partial u - \tfrac{1}{2}\partial f_{0lm}/\partial r - f_{0lm}/2r \\ &\qquad + [(l + 2)(l - 1)/2r^5]\textstyle\int r^3 f_{0lm}\,dr = 0, \\ &\partial f_{1lm}/\partial u - \tfrac{1}{2}\partial f_{1lm}/\partial r - f_{1lm}/r \\ &\qquad + [(l + 1)l/2r^4]\textstyle\int r^2 f_{1lm}\,dr = 0, \\ &\partial f_{2lm}/\partial u - \tfrac{1}{2}\partial f_{2lm}/\partial r - 3f_{2lm}/2r \\ &\qquad + [(l + 1)l/2r^3]\textstyle\int r f_{2lm}\,dr = 0, \\ &\partial f_{3lm}/\partial u - \tfrac{1}{2}\partial f_{3lm}/\partial r - 2f_{3lm}/r \\ &\qquad + [(l + 2)(l - 1)/2r^2]\textstyle\int f_{3lm}\,dr = 0, \end{aligned} \tag{5.3}$$

and

$$f_{4lm} = (1/\sqrt{2}\,r)(l - 1)(l + 2)\textstyle\int f_{3lm}\,dr. \tag{5.4}$$

In order to derive a class of radiative solutions we note the general result that for $K = -1, 0$, positive integer,

$$\textstyle\int r^K \partial^{K+1} f(r)/\partial r^{K+1}\,dr = r^{K+1}\partial^K[f(r)/r]/\partial r^K, \tag{5.5}$$

which can be proven by $K + 1$ integrations by parts. Using this result, we find that Eqs. (5.3) and Eq. (5.4)

are satisfied by[11]

$$\begin{aligned} f_{0lm} &= r^{l-2}D^{l+2}[a(-u-2r)/r^{l-1}], \\ f_{1lm} &= r^{l-2}D^{l+1}[a(-u-2r)/r^{l}], \\ f_{2lm} &= r^{l-2}D^{l}[a(-u-2r)/r^{l+1}], \quad l \geq 2 \\ f_{3lm} &= r^{l-2}D^{l-1}[a(-u-2r)/r^{l+2}], \\ f_{4lm} &= r^{l-2}D^{l-2}[a(-u-2r)/r^{l+3}], \end{aligned} \tag{5.6}$$

where $D \equiv \partial/\partial r$. Using these results the linear theory Eqs. (3.4) and (3.5) are satisfied by

$$\begin{aligned} \psi_0 &= \sum_{lm} 2K_{-2}A_{lm}r^{l-2}D^{l+2}(\tilde{a}_{lm}/r^{l-1})_2Y_{lm}, \\ \psi_1 &= \sum_{lm} \sqrt{2}\, K_{-1}A_{lm}r^{l-2}D^{l+1}(\tilde{a}_{lm}/r^{l})_1Y_{lm}, \quad l \geq 2, \\ \psi_2 &= \sum_{lm} A_{lm}r^{l-2}D(\tilde{a}_{lm}/r^{l+1})_0Y_{lm}, \\ \psi_3 &= \sum_{lm} (1/\sqrt{2})K_1A_{lm}r^{l-2}D^{l-1}(\tilde{a}_{lm}/r^{l+2})_{-1}Y_{lm}, \\ &\qquad\qquad -l \leq m \leq +l, \\ \psi_4 &= \sum_{lm} (\tfrac{1}{2})K_2A_{lm}r^{l-2}D^{l-2}(\tilde{a}_{lm}/r^{l+3})_{-2}Y_{lm}, \end{aligned} \tag{5.7}$$

where

$$K_p \equiv [(l+p)!/(l-p)!]^{\frac{1}{2}}, \quad \tilde{a}_{lm} \equiv a_{lm}(-u-2r),$$

and the A_{lm} are arbitrary complex constants. The interpretation of these solutions as representing advanced radiation follows from the appearance of an arbitrary function whose argument is constant on the past null cones (if u labels future null cones). Calculation of the other first-order quantities (spin coefficients, etc.) is done through Eqs. (3.8). The r integrations can be explicitly carried out despite the arbitrary function of $-u-2r$ that is present. [This is related to the fact that the ψ_A can be put in the convenient total-differential form (5.7).] The initial data for these solutions take an interesting form. Since $\psi_4^\circ = \psi_3^\circ = 0$, Eqs. (2.7) assure us that we have no arbitrary retarded news function. On the other hand, the initial data include $\psi_0(r, \theta, \phi, u_0)$ and, as can be seen from the first of Eqs. (5.7), this tells us the arbitrary function $\tilde{a}_{lm}(-u-2r)$ over a semi-infinite range of its argument ($-u_0$ to ∞). (The rest of this function describes radiation which reached $r=0$ prior to $u=u_0$.) Thus the incoming radiation is "sampled" by the forward null cone, $u=u_0$, and in this way its prescription is included among the initial data.

B. Retarded Solutions

Suppose one has a mathematical solution of a physical theory corresponding to a particular physical situation. If the theory is invariant under time reversal (as in general relativity), one can easily derive a mathematical solution corresponding to the time-reversed physical situation. One simply does the coordinate transformation $t' = -t$ and then ignores the prime on t', i.e. interprets t' as increasing into the future as did the original t. In using the above coordinate transformation method to derive, in null coordinates, the retarded gravitational radiation solutions from the advanced gravitational radiation solutions, there is an added complication. Under $u' = -u$ and the re-interpretation of u' as increasing into the future as did u, the new u (replacing u') labels null cones opening into the past if the original u labeled null cones opening into the future. In order to preserve all characteristics of the reference frame in which we describe the different physical situations we must then change null cones; that is, we must do both the transformation $u' = -u$ and the transformation (in the example of flat space) $u'' = u' - 2r' = -u - 2r$. Now the new coordinate u (replacing u'') increases into the future and labels null cones opening into the future, and is in fact indistinguishable from the original coordinate u. It is clear that the transformations derived in Sec. 4 are exactly the ones needed here to change null cones. If we subject the advanced radiation solutions just derived to the combination of tetrad and coordinate transformations derived in Sec. 4 along with the corresponding transformation of the ψ_A also derived there and then drop all primes and tildes, we will obtain the retarded radiation solutions with the usual coordinate and tetrad conditions holding. This argument is not restricted to the linear theory. If one knows the transformations to order n, one can find the new ψ_A to order $n+1$, and can then use Eqs. (3.8) (with the proper driving terms) to calculate all other quantities to order $n+1$.

It is quite simple to apply the above procedure to the linear theory. Since we are only working with the ψ_A, we need only the flat-space transformations. Thus we subject the ψ_A of Eqs. (5.7) to the transformation $u' = -u - 2r$, $r' = r$, $\theta' = \theta$, $\varphi' = \varphi$, and $\bar{\psi}_0 = 4\psi_4$, $\bar{\psi}_1 = -2\psi_3$, $\bar{\psi}_2 = \psi_2$, $\bar{\psi}_3 = (-\tfrac{1}{2})\psi_1$, and $\bar{\psi}_4 = (\tfrac{1}{4})\psi_0$, and then drop primes and tildes. The resulting retarded solutions are of the form

$$\begin{aligned} \psi_0 &= \sum_{lm} 2K_2R_{lm}r^{l-2}\, d^{l-2}(b_{lm}/r^{l+3})_2Y_{lm}, \quad l \geq 2, \\ \psi_1 &= \sum_{lm} \sqrt{2}\, K_1R_{lm}r^{l-2}\, d^{l-1}(b_{lm}/r^{l+2})_1Y_{lm}, \\ \psi_2 &= \sum_{lm} R_{lm}r^{l-2}\, d^{l}(b_{lm}/r^{l+1})_0Y_{lm}, \quad -l \leq m \leq +l, \\ \psi_3 &= \sum_{lm} (1/\sqrt{2})K_{-1}R_{lm}r^{l-2}\, d^{l+1}(b_{lm}/r^{l})_{-1}Y_{lm}, \\ \psi_4 &= \sum_{lm} (1/2)K_{-2}R_{lm}r^{l-2}\, d^{l+2}(b_{lm}/r^{l-1})_{-2}Y_{lm}, \end{aligned} \tag{5.8}$$

[11] This simple form for the solutions was pointed out by E. Couch.

where $d \equiv -2\partial/\partial u + \partial/\partial r$, $b_{lm} = b_{lm}(u)$, and the R_{lm} are arbitrary complex constants. The solutions (5.8) can be expanded into finite series in $1/r$, namely,

$$\psi_0 = \sum_{n=0}^{l-2} \sum_{ml} 2K_{-2}R_{lm}(-1)^{l-2} \times \left(\frac{2^{l-2-n}}{n!} K_{n+2}^2\right)\left(\frac{(l-2-n)}{b_{lm}}{r^{5+n}}\right)_2 Y_{lm},$$

$$\psi_1 = \sum_{n=0}^{l-1} \sum_{ml} \sqrt{2}\, K_{-1}R_{lm}(-1)^{l-1} \times \left(\frac{2^{l-1-n}}{n!} K_{n+1}^2\right)\left(\frac{(l-1-n)}{b_{lm}}{r^{4+n}}\right)_1 Y_{lm},$$

$$\psi_2 = \sum_{n=0}^{l} \sum_{ml} R_{lm}(-1)^{l} \times \left(\frac{2^{l-n}}{n!} K_n^2\right)\left(\frac{(l-n)}{b_{lm}}{r^{3+n}}\right)_0 Y_{lm}, \tag{5.9}$$

$$\psi_3 = \sum_{n=0}^{l+1} \sum_{ml} (1/\sqrt{2})K_1R_{lm}(-1)^{l+1} \times \left(\frac{2^{l+1-n}}{n!} K_{n-1}^2\right)\left(\frac{(l+1-n)}{b_{lm}}{r^{2+n}}\right)_{-1} Y_{lm},$$

$$\psi_4 = \sum_{n=0}^{l+2} \sum_{ml} (\tfrac{1}{2})K_2R_{lm}(-1)^{l+2} \times \left(\frac{2^{l+2-n}}{n!} K_{n-2}^2\right)\left(\frac{(l+2-n)}{b_{lm}}{r^{1+n}}\right)_{-2} Y_{lm},$$

where $\overset{(K)}{b}_{lm} \equiv \partial^K b_{lm}/\partial u^K$. These are the retarded solutions first derived in JN. The rederivation here yields two improvements. The use of the operator $\eth$ has allowed us to drop the JN assumption of axial symmetry. In addition, by using the time-reversal method, we have obtained the general coefficient in the $1/r$ expansion. The JN general coefficients were more complicated and did not cover the leading term of each series.

6. SECOND-ORDER CALCULATIONS

A small-parameter approximation nethod has been presented, and we make the usual assumption that the approximation converges. In this section we show that nonlinear (at least second-order) calculations can in fact be done in practice. We consider an axially symmetric linear solution consisting of an imploding quadrupole wave [moment $\tilde{a} = a(-u-2r)$] and an exploding quadrupole wave [moment $b = b(u)$], with a mass $-m$ at their common focus. We calculate part of the second-order correction to this linear solution and give it in a form with all r integrations explicitly carried out despite the arbitrary function of $u + 2r$ present. Setting $l = 2$ and $m = 0$ in Eqs. (5.7) and (5.8) (with convenient choices for A_{20} and R_{20}) and adding on the Schwarzschild solution expressed in this language,[6] we get

$$\underset{1}{\psi}_0 = \left(\frac{3b}{2r^5} + \frac{\dddot{\tilde{a}}}{r} + \frac{2\ddot{\tilde{a}}}{r^2} + \frac{3\dddot{\tilde{a}}}{r^3} + \frac{3\dot{\tilde{a}}}{r^4} + \frac{3\tilde{a}}{2r^5}\right)\left(\frac{2P_2^2}{3}\right),$$

$$\underset{1}{\psi}_1 = \left(\frac{3b}{2r^4} + \frac{3b}{r^5} + \frac{\ddot{\tilde{a}}}{r^2} + \frac{3\ddot{\tilde{a}}}{r^3} + \frac{9\dot{\tilde{a}}}{2r^4} + \frac{3\tilde{a}}{r^5}\right)\left(-\frac{2\sqrt{2}\,P_2^1}{3}\right),$$

$$\underset{1}{\psi}_2 = \left(\frac{\ddot{b}}{r^3} + \frac{3\dot{b}}{r^4} + \frac{3b}{r^5} + \frac{\ddot{\tilde{a}}}{r^3} + \frac{3\dot{\tilde{a}}}{r^4} + \frac{3\tilde{a}}{r^5}\right)(2P_2) + \left(\frac{m}{r^3}\right)P_0,$$

$$\underset{1}{\psi}_3 = \left(\frac{2\ddot{b}}{3r^2} + \frac{2\dot{b}}{r^3} + \frac{3\dot{b}}{r^4} + \frac{2b}{r^5} + \frac{\dot{\tilde{a}}}{r^4} + \frac{2\tilde{a}}{r^5}\right)\left(\frac{P_2^1}{\sqrt{2}}\right),$$

$$\underset{1}{\psi}_4 = \left(\frac{2\dddot{b}}{3r} + \frac{4\ddot{b}}{3r^2} + \frac{2\dot{b}}{r^3} + \frac{2\dot{b}}{r^4} + \frac{b}{r^5} + \frac{\tilde{a}}{r^5}\right)\left(\frac{P_2^2}{4}\right), \tag{6.1}$$

where a dot signifies differentiation with respect to the argument, be it u or $-u-2r$, and the P_l^m are the associated Legendre polynomials. One completes the first-order solution using Eqs. (3.8) and

$$2g^{\mu\nu} = l^{(\mu}n^{\nu)} - m^{(\mu}\bar{m}^{\nu)}.$$[12]

We can now go on to the second-order correction, where we restrict our attention to $\underset{2}{\psi}_0$. In order to solve the first of the driven equations analogous to Eqs. (3.7) for $\underset{2}{\psi}_0$, we must know $\underset{2}{D}_0$ and $\underset{2}{\psi}_1^\circ$. The first is obtained directly from Eq. (3.10). The following argument gives us $\underset{2}{\psi}_1^\circ$. Since we give $\underset{2}{\sigma}^\circ = 0$ as initial data Eqs. (2.7) tell us that $\underset{2}{\psi}_3^\circ = \underset{2}{\psi}_4^\circ = 0$. An inspection of the leading terms of $\underset{2}{D}_2$ and $\underset{2}{D}_1$ then enables us to evaluate $\underset{2}{\psi}_2^\circ$ and $\underset{2}{\psi}_1^\circ$.[12] The effective driving term of the equation for $\underset{2}{\psi}_0$ is then

$$\underset{2}{\hat{D}}_0 \equiv \underset{2}{D}_0 - \eth\underset{2}{\psi}_1^\circ/\sqrt{2}\,r^5. \tag{6.2}$$

It is convenient to write D_0 in five parts, that is

$$\underset{2}{\hat{D}}_0 = \underset{2}{\hat{D}}_0(R\times R) + \underset{2}{\hat{D}}_0(R\times A) + \underset{2}{\hat{D}}_0(A\times A) + \underset{2}{\hat{D}}_0(R\times m) + \underset{2}{\hat{D}}_0(A\times m), \tag{6.3}$$

where $\hat{D}_0(R\times A)$, for example, is that part of $\hat{D}_0$ bilinear in $b(u)$ and $a(-u-2r)$. We restrict our attention now to $\hat{D}_0(R\times R)$, $\hat{D}_0(R\times A)$, and $\hat{D}_0(R\times m)$. These quantities have been evaluated[12] and the first of the driven form of Eqs. (3.7) solved with these driving terms. We give here the solutions

[12] For these results see R. J. Torrence, thesis, University of Pittsburgh (1965).

in the three corresponding pieces

$\psi_0(R \times R)$, $\psi_0(R \times m)$, and $\psi_0(R \times A)$:

$$\begin{aligned}
\underset{2}{\psi_0}(R \times R) = &\left[\left(2\int \ddot{b}\ddot{b}\,du + \frac{4}{3}\int f\,du\right)\Big/7r^5\right. \\
&\left. + 30b\dot{b}/7r^7 + 35b\ddot{b}/7r^8\right]P_2^2 \\
&+ \left[\left(-3\int \dddot{b}\ddot{b}\,du - 2\int f\,du\right)\Big/35r^5\right. \\
&+ \left(-4\int \dddot{b}\dot{b}\,du - 3\iint \ddddot{b}\ddot{b}\,du\,du - 2\iint f\,du\,du\right)\Big/5r^6 \\
&+ \left(60b\dot{b} - 105\int b\ddot{b}\,du - 70\int \dddot{b}\dot{b}\,du - 56\iint \ddddot{b}\dot{b}\,du\,du\right. \\
&\left. - 42\iiint \ddddot{b}\ddot{b}\,du\,du\,du - 28\iiint f\,du\,du\,du\right)\Big/35r^7 \\
&\left. + 2b\dot{b}/r^8\right]P_4^2, \qquad (6.4)
\end{aligned}$$

where

$$f \equiv \frac{1}{4}\left[\iint(\ddddot{b}\ddot{b} + \dddot{b}\dddot{b})du\,du + \int(5\ddddot{b}\ddot{b} - \dddot{b}\dddot{b})du\right]$$

and where all integrals are evaluated from u_0 (the initial hypersurface) to u,

$$\underset{2}{\psi_0}(R \times m) = \left(-\frac{m}{2}\right)\left[\frac{\dot{b}}{r^5} + 15\sum_{N=0}^{\infty} C_N(u)/r^{N+6}\right], \qquad (6.5)$$

where

$$C_N(u) \equiv \prod_{n=0}^{N} A_n \overbrace{\int_{u_0}^{u}\cdots\int_{u_0}^{u}}^{N+1} b\,du^{N+1},$$

with $A_0 = 1$ and $A_n = 2/(n+2) - \frac{1}{2}(n+5)$, $n \geq 1$, and

$$\begin{aligned}
&\underset{2}{\psi_0}(R \times A) \\
&= [b(4\dddddot{a}/r^2 + 18\ddddot{a}/r^3 + 48\dddot{a}/r^4 \\
&\quad + 84\ddot{a}/r^5 + 90\dot{a}/r^6 + 45a/r^7)/7 \\
&\quad + b(2\dddddot{a}/r^3 + 14\ddddot{a}/r^4 + 52\dddot{a}/r^5 + 120\ddot{a}/r^6 \\
&\quad + 165\dot{a}/r^7 + 105a/r^8)/7 \\
&\quad + \dot{b}(4\ddddot{a}/r^2 + 6\dddot{a}/r^3 + 6\ddot{a}/r^4 + 3\dot{a}/r^5)/7 \\
&\quad + \ddot{b}(2\dddot{a}/r^3 + 2\ddot{a}/r^4 + \dot{a}/r^5)]P_2^2 \\
&\quad + [b(-6\dddot{a}/r^2 - 27\ddot{a}/r^3 - 72\dot{a}/r^4 - 126a/r^5 \\
&\quad - 135\dot{a}/r^6 - 135a/2r^7)/35 + b(-3\dddot{a}/r^3 - 14\ddot{a}/r^4 \\
&\quad - 22\dot{a}/r^5 + 30a/r^6 + 345\dot{a}/2r^7 + 210a/r^8)/35 \\
&\quad + \dot{b}(-6\ddot{a}/r^2 - 23\dot{a}/r^3 - 65a/r^4 - 261\dot{a}/2r^5 \\
&\quad - 168\dot{a}/r^6 - 105a/r^7)/35 + \ddot{b}(-3\dot{a}/r^3 \\
&\quad - 10\ddot{a}/r^4 - 45\dot{a}/2r^5 - 63a/2r^6 - 21\dot{a}/r^7)/35]P_4^2. \qquad (6.6)
\end{aligned}$$

This completes our explicit second-order calculations.

7. CONCLUSION

We wish to discuss the usefulness of the method outlined in this paper. In Sec. 6 we have calculated only a fragment of the second-order ψ_A, namely $\psi_0(R \times R)$, $\psi_0(R \times m)$, and $\psi_0(R \times A)$. It is clear however that the other $\psi_A(R \times R)$, $\psi_A(R \times m)$, and $\psi_A(R \times A)$ can be obtained from Eqs. (3.6) with the driving terms given by Eqs. (3.9). That the r integrations in Eqs. (3.6) and (3.9) can be done is certain since Eqs. (3.5) would otherwise be inconsistent. Consider, for example, the driven equation corresponding to the first of Eqs. (3.5). It enables us to solve for the r dependence of $\underset{2}{\psi_1}$ in terms of $\underset{2}{\psi_0}$, $(2\partial/\partial u - \partial/\partial r)\underset{2}{\psi_0}$, and a driving term bilinear in first-order quantities. In view of the form of $\underset{2}{\psi_0}$ which we have just given, $\underset{2}{\psi_1}$ must also be free of r integrations, and the same argument applies to $\underset{2}{\psi_2}$, $\underset{2}{\psi_3}$, and $\underset{2}{\psi_4}$. The $\psi_A(A \times A)$ and $\psi_A(m \times A)$ might be very difficult to solve for directly; however, we know they are simply the time-reverse solutions corresponding to the $\psi_A(R \times R)$ and the $\psi_A(R \times m)$. Thus the transformations of Sec. 4 can be used to find the $\psi_A(A \times A)$ and $\psi_A(m \times A)$. [One encounters the r integrations of Eqs. (4.7), but these can again be carried out.[12]] Thus we can obtain the full $\underset{2}{\psi_A}$. It is plausible but not certain that the other second-order quantities can be found. We need the second-order form of Eqs. (3.8), and we must be able to do the r integrations indicated by these equations. This was possible in first order where many of the integrations were precisely those contained in Eqs. (3.7), and it is plausible that the pattern will continue into the second order. In any case, the ψ_A alone are valuable. (It should be noted that the above remarks on r integrations are only necessary when advanced solutions are involved; with pure retarded solutions of any order, our integrands are always finite series in $1/r$, and r integrations pose no problem.)

Thus the usefulness of the method presented is not vitiated by calculational impossibilities. The calculations are long, but when motivated by an explicit question one could work out the exact second-order solution. (It should be emphasized that no asymptotic approximation has been made.) It is the formulation of questions suited to our approximation scheme and choice of coordinates which poses problems.

A few interesting observations can be made despite the incompleteness of our second-order corrections.

Clearly our second-order solutions could be modified by adding to them second-order homogeneous solutions. These homogeneous solutions are formally indistinguishable from the linearized solutions given by Eqs. (5.6) and (5.8); their introduction would therefore introduce second-order news functions in no way determined by the first-order initial data. This flexibility is not surprising since the entire news function is initial data. However, by imposing extra conditions on the solution, this arbitrariness can be decreased. It has been suggested[6] that the $(1/r^5)P_2^2$ part of ψ_0 should be singled out as the quadrupole moment M_2 of the solution. We see from an examination of $\psi_0(R \times R)$ that, if we give M_2 as part of the initial data, there is a correction $\overset{1}{M}_2$. We can obviously make $\overset{2}{M}_2 = 0$ by adding a second-order retarded quadrupole solution with the proper news function. This can be interpreted as telling us that source activity characterized by $M_2 \neq 0$ with $\overset{1}{M}_2 = 0$ results in asymptotic outgoing second-order radiation. If, on the other hand, we insist that there be no outgoing second-order radiation at infinity, then the source must have just that second-order behavior implicit in Eq. (6.4).

A similar interpretation can be applied to $\psi_0(R \times m)$. Once again we have, from Eq. (6.4), a second-order correction to the quadrupole moment (in this case it is proportional to m). Adding the right second-order news function to the initial data will cancel the correction to the moment. One could argue from this that if a first-order spherically symmetric source undertakes the emission of first-order quadrupole radiation, it will simultaneously develop a second-order quadrupole moment. If it is to remain spherically symmetric it must radiate quadrupole radiation in second order as well.

The above interpretations should probably not be taken too seriously; however, they do indicate the potential value of the method. Two well-known results are also consistent with our solutions. The evaluation of ψ_2° described in Sec. 6 gives us the radiation-induced mass loss first derived by Bondi.[1] In addition, the fact that $\psi_0(R \times R)$ is missing a term proportional to P_2^2/r^6 is a direct consequence of the recently discovered conservation laws of Newman and Penrose.[13] One question of particular interest whose investigation may be aided by extension of this work concerns "backscattering." Can we, by imposing reasonable restrictions on our solutions, discover a necessary relationship between, for example, a first-order *advanced* news function and a second-order *retarded* news function? This question is being actively investigated.

[13] E. Newman and R. Penrose, J. Math. Phys. 7, 863 (1966).

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APPENDIX

In this Appendix, we give a brief summary of some useful notation introduced by Newman and Penrose.[13]

In flat space, a quantity η is said to have spin weight s if the tetrad transformation $m^{\mu'} = e^{i\psi}m^\mu$ induces the transformation $\eta' = e^{si\psi}\eta$. Since in linearized gravitational theory the ψ_A are defined with respect to the flat-space tetrad, we may think of the ψ_A as a spin-weighted field in a flat-space background. It follows from their definitions (2.3) that the ψ_A have spin weights $2 - A$. The operator thop, denoted by $\eth$, is then defined by

$$\bar{\eth}\eta = -(\sin\theta)^s\left(\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial\varphi}\right)[(\sin\theta)^{-s}\eta], \quad \text{(A1)}$$

where s is the spin weight of η. We also define

$$\bar{\eth}\eta = -(\sin\theta)^{-s}\left(\frac{\partial}{\partial\theta} - \frac{i}{\sin\theta}\frac{\partial}{\partial\varphi}\right)[(\sin\theta)^{s}\eta]. \quad \text{(A2)}$$

These definitions permit the introduction of thop beginning with Eqs. (3.4).

Spin-weighted spherical harmonics ${}_sY_{lm}$ are defined by

$${}_sY_{lm} = \begin{cases} \left[\dfrac{(l-s)!}{(l+s)!}\right]^{\frac{1}{2}}\eth^s Y_{lm}, & 0 \leq s \leq l, \\ (-1)^s\left[\dfrac{(l+s)!}{(l-s)!}\right]^{\frac{1}{2}}\bar{\eth}^{-s}Y_{lm}, & -l \leq s \leq 0, \end{cases} \quad \text{(A3)}$$

where the ${}_0Y_{lm} \equiv Y_{lm}$ are the ordinary spherical harmonics and the ${}_sY_{lm}$ are of spin weight s. The ${}_sY_{lm}$ form a complete set for quantities of spin weight s, but, more important for our purposes, they satisfy

$$\begin{aligned} \eth_s Y_{lm} &= [(l-s)(l+s+1)]^{\frac{1}{2}}{}_{s+1}Y_{lm}, \\ \bar{\eth}_s Y_{lm} &= -[(l+s)(l-s+1)]^{\frac{1}{2}}{}_{s-1}Y_{lm}, \end{aligned} \quad \text{(A4)}$$

from which it follows that

$$\bar{\eth}\eth_s Y_{lm} = -(l-s)(l+s+1){}_sY_{lm}. \quad \text{(A5)}$$

It is this last relation that is used in obtaining Eqs. (5.2).

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Canonical Form Factors and Current Commutation Relations

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Starting with the vector (or axial vector) currents j^μ and the momentum operators P^ν, we define the canonical operator $\tilde{j}$, such that instead of the four covariantly transforming components of j, we have a scalar $\tilde{j}^0$ and three other components $\tilde{\mathbf{j}}$ undergoing Wigner rotations under Lorentz transformations. We first give a construction of $\tilde{j}$ explicitly in terms of j and P. But, since the transformation properties are not quite the most convenient ones, a subsequent generalized definition, leading to a convenient canonical parametrization of the matrix elements of $\tilde{j}$, is introduced. We then study the physical significances of the canonical form factors thus obtained. For vector currents $\tilde{j}^\nu$ the transformation properties correspond to a separation of the physical charge ($\tilde{j}^0$) and magnetic ($\tilde{\mathbf{j}}$) form factors in any frame (and not only in Breit frame as for j). For nonconserved axial currents we relate the matrix elements of $\tilde{j}^{0A}$ with mass-difference effects and express the partial conservation condition in terms of the canonical form factors. We then study in detail the application of our formalism to the limiting case of infinite momentum and small momentum-exchange, as often introduced in the study of current algebras. Next we give explicitly the canonical form factors for photoproduction processes. In the last section we study the possibility of constructing a canonical spin operator directly in terms of the vector and axial vector charges and the consequences for the "inner orbital" contribution to be added to obtain the total spin of a composite particle. Some useful formulas are collected in Appendixes *A* and *B*.

1. INTRODUCTION AND DEFINITIONS

IN our previous studies[1] of various aspects of the representations of the Poincaré group and, in particular, those of the relativistic properties of spin, we saw how directly "Wigner rotations" are related to physical magnitudes.

Here we try to apply this lesson in a field theoretic context, by relating to vector (and axial vector) currents certain modified operators (defined below) which lead us directly to the desired transformation properties. In this article we restrict ourselves to the physically important case of vector currents and do not consider operators of more general spinorial or tensorial transformation properties.

In quantum mechanics, for a given irreducible representation $[m, s]$ of the Poincaré group, the Pauli–Lubanski 4-vector operator w is related to the canonical (or "physical") spin $\mathbf{S}$ through the momentum operators P^μ (for $m > 0$) as follows:

$$\Lambda_{(\hat{P})} \cdot \omega/m = (0, \mathbf{S}), \tag{1.1}$$

where

$$\Lambda_{(\hat{P})} = I - \frac{(\hat{P} + \hat{K}) \otimes (\hat{P} + \hat{K})}{(\hat{P} + \hat{K}) \cdot \hat{P}} + 2\hat{K} \otimes \hat{P} \tag{1.2}$$

with

$$\hat{P} = P \cdot (P^2)^{-\frac{1}{2}}, \quad \hat{K} = (1, \mathbf{0}), \quad \Lambda_{(\hat{P})} \cdot \hat{P} = \hat{K}.$$

Under Lorentz transformation, $\langle \mathbf{S} \rangle$ undergoes a Wigner rotation R_W about the same axis as the initial momentum $\mathbf{p}$. [For details and notations see Appendix A of Ref. 1(b).] The transition to the case ($m = 0$) is discussed in Ref. 1(a).

Suppose now that we consider a field theoretic vector (or axial vector) current operator $j(x)$ and introduce the operator

$$\tilde{j}(x) = \tfrac{1}{2}(\Lambda_{(\hat{P})} \cdot j(x) + j(x) \cdot \Lambda^{\mathrm{tr}}_{(\hat{P})}), \tag{1.3}$$

where we have symmetrized, since, unlike w^μ, $j^\mu(x)$ does not commute with P^ν. The action of this operator $\tilde{j}(x)$ is well-defined in terms of those of j and P, for all states of nonzero total mass. We have

$$\tilde{j}^0(x) = \tfrac{1}{2}(\hat{P} \cdot j(x) + \text{h.c.}), \tag{1.4}$$

$$\tilde{\mathbf{j}}(x) = j(x) - \tfrac{1}{2}\{[\hat{P}/(1 + \hat{P}^0)](\hat{P} \cdot j(x) + j^0(x)) + \text{h.c.}\}, \tag{1.5}$$

where the terms h.c. are obtained by transposing the P^μ's to the right.

Considering a Lorentz transformation operator $U(\Lambda)$ such that

$$U(\Lambda) j(x) U(\Lambda)^{-1} = \Lambda^{-1} \cdot j(x') \quad (x' = \Lambda \cdot x), \tag{1.6}$$

$$U(\Lambda) P U(\Lambda)^{-1} = \Lambda^{-1} \cdot P, \tag{1.7}$$

we obtain, by definition,

$$U(\Lambda) \tilde{j}(x) U(\Lambda)^{-1} = (\Lambda_{(\hat{P})} \cdot \Lambda \cdot \Lambda^{-1}_{(\Lambda^{-1} \cdot \hat{P})})^{-1} \tilde{j}(x') + \text{h.c.} \tag{1.8}$$

Equation (1.8) has the following content. While $^0(x)$

[1] A. Chakrabarti, (a) J. Math. Phys. 7, 949 (1966); (b) Nuovo Cimento 43A, 576 (1966). These two contain references to our previous articles and other relevant works.

transforms [as is evident from (1.4)] as a scalar, $\tilde{\mathbf{j}}(x)$ is multiplied by a rotation matrix $R_W^{-1}(\Lambda, \mathrm{P})$ involving the operator $\hat{P}$ (and further, the product is to be symmetrized).

The Wigner rotation matrices $R_W(\Lambda, p)$, obtained on replacing the operators P^μ by some momentum eigenvalues p^μ, are given explicitly in Ref. 1(b).

Here we may mention briefly that when Λ is a rotation, $R_W(\Lambda, \hat{p})$ reduces to the same rotation; and when Λ is a pure Lorentz transformation, $R_W(\Lambda, \hat{p})$ denotes a rotation around the axis $\mathbf{u} \times \mathbf{u}''$, where

$$\Lambda \cdot (1, \mathbf{0}) = u'', \quad \Lambda^{-1} \cdot \hat{p} = u,$$
$$\hat{p} \equiv u' = \Lambda\Lambda^{-1} \cdot \hat{p} = \Lambda \cdot u. \tag{1.9}$$

The angle of rotation is given by

$$\sin \omega = \frac{(1 + u^0 + u'^0 + u''^0)}{(1 + u^0)(1 + u'^0)(1 + u''^0)} |\mathbf{u} \times \mathbf{u}''|. \tag{1.10}$$

Comparing (1.4) and (1.5) with (1.1), we notice the following main differences.

First, $\tilde{\mathbf{j}}^0$ is not zero identically. (We discuss the physical significance of this scalar in a following section.) Secondly, the noncommutativity of $j^\mu_{(x)}$ and P^ν has the consequence that when we consider the matrix elements of $\tilde{\mathbf{j}}$ between initial and final states $|p\rangle_i$, $|p'\rangle_f$, such that $\hat{p} \neq \hat{p}'$, then $U(\Lambda)$ leads to the form

$$\tfrac{1}{2}\big(R_w^{-1}(\Lambda, \hat{p}) + R_w^{-1}(\Lambda, \hat{p}')\big) \cdot \tilde{\mathbf{j}}(\Lambda \cdot x). \tag{1.11}$$

Of course, in considering expectation values for the same momentum eigenstate of one particle, or, more generally, for states belonging to the same eigenvalues of the operators $\hat{P}^\mu$ ($\mu = 0, \cdots, 3$) (of which $p' = p$, $m' = m$ is a particular case), these two matrices coincide and we do have a simple Wigner rotation. And in fact, it may be said that, in the case of transition matrix elements between states of different mass and momenta, we cannot *a priori* expect particularly simple transformation properties.

However, formally more convenient properties can be obtained by modifying the definition (1.3) as follows.

Let us now define the operator $\tilde{\mathbf{j}}(x)$ [instead of as in (1.3)] through the relation

$$\langle p', s_3'; [m', s'] | (\tilde{j}x) | p, s_3; [m, s] \rangle$$
$$= \Lambda_{(\hat{k})} \cdot \langle p's_3'; [m', s'] | j(x) | p, s_3; [m, s] \rangle, \tag{1.12}$$

where

$$\hat{k} \equiv (p + p')\{(p + p')^2\}^{-\frac{1}{2}}$$

and

$$\Lambda_{(\hat{k})} \cdot \hat{k} = (1, \mathbf{0}). \tag{1.13}$$

This definition corresponds to the formalism of Cheskov and Shirokov.[2] (See also the subsequent remarks in this section about their parametrization.)

It is to be noted that now we can no longer express $\tilde{j}(x)$ explicitly in terms of the operators $j(x)$ and P, but have to define $\tilde{j}(x)$ simply by defining all the matrix elements between momentum eigenstates forming a complete basis. The matrix elements are all well-defined [as long as those of $j(x)$ and P are so] if we exclude states such that

$$(p + p')^2 = 0.$$

Such a case can arise only when we consider initial and final states of zero-mass particles only, with collinear momenta. As for vacuum state expectation values, if we adopt the convention of considering the limiting processes $\mathbf{p} \to 0$ first and then $m \to 0$, then

$$\langle 0 | \tilde{j} | 0 \rangle = \langle 0 | j | 0 \rangle,$$

the right-hand side vanishes if an ordered form is implied. Since, however, we are interested in cases where at least one positive mass particle is involved, the above formal difficulties are not present.

As to the transformation property, we now have, as a consequence of (1.12),

$$\langle p', s_3' | \big(U(\Lambda) \tilde{j}(x) U(\Lambda)^{-1}\big) | p, s_3 \rangle$$
$$= (\Lambda_{(\hat{k}')} \cdot \Lambda \cdot \Lambda^{-1}_{(\Lambda^{-1}(\hat{k}))})^{-1} \cdot \langle p', s_3' | \tilde{j}(x') | p, s_3 \rangle. \tag{1.14}$$

Thus we now have our scalar ($\tilde{j}^0$) and three other components ($\tilde{\mathbf{j}}$) undergoing spinlike Wigner rotations.

Again from (1.12) we have

$$\left\langle \begin{matrix} -\mathbf{p}, s_3' \\ [m', s'] \end{matrix} \middle| j(x) \middle| \begin{matrix} \mathbf{p}, s_3 \\ [m, s] \end{matrix} \right\rangle = \left\langle \begin{matrix} -\mathbf{p}, s_3' \\ [m', s'] \end{matrix} \middle| j(x) \middle| \begin{matrix} \mathbf{p}, s_3 \\ [m, s] \end{matrix} \right\rangle. \tag{1.15}$$

Thus we can always establish a direct connection with the usual covariant formalism. But in fact the equality (1.15) can be generalized. Since the spin indices S_3, S_3' are always taken to refer to the projections of the "canonical spin operator" (1.1), we have for any pure Lorentz transformation Λ, *collinear to* $\mathbf{p}$,

$$\langle -\mathbf{p}, s_3' | j(0) | \mathbf{p}, s_3 \rangle = \langle -\mathbf{p}, s_3' | j(0) | \mathbf{p}, s_3 \rangle$$
$$= \langle \mathbf{p}''', s_3' | j(0) | \mathbf{p}'', s_3 \rangle, \tag{1.16}$$

where

$$\Lambda \cdot \big((\mathbf{p}^2 + m^2)^{\frac{1}{2}}, \mathbf{p}\big) = p'',$$
$$\Lambda \cdot \big((\mathbf{p}^2 + m'^2)^{\frac{1}{2}}, -\mathbf{p}\big) = p''', \tag{1.17a}$$

[2] A. A. Cheskov and Ju. M. Shirokov, (a) Nucl. Phys. **49**, 108 (1963); (b) Zh. Eksperim. i Teor. Fiz. **44**, 1982 (1963) [English transl.: Soviet Phys.—JETP **17**, 1333 (1963)] (Sec. 6, in particular).

all the 3-momenta being collinear and the covariant normalization

$$\langle p', s_3' \mid p, s_3\rangle = 2p^0\delta(\mathbf{p}' - \mathbf{p})\delta s_3 s_3' \qquad (1.17b)$$

being implied.

As a particular case, we have

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j(0)\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = \langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ \tilde{j}(0)\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = \langle \mathbf{0}, s_3'|\ \tilde{j}(0)\ |\eta\mathbf{k}, s_3\rangle, \qquad (1.18)$$

where

$$\eta = (1/2m')[(\tfrac{1}{4}\mathbf{k}^2 + m'^2)^{\frac{1}{2}} + (\tfrac{1}{4}\mathbf{k}^2 + m^2)^{\frac{1}{2}}]. \qquad (1.19)$$

Putting

$$-q^2 = (p' - p)^2 = [(\tfrac{1}{4}\mathbf{k}^2 + m'^2)^{\frac{1}{2}} - (\tfrac{1}{4}\mathbf{k}^2 + m^2)^{\frac{1}{2}}]^2 - \mathbf{k}^2, \qquad (1.20)$$

we have

$$\mathbf{k}^2 = \frac{[q^2 + (m' - m)^2][q^2 + (m' + m)^2]}{[q^2 + 2(m'^2 + m^2)]}, \qquad (1.21a)$$

$$= q^2, \text{ for } m' = m. \qquad (121.b)$$

For $m' \neq m$, $\mathbf{k}^2 \neq q^2$, but [as is besides evident from (1.21)] $\tilde{k}^2$ is still invariant for the trivial reason that it is *defined* to be the square of the 3-momentum exchange in the Breit frame and since $\mathbf{k}$ can differ at most by a rotation from its previous value when we come back to the Breit frame after arbitrary intermediate transformations.

Let us now develop the matrix element on the extreme right-hand side of (1.18), using the following notations:

$$\tilde{j}^0 = \tilde{j}^{(0)}, \qquad (1.22)$$

$$\tilde{j}^{(1)}_{(0)} = \tilde{j}^3, \quad \tilde{j}^{(1)}_{(\pm)} = \mp\frac{(\tilde{j}^1 \pm i\tilde{j}^2)}{\sqrt{2}}. \qquad (1.23)$$

[It is implied henceforth that we have $x = (0, 0, 0, 0)$ as argument.]

Developing $|\lambda\mathbf{k}, S_3\rangle$ in a series of products of spin and angular momentum eigenstates and using the standard CG coupling coefficients, we obtain (taking account of the transformation properties of $\tilde{j}^{(0)}$ and $\tilde{j}^{(1)}$ and noting that at left $\langle \mathbf{0}, S_3'|$ can have only zero orbital angular momentum),

$$\langle \mathbf{0}, s_3'|\ \tilde{j}(0)\ |\eta\mathbf{k}, s_3\rangle = \frac{1}{(2\pi)^3}\sum_L (-1)^M\left(\frac{4\pi}{2L+1}\right)^{\frac{1}{2}}(ss_3, LM \mid s's_3')\times \mathcal{F}^{(0)}_{ss',L}(\mathbf{k}^2)\mathcal{Y}^M_L(\mathbf{k}) \quad (M = s_3' - s_3), \qquad (1.24a)$$

$$\langle \mathbf{0}, s_3'|\ \tilde{j}^{(1)}_{(m)}\ |\eta\mathbf{k}, s_3\rangle = \frac{1}{(2\pi)^3}\sum_{L,j'} (-1)^M\left(\frac{4\pi}{2L+1}\right)^{\frac{1}{2}}(ss_3, LM \mid j'j_3')\times (j'j_3', 1m \mid s's_3')\mathcal{F}^{(1)'}_{ss',Lj'}(\mathbf{k}^2)\mathcal{Y}^M_L(\mathbf{k}) \quad (m = 0, \pm 1;\ j_3' = s_3' - m,\ M = j_3' - s_3) \qquad (1.24b)$$

(we do not indicate explicitly the dependence of the $\mathcal{F}$'s on the masses and other possible internal quantum numbers).

In the above definitions we have introduced the solid spherical harmonics [$\mathcal{Y}^M_L(\mathbf{k}) = |\tilde{k}|^L Y^M_L(\mathbf{k})$]. This amounts merely to a particular convention as regards the normalization of the form factors $\mathcal{F}(\mathbf{k}^2)$ [$= F(q^2)$, say, due to (1.21)], an invariant factor [see (1.21)] being extracted explicitly from the coefficient. [Introducing, for example, $\mathcal{Y}^M_L(\eta\mathbf{k})$ instead of $\mathcal{Y}^M_L(\mathbf{k})$, we again obtain a modified invariant factor, since η is a function of $\mathbf{k}^2$ and hence of q^2.]

Now from (1.16), (1.18), we note that *the same expressions* (1.24a), (1.24b) *hold also for the Breit frame matrix elements of* $\tilde{j}$ *and* j—and in fact for $\tilde{j}$ after any collinear pure Lorentz transformation, $\mathbf{k}$ being always defined to be the momentum obtained on reducing to the Breit frame through a pure Lorentz transformation.

It is, of course, possible to couple the angular momenta involved in (1.24b) in different ways. For example, using the formula (6.26) of Ref. 3, p. 95, we can rewrite (1.24b) as

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ \tilde{j}^{(1)}_{(m)}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\sum_{L,j}\frac{(-1)^M}{(2L+1)^{\frac{1}{2}}}(LM, 1m \mid jj_3)(ss_3, jj_3 \mid s's_3)\times \mathcal{F}^{(1)}_{ss',Lj}(\mathbf{k}^2)\mathcal{Y}^{-M}_L(\mathbf{k}) \quad (j^3 = s_3' - s_3), \qquad (1.25)$$

where the new form factors are linear combinations of the $\mathcal{F}^{(1)\prime}$s involving $6 - j$ symbols.

This is the form proposed in Ref. 2 (see, however, Ref. 4) and as compared to (1.24b) it has the merit that the matrix elements of the divergence ($\partial_\mu j^\mu$) assume a simpler form (see Appendix A), leading to a more direct physical significance of the form factors $\mathcal{F}^{(1)}$. For this reason we adopt (1.25).

Since we are dealing with states labeled with canonical spin indices, in an arbitrary frame we have [as a consequence of (1.14)]

$$\langle p', s_3'|\ \tilde{j}\ |p, s_3\rangle = \sum_{\sigma_3\sigma_3'}\mathcal{D}^{*(s')}_{\sigma_3's_3'}(\Lambda, \hat{p}')\mathcal{D}^{(s)}_{\sigma_3 s_3}(\Lambda, \hat{p})\times \langle -\tfrac{1}{2}\mathbf{k}, \sigma_3'|\ \tilde{j}\ |\tfrac{1}{2}\mathbf{k}, \sigma_3\rangle, \qquad (1.26)$$

where

$$\Lambda\cdot(p' + p) = ([(p' + p)^2]^{\frac{1}{2}}, \mathbf{0}),$$
$$(\mathbf{p}', \mathbf{p}) \xrightarrow{\Lambda} (-\tfrac{1}{2}\mathbf{k}, \tfrac{1}{2}\mathbf{k}).$$

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[3] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[4] In comparing (1.25) with Eq. (47) of Ref. 2 it should be noted that apart from other differences of convention we have a negative sign of $M(Y^{-M}_L)$ instead of Y_{LM} of Ref. 2. A positive sign would lead to quite incorrect results. In fact, though different couplings are possible, we should be careful about the corresponding sign of M. For example, it is indeed possible to have Y^M_L [or rather $Y^{-M}_L(-\mathbf{k})^*$] if, instead of (1.18), we start equivalently from $\langle -\eta\mathbf{k}, s_3'|\ j\ |\mathbf{0}, S_3\rangle$, corresponding to the coupling $(S's_3', LM\,|\,j''j_3'')(Ss_3, 1m\,|\,j''j_3'')$.

The corresponding matrix elements of the covariant vector operator are

$$\langle p', s_3'|\ j\ |p,s_3\rangle = \sum_{\sigma_3\sigma_3'} \mathfrak{D}^{(s')*}_{\sigma_3's_3'}(\Lambda, \hat{p}')\mathfrak{D}^{(s)}_{\sigma_3s_3}(\Lambda, \hat{p}) \times (\Lambda^{-1}\cdot\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle). \quad (1.27)$$

If j is taken to be a pure vector or pseudo-vector current, j, as may easily be verified, will have the same behavior under space and time reversals. Thus in the series (1.24a), (1.25) only odd or even harmonics appear, depending on the intrinsic parities of the initial and final states (assuming them to be pure parity states).

Time-reversal invariance leads to the usual reality conditions on the form factors. For conserved currents, we have again further restrictions. Some examples are discussed in Appendix A.

We have already noted that if we want to construct the operators explicitly in terms of j^μ and P^ν [as in (1.4), (1.5)], we cannot have the properties corresponding to (1.12). Considering, however, matrix elements *between states of equal mass*, we have in the Breit frame [denoting the right-hand side of (1.3) by j' in order to distinguish it from (1.12)], from (1.4), (1.5),

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j'^{(0)}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{k^0}{m}\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j^0\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle, \quad (1.28)$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ \tilde{\mathbf{j}}'^{(1)}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = \langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ \mathbf{j} - \frac{\mathbf{k}(\mathbf{k}\cdot\mathbf{j})}{4(m+k^0)}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle \quad [k^0 = (\tfrac{1}{4}\mathbf{k}^2 + m^2)^{\frac{1}{2}}]. \quad (1.29)$$

Thus we see that for *conserved currents*, we have effectively the same equality as (1.16) between the matrix elements of j' and j. Only there is the extra factor k^0/m in (1.28). Hence, in particular, the electromagnetic form factors, as studied in Sec. 2, have a simple interpretation in terms of j' also. For the general cases, j' leads to more complicated behavior. As for the matrix elements of j' between states of the same mass and momenta, they are just equal to the corresponding rest frame matrix elements of j (or j).

In Sec. 5 we again consider an explicit construction (for the canonical spin operator) in terms of the covariant current and momentum operators.

2. COMPARISON WITH THE COVARIANT FORMALISM AND PHYSICAL INTERPRETATIONS

A. Nucleon Electromagnetic Form Factors

In order to compare our formalism with more familiar ones, let us start by considering the simple but important case of nucleon electromagnetic form factors.

For $s' = s = \frac{1}{2}$, we have [from (1.24, 1.25)], utilizing the parity restrictions (and the covariant normalization) for the vector current j^v,

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j^{(0)v}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle = [1/(2\pi)^3]\mathcal{F}^{(0)v}_{\frac{1}{2}\frac{1}{2},0}(\mathbf{k}^2)\delta_{s_3s_3'} \quad (2.1)$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\ j^{(1)v}_{(m)}\ |\tfrac{1}{2}\mathbf{k}, s_3\rangle, = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\frac{(-1)^M}{\sqrt{3}}[(1M, 1m\mid 00)\delta_{s_3s_3'}\mathcal{F}^{(1)v}_{\frac{1}{2}\frac{1}{2},10}(\mathbf{k}^2) + (1M, 1m\mid 1s_3' - s_3)(\tfrac{1}{2}s_3', 1s_3' - s_3\mid \tfrac{1}{2}s_3') \times \mathcal{F}^{(1)v}_{\frac{1}{2}\frac{1}{2},11}(\mathbf{k}^2)]\mathcal{Y}_1^{-M}(\mathbf{k}). \quad (2.2)$$

When we have the same particle (such as a nucleon) as initial and final states ($m' = m$ and similarly for other internal quantum numbers), the combined restrictions due to Hermiticity and T invariance lead to

$$\mathcal{F}^{(1)v}_{\frac{1}{2}\frac{1}{2},10}(\mathbf{k}^2) = 0. \quad (2.3)$$

In this particular case, this restriction coincides with that due to the conservation condition

$$k_{(0)}\langle j^{(1)}_{(0)}\rangle - k_{(+)}\langle j^{(1)}_{(-)}\rangle - k_{(-)}\langle j^{(1)}_{(+)}\rangle = 0. \quad (2.4)$$

(See Appendix A for more general considerations on this point for arbitrary spin.)

Thus for

$$s_3' = s_3 = +\tfrac{1}{2}$$

we have

$$+\langle j^{(0)v}\rangle_+ = \frac{1}{(2\pi)^3}\mathcal{F}^{(0)v}_{\frac{1}{2}\frac{1}{2},0}(\mathbf{k}^2), \quad +\langle j^{(1)v}_{(0)}\rangle_+ = 0, \quad +\langle j^{(1)}_{(\pm)}\rangle_+ = \pm\frac{\mathcal{F}^{(1)v}_{\frac{1}{2}\frac{1}{2},11}(\mathbf{k}^2)}{(2\pi)^3}\frac{k_{(\pm)}}{6^{\frac{1}{2}}}. \quad (2.5)$$

Now, in order to compare, let the covariant form factors be defined [corresponding to the covariant normalization (1.17b)] as

$$\langle p', s_3|\ j_\mu\ |p, s_3\rangle = \frac{1}{(2\pi)^3}\bar{u}_{s_3'}(\mathbf{p})(F_1(q^2)\gamma_\mu + iF_2(q^2)\sigma_{\mu\nu}q_\nu)u_{s_3}(\mathbf{p}) \quad (q = p' - p). \quad (2.6)$$

For the purpose of explicit calculations we can write the solutions corresponding to the canonical spin indices (s_3', s_3) in a rather symmetrical form as

$$u_+(p) = \frac{1}{2[m(p^0+m)]^{\frac{1}{2}}}\begin{vmatrix} m + p^0 + p^3 \\ p^1 + ip^2 \\ m + p^0 - p^3 \\ -p^1 - ip^2 \end{vmatrix}, \qquad u_-(p) = \frac{1}{2[m(p^0+m)]^{\frac{1}{2}}}\begin{vmatrix} p^1 - ip^2 \\ m + p^0 - p^3 \\ -p^1 + ip^2 \\ m + p^0 + p^3 \end{vmatrix}, \quad (2.7)$$

where we have utilized the following representation of the γ matrices,

$$\gamma^0 = \begin{vmatrix} & I_2 \\ I_2 & \end{vmatrix}, \quad \boldsymbol{\gamma} = \begin{vmatrix} & -\boldsymbol{\tau} \\ \boldsymbol{\tau} & \end{vmatrix}, \quad \gamma^5 = \begin{vmatrix} I_2 & \\ & -I_2 \end{vmatrix}, \tag{2.8}$$

and the normalization is

$$\bar{u}(p)u(p) = 1, = (m/p^0)u^*(p)u(p). \tag{2.9}$$

Comparing (2.2), (2.5), and (2.6) we have

$$\mathcal{F}^{(0)v}_{\frac{1}{2}\frac{1}{2},0}(q^2) = F_1(q^2) + (q^2/2m)F_2(q^2) = F_{\text{ch}}(q^2),$$
$$\mathcal{F}^{(1)v}_{\frac{1}{2}\frac{1}{2},11}(q^2) = 6^{\frac{1}{2}}\{[F_1(q^2)/2m] + F_2(q^2)\} = 6^{\frac{1}{2}}F_{\text{mag}}(q^2). \tag{2.10}$$

The appearence of such a factor as $6^{\frac{1}{2}}$, of course, depends upon the conventions adopted [such as the explicit appearance of the factor $(2L+1)^{-\frac{1}{2}}$ in (1.25)]. What is important for our purpose is the direct proportionality with the famous linear combinations of F_1 and F_2, giving F_{ch} and F_{mag}, respectively.

In our formalism $j^{(0)}$ is a scalar and $j^{(1)}$ has spin-like transformation properties (Wigner rotations). As we have seen above, this automatically separates out the electric and magnetic properties corresponding to the familiar combinations (2.10). This is more than merely a technique for carrying through spherical harmonic expansions for the matrix elements of j^μ in one particular frame (namely, the Breit frame). The electric charge being a scalar, and the magnetic properties being related to spin, they correspond [and that not only in one particular reference frame, as is seen from (1.16) and (1.21)] directly to $j^{(0)}$ and $j^{(1)}$, respectively.

Thus, the separation of $j(x)$ into $j^{(0)}(x)$ and $j^{(1)}(x)$ has a significant physical basis.

Some other examples for different spins are considered in Appendix A. We now pass on to the case of the axial currents.

B. Axial Form Factors

For spin $\frac{1}{2}$ ($s' = s = \frac{1}{2}$), we have for the matrix elements of axial currents *between states of the same parity*:

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3' | \, j^{(0)A} | \tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\frac{(-1)^M}{\sqrt{3}}(\tfrac{1}{2}s_3, 1M \mid \tfrac{1}{2}s_3')\mathcal{F}^{(0)A}_{\frac{1}{2}\frac{1}{2},1}(\mathbf{k}^2)\mathcal{Y}_1^{-M}(\mathbf{k}) \qquad (M = s_3' - s_3) \tag{2.11}$$

and

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3' | \, j^{(0)A}_{(m)} | \tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\Big\{(\tfrac{1}{2}s_3, 1m \mid \tfrac{1}{2}s_3')\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},01}(\mathbf{k}^2)\mathcal{Y}_0^0(\mathbf{k}) + \frac{(-1)^M}{5^{\frac{1}{2}}} \times (2M, 1m \mid 1j_3)(\tfrac{1}{2}s_3, 1j_3 \mid \tfrac{1}{2}s_3')\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},21}(\mathbf{k}^2)\mathcal{Y}_2^{-M}(\mathbf{k})\Big\}. \tag{2.12}$$

When the initial and final states correspond to the same particle, Hermiticity and T-invariance restrictions lead to

$$\mathcal{F}^{(0)A}_{\frac{1}{2}\frac{1}{2},1}(\mathbf{k}^2) = 0. \tag{2.13}$$

The corresponding feature in the covariant formalism consists in writing the nucleon matrix elements in the form

$$\langle p', s_3' | \, j_\mu^A | p, s_3\rangle = \bar{u}_{s_3'}(p') \times [F_1^A(\mathbf{k}^2)\gamma_\mu + F_2^A(\mathbf{k}^2)(p'-p)^\mu]\gamma^5 u_{s_3}(p) \tag{2.14}$$

and suppressing such a term as

$$\bar{u}_{s_3'}(p')\sigma_{\mu\nu}(p'-p)_\nu\gamma^5 u_{s_3'}(p). \tag{2.15}$$

[Sometimes G parity is invoked (p. 307, Ref. 5) in order to eliminate this term.]

Thus we see that our formalism brings to attention in a very natural way the *symmetrized* scalar (corresponding $j^{(0)}$)

$$(P\cdot j + j\cdot P) \tag{2.16}$$

and displays its physical significance. Usually only the antisymmetrized scalar

$$i(P\cdot j - j\cdot P) \tag{2.17}$$

is singled out through the conservation or partial conservation condition.

Considering electromagnetic vector currents, we have seen that (2.16) leads to the charge form factors in any frame. Now, for axial currents we find that the restrictions due to Hermiticity and T invariance have the very simple consequence of reducing the expectation values of (2.16) to zero. These features hold for arbitrary spin. Some cases are treated explicitly in Appendix A.

We may also note that the matrix elements of $j^{(0)}A$ between states of the same 4-velocity p/m (or in particular, the same momentum $\mathbf{p}$ and mass m) and the same intrinsic parity, are always zero, since such elements

$$\langle \hat{p}, s_3' | \, j^{(0)A} | \hat{p}, s_3\rangle = \langle \mathbf{0}, s_3' | \, j^{(0)A} | \mathbf{0}, s_3\rangle = 0 \tag{2.18}$$

through parity restrictions.

[5] J. D. Jackson, in *Elementary Particle Physics and Field Theory* (W. A. Benjamin Inc., New York, 1963), Vol. 1.

More generally, we may say that, separating a nonconserved current into its so-called "transverse" and "longitudinal" parts, is

$$j_\mu = \{j_\mu - \partial\mu(\partial_\nu j_\nu/\Box)\} + \partial\mu(\partial_\nu j_\nu/\Box); \quad (2.19)$$

we have for the longitudinal part

$$[P^\mu, [P_\mu, (\partial_\nu j_\nu/\Box)]_-]_+ = [P^2, (\partial_\nu j_\nu/\Box)]. \quad (2.20)$$

Hence for the nonconserved longitudinal part, the matrix elements of the symmetrized scalar are *proportional to the mass difference* between the initial and the final states.

If corresponding to the anticommutator in (2.16) [instead of the commutator in (2.17)] we introduce the term "anticonservation," that the axial current cannot be fully "anticonserved" follows immediately by considering the matrix element

$$\langle 0|\,(P\cdot j^A + j^A\cdot P)\,|\pi\rangle \quad (2.21)$$

exactly as for the divergence (Ref. 5, p. 313). In fact we have already seen that (2.16) is directly related to the mass difference.

Let us now consider the form factors $\mathcal{F}^{(1)A}$. Comparing (2.12) and (2.14) we obtain

$$\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},01}(\mathbf{k}^2) = \frac{\sqrt{3}}{2m}\Big[F_1^A(\mathbf{k}^2)(k^0+m) + \left(\frac{F_1^A(\mathbf{k}^2)}{4(k^0+m)} - F_2^A(\mathbf{k}^2)\right)\frac{\mathbf{k}^2}{3}\Big], \quad (2.22)$$

$$\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},21}(\mathbf{k}^2) = \left(\frac{5}{6}\right)^{\frac{1}{2}}\frac{1}{m}\left\{\left[\frac{F_1^A(\mathbf{k})}{2(k^0+m)} + F_2^A(\mathbf{k})^2\right]\right\}. \quad (2.23)$$

For small momentum exchange, keeping terms only up to $\mathbf{k}^2$, we obtain

$$\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},01}(\mathbf{k}^2) = \frac{\sqrt{3}}{2m}\Big[2mF_1^A(0) + \mathbf{k}^2\left\{\frac{1}{6m}F_1^A(0) - \tfrac{1}{3}F_2^A(0) + 2mF_1^{A\prime}(0)\right\}\Big], \quad (2.24)$$

$$\mathcal{F}^{(1)A}_{\frac{1}{2}\frac{1}{2},21}(\mathbf{k}^2) = \frac{1}{m}\left(\frac{5}{6}\right)^{\frac{1}{2}}\Big[\left(\frac{F_1^A(0)}{4m} + F_2^A(0)\right) + \mathbf{k}^2\left\{-\frac{F_1^A(0)}{64m^2} + \frac{F_1^{A\prime}(0)}{4m} + F_2^{A\prime}(0)\right\}\Big] \quad \left(F'_{1,2}(0) = \frac{\partial}{\partial\mathbf{k}^2}F_{1,2}(\mathbf{k}^2)\Big|_{\mathbf{k}^2=0}\right). \quad (2.25)$$

If we postulate the usual "partial conservation" condition

$$\partial_\mu j^{\mu A}_{(x)} = C\varphi(x), \quad (2.26)$$

then, taking the matrix elements of both sides between proton and neutron states in the Breit frame, we have from (2.12) (neglecting $M_p - M_n$),

$$C_{(p)}\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,\varphi(0)\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle_{(n)} = -i\mathbf{k}\cdot{}_{(p)}\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,\hat{j}^{(A)}_{(0)}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle_{(n)}, = \frac{i(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\frac{(-1)^M}{\sqrt{3}}(\tfrac{1}{2}s_3, 1M\,|\,\tfrac{1}{2}s_3') \times \left(\mathcal{F}^{(1)A}_{np,01}(\mathbf{k}^2) - (\tfrac{2}{5})^{\frac{1}{2}}\mathcal{F}^{(1)A}_{np,21}(\mathbf{k}^2)\cdot\mathbf{k}^2\right)\mathcal{Y}_1^{-M}(\mathbf{k}). \quad (2.27)$$

If we want to express the combination of canonical form factors appearing in (2.27) in terms of the covariant ones, we have from (2.22) and (2.23),

$$\left(\mathcal{F}^{(1)A}_{np,01}(\mathbf{k}^2) - (\tfrac{2}{5})^{\frac{1}{2}}\mathcal{F}^{(1)A}_{np,21}(\mathbf{k}^2)\right) = \frac{\sqrt{3}}{2m}\Big[(k^0+m)F^A_{(np)1}(\mathbf{k}^2) - \frac{1}{4(k^0+m)}F^A_{(np)1}(\mathbf{k}^2) - F^A_{(np)2}(\mathbf{k}^2)\Big]. \quad (2.28)$$

Thus even in the simplest cases the explicit momentum dependence comes out in a simpler and neater form in the canonical formalism, leading to a more direct physical significance of the form factors. Besides, quite generally (i.e., whenever we can exclude extremely steep variations of the form factors concerned with respect to the momentum exchange), the predominance of each term over the succeeding one is very evident in our formalism for sufficiently small momentum exchange.

The general formula for the matrix elements of the divergence along with some particular cases is given in Appendix A.

3. APPLICATIONS TO THE LIMITING CASE OF INFINITE MOMENTUM AND SMALL MOMENTUM EXCHANGE

With a view to subsequent applications to current algebras[6] we now work out the necessary canonical kinematics of the above-mentioned case.

Consider first the matrix element

$$\left\langle \begin{matrix}\mathbf{K}-\frac{1}{2}\mathbf{k}, s_3' \\ [m', s']\end{matrix}\right|\hat{j}\left|\begin{matrix}\mathbf{K}+\frac{1}{2}\mathbf{k}, s_3 \\ [m, s]\end{matrix}\right\rangle, \quad (3.1)$$

where j stands for any one of $j^{(0)}$ or $j^{(1)}_{(m)}$ $(m = 0, \pm 1)$. We are not concerned, for the moment, with other possible internal quantum numbers.

Our purpose is to express (3.1) in terms of the Breit frame matrix elements through (1.26), in the limit when

$$|\mathbf{K}| \to \infty$$

and keeping terms only up to $\mathbf{k}^2$ ($|\mathbf{k}|$ is supposed to be sufficiently small for $|\mathbf{k}^3|$ and higher powers are neglected).

[6] R. Dashen and M. Gell-Mann, (a) *Proceedings of the Third Coral Cables Conference* (W. H. Freeman and Company, San Francisco California, 1966); (b) Phys. Rev. Letters 17, 340 (1966).

The components of $\mathbf{k}$ parallel and perpendicular to $\mathbf{K}$ are denoted, respectively, by $\mathbf{k}_{\|}$ and $\mathbf{k}_{\perp}$. We need not suppose $\mathbf{k}_{\|} = 0$ to start with; it will automatically be eliminated in the limit considered.

The transformation to the Breit frame corresponds to a pure Lorentz transformation $\Lambda(u)$ corresponding to the 4-velocity u, having the limiting form

$$\mathbf{u} = \mathbf{K}/\lambda, \quad u^0 = |\mathbf{K}|/\lambda + \lambda/2\,|\mathbf{K}|, \tag{3.2}$$

where

$$\lambda = [\tfrac{1}{2}(m'^2 + m^2) + (\tfrac{1}{2}\mathbf{k}_{\perp})^2]^{\frac{1}{2}} = \kappa\big(1 - (\tfrac{1}{2}\mathbf{k}_{\perp})^2/2\kappa\big) \tag{3.3a}$$

with

$$\kappa = [\tfrac{1}{2}(m'^2 + m^2)]^{\frac{1}{2}}. \tag{3.3b}$$

The limiting forms of the Wigner-rotation matrices appearing in (1.26) are quite simple. We have, for the above $\mathbf{u}$ and $(\mathbf{p}, \mathbf{p}') = (\mathbf{K} \pm \tfrac{1}{2}\mathbf{k})$,

$$(\mathbf{\Lambda}(u)\cdot\mathbf{p}) = \tfrac{1}{2}\mathbf{k}_{\perp} - \frac{m^2 - m'^2}{4\lambda}\hat{K} = -(\mathbf{\Lambda}(u)\cdot\mathbf{p}') \qquad (\hat{K} = \mathbf{K}/|\mathbf{K}|), \tag{3.4}$$

$$\mathfrak{D}^{(s)}(\Lambda, \hat{p}) = I_s + (1/2\xi)\{i(\mathbf{s}\times\mathbf{k}_1)\cdot\hat{K}\} + (1/8\xi^2)\{i(\mathbf{s}\times\mathbf{k}_{\perp})\cdot\hat{K}\}^2. \tag{3.5}$$

Where, for example, for $\mathbf{K} \to (0, 0, \infty)$, we have

$$i(\mathbf{s}\times\mathbf{k}_{\perp})\cdot\hat{K} = i(s^1k^2 - s^2k^1) \tag{3.6a}$$

$$= (s_{(+)}k_{(-)} - s_{(-)}k_{(+)}), \tag{3.6b}$$

and we have used the notation

$$\frac{1}{\xi} = \frac{4(\kappa + m)}{4\kappa(\kappa + m) + (m^2 - m'^2)} \tag{3.7}$$

$$= 1/m \quad (\text{for } \kappa = m' = m). \tag{3.8}$$

For $D^{(s')}(\Lambda, \hat{p}')$ we have to change the sign of $\mathbf{k}$ and interchange m and m', leading to

$$\frac{1}{\xi'} = \frac{4(\kappa + m')}{4\kappa(\kappa + m) + (m'^2 - m^2)}. \tag{3.9}$$

The explicit formulas for $D^{(s)}$ for $s = \frac{1}{2}, 1, \frac{3}{2}$ are given in Appendix B. In fact, due to the simple forms of the matrices $S_{(\pm)}$, the general case presents no difficulty, the only nonzero elements being $D^{(s)}_{(m,n)}$ $(n = m, m \pm 1, m \pm 2; m = -s, \cdots, s)$.

Remembering the transformation properties of $\tilde{j}$, we obtain, up to second order in $\mathbf{k}$, the general expression,

$$\begin{aligned}
\langle \mathbf{K} - \tfrac{1}{2}\mathbf{k}, s_3'|\,\tilde{j}\,|\,\mathbf{K} + \tfrac{1}{2}\mathbf{k}, s_3\rangle &= \langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3'|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3\rangle + \sum_{\pm}\frac{k_{(\pm)}}{2\sqrt{2}\,\xi}\{(s \pm s_3)(s \mp s_3 + 1)\}^{\frac{1}{2}}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3'|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3 \mp 1\rangle \\
&+ \sum_{\pm}\frac{k_{(\pm)}}{2\sqrt{2}\,\xi'}\{(s' \mp s_3')(s' \pm s_3' + 1)\}^{\frac{1}{2}}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3' \pm 1|\,\tilde{j}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle \\
&+ \sum_{\pm}\frac{(k_{\pm})^2}{8\xi^2}\{(s \mp s_3 + 1)(s \mp s_3 + 2)(s \pm s_3 - 1)(s \pm s_3)\}^{\frac{1}{2}}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3'|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3 \mp 2\rangle \\
&+ \sum_{\pm}\frac{(k_{\pm})^2}{8\xi^2}\{(s' \pm s_3' + 1)(s' \pm s_3' + 2)(s' \mp s_3' - 1)(s' \mp s_3')\}^{\frac{1}{2}}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3' \pm 2|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3\rangle \\
&+ \sum_{\pm}\frac{k_{-}k_{+}}{8\xi\xi'}\{(s \pm s_3)(s \mp s_3 + 1)(s' \pm s_3')(s' \mp s_3' + 1)\}^{\frac{1}{2}}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3' \mp 1|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3 \mp 1\rangle \\
&+ \frac{k_{-}k_{+}}{8}\left\{\frac{1}{\xi^2}[s(s+1) - s_3^2] + \frac{1}{\xi_2'}[s'(s'+1) - s_3'^2]\right\}\langle -\tfrac{1}{2}\tilde{\mathbf{k}}, s_3'|\,\tilde{j}\,|\tfrac{1}{2}\tilde{\mathbf{k}}, s_3\rangle.
\end{aligned} \tag{3.10a}$$

Here

$$\tilde{\mathbf{k}} = \mathbf{k}_{\perp} - [(m^2 - m'^2)/\lambda]\hat{K}$$

and the invariant momentum exchange

$$-q^2 = -\mathbf{k}_{\perp}^2.$$

In the matrix elements appearing as the coefficients of $k_{-}k_{+}$ or $(k_{\pm})^2$, only terms of order zero in $|\mathbf{k}|$ are to be retained and so on. Thus in the usual cases, most of these terms are automatically eliminated.

As an illustrative example, let us (with a view to subsequent applications) write down explicitly (3.10a) up to second order for a particular case.

With the further supposition that not only $|\mathbf{k}|^3$ but also $|\tilde{\mathbf{k}}|^3$ in (3.10a) is small enough to be neglected, namely, *supposing that we need take into account the mass-difference effects only up to second order*, we

obtain (for states of the same parity)

$$\left\langle \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, s_3+1 \\ [m', s'] \end{matrix} \middle| (j^{(0)v} + j^{(1)v}_{(0)}) \middle| \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, s_3 \\ [m, s] \end{matrix} \right\rangle$$

$$= \frac{k_{(-)}}{(2\pi)^3}\Big[\delta_{ss'}\{(s-s_3)(s+s_3+1)\}^{\frac{1}{2}}\frac{1}{2}\Big(\frac{1}{\xi}+\frac{1}{\xi'}\Big)(\mathcal{F}^{(0)v}_{ss,0}(0) - \zeta\mathcal{F}^{(1)v}_{ss,10}(0))$$

$$- (ss_3, 11 \mid s's_3+1)\frac{1}{\sqrt{2}}\mathcal{F}^{(1)v}_{ss',11}(0) - (ss_3, 21 \mid s's_3+1)\Big(\frac{1}{\sqrt{2}}\mathcal{F}^{(1)v}_{ss',12}(0) + \frac{\zeta}{2}\mathcal{F}^{(0)v}_{ss',2}(0)\Big)$$

$$+ \Big\{\frac{1}{2\sqrt{2}\,\xi}[(s-s_3)(s+s_3+1)]^{\frac{1}{2}}(ss_3+1, 20 \mid s's_3+1)$$

$$+ \frac{1}{2\sqrt{2}\,\xi'}[(s'-s_3')(s'+s_3'+1)]^{\frac{1}{2}}(ss_3, 20 \mid s's_3)\Big\}\zeta\mathcal{F}^{(1)v}_{ss',12}(0), \qquad (3.10b)$$

where

$$\zeta = (m^2 - m'^2)/2[\tfrac{1}{2}(m^2+m'^2)]^{\frac{1}{2}}.$$

Further, when we have the same initial and final particle, all but one $\mathcal{F}^{(1)v}$ terms disappear (since only $L = j$ terms survive due to Hermiticity and T invariance, as noted in Appendix A).

Before proceeding further we must decide whether or not we choose to retain the covariant normalization for scalar product (1.17b).

In connection with the infinite momentum limit the normalization usually adopted is

$$\langle p', s_3' \mid p, s_3\rangle = \delta(\mathbf{p}'-\mathbf{p})\delta s_3' s_3. \qquad (3.11)$$

The reason is that the commutation relations and the definitions of such operators as the multipole moments are written down in terms of the covariant components of j, and corresponding to transformation $\Lambda_{(u)}$ of (3.2), we have

$$\lim_{K\to(0,0,\infty)} \Lambda^{-1}_{(u)}\cdot j = \frac{|\mathbf{K}|}{\lambda}(j^0+j^3, 0, 0, j^0+j^3). \qquad (3.12)$$

Hence in calculating for the covariant components

$$\langle \mathbf{K}-\tfrac{1}{2}\mathbf{k}, s_3' \mid j \mid \mathbf{K}+\tfrac{1}{2}\mathbf{k}, s_3\rangle,$$

we have to replace j^μ in the Breit frame matrix elements on the right-hand side of (3.10a) by (3.12) if we use the covariant normalization. But if instead we adopt (3.11), then (3.12) is replaced by

$$\frac{(\tilde{k}^0\tilde{k}'^0)^{\frac{1}{2}}}{\lambda}(j^0+j^3, 0, 0, j^0+j^3)$$
$$[\tilde{k}^0 = (\tilde{\mathbf{k}}^2+m^2)^{\frac{1}{2}}, \tilde{k}'^0 = (\tilde{\mathbf{k}}^2+m'^2)^{\frac{1}{2}}], \qquad (3.13)$$

and thus the infinite factor is eliminated. So far as the extraction of information from the current commutation relations is concerned, the question of normalization is not an essential one, since in either case what we effectively retain is the coefficient (nonzero) of the highest power of $|\mathbf{K}|$. On the other hand, in defining a physical magnitude (such as a multipole moment), the normalization must be chosen to assure a correct physical behavior in the limiting case.

In any case, in what follows *in this section*, we adopt (3.11) in order to conform to usual practice.

Let us illustrate the possible applications of our formalism to current algebras by considering the expression

$$\lim_{K\to(0,0,\infty)} \left\langle \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, s_3' \\ [m, s] \end{matrix} \right| \times \Big[\int_{t=0} j^{0A}_{(x)}\, d^3x, \epsilon\cdot j^v(0)\Big] \left| \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, s_3 \\ [m, s] \end{matrix} \right\rangle = 0, \qquad (3.14)$$

where ϵ is an arbitrary 4-vector.

In the dispersion treatment in Ref. 7 studying the magnetic moment of the baryons, the authors assume that the integral over the intermediate states can be approximated by two discrete contributions.

Let us suppose that in a more general case the intermediate states are saturated by a certain number (say n) of states, each of a definite total mass and spin ($[m_i, \Sigma_i]$, $i = 1, 2, \cdots, n$). (We do not write explicitly other indices of internal symmetry. We may suppose, for example, that j^v_μ are the components of the isoscalar or isovector electromagnetic current and the integral is the corresponding axial charge.) Thus we have,

$$\sum_i \Big[\left\langle \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, s_3' \\ [m, s] \end{matrix} \right| j^{0A} \left| \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right| \epsilon\cdot j^v \left| \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, s_3 \\ [m, s] \end{matrix} \right\rangle$$
$$- \left\langle \begin{matrix} \mathbf{K}-\frac{1}{2}\mathbf{k}, s_3' \\ [m, s] \end{matrix} \right| \epsilon\cdot j^v \left| \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right| j^{0A} \left| \begin{matrix} \mathbf{K}+\frac{1}{2}\mathbf{k}, s_3 \\ [m, s] \end{matrix} \right\rangle\Big] = 0 \qquad (3.15)$$

[7] S. Fubini, G. Furlan, and C. Rossetti, Nuovo Cimento **43A**, 161 (1966); S. V. Mathur and L. K. Pandit, Phys. Rev. **147**, 965 (1966).

(σ_i is the z comp. of Σ_i). In order to express the matrix elements of j^{0A} (corresponding to the space integral) in terms of the Breit frame matrix elements, we have only to put $\mathbf{k}_\perp = 0$ in the expressions found for (3.1). This may easily be verified. [In fact, if we replace the charge by a more general Fourier transform of the density, it is useful to note that in (3.10a) we may add a finite $\mathbf{k}'$ to $\mathbf{K}$ without changing anything essential, since such a $\mathbf{k}$ may be absorbed in $\mathbf{K}$ without affecting its previous limiting behavior.] Thus we have the simple results,

$$\lim \left\langle \begin{matrix} \mathbf{K} + \tfrac{1}{2}\mathbf{k}, s_3' \\ [m, s] \end{matrix} \middle| j^{0A} \middle| \begin{matrix} \mathbf{K} + \tfrac{1}{2}\mathbf{k}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right\rangle = \left(\frac{2mm_i}{m^2 + m_i^2}\right)^{\frac{1}{2}} \left\langle \begin{matrix} -\tfrac{1}{2}\zeta_i \hat{K}, s_3' \\ [m, s] \end{matrix} \middle| (j^{0A} + j^{3A}) \middle| \begin{matrix} \tfrac{1}{2}\zeta_i \hat{K}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right\rangle, \tag{3.16}$$

where

$$\zeta_i = \frac{m^2 - m_i^2}{2[\frac{1}{2}(m^2 + m_i^2)]^{\frac{1}{2}}} = \frac{\frac{1}{2}(m^2 + m_i^2) - m_i^2}{[\frac{1}{2}(m^2 + m_i^2)]^{\frac{1}{2}}}. \tag{3.17a}$$

For the momentum exchange, we have, instead of (3.10b),

$$q^2 = 0. \tag{3.17b}$$

If we suppose [as for (3.10b)] that the effects of mass difference need only to be taken into account up to second order, we obtain *for states of the same intrinsic parity*,

$$\begin{aligned} &\left\langle \begin{matrix} -\tfrac{1}{2}\zeta_i \hat{K}, s_3' \\ [m, s] \end{matrix} \middle| (j^{0A} + j^{3A}) \middle| \begin{matrix} \tfrac{1}{2}\zeta_i \hat{K}, \sigma_i \\ [m_i, \Sigma_i] \end{matrix} \right\rangle \\ &= \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3} \left[\frac{1}{\sqrt{3}} (\Sigma_i \sigma_i, 10 \mid s s_3') \mathcal{F}^{(0)A}_{\Sigma_i S,1} \mathcal{Y}^0_1(\zeta_i \hat{K}) \right. \\ &\quad + (\Sigma_i \sigma_i, 10 \mid s s_3') \mathcal{F}^{(1)A}_{\Sigma_i S,01} \mathcal{Y}^0_1(\zeta_i \hat{K}) \\ &\quad \left. + \frac{1}{5^{\frac{1}{2}}} \left(\sum_{j=1,3} (20, 10 \mid j0)(\Sigma_i \sigma_i, j0 \mid s s_3') \mathcal{F}^{(1)A}_{\Sigma_i S,2j} \right) \mathcal{Y}^0_2(\zeta_i \hat{K}) \right]. \end{aligned} \tag{3.18}$$

(All the other necessary indices of the $\mathcal{F}$'s are supposed to be implied through i, and for k^2 we have zero. This should be taken into account in expressing $\mathcal{F}_{S\Sigma_i}$ in terms of $\mathcal{F}_{\Sigma_i S}$ through Hermiticity.) Thus no spin index summation is needed over σ_i, since always (independently of the approximation concerning ζi),

$$\sigma_i = s_3'$$

[similarly $\sigma_i = s_3$ in the second term of (3.15)]. Considering the products of expression (3.18) and (3.10b), we find that up to second order of smallness we need only retain the terms

$$\Sigma_i = s, \quad s \pm 1.$$

For states of opposite intrinsic parity, the odd and even harmonics are associated with $\mathcal{F}^{(1)A}$ and $\mathcal{F}^{(2)A}$, respectively.

From (3.10a) [of which (3.10b), is a particular example], (3.18b), we can develop (3.15) in powers of $|\mathbf{k}_\perp|$ by just collecting together the appropriate coefficients keeping systematically terms up to second order $|\mathbf{k}_\perp|^l$ ($l = 0, 1, 2$). We get the necessary restriction of the form factors implied by the current algebras in this limiting case.

4. CANONICAL FORM FACTORS FOR PHOTOPRODUCTION AMPLITUDES

We have discussed elsewhere [Ref. 1(a)] how to treat particles of zero and positive rest masses in a unified manner in the canonical formalism. Here, as an illustrative example, we give the canonical parametrization of the process

$$\gamma + A \to B + A, \tag{4.1}$$

where A is a particle of spin Σ_a and B of spin zero. [In Ref. 7 such a photoproduction amplitude is related to the commutator (3.14) through the partial conservation hypothesis.]

In fact, the representation proposed in Ref. 1(a) gives directly the vector potential A for photons, *in the Coulomb gauge*. The relation between the Wigner representation and Coulomb gauge vector potentials has been discussed by Weinberg and also by Moses.[8] We would like to point out that if instead of passing via the little group (two-dimensional Euclidean) one uses our representation, the correspondence with the potentials (for any spin) takes the most direct form possible. (The details of the uses of the Coulomb gauge potential, where one no longer needs indefinite metric, are discussed in Ref. 9.)

For circularly polarized photons, for example, we get in our representation the wavefunctions[10]

$$\psi_\pm(\mathbf{p}) = \pm \frac{1}{\sqrt{2}} \begin{vmatrix} (\hat{n}_1 \pm i\hat{n}_2)_{(-)} \\ -(\hat{n}_1 \pm i\hat{n}_2)_{(0)} \\ (\hat{n}_1 \pm i\hat{n}_2)_{(+)} \end{vmatrix}, \tag{4.2}$$

where $\hat{n}_1$, $\hat{n}_2$, and $\hat{p}$ ($= \mathbf{p}/|\mathbf{p}|$) are mutually orthogonal unit vectors. The spherical components of $\hat{n}_{1,2}$ are defined in terms of $\hat{p}(\theta, \varphi)$ as

$$\begin{aligned} \hat{n}_{1(0)} &= -\sin\theta, & \hat{n}_{1(\pm)} &= \mp(e^{\pm i\varphi}/\sqrt{2}) \cos\varphi, \\ \hat{n}_{2(0)} &= 0, & \hat{n}_{2(\pm)} &= -(i/\sqrt{2}) e^{\pm i\varphi}. \end{aligned} \tag{4.3}$$

[8] S. Weinberg, Brandeis Lectures (1964) p. 405 ; H. E. Moses, Nuovo Cimento **42A**, 757 (1966).

[9] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (McGraw-Hill Book Company, Inc., New York, 1965).

[10] It should be noted that for helicity $\pm S$, the apparently slight difference between our canonical and the spinor representation [namely, transformation by $(P^0)^{\pm S}$] plays a decisive role in distinguishing the respective transformation properties.

The components of $\psi_{\pm(\mathbf{P})}$ are nothing but the spherical components of the Fourier transforms of the Coulomb gauge potential for circularly polarized photons $[0, \mathbf{A}(\mathbf{p})]$.

Maxwell's equations are often cast into the spinor form through combinations $(\mathbf{E} \pm i\mathbf{B})$. Here we are dealing directly with the three components of $\mathbf{A}$.

Following the technique indicated in Sec. V of Ref. 1(a), we obtain for the process (4.1) the following parametrization of the S-matrix elements in the center-of-mass system:

$$\left\langle \begin{matrix} \mathbf{p}', \sigma_a'; -\mathbf{p}', 0 \\ [m_a, \Sigma_a]; [m_b, 0] \end{matrix} \middle| S \middle| \begin{matrix} \mathbf{p}, \lambda; -\mathbf{p}, \sigma_a \\ [0, 1]; [m_a, \Sigma_a] \end{matrix} \right\rangle$$
$$= \sum_{\Sigma,(\Sigma' L),L'} 4m(m^2 - m_a^2)^{-\frac{1}{2}} \lambda^{-\frac{1}{4}}(m^2, m_a^2, m_b^2) \left(\frac{2L+1}{4\pi}\right)^{\frac{1}{2}}$$
$$\times (1\lambda, \Sigma_a\sigma_a \,|\, \Sigma'\sigma')(\Sigma'\sigma', L0 \,|\, \Sigma\sigma)$$
$$\times (\Sigma_a\sigma_a', L'M' \,|\, \Sigma\sigma) Y_{L'}^{M'}(\hat{p}') S_{\Sigma,(\Sigma' L),L'}, \tag{4.4}$$

where

$$m = (\mathbf{p}^2 + m_a^2)^{\frac{1}{2}} + |\mathbf{p}|; \quad \lambda = \pm 1,$$
$$\lambda(m^2, m_a^2, m_b^2) = m^4 + m_a^4 + m_b^4 - 2(m_a^2 m_b^2 + m_b^2 m^2 + m_a^2 m^2),$$

and by choice of axis, $p_x = p_y = 0$. Corresponding to the crossed process

$$\gamma + \bar{B} \to A + \bar{A} \tag{4.5}$$

we have

$$\left\langle \begin{matrix} \mathbf{p}', \sigma_a'; -\mathbf{p}', \sigma_a'' \\ [m_a, \Sigma_a]; [m_a, \Sigma_a] \end{matrix} \middle| S \middle| \begin{matrix} \mathbf{p}, \lambda; -\mathbf{p}, 0 \\ [0, 1]; [m_b, 0] \end{matrix} \right\rangle$$
$$= \sum_{\Sigma,L,(\tilde{\Sigma}L')} 4m'^{\frac{1}{2}}(m'^2 - m_b^2)^{-\frac{1}{2}}(m'^2 - 4m_a^2)^{-\frac{1}{4}} \left(\frac{2L+1}{4\pi}\right)^{\frac{1}{2}}$$
$$\times (1\lambda, L0 \,|\, \Sigma\lambda)(\Sigma_a\sigma_a', \Sigma_a\sigma_a'' \,|\, \tilde{\Sigma}\tilde{\sigma})$$
$$\times (\tilde{\Sigma}\tilde{\sigma}, L'M' \,|\, \Sigma\lambda) Y_{L'}^{M'}(\hat{p}') S'_{\Sigma,L,(\tilde{\Sigma}L')}$$
$$(m' = (\mathbf{p}^2 + m_b^2)^{\frac{1}{2}} + |\mathbf{p}|). \tag{4.6}$$

5. CANONICAL SPIN AND CHARGE COMMUTATION RELATIONS

Let us consider the operator

$$\mathbf{\Sigma} = \frac{1}{M}\left(P^0\mathbf{A} - \frac{1}{P^0 + M}\mathbf{P}(\mathbf{P}\cdot\mathbf{A}) - \mathbf{P}\times\mathbf{V}\right), \tag{5.1}$$

where $\mathbf{A}$, $\mathbf{V}$ are the charges

$$\mathbf{A} = \frac{1}{(2\pi)^3}\int_{x^0=t} \mathbf{j}_{(x)}^{(A)}\, d^3x, \quad \mathbf{V} = \frac{1}{(2\pi)^3}\int_{x^0=t} \mathbf{j}_{(x)}^{(v)}\, d^3x \tag{5.2}$$

and are supposed to have their quark model commutation properties.

In (5.1) M is supposed to be the "mass operator" and in fact $\mathbf{\Sigma}$ should be symmetrized with respect to M and P^0 to ensure Hermiticity. But let us suppose that $\mathbf{\Sigma}$, acting on a state of definite total mass, leads to states of the same total mass as the initial one, or rather that the mass differences between the initial and final states can be neglected up to a certain approximation. To this approximation we may suppose that $\mathbf{A}$ and $\mathbf{V}$ commute, not only with $\mathbf{P}$, but also with M and P^0. With this assumption we have,

$$[\Sigma^i, \Sigma^j] = i\epsilon_{ijk}\Sigma^k. \tag{5.3}$$

Moreover, for initial and final states of the same mass, momentum, and parity, we obtain

$$\langle \mathbf{p}, s_3' | \mathbf{\Sigma} | \mathbf{p}, s_3 \rangle = \langle \mathbf{0}, s_3' | \mathbf{\Sigma} | \mathbf{0}, s_3 \rangle = \langle \mathbf{0}, s_3' | \mathbf{A} | \mathbf{0}, s_3 \rangle, \tag{5.4}$$

where the normalization (3.11) is implied.[11]

It follows that the expectation values (5.4) of $\mathbf{\Sigma}$ do have the correct transformation properties of the canonical spin,[1a] namely, they transform through Wigner rotations. Transition matrix elements (between different mass and parity states, if we cannot neglect them) would have a more complicated behavior, but neither can we expect, *a priori*, a simple transformation law for such cases.

Our definition (5.1) directly in terms of the currents and the momentum operators may be compared with Gürsey's construction[12] of the spin operator for a free quark.

Of course, $\langle \mathbf{\Sigma} \rangle$ need not necessarily give the total spin of a particle. In Gell-Mann's model [Ref. 6, includes previous references], $\mathbf{A}$ gives the quark spin contribution to the total spin of a composite particle, to which we have to add the "inner orbital" contribution $\mathbf{L}$.

The canonical coupling scheme (which we may call "spin-symmetric" coupling), introduced in Ref. 13 and already used in Sec. 4, provides a particularly suitable technique for displaying the inner orbital contribution since the complementary contribution due to the spins is separated out in the simplest possible fashion. The essential point that emerges from formula (2.30) of Ref. 13 is that

$$(\mathbf{L} \equiv)\mathbf{S}_{or} = \mathbf{S} - \mathbf{S}_{\Sigma}, \tag{5.5}$$

where both $\mathbf{S}$ and $\mathbf{S}_{\Sigma}$ and hence also $\mathbf{S}_{or}$ transform through Wigner rotations.

Thus we see that if the correct canonical transformation properties are ensured, then the respective

[11] That the normalization (3.11) corresponds to the result (5.4) is related to the fact that quark model *charges* appear in (5.1) and not the *densities*.

[12] F. Gürsey, in *High Energy Physics*, C. de Witt and M. Jacob, Eds. (Gordon and Breach Science Publishers, Inc., New York, 1965).

[13] A. Chakrabarti, J. Math. Phys. 5, 922 (1964).

contributions $\mathbf{S}_\Sigma$, $\mathbf{S}_{or}$ remain the same, whatever value we take for $\mathbf{p}$ in (5.4). The varying mixtures discussed in Ref. 6 as one passes from $\mathbf{p} = 0$ to $|\mathbf{p}| \to \infty$, are only consequences of defining as "spin," operators with unphysical transformation properties.

APPENDIX A

Here we write down explicitly the form factors for some useful particular cases and discuss the restrictions due to combined Hermiticity and T invariance on the matrix elements of the currents and their divergence for such cases.

We have already noted (Sec. 2) that for the same initial and final particle of spin $\frac{1}{2}$ (or rather, more generally, for such spin $\frac{1}{2}$ particles as may be grouped into a multiplet, their mass differences being neglected) the above-mentioned restrictions coincide for vector currents with those due to the conservation condition.

From (1.24), (1.25) we can write the matrix elements of the divergence as

$$-i\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,(P\cdot j - j\cdot P)\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = -i(4\pi)^{\frac{1}{2}}\frac{1}{(2\pi)^3}\sum_{L'}\frac{(-1)^{M'}}{(2L'+1)^{\frac{1}{2}}}(ss_3, L'M'\,|\,s's_3') \times \mathcal{F}^{(\mathfrak{D})}_{ss',L'}(\mathbf{k}^2)\mathcal{Y}^{-M'}_{L'}(\mathbf{k}), \quad \text{(A1)}$$

where

$$\mathcal{F}^{(\mathfrak{D})}_{ss',L'} = \left\{(k'^0 - k^0)\mathcal{F}^{(0)}_{ss',L'} + \left[\left(\frac{L'}{2L'-1}\right)^{\frac{1}{2}}\mathcal{F}^{(1)}_{ss',(L'-1)L'} - \mathbf{k}^2\left(\frac{L'+1}{2L'+3}\right)^{\frac{1}{2}}\mathcal{F}^{(1)}_{ss',(L'+1)L'}\right]\right\}$$
$$[k'^0 = (\tfrac{1}{4}k^2 + m'^2)^{\frac{1}{2}},\ k^0 = (\tfrac{1}{4}\mathbf{k}^2 + m^2)^{\frac{1}{2}}]. \quad \text{(A2)}$$

Thus it is quite easy to derive the effects of conservation or partial conservation conditions imposed on the divergence and to compare them with the consequences of other restrictions.

(i) $\qquad S' = S = 1$

For the elastic case (by which we mean the same initial and final particles, which may, however, have different $\mathbf{p}$ and S_3), Hermiticity of the current operator and T invariance lead for vector currents to the conditions

$$\mathcal{F}^{(1)v}_{11,10}(\mathbf{k}^2) = \mathcal{F}^{(1)v}_{11,12}(\mathbf{k}^2) = \mathcal{F}^{(1)v}_{11,32}(\mathbf{k}^2) = 0, \quad \text{(A3)}$$

reducing the corresponding $\mathcal{F}^{(\mathfrak{D})v}$'s to zero. The matrix elements are reduced to

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(0)v}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\left[\mathcal{F}^{(0)v}_{11,0}(\mathbf{k}^2)\mathcal{Y}^0_0(\mathbf{k})\delta_{s_3s_3'} + \frac{(-1)^M}{5^{\frac{1}{2}}} \times (1s_3, 2M\,|\,1s_3')\mathcal{F}^{(0)v}_{11,2}(\mathbf{k}^2)\mathcal{Y}^{-M}_2(\mathbf{k})\right], \quad \text{(A4)}$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(1)v}_{(m)}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}(-1)^M}{(2\pi)^3\sqrt{3}}(1M, 1m\,|\,1j_3)(1s_3, 1j_3\,|\,1s_3') \times \mathcal{F}^{(1)v}_{11,11}(\mathbf{k}^2)\mathcal{Y}^{-M}_1(\mathbf{k}). \quad \text{(A5)}$$

For the axial currents, we obtain, corresponding to (A3),

$$\mathcal{F}^{(0)A}_{11,1}(\mathbf{k}^2) = 0 = \mathcal{F}^{(1)A}_{11,22}(\mathbf{k}^2), \quad \text{(A6)}$$

and hence

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(0)A}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = 0, \quad \text{(A7)}$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(1)A}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\left[(1s_3, 1m\,|\,1s_3')\mathcal{F}^{(1)A}_{11,01}(\mathbf{k}^2)\mathcal{Y}^0_0(\mathbf{k}) + \frac{(-1)^M}{5^{\frac{1}{2}}} \times (2M, 1m\,|\,1j_3)(1s_3, 1j_3\,|\,1s_3')\mathcal{F}^{(1)A}_{11,21}(\mathbf{k}^2)\mathcal{Y}^{-M}_2(\mathbf{k})\right]. \quad \text{(A8)}$$

The divergence is now given by

$$\mathcal{F}^{(\mathfrak{D})A}_{11,1}(\mathbf{k}^2) = [\mathcal{F}^{(1)A}_{11,01}(\mathbf{k}^2) - (\tfrac{2}{5})^{\frac{1}{2}}\mathbf{k}^2\mathcal{F}^{(1)A}_{11,21}(\mathbf{k}^2)]. \quad \text{(A9)}$$

(ii) $\qquad S' = S = \frac{3}{2}$

Corresponding to (A3), we obtain (for the elastic case)

$$\mathcal{F}^{(1)v}_{\frac{3}{2}\frac{3}{2},10}(\mathbf{k}^2) = \mathcal{F}^{(1)v}_{\frac{3}{2}\frac{3}{2},12}(\mathbf{k}^2) = \mathcal{F}^{(1)v}_{\frac{3}{2}\frac{3}{2},32}(\mathbf{k}^2) = 0, \quad \text{(A10)}$$

reducing $\mathcal{F}^{(\mathfrak{D})v}_{\frac{3}{2}\frac{3}{2},0}$ and $\mathcal{F}^{(\mathfrak{D})v}_{\frac{3}{2}\frac{3}{2},2}$ to zero again. The final forms are

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(0)v}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\left[\delta_{s_3s_3'}\mathcal{F}^{(0)v}_{\frac{3}{2}\frac{3}{2},0}(\mathbf{k}^2)\mathcal{Y}^0_0(\mathbf{k}) + \frac{(-1)^M}{5^{\frac{1}{2}}} \times (\tfrac{3}{2}s_3, 2M\,|\,\tfrac{3}{2}, s_3')\mathcal{F}^{(0)v}_{\frac{3}{2}\frac{3}{2},2}(\mathbf{k}^2)\mathcal{Y}^{-M}_2(\mathbf{k})\right], \quad \text{(A11)}$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(1)v}_{(m)}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\left[\frac{(-1)^M}{\sqrt{3}}(1M, 1m\,|\,1j_3)(\tfrac{3}{2}s_3, 1j_3\,|\,\tfrac{3}{2}s_3') \times \mathcal{F}^{(1)v}_{\frac{3}{2}\frac{3}{2},11}(\mathbf{k}^2)\mathcal{Y}^{-M}_1(\mathbf{k}) + \frac{(-1)^M}{7^{\frac{1}{2}}}(3M, 1m\,|\,3j_3) \times (\tfrac{3}{2}s_3, 3j_3\,|\,\tfrac{3}{2}s_3')\mathcal{F}^{(1)v}_{\frac{3}{2}\frac{3}{2},33}(\mathbf{k}^2)\mathcal{Y}^{-M}_3(\mathbf{k})\right]. \quad \text{(A12)}$$

For the axial currents, we obtain, for the elastic case

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(0)A}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = 0, \quad \text{(A13)}$$

$$\langle -\tfrac{1}{2}\mathbf{k}, s_3'|\,j^{(1)A}_{(m)}\,|\tfrac{1}{2}\mathbf{k}, s_3\rangle = \frac{(4\pi)^{\frac{1}{2}}}{(2\pi)^3}\left[(\tfrac{3}{2}s_3, 1m\,|\,\tfrac{3}{2}s_3')\mathcal{F}^{(1)A}_{\frac{3}{2}\frac{3}{2},01}(\mathbf{k}^2)\mathcal{Y}^0_0(\mathbf{k}) + \frac{(-1)^M}{5^{\frac{1}{2}}} \times \sum_{j=1,3}(2M, 1m\,|\,jj_3)(\tfrac{3}{2}s_3, jj_3\,|\,\tfrac{3}{2}s_3')\mathcal{F}^{(1)A}_{\frac{3}{2}\frac{3}{2},2j}(\mathbf{k}^2)\mathcal{Y}^{-M}_2(\mathbf{k}) + \frac{(-1)^M}{9^{\frac{1}{2}}}(4M, 1m\,|\,3j_3)(\tfrac{3}{2}s_3, 3j_3\,|\,\tfrac{3}{2}s_3') \times \mathcal{F}^{(1)A}_{\frac{3}{2}\frac{3}{2},43}(\mathbf{k}^2)\mathcal{Y}^{-M}_4(\mathbf{k})\right]. \quad \text{(A14)}$$

We may note [(A5), (A12)] that for $j^{(1)v}$ only the terms with $L = j$ survive (implying $\mathcal{F}^{(\mathfrak{D})v} = 0$). This is a general rule and follows, for arbitrary spin, from the properties of the CG coefficients. For $j^{(1)A}$ on the contrary, the terms with $L = j$ disappear.

APPENDIX B

We first give the explicit forms of the matrix (3.5) for the particular cases $s = \frac{1}{2}, 1, \frac{3}{2}$, for the limit $\mathbf{K} \to (0, 0, \infty)$. The parameter ξ is given by (3.7).

(i) $S = \frac{1}{2}$

$$\lim_{\mathbf{k}\to(0,0,\infty)} \mathfrak{D}^{(\frac{1}{2})}(\Lambda, \mathbf{K} + \tfrac{1}{2}\mathbf{k}) = \begin{vmatrix} \left(1 + \dfrac{k_-k_+}{16\xi^2}\right) & -\dfrac{1}{2\sqrt{2}\,\xi}\,k_- \\ -\dfrac{1}{2\sqrt{2}\,\xi}\,k_+ & \left(1 + \dfrac{k_-k_+}{16\xi^2}\right) \end{vmatrix}. \tag{B1}$$

(ii) $S = 1$

$$\mathfrak{D}^{(1)} \to \begin{vmatrix} \left(1 + \dfrac{k_-k_+}{8\xi^2}\right) & -\dfrac{k_-}{2\xi} & \dfrac{k_-k_-}{8\xi^2} \\ -\dfrac{k_+}{2\xi} & \left(1 + \dfrac{2k_-k_+}{8\xi^2}\right) & -\dfrac{k_-}{2\xi} \\ \dfrac{k_+k_+}{8\xi^2} & -\dfrac{k_+}{2\xi} & \left(1 + \dfrac{k_-k_+}{8\xi^2}\right) \end{vmatrix}. \tag{B2}$$

(iii) $S = \frac{3}{2}$

$$\mathfrak{D}^{(\frac{3}{2})} \to \begin{vmatrix} \left(1 + \dfrac{3k_-k_+}{16\xi^2}\right) & \dfrac{-\sqrt{3}\,k_-}{2\sqrt{2}\,\xi} & \dfrac{\sqrt{3}\,k_-k_-}{8\xi^2} & 0 \\ \dfrac{-\sqrt{3}\,k_+}{2\sqrt{2}\,\xi} & \left(1 + \dfrac{7k_-k_+}{16\xi^2}\right) & -\dfrac{k_-}{\sqrt{2}\,\xi} & \dfrac{\sqrt{3}\,k_-k_-}{8\xi^2} \\ \dfrac{\sqrt{3}\,k_+k_+}{8\xi^2} & -\dfrac{k_+}{\sqrt{2}\,\xi} & \left(1 + \dfrac{7k_-k_+}{16\xi^2}\right) & \dfrac{-\sqrt{3}\,k_-}{2\sqrt{2}\,\xi} \\ 0 & \dfrac{\sqrt{3}\,k_+k_+}{8\xi^2} & \dfrac{-\sqrt{3}\,k_+}{2\sqrt{2}\,\xi} & \left(1 + \dfrac{3k_-k_+}{16\xi^2}\right) \end{vmatrix}. \tag{B3}$$

Finally we write down, as the essential step in calculating (in terms of the canonical form factors in the infinite momentum limit) the magnetic moment, the electric dipole moment and the charge radius of a particle, the derivatives

$$\lim_{|\mathbf{k}|\to 0}\left[\frac{\partial}{\partial k_{(\pm)}}, \frac{\partial^2}{\partial k_{(-)}\partial k_{(+)}}\right] \times \left\{\lim_{\mathbf{k}\to(0,0,\infty)} \left\langle \begin{matrix}\mathbf{K} - \frac{1}{2}\mathbf{k}, s_3' \\ [m, s]\end{matrix}\middle| (\tilde{j}^{(0)v} + \tilde{j}^{(1)v}_{(0)}) \middle| \begin{matrix}\mathbf{K} + \frac{1}{2}\mathbf{k}, s_3 \\ [m, s]\end{matrix}\right\rangle\right\}$$
$$\left[\frac{\partial}{\partial k_{(\pm)}} = -\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial k^1} \pm \frac{1}{i}\frac{\partial}{\partial k^2}\right)\right]. \tag{B4}$$

These results would be sufficient in view of (B3) and the fact that k_3 disappears in the limit considered. [For the charge radius we have also to take into account the term arising from the derivation of the normalization factor in (3.13) multiplied by $1/(2\pi)^3 \times \mathcal{F}^{(0)v}_{SS,0}$.]

In applying (3.10a) we note that in this case $\tilde{\mathbf{k}} = \mathbf{k}$ and (as noted in Appendix A)

$$\mathcal{F}^{(1)v}_{ss,Lj}(\mathbf{k}^2) = 0, \quad \text{for } L \neq j \tag{B5}$$

since we have the same initial and final particle, whose moments we calculate.

Thus, finally we have, corresponding to the derivatives $\partial/\partial k_{(\pm)}$,

$$\delta_{s_3',s_3\mp 1}\{(s \pm s_3)(s \mp s_3 + 1)\}^{\frac{1}{2}} \frac{1^{\perp}}{\sqrt{2}} \frac{1}{(2\pi)^3} \times \left[\frac{1}{m}\mathcal{F}^{(0)v}_{ss,0}(0) + \frac{\mathcal{F}^{(1)v}_{ss,11}(0)}{[2s(s+1)]^{\frac{1}{2}}}\right]. \tag{B6}$$

Corresponding to $\partial^2/\partial k_{(-)}\partial k_{(+)}$, we obtain

$$\delta_{s_3's_3}\frac{1}{(2\pi)^3}\left[-\frac{1}{2}\left(\frac{\partial}{\partial k_{\perp}^2}\mathcal{F}^{(0)v}_{ss,0}(\mathbf{k}_{\perp}^2)\right)_{\mathbf{k}_{\perp}^2=0} + \tfrac{1}{4}(ss_3, 20 \mid Ss_3)\mathcal{F}^{(0)v}_{ss,0}(0) + \frac{1}{m}\{s(s+1) - s_3^2\} \times \left\{\frac{1}{2m}\mathcal{F}^{(0)v}_{ss,0}(0) + \frac{\mathcal{F}^{(1)v}_{ss,11}(0)}{[2s(s+1)]^{\frac{1}{2}}}\right\}\right]. \tag{B7}$$

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Remarks on Relativistic Statistical Mechanics. II. Hierarchies for the Reduced Densities

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In Paper I the basis of relativistic statistical mechanics was discussed and notions such as phase space, Gibbs ensemble, distribution functions were defined. Paper II deals with hierarchies of equations for the reduced densities. Extensive use is made of the beautiful methods of Klimontovich. In this way "classical mesic interactions" are dealt with neglecting "radiation" effects (i.e., "classical" emission of mesons). It is shown how the "renormalization of mass" affects the hierarchies obtained. Electromagnetic interactions are dealt with: (a) neglecting radiation effects, (b) including radiation effects. The latter case is treated on the basis of the Lorentz–Dirac equations and with the help of suitable modifications of the formalism. In this way a new approach to radiation phenomena (for instance, in plasmas) is obtained. Finally, as a matter of illustration, several well-known relativistic kinetic equations are rederived in a slightly improved manner (i.e., Vlasov and Landau equations).

1. INTRODUCTION

In a preceding paper,[1] hereafter referred to as Paper I, we have developed a possible general framework for relativistic statistical mechanics. In particular, notions such as Γ space, densities, and reduced densities were defined in a *strictly covariant manner*. With respect to the latter point our general philosophy was to define relativistic notions only within the framework of the geometry of Minkowski space–time and of the system under study: no objects, such as 3-planes $t = \text{const}$, extraneous to these geometries need to be used. In this paper, we adopt again such an approach which, in our opinion, corresponds deeply to the geometrical nature of the special theory of relativity. In Paper I, the results obtained (at least the definitions of densities, etc.) were, to a large extent, independent of dynamics and therefore were of kinematical nature.

This paper is devoted to some considerations of a more dynamical character. In particular, we derive equations for the various densities of Paper I. In the following, we mostly consider electromagnetic interactions because of their importance in plasma physics. However, we do not completely neglect the so-called classical mesic forces since they may be of importance in the study of neutron stars. The extension of the results obtained, to the case of gravitational *collective* forces being straightforward, is not considered here.

The methods developed below were initiated by Klimontovich in the nonrelativistic case,[2] and also in the relativistic case (although not in a completely correct form). These methods, which we use to a large extent in the following, are most elegant and particularly well adapted to relativistic statistical mechanics: whatever the point of view adopted (either action-at-a-distance or field) and whatever the further developments of nonquantal relativistic dynamics of interacting particles may be (e.g., the Van Dam–Wigner theory[3] or the consideration of extended[4] or spinning[5] particles) Klimontovich's methods can be applied. The main idea developed hereafter is the following: The consideration of the equations of motion given by Rohrlich in his book,[6] shows that one is led *to extend the usual phase space*[7] so as to include the accelerations of the particles and hence to define generalized densities on this extended phase space. Doing so, all radiation effects are included in the densities and in the equations they satisfy. Therefore, we are led to deal with a theory which is *renormalized ab initio* and has all standard properties of usual statistical mechanics with the advantage that it also *includes radiation phenomena* without using the so-called field oscillators.

Section 2 is devoted to the study of the one-particle problem. This section is of particular importance because it contains the main characteristic features of the theory and more particularly it yields a kinetic equation for the particle in presence of its "self-field" and shows how radiation phenomena can be dealt

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[7] In Paper I, we have seen that the phase-space of particles is a $8N$-dimensional space. In what follows, it is extended to a $12N$-dimensional space.

with. In Sec. 3 we treat the case of classical "mesic forces" and give a hierarchy of equations for the different reduced densities. Section 4 is devoted to electromagnetic interactions which are *formally* considered from the field point of view on the one hand, and from the Rohrlich equations on the other hand. In Sec. 5 we rederive some well-known kinetic equations.

Applications of the present *formalism* are to be given in Paper III, where, for example, kinetic equations including radiation effects are given.

Finally, let us emphasize that the results obtained in this paper are merely *plausible* results and will remain so until a completely satisfactory relativistic dynamics is found.[8] Although the research of a nonquantal relativistic statistical mechanics be interesting on merely theoretical grounds, although it may be useful in plasma physics (for instance, radiation effects for frequencies below the far infrared can be treated in a nonquantal framework), we believe that a fully satisfactory theory may be found in the only well-studied relativistic dynamics, i.e., in quantum electrodynamics.

Notations and Conventions

Throughout this paper, we adopt the notations and conventions used in Paper I. Let us recall, however, that we use the metric $+ - - -$ and a system of units where the speed of light is equal to one.

2. A ONE-PARTICLE PROBLEM

In this section we treat the statistical problem of a charged particle embedded in an external force field. Its equations of motion thus are the Lorentz–Dirac equations. Hence we generalize relativistic kinetic theories so as to include radiation phenomena. We show, in another section, that the generalization to many-interacting particle systems is straightforward.

A. Basic Equations and Definitions.

As is well known (see, e.g., Paper I), the equations of motion of a charged particle immersed in an external force field $F^\mu(x_\nu, u_\nu)$ and taking radiation reaction into account, are[9]

$$m\frac{d^2x^\mu}{d\tau^2} = F^\mu(x_\nu, u_\nu) + \tfrac{2}{3}e^2\left\{\frac{d^3x^\mu}{d\tau^3} + \frac{d^2x^\nu}{d\tau^2}\cdot\frac{d^2x_\nu}{d\tau^2}\cdot\frac{dx^\mu}{d\tau}\right\}, \tag{2.1}$$

where m is the renormalized mass of the particle.

[8] The same "plausible" character occurs also in other theories such as the one developed by the Brussels school (see Paper I, Ref. 10).

[9] Or equivalently, ... interacting with its self-field and *after* a mass renormalization ....

To Eq. (1) we must add the *asymptotic conditions*

$$\lim_{\tau\to\pm\infty}\gamma^\mu(\tau) = 0, \tag{2.2}$$

where we have set

$$\gamma^\mu = d^2x^\mu/d\tau^2$$

(in what follows we also use the notation $u^\mu = dx^\mu/d\tau$).

The fact that Eq. (2.1) is a third-order differential equation implies that the general solution depends on three arbitrary constants: x_0^μ, u_0^μ, and γ_0^μ. Condition (2.2) ensures that only physical solutions of Eq. (2.1) are kept among the three possible classes of solutions. Hence there is no runaway solution.

Let us now consider the statistical problems: The initial data of the particle are distributed with a given density of probability. From the third-order character of Eq. (2.1) follows the nature of the μ-phase space of the particle: it is twelve dimensional. Indeed we have

$$\mu = \mathcal{M}^4 \times \mathbf{U}^4 \times \boldsymbol{\gamma}^4, \tag{2.3}$$

where $\mathcal{M}^4$ is the Minkowski space–time, $\mathbf{U}^4$ is the 4-velocity space and $\boldsymbol{\gamma}^4$ the 4-acceleration space. It should be noted that we have considered a *flat* μ-space which contains the *actual curved* μ-space, which is a 10-dimensional space. Indeed we must bear in mind the two following relations:

$$\begin{aligned} u^\mu u_\mu &= 1, \\ u^\mu\gamma_\mu &= 0, \end{aligned} \tag{2.4}$$

which restrict the dimensionality of μ. Definition (2.3) is used only for the sake of simplicity and we also impose conditions (2.4). Taking into account this new dimensionality (12) of μ-space, the microscopic random density is defined as being

$$\begin{aligned} R(x_\nu, u_\nu, \gamma_\nu; \tau) = {} & \delta[x_\nu - x_\nu(\tau, x_0^\rho, u_0^\rho, \gamma_0^\rho)] \\ & \otimes \delta[u_\nu - u_\nu(\tau, x_0^\rho, u_0^\rho, \gamma_0^\rho)] \\ & \otimes \delta[\gamma_\nu - \gamma_\nu(\tau, x_0^\rho, u_0^\rho, \gamma_0^\rho)]. \end{aligned} \tag{2.5}$$

This density is obviously normalized by

$$\int_\mu R\, d\mu = 1. \tag{2.6}$$

By taking the average value of R over the initial data of the particle, we determine a generalized distribution function

$$\begin{aligned} D(x^\mu, u^\mu, \gamma^\mu; \tau) = {} & \int_\mu R(x^\mu, u^\mu, \gamma^\mu, \tau; x_0^\mu, u_0^\mu, \gamma_0^\mu) \\ & \times D_0(x_0^\mu, u_0^\mu, \gamma_0^\mu)\, d\mu_0, \end{aligned} \tag{2.7}$$

where we have made the initial data apparent in the argument of R. However, the situation is not so simple as the one indicated in Eq. (2.7). Indeed, we

must take the asymptotic condition (2.2) into account. This condition implies that the only physically admissible generalized distribution function D should satisfy

$$\lim_{\tau\to+\infty} D(x^\mu, u^\mu, \gamma^\mu; \tau) = \Phi(x^\mu, u^\mu) \otimes \delta(\gamma^\mu), \quad (2.8)$$

which, of course, expresses the fact that, at infinity, the acceleration is well determined to the value zero. There is another interesting consequence of Eq. (2.2). It reads

$$\lim_{\tau\to\infty} \gamma^\mu(\tau; x_0^\mu, u_0^\mu, \gamma_0^\mu) = 0$$

or

$$\gamma^\mu(+\infty, x_0^\mu, u_0^\mu, \gamma_0^\mu) = 0 \quad (2.9)$$

and allows the determination of γ_0^μ *provided the Jacobian*

$$\mathrm{Det}\left\| \frac{\partial \gamma^\mu(+\infty, x_0^\mu, u_0^\mu, \gamma_0^\mu)}{\partial \gamma_0^\nu} \right\| \quad (2.10)$$

is different from zero for all (x_0^ν, u_0^ν). Note that in Eqs. (2.8) and (2.9) we have only considered the limit $\tau \to +\infty$, for we are mainly interested in *prediction problems* not also in *retrodiction problems.*

The existence of solutions of the Lorentz–Dirac equations satisfying the asymptotic conditions has been proved by Hale and Stokes[10] for large classes of external forces.[11] Unfortunately they have not proved their uniqueness, which property would ensure that the Jacobian (2.10) would be nonvanishing. In the following, we *assume* that the external force field F^μ is such that the Jacobian (2.10) is nonvanishing.

Conditions (2.9) and (2.10) show that the average (2.7) is incorrect and $D_0(x_0^\nu, u_0^\nu, \gamma_0^\nu)$ necessarily includes a factor $\delta(\gamma_0^\mu - \gamma_0^\mu(x_0^\nu, u_0^\nu))$.

Consequently, instead of Eq. (2.7) we should write

$$D(x^\mu, u^\mu, \gamma^\mu; \tau) = \int_{\mathcal{M}^4\times U^4} d_4x_0\, d_4u_0 R_1(x^\mu, u^\mu, \gamma^\mu, \tau; x_0^\nu, u_0^\nu) D_0(x_0^\nu, u_0^\nu), \quad (2.11)$$

where the D_0 occurring in Eq. (2.11) is *the same* as the one used in Sec. 2 of Paper I.

Exactly as in Paper I, we can introduce a proper time-independent density $\mathcal{N}(x_\nu, u_\nu, \gamma_\nu)$ through

$$\mathcal{N}(x_\nu, u_\nu, \gamma_\nu) = \int_{-\infty}^{+\infty} d\tau D(x_\nu, u_\nu, \gamma_\nu; \tau) \quad (2.12)$$

and a current in the generalized μ-space (2.3) as

$$J^A(x_B) = \mathcal{N}(x_B)\eta^A(x_B), \quad A = 1, \cdots, 12, \quad (2.13)$$

where we have set

$$x_B = (x_\nu, u_\nu, \gamma_\nu)$$

and

$$\eta^A = \dot{x}^A. \quad (2.14)$$

In the new μ-space $\mathcal{N}(x_A)$ is normalized by

$$\int_{S\subset\mu} \mathcal{N}(x_B)\eta^A(x_B)\, dS_A = 1, \quad (2.15)$$

where S is an arbitrary 11-dimensional surface in μ-space which is crossed by all possible world lines solutions of the equations of motion. With the usual choice of coordinates $(x_\nu, u_\nu, \gamma_\nu)$ and by making apparent[12] in Eq. (2.15) the constraints (2.4), the normalization integral reduces to

$$\int_{\Sigma\times V^+\times\Pi} \mathcal{N}(x_\nu, u_\nu, \gamma_\nu) u^\mu\, d\Sigma_\mu \cdot \frac{d_3u}{u^0}\frac{d_3\gamma}{u^0} = 1, \quad (2.16)$$

where we have set Σ equal to the arbitrary spacelike three-surface; V^+ equal to the velocity three-space: $u^\mu u_\mu = +1$, $u^0 > 0$; Π equal to the acceleration spacelike three-plane: $u^\mu\gamma_\mu = 0$. The arbitrariness of S (or Σ) implies the integrability condition

$$\nabla_A\{\mathcal{N}(x_B)\eta^A\} = 0, \quad (2.17)$$

which is nothing but the continuity equation in μ-space.

B. The Generalized Liouville Equation

We are now able to derive an equation for $D(x_B, \tau)$. To this end we first derive an equation for the random density $R(x_B, \tau)$. First we start from the continuity equation in μ-space:

$$\frac{\partial}{\partial\tau} R(x_B, \tau) + \partial_\mu\{u^\mu R(x_B, \tau)\} + \frac{\partial}{\partial u^\mu}\{\gamma^\mu R(x_B, \tau)\} + \frac{\partial}{\partial\gamma^\mu}\{\dot{\gamma}^\mu R(x_B, \tau)\} = 0. \quad (2.18)$$

Next, taking the equations of motion (2.1) into account and remarking that the independent variables are $(x_\nu, u_\nu, \gamma_\nu)$, we obtain

$$\frac{\partial}{\partial\tau} R(x_B, \tau) + u^\mu\partial_\mu R(x_B, \tau) + \gamma^\mu \frac{\partial}{\partial u^\mu} R(x_B, \tau) + \left\{(m\gamma^\mu - F^\mu(x_\nu, u_\nu))\frac{3}{2e^2} - \gamma^\rho\gamma_\rho u^\mu\right\}\frac{\partial}{\partial\gamma^\mu} R(x_B, \tau) + \frac{6m}{e^2} R(x_B, \tau) = 0, \quad (2.19)$$

where we have used the relation $u^\mu\gamma_\mu R = 0$ occurring because of the δ factors included in R and due to the fact that $\gamma^\mu(\tau)\, u_\mu(\tau) = 0$ as follows trivially from Eq. (2.1).

[10] J. K. Hale and A. P. Stokes, J. Math. Phys. **3**, 70 (1962).

[11] This, for usual initial data (x_0^μ, u_0^μ).

[12] In fact, S is actually a nine-dimensional surface because of the constraints (2.4).

The equation for D is obtained by averaging Eq. (2.19), and we get the very similar equation

$$\frac{\partial}{\partial\tau} D + u^\mu \partial_\mu D + \gamma^\mu \frac{\partial}{\partial u^\mu} D + \left\{(m\gamma^\mu - F^\mu)\frac{3}{2e^2} - \gamma^\rho \gamma_\rho u^\mu\right\}\frac{\partial}{\partial \gamma^\mu} D + \frac{6m}{e^2} D = 0. \tag{2.20}$$

Integrating now this last equation over τ, we obtain an equation for $\mathcal{N}$:

$$u^\mu \partial_\mu \mathcal{N} + \gamma^\mu \frac{\partial}{\partial u^\mu}\mathcal{N} + \left\{(m\gamma^\mu - F^\mu)\frac{3}{2e^2} - \gamma^\rho\gamma_\rho u^\mu\right\}\frac{\partial}{\partial\gamma^\mu}\mathcal{N} + \frac{6m}{e^2}\mathcal{N} = 0, \tag{2.21}$$

which could as well have been derived from Eq. (2.1) and the continuity equation (2.17).

C. Remarks and Discussion

(1) Equations (2.20) or (2.21) have been called "Liouville equations" because they are equivalent both to the continuity equations in μ-space and to the equations of motion. In fact, we no longer have a Liouville theorem due to

$$\partial\dot{\gamma}^\mu/\partial\gamma_\mu \neq 0.$$

Consequently, the μ-phase space volume element is not conserved during the motion. This can be roughly shown by rewriting Eq. (2.20) under the form

$$(dD/d\tau) + (6m/e^2)D = 0,$$

which implies

$$D(\tau) \sim \exp\,[-(6m/e^2)\tau]\cdot D(0);$$

and since

$$D(\tau)\delta\mu(\tau) = D(0)\delta\mu(0) \Leftrightarrow \frac{d}{d\tau}\{D(\tau)\delta\mu(\tau)\} = 0$$

(conservation of the number of particles), it follows that

$$\delta\mu(\tau) \sim \exp\,[+(6m/e^2)\tau]\cdot\delta\mu(0).$$

Hence, the μ-space volume element increases exponentially with "time." This renders troublesome the definition of equilibrium.

(2) It is easy to verify that the solution of Eq. (2.20) satisfying the asymptotic conditions (2.2) in the absence of external force field is

$$D(x^\mu, u^\mu, \gamma^\mu; \tau) = f(x^\mu, u^\mu, \tau) \otimes \delta(\gamma^\mu),$$

where $f(x^\mu, u^\mu, \tau)$ is given by

$$f(x^\mu, u^\mu, \tau) = \langle\delta[x^\mu - x^\mu(\tau)] \otimes \delta[u^\mu - u^\mu(\tau)]\rangle = \langle\delta(x^\mu - x_0^\mu - u_0^\mu\tau)\otimes\delta(u^\mu - u_0^\mu)\rangle \tag{2.22}$$

and represents what we called $D_1(x_\mu, u_\mu; \tau)$ in Paper I.

(3) The passage from Eq. (2.20) to Eq. (2.21) has eliminated the term $(\partial/\partial\tau)D$. However, when an initial-value problem is dealt with, Eq. (2.21) involves a source term and reads

$$u^\mu\partial_\mu\mathcal{N}(x_B) + \gamma^\mu\frac{\partial}{\partial u^\mu}\mathcal{N}(x_B) + \left\{(m\gamma^\mu - F^\mu)\frac{3}{2e^2} - \gamma^\rho\gamma_\rho u^\mu\right\}\frac{\partial}{\partial\gamma^\mu}\mathcal{N}(x_B) + \frac{6m}{e^2}\mathcal{N} = D_0(x^\mu, u^\mu)\otimes\delta(\gamma^\mu - \gamma_0^\mu(u^\mu, x^\mu)). \tag{2.23}$$

(4) In fact, statistical mechanics derived from the Lorentz–Dirac equations are not completely satisfactory as far as Lorentz–Dirac equations are *not* the equations of motion for the particle. The correct equations of motion are, as remarked by Rohrlich, equivalent to *both* Lorentz–Dirac equations and the asymptotic conditions, which prevent the possibility of runaway solutions. In our model, we must *impose* the asymptotic conditions to the various densities involving acceleration variables. Had we used the correct equation of motion,[6]

$$m\gamma^\mu(\tau) = \int_0^\infty K^\mu(\tau + \alpha\tau_0)\exp\,[-\alpha]\,d\alpha, \tag{2.24}$$

$$K^\mu(\tau) = m\gamma^\mu(\tau) - \tau_0\dot{\gamma}^\mu(\tau), \tag{2.25}$$

the situation would have been much more complicated. Indeed, the highly *nonlocal* character of Eq. (2.1) shows that the μ-space which should be used is an infinite dimensional space

$$\tilde{\mu} = \mathcal{M}^4 \times \mathbf{U}^4 \times \bigtimes_{i=1}^{\infty} \boldsymbol{\gamma}^{(n)4}, \tag{2.26}$$

where $\boldsymbol{\gamma}^{(n)4}$ is the four-dimensional space of the nth derivatives of γ^μ. In this μ-space the continuity equation would *formally* read

$$\frac{\partial}{\partial\tau}\tilde{D} + u^\mu\partial_\mu\tilde{D} + \sum_{n=-1}^{\infty}\frac{\partial}{\partial\gamma_\rho^{(n)}}\{\gamma^{\rho(n+1)}\tilde{D}\} = 0, \tag{2.27}$$

where $\tilde{D}$ is a *pseudo-density* on this μ-space, which is of the same nature as the one considered when dealing with field oscillators. In Eq. (2.27) the various $\gamma^{\mu(n)}$ $(n \geq 1)$ can be obtained, at least in principle, from the equations of motion (2.24), (2.25) or from Eq. (2.1). Besides the mathematical difficulties raised by Eq. (2.27), the variables $\gamma^{\mu(n)}$ are interrelated by means of the constraints obtained by derivations of $u^\mu u_\mu = +1$, in such a way that the situation becomes rather involved. These are the reasons why it is preferable to start directly from the Lorentz–Dirac equations and *next* to impose the asymptotic condition (2.8) to the densities.

(5) It is interesting to compare the theory presented here with the results obtained by Hénin,[13] who dealt with a similar problem. Hénin's approach consists in writing a Liouville equation for a pseudo-density involving both particle and field variables and giving a perturbative treatment.

(a) Our approach is manifestly covariant while the transformation properties of Hénin's are not completely clear and need a special (and not given) proof.

(b) We have dealt only with particle variables so that our density has a well-defined meaning. Another consequence is that we have no problem of choosing a gauge.

(c) The Lorentz–Dirac equations include only a finite mass and hence our theory is renormalized *ab initio*. On the contrary, Hénin's theory is not free from self-energy infinities and the renormalization procedure effected on the terms of the perturbative developments of the pseudo-density is much more complicated. Furthermore, Lorentz–Dirac equations have to be derived in her approach.

(d) As we see in what follows, a manifestly covariant perturbation expansion of Eqs. (2.20) and (2.21) can be obtained, while in Hénin's work, it is not so. Accordingly we are able to derive easily covariant kinetic equations taking radiation phenomena into account while Hénin's methods give rise to rather lengthy calculations.

(6) The distribution functions $D(x_B, \tau)$ or $\mathcal{N}(x_B)$ contain the effects of radiation in their γ^μ dependence. This is particularly interesting since the use of the field oscillators is avoided. Let us give several examples of radiation quantities[6,14]:

$$dP^\mu/d\tau = \tfrac{2}{3}e^2\gamma^\nu\gamma_\nu u^\mu \quad \text{(momentum energy of the radiation emitted per unit proper time)}, \tag{2.28}$$

$$F^{\mu\nu}_{\text{rad}} = -\tfrac{2}{3}e\{u^\mu\dot{\gamma}^\nu - u^\nu\dot{\gamma}^\mu\} \quad \text{(radiation field)}, \tag{2.29}$$

$$F^{\mu\nu}_{\text{rad}\,\infty} = (e/R^3)\{(X^\mu\gamma^\nu - X^\nu\gamma^\mu)R - (X^\mu u^\nu - X^\nu u^\mu)Q\}, \tag{2.30}$$

with

$$X^\mu = x^\mu - z^\mu,$$
$$R = X^\mu u_\mu,$$
$$Q = X^\mu\gamma_\mu,$$

z^μ is the position of the particle, and x^μ is the event where the field is observed. $F^{\mu\nu}_{\text{rad}\,\infty}$ is the *far field* [see Ref. 14, p. 168, Eq. (5–8)]. An alternative form is given by Rohrlich.[6] In fact, it is rather Eq. (2.30) which is at the basis of all radiation quantities. By applying the methods given in Paper I we are able to compute the average radiation quantities. However, it must be remarked that *all* radiation quantities *cannot* be obtained from *only* the distribution function.

For instance, it is well known in the nonrelativistic case that the spectral density of radiation is connected to the Fourier transform of the second-order momentum of the stochastic process $\boldsymbol{\gamma}(t)$[15]

$$I(\omega, t) \sim \int e^{i\omega\tau}\langle\boldsymbol{\gamma}(t)\cdot\boldsymbol{\gamma}(t+\tau)\rangle\, d\tau$$

[of course $I(\omega, t)$ does not depend on t in the case of a stationary process]. This last relation involves the knowledge of the joint probability that the particle be in the state $(\mathbf{x}, \mathbf{v}, \boldsymbol{\gamma})$ at time t *and* be in the state $(\mathbf{x}', \mathbf{v}', \boldsymbol{\gamma}')$ at time $t + \tau$.

In the relativistic case, we need a similar density of probability, say

$$W_2(x_B, \tau; x_B + y_B, \tau + \theta) = \langle R(x_B, \tau) \otimes R(x_B + y_B, \tau + \theta)\rangle, \tag{2.31}$$

where the angular brackets denote an average over the initial data. The preceding density W_2 must satisfy the relations

$$-W_2(x_B, \tau; x_B + y_B, \tau + \theta) = 0 \quad \forall y^\mu \notin \Gamma^+(x^\mu) \text{ (causality)}, \tag{2.32}$$

$$-\lim_{\theta\to 0} W_2(x_B, \tau; x_B + y_B, \tau + \theta) = D(x_B, \tau)\delta(y_B), \tag{2.33}$$

$$-\int_\mu W_2(x_B, \tau; x_B + y_B, \tau + \theta)\, d\mu(y_B) = D(x_B, \tau). \tag{2.34}$$

We return to these questions later.[16]

(7) Another feature of the theory is that kinetic equations including radiation effects are obtained without difficulty: in order to recover a usual distribution function $f(x^\mu, u^\mu; \tau)$ it is sufficient to integrate $D(x_B, \tau)$ over the acceleration variables. This is done in a following paragraph.

(8) Finally, let us also note that the introduction of interaction is not extremely difficult when one considers the external force field as given by the action of the other particles.

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[13] F. Hénin, Physica **29**, 1233 (1963).

[14] A. O. Barut, *Electrodynamics and Classical Theory of Fields and Particles* (The Macmillan Company, New York, 1964).

[15] It is often considered that the brackets below have the meaning of a time average. This is, however, neither completely general nor completely exact (see the brief discussion at the end of this section).

[16] It is clear that if we want to know something about higher-order moments of the radiation field, then it is necessary to have more general densities, say W_n.

D. Kinetic Equations and Perturbation Expansion

In order to obtain a kinetic equation for the reduced (and usual)[17] distribution function

$$f(x_\mu, u_\mu; \tau) \underset{\text{def}}{\equiv} PD(x_\mu, u_\mu, \gamma_\mu; \tau) = \int d_4\gamma D(x_\mu, u_\mu, \gamma_\mu; \tau), \quad (2.35)$$

a first idea would consist in using Zwanzig's techniques.[18] However, the operator P is *not* a projector so that they cannot be easily applied ($P^2 = \infty!$). Consequently we start directly from Eq. (2.20) and integrate it over the acceleration variables. We get

$$\frac{\partial}{\partial\tau} f(x_\nu, u_\nu; \tau) + u^\mu \partial_\mu f(x_\nu, u_\nu; \tau) + \frac{\partial}{\partial u^\mu} \int d_4\gamma \cdot \gamma^\mu D(x_\nu, u_\nu, \gamma_\nu; \tau) = 0, \quad (2.36)$$

where the term $(\partial/\partial\gamma^\mu)\dot{\gamma}^\mu_D(x_\nu, u_\nu, \gamma_\nu; \tau)$ goes to zero if we assume a sufficiently decreasing behavior of D at infinity in the γ^μ variables (i.e., in the three-plane Π). At first sight Eq. (2.36) seems to be very strange since the external force field has disappeared. In fact it is *implicitly* contained in D. Let us now give a perturbative treatment of Eq. (2.36). To this end, use is made of the perturbation expansion of the solution of the Lorentz–Dirac equation, as given by Rohrlich.[6] To the order zero in τ_0, where radiation reaction is completely neglected, we have $F^\mu = m\gamma^\mu$, and hence, at zeroth order f is given by the solution of the usual equation

$$\frac{\partial}{\partial\tau} f^{(0)}(x_\nu, u_\nu; \tau) + u^\mu \partial_\mu f^{(0)}(x_\nu, u_\nu; \tau) + \frac{\partial}{\partial u^\mu}\left\{\frac{F^\mu}{m}(x^\nu, u^\nu) f^{(0)}(x^\nu, u^\nu)\right\} = 0, \quad (2.37)$$

which reduces to a true Liouville equation when the external force field is "conservative":

$$(\partial/\partial u^\mu) F^\mu(x^\nu, u^\nu) = 0,$$

which case occurs with electromagnetic forces.

For the sake of simplicity, the next order (order one in τ_0) is studied in the case of an external electromagnetic force field:

$$F^\mu(x^\nu, u^\nu) = eF^{\mu\nu}(x_\rho)u_\nu.$$

According to Rohrlich [Ref. 6, Eq. (6-91)] at order one in τ_0, $m\gamma^\mu$ can be approximated by[19]:

$$m\gamma^{\mu[1]} = F^\mu(x_\nu, u_\nu) + \tau_0\left\{\frac{d}{d\tau} F^\mu(x^\nu, u^\nu) + m\gamma^\rho\gamma_\rho u^\mu\right\}^{[0]}, \quad (2.38)$$

which can be rewritten as

$$m\gamma^{\mu[1]} = F^\mu(x^\nu, u^\nu) + \tau_0\left\{u^\rho\partial_\rho F^\mu(x^\nu, u^\nu) + \gamma^\rho \frac{\partial}{\partial u^\rho} F^\mu(x^\nu, u^\nu) + m\gamma^\rho\gamma_\rho u^\mu\right\}^{[0]}.$$

In the case of an electromagnetic force field, this last equation reads

$$\begin{aligned} m\gamma^{\mu[1]} &= eF^{\mu\nu}(x_\rho)u_\nu + \tau_0\{eu_\nu u^\rho \partial_\rho F^{\mu\nu}(x_\rho) + e\gamma^{[0]}_\rho F^{\mu\rho}(x_\alpha) + m\gamma^{\rho[0]}\gamma^{[0]}_\rho u^\mu\} \\ &= eF^{\mu\nu}\cdot u_\nu + \tau_0\left\{eu_\nu u^\rho\partial_\rho F^{\mu\nu} + \frac{e^2}{m} u^\nu F_{\rho\nu}\cdot F^{\mu\rho} + \frac{e^2}{m} u_\alpha u^\beta u^\mu F^{\rho\alpha}\cdot F_{\rho\beta}\right\}. \end{aligned} \quad (2.39)$$

Taking into account the fact that $\partial_\mu F^{\mu\nu} = 0$ (the external force field is a free field),[20] one finds easily

$$\frac{\partial}{\partial u^\mu}\gamma^{\mu[1]}(x_\rho \cdot u_\rho) = \tau_0\left\{\frac{e^2}{m} F_{\rho\nu}F^{\nu\rho} + \frac{6e^2}{m} u^\beta u_\alpha F^{\rho\alpha}F_{\rho\beta}\right\}, \quad (2.40)$$

so that the kinetic equation looked for is

$$\frac{\partial}{\partial\tau} f^{[1]}(x_\mu, u_\nu; \tau) + u^\mu\partial_\mu f^{[1]}(x_\nu, u_\nu; \tau) + \frac{e}{m} F^{\mu\nu}(x_\alpha)u_\nu \frac{\partial}{\partial u^\mu} f^{[1]}(x_\nu, u_\nu; \tau) = \frac{\partial}{\partial u^\mu}\{\gamma^{\mu[1]'}(x_\alpha, u_\alpha) f^{[0]}(x_\alpha, u_\alpha)\}, \quad (2.41)$$

where $\gamma^{\mu[1]'}$ denotes the part of $\gamma^{\mu[1]}$ which is actually proportional to τ_0. The right-hand side of Eq. (2.41) involves $f^{[0]}$ and not $f^{[1]}$ since we are dealing with order one in τ_0. However, we could perfectly replace $f^{[0]}$ by $f^{[1]}$ in Eq. (2.41) since in doing it we should add term of order τ_0^2 and hence negligible terms.

E. Remarks

(1) In deriving Eq. (41) it could be argued that we have done an approximation on the *variables* γ^μ and that does not make sense. This procedure can, however, be justified with the help of the random density $R(x_\nu, u_\nu, \gamma_\nu; \tau)$. It is sufficient to note that

$$\gamma^\mu R(x_\nu, u_\nu, \gamma_\nu; \tau) = \gamma^\mu(\tau)\, R(x_\nu, u_\nu, \gamma_\nu; \tau)$$

because of the δ factors occurring in the definition of R. *Next*, we may write: $\gamma^{\mu[n]}(\tau) = \gamma^{\mu[n]}[x_\nu(\tau), u_\nu(\tau)]$ and use again the δ factors included in R. Finally, Eq. (2.41) follows after taking the average value in the equations obtained for $R^{[1]}$ and $R^{[0]}$.

[17] In Paper I, we used $D(x_\mu, u_\mu; \tau)$ instead of $f(x_\mu, u_\mu; \tau)$.

[18] R. Zwanzig, in *1960 Boulder Summer School* (Interscience Publishers, Inc., New York, 1961), Vol. 3.

[19] $\gamma^{\mu[n]}$ denotes the nth-order approximation, while $\gamma^{\mu(n)}$ is the nth derivative of γ^μ.

[20] This assumption is not necessary. It only allows us to drop a term in Eq. (2.40).

(2) We want to emphasize that the expansion given above is a series in powers of τ_0 and *not* of e^2. Because of the occurrence in the relativistic framework of a new universal constant (i.e., the velocity of light), it is clear that we have a new expansion parameter at our disposal.

(3) We could perfectly obtain other kinetic equations valid at higher orders in τ_0. However, according to Rohrlich,[6] it is "empirically well-known that only the first order in τ_0 is physically significant."

F. Use of Another μ-Space

We have already seen that, when neglecting radiation effects, the usual relativistic kinetic equation for $f(x_\nu, u_\nu; \tau)$ is recovered. However, it would be interesting to obtain a *rigorous* equation resembling the usual one but having a second member involving τ_0 so that the "no-radiation approximation" would be recovered simply by setting $\tau_0 = 0$. To do so we use a modified formalism which is based on an alternative form of the Lorentz–Dirac equation.

It can be rewritten as[14]

$$m\gamma^\mu(\tau) = F^\mu(x_\nu, u_\nu) + m\tau_0\Delta^{\mu\nu}(u_\rho)\dot{\gamma}_\nu(\tau), \quad (2.42)$$

where $\Delta^{\mu\nu}(u_\rho)$ has been defined in Paper I. This expression shows that γ^μ depends linearly on $\dot{\gamma}^\mu$, the converse property being not true as shown by Eq. (2.1):

$$\dot{\gamma}^\mu(\tau) = \tau_0^{-1}\left\{\gamma^\mu(\tau) - \frac{F^\mu}{m}\right\} - \gamma^\rho(\tau), \gamma_\rho(\tau)u^\mu. \quad (2.43)$$

Equations (2.42) and (2.43) indicate that we have the possibility of using either $(x_\nu, u_\nu, \gamma_\nu)$ or $(x_\nu, u_\nu, \dot{\gamma}_\nu)$ as independent variables. As a consequence, we define another μ-space:

$$\hat{\mu} = \mathcal{M}^4 \times \mathbf{U}^4 \times \dot{\Gamma}^4 \quad (2.44)$$

and hence a new random density

$$\hat{R}(x_\nu, u_\nu, \dot{\gamma}_\nu; \tau) = \delta[x_\nu - x_\nu(\tau)] \otimes \delta[u_\nu - u_\nu(\tau)] \otimes \delta[\dot{\gamma}_\nu - \dot{\gamma}_\nu(\tau)]. \quad (2.45)$$

In this new μ-space, let us start again from the continuity equation:

$$\frac{\partial}{\partial\tau}\hat{R} + \partial_\mu\{u^\mu R\} + \frac{\partial}{\partial u^\mu}\{\gamma^\mu(x_\nu, u_\nu, \dot{\gamma}_\nu)\hat{R}\} + \frac{\partial}{\partial\dot{\gamma}^\mu}\{\dot{\gamma}^\mu(x_\nu, u_\nu, \dot{\gamma}_\nu)\hat{R}\} = 0. \quad (2.46)$$

In Eq. (2.46), γ^μ is to be replaced by its expression (2.42) while $\dot{\gamma}^\mu$ is obtained by deriving Eq. (2.43) and taking Eq. (2.42) into account. Of course, a similar equation may be obtained for

$$\hat{D}(x_\nu, u_\nu, \dot{\gamma}_\nu; \tau) = \langle\hat{R}(x_\nu, u_\nu, \dot{\gamma}_\nu; \tau)\rangle. \quad (2.47)$$

Explicitly, it reads

$$\frac{\partial}{\partial\tau}\hat{D} + u^\mu\partial_\mu\hat{D} + \frac{F^\mu}{m}\frac{\partial}{\partial u^\mu}\hat{D} + \tau_0\left\{\frac{\partial}{\partial u^\mu}[\Delta^{\mu\nu}(u_\rho)\dot{\gamma}_\nu\hat{D}]\right\} + \frac{\partial}{\partial\dot{\gamma}^\mu}\{\dot{\gamma}^\mu\hat{D}\} = 0. \quad (2.48)$$

Integrating Eq. (2.48) over the variables $\dot{\gamma}^\mu$ and under the assumption that $\hat{D}$ vanishes sufficiently rapidly at infinity (in these variables), we obtain a *rigorous* equation satisfied by $f(x_\nu, u_\nu; \tau)$,[21]

$$\frac{\partial}{\partial\tau}f + u^\mu\partial_\mu f + \frac{F^\mu}{m}\frac{\partial}{\partial u^\mu}f = -\tau_0\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d_4\dot{\gamma}\cdot\dot{\gamma}_\nu\hat{D}\right\}. \quad (2.49)$$

This equation has the required form we were looking for.[22] In order to obtain a kinetic equation at order one in τ_0, it is sufficient to replace $\dot{\gamma}_\nu$ by $\dot{\gamma}_\nu^{[0]}$ and use the same techniques as those used above. As a consequence we reobtain the kinetic equation (2.41). One easily verifies that setting $\tau_0 = 0$ in Eq. (2.49) yields the "no-radiation approximation."

G. Transport Equations

(1) Let us now integrate the (rigorous) equation (2.36) over the proper time and 4-velocity variables. Due to the vanishing of D (or $\mathcal{N}$) at infinity in the velocity space, we get

$$\partial_\mu\iint d\tau\, d_4u f(x_\nu, u_\nu; \tau)u^\mu = \partial_\mu\int d_4u\mathcal{N}(x_\nu, u_\nu)u^\mu = \partial_\mu j^\mu(x_\nu) = 0, \quad (2.50)$$

i.e., the conservation of the numerical current of particles, as expected. The same result can be obtained from Eq. (2.49) as well.

(2) Multiplying Eq. (2.36) by u_θ and integrating again over both the 4-velocity and the proper time variables, we obtain the transport equation for the energy and momentum:

$$\partial_\mu\int_{\mathbf{U}^4}u^\mu u^\alpha\mathcal{N}(x_\rho, u_\rho)\, d_4u - \int_{\Gamma^4\times\mathbf{U}^4}d_4u\, d_4\gamma\cdot\gamma^\alpha\mathcal{N}(x_\rho, u_\rho, \gamma_\rho) = 0. \quad (2.51)$$

The first term of this last equation is the divergence of the momentum-energy tensor of the particles while the second term contains the effects of the external field of force and of the radiation. To the zeroth order in τ_0 Eq. (2.51) reduces to the usual equation

$$\partial_\mu T^{\mu\nu}(x_\alpha) = (e/m)F^{\mu\nu}(x_\alpha)\cdot j_\nu(x_\alpha). \quad (2.52)$$

[21] Indeed we have $\int d_4\gamma\cdot D = \int d_4\dot{\gamma}\cdot\hat{D} = f$.

[22] We have again assumed that $(\partial/\partial u^\mu)F^\mu = 0$.

To the first order in τ_0, we obtain [from Eq. (2.41)]:

$$\partial_\mu T^{\mu\nu}(x_\rho) - (e/m)F^{\mu\nu}(x_\rho)\cdot\partial_\nu(x_\rho) = \frac{\tau_0}{m}\left\{e\partial_\rho F^{\nu\beta}\cdot T^\rho_\beta + \frac{e^2}{m}F^{\nu\beta}\cdot F_{\beta\rho}\cdot j^\rho + e^2\frac{F^{\alpha\rho}F_{\alpha\lambda}}{m}\overline{u_\rho u^\lambda u^\mu}\right\}, \quad (2.53)$$

where the bar over $u_\rho u^\lambda u^\mu$ indicates a "local average" over u. Expression (2.53) shows clearly that in addition to the conventional terms (left-hand side) an extra term representing the *force density due to the radiation reaction*, should be added. Of course, Eq. (2.53) could have been obtained from Eq. (2.49).

(3) As is well known, the frequency distribution in a given direction is closely related to the *correlation function* of the radiation field through its Fourier transform. In fact, all *observable* spectra can be derived from this "basic" spectrum:

$$I(\mathbf{x}, t; \omega, \mathbf{k}) \sim \int e^{i\omega\tau - i\mathbf{k}\mathbf{y}}\{\langle\mathbf{E}^+(\mathbf{x}, t)\cdot\mathbf{E}^-(\mathbf{x}+\mathbf{y}, t+\tau)\rangle - \langle\mathbf{E}^+(\mathbf{x}, t)\rangle\langle\mathbf{E}^-(\mathbf{x}+\mathbf{y}, t+\tau)\rangle\}\, d\tau\, d_3y \quad (2.54)$$

(where the $\langle\ \rangle$ denotes an *ensemble* average). In Eq. (2.54) $\mathbf{E}^\pm$ symbolizes the positive or negative frequency part of $\mathbf{E}$.

For instance, it is usually stated that the *observable* spectrum is obtained from the above one (see, e.g., Ref. 23) by averaging over t *and* x:

$$I_{\text{obs}}(\omega, \mathbf{k}) \lim_{V\to\infty, T\to\infty} \frac{1}{VT}\int_V d_3x \int_0^T dt I(\mathbf{x}, t; \omega, \mathbf{k}); \quad (2.55)$$

of course, Eqs. (2.54) and (2.55) are equivalent when the stochastic process $\mathbf{E}(\mathbf{x}, t)$ is *stationary* and *homogeneous*.

However, there exists an infinity of possible averaging operations, the one chosen depending on the experiment under consideration. This shows that it is rather expression (2.54) which is basic.

Furthermore, it is rather definition (2.54) which is useful in order to derive a transport equation for radiation phenomena, and hence to find *emission and absorption coefficients*.

In the relativistic case, it has been shown that the "intensity" I has no invariant (or covariant) meaning.[24] Despite this slight trouble, it is possible, however, to derive a transport equation for the quantity from which a spectral distribution can be derived in every Galilean frame, say, the correlation tensor of the radiation field

$$\langle F^{\mu_1\nu_1}(x_\rho)\cdot F^{\mu_2\nu_2}(x_\rho + y_\rho)\rangle.$$

In fact, as pointed out by Marshall,[25] it is not this quantity which is of interest for the momentum-energy spectrum; it is rather a contraction of this tensor. This contracted correlation tensor is[25]

$$\Gamma_{\mu\nu}(x_\rho, x_\rho + y_\rho) = \langle F_{\mu\alpha}(x_\rho)F^\alpha_\nu(x_\rho + y_\rho)\rangle - \tfrac{1}{4}g_{\mu\nu}\langle F^{\alpha\beta}(x_\rho)F_{\alpha\beta}(x_\rho + y_\rho)\rangle \quad (2.56)$$

and the spectrum can be derived from $\Gamma_{\mu\nu}$ (see Ref. 25). Therefore, we shall derive (in Paper III) transport equations for $\Gamma_{\mu\nu}$ or rather for

$$K_{\mu\nu}(x_\rho, k_\rho) = \int \exp\{ik^\mu y_\mu\} \times \Gamma_{\mu\nu}(x_\rho, x_\rho + y_\rho)\, d_4y. \quad (2.57)$$

The radiation field is given by (Ref. 14, p. 171)

$$F_{\text{rad}} = \tfrac{2}{3}e\{u^\mu\dot\gamma^\nu - u^\nu\dot\gamma^\mu\}, \quad (2.58)$$

while the far field, which is of special interest in view of applications, is given by Eq. (2.30), so that its various transport properties will be obtained easily (at least in principle) from the distribution $\hat D$ [or D in condition to express $\dot\gamma^\mu$ in term of γ^μ in Eq. (2.58)] and from distributions W_n, similar to W_2.

H. A Remark on Irreversibility

The fact that radiation is emitted in an *irreversible way* and more particularly the fact that it implies the use of *retarded actions*, has led a number of physicists[26] to state a "postulate of equivalence of retarded actions and Carnot principle." Since the theory developed here contains all the effects of the irreversible emission of radiation, it would be interesting to study whether this conjecture is verified or not.

To this end, we have to calculate the entropy 4-current of the system, and if the above conjecture is verified we must have

$$\partial_\mu S^\mu(x_\rho) > 0, \quad (2.59)$$

which expresses (as shown in Paper I) the increase of entropy and hence (in a sense) irreversibility.

Let us start again from Eq. (2.40) and multiply it by $\log \mathcal{N}(x_\rho, u_\rho)$. After an integration over the velocity variables, we get

$$\partial_\mu \int \mathcal{N}(x_\rho, u_\rho)\log\mathcal{N}(x_\rho, u_\rho)u^\mu\, d_4u = \partial_\mu S^\mu(x_\rho) = 0 \quad (2.60)$$

(where we have assumed that the electromagnetic

[23] J. D. Jackson, *Classical Electrodynamics* (John Wiley & Sons, Inc., New York, 1962).

[24] J. L. Synge, *The Relativistic Gas* (North-Holland Publishing Company, Amsterdam, 1957).

[25] T. W. Marshall, Proc. Cambridge Phil. Soc. **61**, 537 (1965).

[26] O. Costa de Beauregard, *La théorie synthétique de la relativité et des quantas* (Gauthiers-Villars, Paris, 1957), Chap. 13.

field is weak, i.e., $|\mathbf{F} \otimes \mathbf{F}| \ll |\mathbf{F}|$), which shows that the total entropy of the system remains constant with or without radiation emission . Therefore the system seems to have a reversible behavior and this is certainly in agreement with the symmetry properties of the subjacent dynamics (see Ref. 6, p. 245). In other words, the gas radiates without loss of entropy: radiation is emitted *adiabatically*.[27] Let us also remark that the same result would not have been obtained by using the entropy defined by $\mathcal{N}'(x_\rho, u_\rho, \gamma_\rho)$ instead of the one derived from $\mathcal{N}'(x_\rho, u_\rho)$ and using the exact Eq. (2.21).

In fact, these curious properties do not prove that the above conjecture is false, especially because of the too simple character of the model (noninteracting[28] charged particles!).

The problem should be reconsidered in a more involved context.

3. KLIMONTOVICH HIERARCHY FOR SCALAR INTERACTIONS

In this section we deal with a many-particle system whose interactions occur through a *scalar field.* Such a system is not of mere academic interest since it is sometimes considered as describing neutron stars[29] as far as quantum effects are not concerned. We give a hierarchy of equations for the successive reduced distribution functions $D_1, D_2, \cdots$ introduced in Part I. We use the most elegant method due to Klimontovich,[30] which is generalized in the following sense: (1) it deals with *scalar interactions*; (2) it is *renormalized*; (3) the densities used are the *proper time dependent densities* D_k rather than $\mathcal{N}_k$. In this section "radiation" effects (i.e., emission of mesons) are *neglected* since they are out of the scope of a classical (i.e., nonquantal) theory. We first derive an unrenormalized hierarchy and next show how the renormalization procedure may be introduced.

We mainly deal with the action-at-a-distance point of view although we always have an eye on the field viewpoint.[31]

A. Unrenormalized Hierarchy

The one-particle random density

$$R_1(x_\nu, u_\nu; \tau) = \sum_{i=1}^{i=N} \delta[x_\nu - x_{\nu_i}(\tau)] \otimes \delta[u_\nu - u_{\nu_i}(\tau)] \tag{3.1}$$

satisfies the following continuity equation in μ-space:

$$\frac{\partial}{\partial \tau} R_1 + \partial_\mu \{u^\mu R_1\} + \frac{\partial}{\partial u^\mu}\left\{\frac{du^\mu}{d\tau} R_1\right\} = 0. \tag{3.2}$$

Using the equations of motion of the particles (see Paper I):

$$m_0(du^\mu/d\tau) = \lambda \Delta^{\mu\nu}(u_\rho)\partial_\nu \phi, \tag{3.3}$$

where m_0 is the *bare* mass, λ the coupling constant and ϕ the *total* scalar field[31] due to the system: $\Delta^{\mu\nu}$ has been defined in Paper I. Equation (3.2) can be rewritten as

$$\frac{\partial}{\partial \tau} R_1 + u^\mu \partial_\mu R_1 + \frac{\lambda}{m_0} \frac{\partial}{\partial u^\mu} \{\Delta^{\mu\nu}(u_\rho) \cdot \partial_\nu \phi \cdot R_1\} = 0. \tag{3.4}$$

Note that we have typically a "nonconservative" force; i.e., $(\partial/\partial u^\mu) F^\mu \neq 0$.

[Let us remark that $m_0 u^\mu$ is *not* the variable canonically conjugated to x^μ; it is rather $p^\mu = (m_0 + \lambda\phi)u^\mu$. Had we used x^μ and p^μ as independent variables and a random density $\tilde{R}_1$, we should have found an equation which would have read

$$\frac{\partial}{\partial \tau} \tilde{R}_1 + \frac{p^\mu}{(m_0 + \lambda\phi)} \partial_\mu \tilde{R}_1 + \lambda \partial_\mu \phi \cdot \frac{\partial}{\partial p^\mu} \tilde{R}_1 \equiv \frac{d\tilde{R}_1}{d\tau} = 0 \tag{3.4'}$$

because of the formally Hamiltonian character of this equation of motion (see Paper I). This equation may be considered as the expression of a relativistic Liouville theorem. With the choice of (x^μ, u^μ) as independent variables, Eq. (3.4) is equivalent to

$$dR_1/d\tau = -\frac{\lambda}{m_0} u^\nu \partial_\nu \phi \cdot R_1 \neq 0 \tag{3.4''}$$

and hence this "Liouville property" is no longer valid.]

To Eq. (3.4) we must add the equation satisfied by the "field" ϕ; for instance,

$$\Box \phi + M_0^2 \phi = \lambda \iint R_1(x_0, u'_\nu; \tau')\, d_4u'\, d\tau'. \tag{3.5}$$

Then using the solution of Eq. (3.5) given in Paper I (with $\phi_{1n} = 0$ since we are dealing with action at a

[27] E. G. Harris and A. Simon [Phys. Fluids 3, 255 (1960)] give a similar result.

[28] If we consider collective interactions, we would no longer have $\partial_\mu F^{\mu\nu} = 0$ but rather $\partial_\mu F^{\mu\nu} = j^\nu$. As a consequence we would find $\partial_\mu S^\mu > 0$. In the same way, if the *external* field $F^{\mu\nu}$ is *not* a free field, we also have this irreversible behavior, provided the field is weak.

[29] G. Szamosi in "Varenna Summer School: High Energy Astrophysics" (1965) (to be published) and references quoted therein.

[30] Yu. L. Klimontovich, Zh. Eksperim. i Teor. Fiz. 33, 982 (1957); 34, 173 (1958). [English transl.: Soviet Phys.—JETP 6, 753; 7, 119 (1958).]

[31] In the following when employing the word "field" in dealing with the action-at-a-distance point of view, it will be intended that the "field" is nothing but a complicated expression involving *only* particle variables which may be identified with the field in the field viewpoint.

distance) and substituting in Eq. (3.4), we find

$$\frac{\partial}{\partial\tau}R_1(x_\nu, u_\nu; \tau) + u^\mu\partial_\mu R_1(x_\nu, u_\nu; \tau) = -\frac{\lambda^2}{m_0}\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d\tau'\, d_4x'\, d_4u' R_1(x'_\nu, u'_\nu; \tau') \times R_1(x_\nu, u_\nu; \tau)\partial_\nu\Delta(x_\rho - x'_\rho)\right\}, \quad (3.6)$$

where $\Delta(x_\rho)$ is an appropriate[32] Green function of Eq. (3.5).

This equation is the fundamental equation generating the relativistic hierarchy for the reduced densities. It is an exact and rigorous equation: no approximation has been used in its derivation.

Let us now proceed with the derivation of this hierarchy. We first recall that both sides of Eq. (3.6) are random because of the random character of R_1; R_1 is random because of the random character of the trajectories or of the (unknown) "initial data" (see the discussion given in Paper I). Assuming[33] now the existence of an averaging operation denoted $\langle\ \rangle$, let us average both sides of Eq. (3.6). We get

$$\frac{\partial}{\partial\tau}D_1(x_\nu, u_\nu; \tau) + u^\mu\partial_\mu D_1(x_\nu, u_\nu; \tau) = -\frac{\lambda^2}{m_0}\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d\tau'\, d_4x'\, d_4u'\partial_\nu\Delta(x_\rho - x'_\rho) \times [(N-1)D_2(x_\nu, u_\nu; \tau; x'_\nu, u'_\nu, \tau') + P_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')]\right\}. \quad (3.7)$$

In the derivation of Eq. (3.7) use has been made of the following relations[1]:

$$\langle R_1\rangle = ND_1,$$
$$\langle R_1 \otimes R_1\rangle = N(N-1)D_2 + NP_2.$$

As we see in a following paragraph P_2 represents nothing but a *self-action* term. In what follows we assume that $N \gg 1$, which only slightly simplifies the equations obtained. The second equations of the hierarchy (i.e., the equation connecting D_2 with higher-order distributions) may be obtained by two different ways. First we may use again Eq. (3.6) by multiplying it by $R_1(x''_\nu, u''_\nu; \tau'')$ and taking the average value. Second, we may obtain an equation for R_2 directly [it is very similar to Eq. (3.6)] and take again the average value. In both cases the same result is found (as expected). Using, for instance, the first procedure, we find

$$\frac{\partial}{\partial\tau}[N^2D_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')] + u^\mu\partial_\mu[N^2D_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')] + \frac{\partial}{\partial\tau}[NP_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')] + u^\mu\partial_\mu[NP_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')] + \frac{\lambda^2}{m_0}\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d\tau''\, d_4x''\, d_4u''\partial_\nu\Delta(x_\rho - x''_\rho) \times [N^3D_3(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau'; x''_\rho, u''_\rho, \tau'') + N^2\mathfrak{T}W_3^2(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau'; \{x''_\rho, u''_\rho, \tau''\}) + NP_3(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau'; x''_\rho, u''_\rho, \tau'')]\right\} = 0. \quad (3.8)$$

In the same way D_2 satisfies another equation in the primed variables. In Eq. (3.8) the symbol $\mathfrak{T}$ means a sum over the permutations of the sets of variables (x_ρ, u_ρ, τ). The term between the brackets [ ] under the sign integral occurs because of the decomposition:

$$\sum_{i,j,k} = \sum_{\substack{i,j,k\\ \text{all different}}} + \sum_{(i=j)\neq k} + \sum_{(i=k)\neq j} + \sum_{(j=k)\neq i} + \sum_i \quad (3.9)$$

each term of this last equality giving rise to D_3, $\mathfrak{T}W_3^2$, P_3, respectively, after the averaging process.[34]

In fact, the two equations verified by D_2 are not sufficient to determine D_1 especially because Eq. (3.7) involves the knowledge of P_2. Therefore, we have to derive the *two* equations verified by P_2: They are very similar and obtained from each other simply by exchanging the primed and unprimed variables.

An equation for P_2 is easily obtained by passing through the intermediate step of the random density.[1] It is found to be

$$\frac{\partial}{\partial\tau}P_2(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau') + u^\mu\partial_\mu P_2(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau') + \frac{\lambda^2}{m_0}\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d\tau''\, d_4x''\, d_4u''\partial_\nu\Delta(x_\rho - x''_\rho) \times [NW_3^2(x_\rho, u_\rho, \tau; x'_\rho, u'_\rho, \tau'; \{x''_\rho, u''_\rho, \tau''\}) + P_3(x_\rho, u_\rho, \tau; x'_\rho; u'_\rho; \tau'; x''_\rho; u''_\rho; \tau'')]\right\} = 0. \quad (3.10)$$

[32] At this stage there is no particular need to specify Δ more precisely.

[33] This assumption is in fact very weak. It is similar to the basic statistical assumption (existence of an initial distribution) of classical statistical mechanics. What we actually assume are some simple mathematical properties like:

$$\partial_\mu\langle\ \rangle = \langle\partial_\mu\rangle, \qquad \int\langle\ \rangle = \langle\int\rangle, \text{ etc.}$$

[34] The physical interpretation of these densities appears to be obvious when coming back to the subjacent random densities. For instance,

$$W_3^2(X, X'; \{X''\}) = \sum_{i\neq j}\delta[X - X_i(\tau)] \otimes \delta[X' - X_i(\tau')] \otimes \delta[X'' - X_j(\tau'')]$$

may be interpreted as follows. It is the probability density that a particle be in state X at τ *and* that the *same* particle undergoes a transition to state X' at τ' *while* another particle be in state X'' at τ''. Of course, the "physical" densities are rather the densities obtained after integration over the proper time variables. However, the physical interpretation of the latter is quite similar. Furthermore, W_3^2 satisfies the following consistency relations:

$$\int W_3^2(X, X'; \{X''\})\, dX'' = P_2(X, X'),$$
$$\int W_3^2(X, X'; \{X''\})\, dX = D_2(X', X'').$$

With the help of Eq. (3.10) we can simplify Eq. (3.8) further and we get

$$\frac{\partial}{\partial\tau} D_2 + u^\mu \partial_\mu D_2 + \frac{\lambda^2}{m_0}\frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d\tau''\, d_4x''\, d_4u''\partial_\nu\Delta(x_\rho - x''_\rho) \times [ND_3 + W_3^2(x_\rho, u_\rho, \tau; x''_\rho, u''_\rho, \tau''; \{x'_\rho, u'_\rho, \tau'\}) + W_3^2(x''_\rho, u''_\rho, \tau''; x'_\rho, u'_\rho, \tau'; \{x_\rho, u_\rho, \tau\})]\right\} = 0. \tag{3.11}$$

For a wide domain of applications the first two equations of the hierarchy are sufficient, although equations for $D_3, D_4, \cdots$ may also be obtained in the same way. Of course, D_2 will be determined by W_3^2 itself satisfying other equations which may be obtained easily. These equations involve higher-order densities of the type W_i^j $(i, j > 3)$.

B. Remarks and Discussion

Let us now discuss the preceding results.

(1) The usual BBGKY hierarchy involves only densities similar to the D_k's while the relativistic hierarchy involves much more complicated densities such as the P_k or W_l^k. Furthermore the classical hierarchy stops at N while the relativistic one is *denumerably infinite* [for orders higher than N, of course, the hierarchy does not involve densities such as D_k but only P_k and W_k^l $(k, l = \cdots \infty)$].

(2) The various equations of the relativistic hierarchy are by essence nonlocal, contrary to what occurs in the classical case [notice the sign sum in Eqs. (3.7), (3.8), and (3.10)]. This corresponds to the fact that, in the action-at-a-distance formalism, the equations of motion are nonlocal. Note that the infinite number of equations of the hierarchy is also due to this circumstance: the occurrence of the distribution P_k, W_k^l is necessary due to the fact that they describe the detailed structure of the system whose knowledge is in principle needed to solve the equations of motion.[1]

(3) So far we have dealt with an action-at-a-distance point of view and it would be interesting to obtain results in the field viewpoint. In Paper I we noted that the statistical problem may be set in different ways. We also remarked that the only one which seems to be compatible both with the nature of the field equation (difficulty of solving the Cauchy problem without an extra assumption) and with the requirement of full Lorentz invariance (i.e., avoiding the introduction of objects extraneous to the geometries of the system and of Minkowski space–time) consists in setting the statistical problem in the following way: the random elements which are at our disposal are (a) R_1 and (b) ϕ_{in} the incident field appearing when solving the Cauchy problem for the field *at infinity*; i.e.,

$$\phi(x_\rho) = \iint_{-\infty}^{+\infty} d_4u'\, d\tau' R_1(x'_\rho, u'_\rho; \tau')\Delta(x_\rho - x'_\rho) + \phi_{\text{in}}(x_\rho), \tag{3.12}$$

where ϕ_{in} is a free field solution.

In the field point of view, Eq. (3.6) would be modified by simply adding a term of the form

$$\frac{\partial}{\partial u^\mu}\{\Delta^{\mu\nu}(u_\rho)\partial_\nu\phi_{\text{in}}R_1\}. \tag{3.13}$$

The relativistic hierarchy would then also imply terms like

$$\langle\phi_{\text{in}} \otimes \cdots \otimes \phi_{\text{in}} \otimes R_1 \otimes \cdots \otimes R_1\rangle \tag{3.14}$$

and would be slightly more complicated. In fact, in the field point of view it is even not necessary to eliminate[35] a part of the field (the one depending on the source R_1) and we might perfectly deal with the total field. In such a case (which is treated as a matter of illustration in the case of electromagnetic interactions in the next section) the hierarchy involves only the "moments":

$$\langle\phi \otimes \cdots \otimes \phi \otimes R_1 \otimes \cdots \otimes R_1\rangle. \tag{3.15}$$

In such a case the hierarchy obtained consists of *local* equations.

It should be noted that all other possibilities indicated in Paper I may also be treated with the same methods.

C. Renormalized Hierarchy

In the preceding developments we were concerned with the unrenormalized equations of motion and the subsequent hierarchies. In particular, the bare mass m_0 and the self-fields were dealt with. Let us try to look at the self-action terms in the various equations of the hierarchy. For instance, in Eq. (3.7) P_2 was a self-action term, i.e., the same particle interacts later with itself. In Eq. (3.8), P_3 may be interpreted in a similar fashion. However, the various terms W_3^2 cannot be interpreted so easily. In order to show their signification let us introduce a "visualization" of the various densities by means of diagrams. We denote by X the set of variables (x_ν, u_ν, τ). Each set X will be represented by a vertex and two solid lines. Hence $D_1(X)$ or $D_2(X, X')$ will be represented as shown in

[35] If instead of Eq. (3.5) we had a nonlinear or a non-exactly solvable equation for the field, this elimination could not be performed.

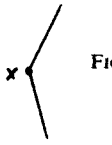


FIG. 1. Diagrammatic representation of $D_1(X)$, $(X \equiv \{x_\nu, u_\nu\tau;\})$.

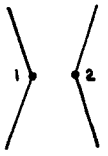


FIG. 2. Diagrammatic representation of $D_2(X_1, X_2)$.

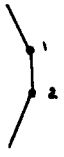


FIG. 3. Diagrammatic representation of $P_2(X_1, X_2)$.

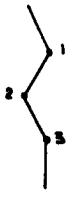


FIG. 4. Diagrammatic representation of $P_3(X_1, X_2, X_3)$.

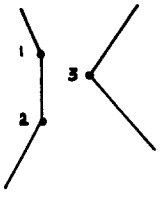


FIG. 5. Diagrammatic representation of $W_3^2(X_1, X_2; \{X_3\})$.

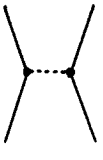


FIG. 6. Diagrammatic representation of $(\lambda^2/m_0)(\partial/\partial u^\mu)\{\Delta^{\mu\nu} \int \partial_\nu \Delta \cdot D_2\}$.

Figs. 1 and 2. A solid line between two vertices indicates that the two vertices refer to the *same* particle. Figures 3 and 4, respectively, represent $P_2(X, X')$ and $P_3(X, X', X'')$. With these conventions $W_3^2(X, X', \{X''\})$ is represented as indicated on Fig. 5. These diagrams symbolize in a simple way all possible densities. Let us now analyze the last term of Eq. (3.7) or (3.8) or of any equation of the hierarchy. These terms are characteristic of dynamics and it is important to represent them in a suitable way if we want to separate the self-action parts. Therefore, given two vertices, we represent by a dotted line an "interaction" between the vertices. By interaction we mean that (a) the first vertex concerns the variables involved in the derivations of the first terms of the equation [as, for instance (x_ν, u_ν, τ) with respect to which D_1 (or D_2) is derived in Eq. (3.7) [or Eq. (3.8)]] and (b) the vertex corresponding to the integration variables. In Figs. 6 and 7 we show how the two terms involving D_2 and P_2 of Eq. (3.7) are visualized. With this method the last terms of Eq. (3.8) may be represented by the sum of the diagrams given in Figs. 8–12.

FIG. 7. Diagrammatic representation of $(\lambda^2/m_0)(\partial/\partial u^\mu)\{\Delta^{\mu\nu} \int \partial_\nu \Delta \cdot P_2\}$.

FIG. 8. Diagrammatic representation of the term involving $W_3^2(1, 2, \{3\})$. $(1, 2, 3 \sim X_1, X_2, X_3)$.

FIG. 9. Diagrammatic representation of the term involving $W_3^2(3, 2; \{1\})$.

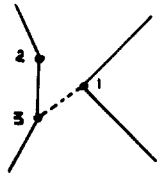
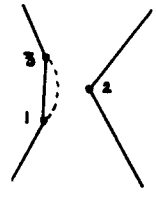


FIG. 10. Diagrammatic representation of the term involving $W_3^2(1, 3; \{2\})$.



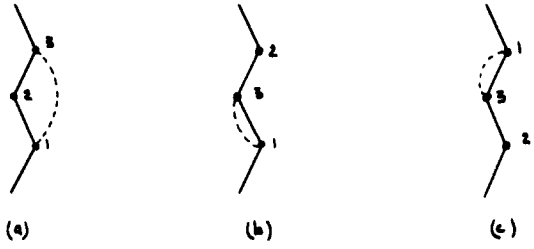
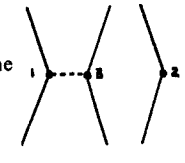


FIG. 11. Diagrammatic representations of the term involving P_3. Note that diagrams (a), (b), and (c) are equivalent. In the same way, other terms admit equivalent diagrams which are not represented.

FIG. 12. Diagrammatic representation of the term involving D_3.



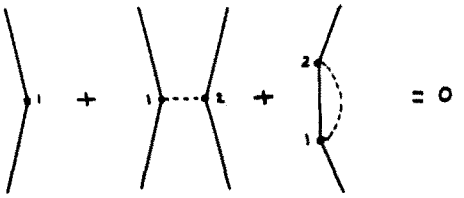


FIG. 13. Diagrammatic representation of Eq. (3.7). The term that does not include a dotted line now represents $\{(\partial/\partial\tau_1) + u_1^\mu \partial_{\mu_1}\} D_1(1)$. Note that the "dynamical term" contains always one more vertex: here, it is labeled 2.

Notice that only an even number of solid lines can pass by one vertex. Note also that this diagrammatic method allows one to write down easily the terms corresponding to the "dynamical term" of the equation verified by a density of order k: it is sufficient to write down $(k + 1)$ vertices and to join them by (connected or not) solid lines in all possible different ways, the dotted line[36] must *always* link a pair of vertices the label of which is chosen once and for all (e.g., in Figs. 8–12 only the vertices numbers 1 and 3 are linked by a dotted line); the choice of other pairs corresponds to writing down the *other* equations satisfied by the density of order k. The power of N to be put before each term is equal to the number of unconnected (by a solid line) solid lines. We have symbolized Eq. (3.7) in Fig. 13.

At this point we want to emphasize strongly that these diagrams are *not* (by definition) representations of a perturbation expansion: They are merely a helpful tool and, as all diagrams, not indispensable. However, they may also be used in a perturbative treatment, but at this stage it is not necessary to go into all the details.

Let us now come back to the self-action terms. A brief examination of Figs. 6–12 shows that the only self-action terms are those represented by Figs. 7, 10, and 11. It seems therefore that a renormalized hierarchy may be obtained by eliminating these terms while replacing the bare mass m_0 by m, the observable mass. We verify this property below.

Let us now derive the fundamental equation of the *renormalized* hierarchy. To this end let us consider the unrenormalized Eq. (3.6). Its right-hand side involves a product $R_1 R_1'$ which corresponds to a sum over two indices, each of them running from 1 to N. This double sum arises from the fact that Eq. (3.5) yields the *total field* acting on the ith particle and thus also its self-field. It is well known that the subtraction of this self-field is equivalent to a *mass renormalization*.[37]

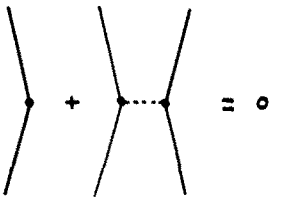


FIG. 14. Diagrammatic representation of Eq. (3.17).

Therefore we are led to perform the substitutions

$$R_1 R_1' = \sum_{i,j} \rightarrow R_2 = \sum_{i \neq j}$$

$$m_0 \rightarrow m$$

(bare mass) (observable mass)

in Eq. (3.6). Hence we obtain

$$\frac{\partial}{\partial\tau} R_1 + u^\mu \partial_\mu R_1 + \frac{\lambda^2}{m} \frac{\partial}{\partial u^\mu} \left\{ \Delta^{\mu\nu}(u_\rho) \int d\tau'\, d_4x'\, d_4u' \partial_\nu \Delta(x_\rho - x'_\rho) R_2 \right\} = 0, \tag{3.16}$$

which constitutes the fundamental equation generating the renormalized hierarchy. Now the first two equations of the renormalized hierarchy are

$$\frac{\partial}{\partial\tau} D_1 + u^\mu \partial_\mu D_1 + \frac{\lambda^2}{m} \frac{\partial}{\partial u^\mu} N \left\{ \Delta^{\mu\nu}(u_\rho) \times \int d\tau'\, d_4x'\, d_4u' \partial_\nu \Delta(x_\rho - x'_\rho) D_2 \right\} = 0 \tag{3.17}$$

and

$$\frac{\partial}{\partial\tau} D_2 + u^\mu \partial_\mu D_2 + \frac{2}{m} \frac{\partial}{\partial u^\mu} \left\{ \Delta^{\mu\nu}(u_\rho) \int d\tau'\, d_4x'\, d_4u' \partial_\nu \Delta(x_\rho - x'_\rho) \times [N D_3 + W_3^2] \right\} = 0, \tag{3.18}$$

and they are represented by Figs. 14 and 15, respectively. The similar second equation verified by D_2 is obtained by exchanging the labels 1 and 2 of the vertices appearing in Fig. 15.

4. ELECTROMAGNETIC INTERACTIONS

In this section we consider first the *renormalized* Klimontovich hierarchy and compare it with the one

[36] The diagrams presented here have only one dotted line. This is due to the fact that in our dynamical model occur only two-body forces.

[37] This renormalization procedure is, of course, not valid whatever the "field" equation (or whatever the equations of motion). It is, however, valid when using Eq. (3.5). Furthermore it is only the part of the self-field that possesses the symmetry past–future, which plays a role in the renormalization, the antisymmetrical part being related to "radiation." Since we are neglecting "radiation" here, we may directly use the symmetrical Green function as $\Delta(x_\rho)$. For the electromagnetic case, see, e.g., P. G. Bergmann, *Handbuch der Physic*, S. Flugge, Ed. (Springer-Verlag, Berlin, 1960), Vol. IV.

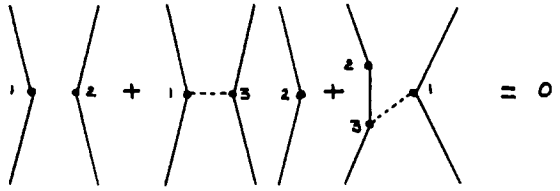


FIG. 15. Diagrammatic representation of Eq. (3.18).

actually given by this author.[38] These hierarchies neglect radiation phenomena so that we must give a more general hierarchy. This hierarchy is a generalization of what has been done in Sec. 2. Finally, for the sake of completeness, we give a formal treatment of both fields and particles by using the elegant methods due to Klimontovich.[2]

A. Renormalized Klimontovich Hierarchy

In the case where radiation phenomena are completely neglected (or rather at zeroth order in τ_0) the same methods as those used in Sec. 3 again yield a renormalized hierarchy whose fundamental equation (in the absence of an external field) is

$$\frac{\partial}{\partial\tau}R_1 + u^\mu\partial_\mu R_1 + \frac{e^2}{m}\int G(x_\rho - x'_\rho, u_\rho)R_2\, d_4x'\, d_4u'\, d\tau' = 0, \quad (4.1)$$

where G is the following operator:

$$G \equiv \{u'^\nu\partial^\mu - u'^\mu\partial^\nu\}D_{\text{ret}}(x_\rho - x'_\rho)u_\nu\frac{\partial}{\partial u^\mu}, \quad (4.2)$$

which is easily found by solving formally Maxwell equations. In Eq. (4.1) D_{ret} is the usual retarded photon propagator.[39]

From Eq. (4.1), the first two equations of the hierarchy are found to be

$$\frac{\partial}{\partial\tau}D_1 + u^\mu\partial_\mu D_1 + \frac{e^2}{m}N\int G\cdot D_2\, d_4x'\, d_4u'\, d\tau' = 0, \quad (4.3)$$

$$\frac{\partial}{\partial\tau}D_2 + u^\mu\partial_\mu D_2 + \frac{e^2}{m}N\int G\cdot\{D_3 + N^{-1}W_3^2\}\, d_4x'\, d_4u'\, d\tau' = 0, \quad (4.4)$$

which may also be represented by Figs. 14 and 15.

To compare this hierarchy to the one given by Klimontovich, we first define

$$Q_k = \int_{-\infty}^{+\infty}\cdots_{k\text{ times}}\int_{-\infty}^{+\infty}R_k\, d\tau_1\cdots d\tau_k.$$

(Note that $Q_1 = N_{q_iu_i}$, with the notations of Klimontovich.) Then, Eq. (4.1) reads (after integrating over τ):

$$u^\mu\partial_\mu Q_1 + \frac{e^2}{m}\int GQ_2\, d_4x'\, d_4u' = 0, \quad (4.5)$$

while the fundamental equation of Klimontovich is

$$u^\mu\partial_\mu Q_1 + \frac{e^2}{m_0}\int GQ'_1Q_1\, d_4x'\, d_4u' = 0. \quad (4.6)$$

The difference between Eqs. (4.5) and (4.6) is obviously due to the fact that Eq. (4.5) is *renormalized* whereas Eq. (4.6) is not. Eq. (4.5) is used in Sec. 5.

B. A Hierarchy Including Radiation Effects

We proceed exactly as in Sec. 2 with the difference that we are dealing now with N particles instead of one. We start with the equations of motion as given by Rohrlich[6]:

$$m\frac{d}{d\tau_i}u_i^\mu = e\overset{(i)}{F}{}^{\mu\nu}_{\text{ret}}(x_i^\rho)u_{\nu_i} + \tfrac{2}{3}e^2(\dot\gamma_i^\mu + \gamma_i^\rho\gamma_{\rho i}u_i^\mu), \quad (4.7)$$

$$\partial_\mu\overset{(i)}{F}{}^{\mu\nu}_{\text{ret}}{}^*(x_{\rho_i}) = 0, \quad (4.8)$$

$$\partial_\mu\overset{(i)}{F}{}^{\mu\nu}_{\text{ret}}(x_i) = e\int_{-\infty}^{+\infty}\sum_{j\neq i}\delta[x_i^\rho - x_j^\rho(\tau_j)]u_j^\nu(\tau_j)\, d\tau_j, \quad (4.9)$$

where we have assumed, *for the sake of simplicity*, that the system under consideration is constituted of identical particles, that there is no external force field.

To Eqs. (4.7), (4.8), and (4.9) must be added the *asymptotic conditions*:

$$\lim_{\tau\to\pm\infty}\gamma_i^\mu(\tau) = 0, \quad i = 1, 2, \cdots, N. \quad (4.10)$$

Equation (4.7) shows that the particle $\mathbf{\Gamma}$ space is

$$\mathbf{\Gamma} = \boldsymbol{\mu}^N = \mathcal{M}^{4N}\times\mathbf{U}^{4N}\times\boldsymbol{\gamma}^{4N}. \quad (4.11)$$

On this $\mathbf{\Gamma}$ space, we can define microscopic random densities exactly as in Paper I; for instance, $R_1(x_\nu, u_\nu, \gamma_\nu; \tau)$ is defined by

$$R_1(x_\nu, u_\nu, \gamma_\nu; \tau) = \sum_{i=1}^{i=N}\delta[x_\nu - x_{\nu i}(\tau)] \otimes \delta(u_\nu - u_{\nu i}(\tau)] \otimes \delta[\gamma_\nu - \gamma_{\nu i}(\tau)]. \quad (4.12)$$

Exactly as in Paper I and in Sec. 2, densities are average values over the "initial condition" [40] of the random

[38] Yu. L. Klimontovich, Zh. Eksperim. i Teor. Fiz., **37**, 535 (1959); **38**, 1212 (1960). [English transl.: Soviet Phys.—JETP **10**, 524 (1960); **11**, 876 (1960).]

[39] Note that we deal with an action-at-a-distance point of view, in the sense that the incident field is taken to be identically null. (See the remarks of the preceding section and of Part I.)

[40] The discussion given in Paper I on "initial conditions" may entirely be reproduced here.

densities; e.g., we have

$$ND_1(x_\nu, u_\nu, \gamma_\nu, \tau) = \langle R_1(x_\nu, u_\nu, \gamma_\nu; \tau)\rangle. \quad (4.13)$$

The asymptotic conditions (4.10) imply that the densities D_k satisfy the following conditions:

$$\lim_{(\tau_1 \cdots \tau_k)\to\pm\infty} D_k(\tau_1, \cdots, \tau_k) = \varphi(x_1^\nu, u_1^\nu \cdots x_k^\nu u_k^\nu) \overset{i=k}{\underset{i=1}{\otimes}} \delta(\gamma_k^\mu). \quad (4.14)$$

The various densities D_k generate proper time-independent densities whose normalization is a straightforward generalization of the ones given in Paper I and Sec. 2. For instance, the normalization of $\mathcal{N}_1(x_\rho, u_\rho, \gamma_\rho)$ is already given in Sec. 2.

Let us now derive the fundamental equation generating the new hierarchy. Starting from the continuity equation in the new μ-space

$$\frac{\partial}{\partial\tau} R_1 + \partial_\mu\{R_1 u^\mu\} + \frac{\partial}{\partial u^\mu}\{R_1 \dot{\gamma}^\mu\} + \frac{\partial}{\partial\gamma^\mu}\{R_1 \dot{\gamma}^\mu\} = 0 \quad (4.15)$$

(which has the same form as the one already derived in Sec. 2) and the equations of motion (7), one finds (in the same way as in Sec. 2)[41]

$$\frac{\partial}{\partial\tau} R_1 + u^\mu \partial_\mu R_1 + \gamma^\mu \frac{\partial}{\partial u^\mu} R_1 + \left\{\frac{3}{2e^2}[m\gamma^\mu - eF^{\mu\nu}u_\nu] - \gamma^\rho\gamma_\rho u^\mu\right\}\frac{\partial}{\partial\gamma^\mu} R_1 - \frac{3m}{2e^2} R_1 = 0. \quad (4.16)$$

In Eq. (4.16) $F^{\mu\nu}$ is, of course, the electromagnetic field which is responsible for interactions,[42] i.e., it does not contain self-fields. The effects of the latter are implicitly included in the renormalized mass *and* in the radiation reaction terms. Eliminating now the field $F^{\mu\nu}$ between Eqs. (4.9) and (4.16), we obtain the fundamental equation generating the *renormalized hierarchy taking account of radiation effects:*

$$\frac{\partial}{\partial\tau} R_1 + u^\mu \partial_\mu R_1 + \gamma^\mu \frac{\partial}{\partial u^\mu} R_1 + \frac{\partial}{\partial\gamma^\mu}\left\{\left[\frac{\gamma^\mu}{\tau_0 m} - \gamma^\nu\gamma_\nu u^\mu\right] R_1\right\} = \frac{e^2}{m\tau_0}\frac{\partial}{\partial\gamma^\mu}\left\{u_\nu \int d\tau'\, d_4x'\, d_4u'\, d_4\gamma' [u'^\nu \partial^\mu - u'^\mu \partial^\nu] \times D_{\text{ret}}(x_\rho - x'_\rho) R_2\right\}. \quad (4.17)$$

Taking now the average value of both sides of this last equation, one finds the first equation of the hierarchy:

$$\frac{\partial}{\partial\tau} D_1 + u^\mu \partial_\mu D_1 + \gamma^\mu \frac{\partial}{\partial\gamma^\mu} D_1 + \frac{\partial}{\partial\gamma^\mu}\left\{\left[\frac{\gamma^\mu}{\tau_0 m} - \gamma^\nu\gamma_\nu u^\mu\right] D_1\right\} = \frac{Ne^2}{m\tau_0}\frac{\partial}{\partial\gamma^\mu}\left\{u_\nu \int d\tau'\, d_4x'\, d_4u'\, d_4\gamma' [u'^\nu \partial^\mu - u'^\mu \partial^\nu] \times D_{\text{ret}}(x_\rho - x'_\rho) D_2\right\}, \quad (4.18)$$

which may be visualized by Fig. 14. The second equations of the hierarchy are obtained in the same way as in the preceding section:

$$\frac{\partial}{\partial\tau} D_2 + u^\mu \partial_\mu D_2 + \gamma^\mu \frac{\partial}{\partial u^\mu} D_2 + \frac{\partial}{\partial\gamma^\mu}\left\{\left[\frac{\gamma_\mu}{\tau_0 m} - \gamma^\nu\gamma_\nu u^\mu\right] D_2\right\} = \frac{Ne^2}{m\tau_0}\frac{\partial}{\partial\gamma^\mu}\left\{u_\nu \int d\tau'\, d_4x'\, d_4u'\, d_4\gamma' [u'^\nu \partial^\mu - u'^\mu \partial^\nu] \times D_{\text{ret}}(x - x') \times [D_3 + W_3^2 N^{-1}]\right\}, \quad (4.19)$$

which may be represented by Fig. 15. Of course, another similar equation is obtained for the other set of variables involved in D_2, etc.

C. An Alternative Form of the Preceding Hierarchy

Exactly as in Sec. 2, it is again possible to use another phase space:

$$\hat{\Gamma} = \hat{\mu}^N = \mathcal{M}^{4N} \times \mathbf{U}^{4N} \times \dot{\gamma}^{4N}. \quad (4.20)$$

On this phase space, densities such as the ones given in Paper I may be defined; for instance, we have

$$\hat{R}_1(x_\nu, u_\nu, \dot{\gamma}_\nu; \tau) = \sum_{i=1}^{i=N} \delta[x_\nu - x_{\nu i}(\tau)] \otimes \delta[u_\nu - u_{\nu_i}(\tau)] \otimes \delta(\dot{\gamma}_\nu - \dot{\gamma}_{\nu_i}(\tau)], \quad (4.21)$$

which satisfies the continuity equation in $\hat{\mu}$-space:

$$\frac{\partial\hat{R}_1}{\partial\tau} + \partial_\mu\{u^\mu \hat{R}_1\} + \frac{\partial}{\partial u^\mu}\{\gamma^\mu \hat{R}_1\} + \frac{\partial}{\partial\gamma^\mu}\{\dot{\gamma}^\mu R_1\} = 0. \quad (4.22)$$

After using the equations of motion (4.7), (4.8), and (4.9), elimination of the interaction field, Eq. (4.22) leads immediately to the fundamental equation generating the hierarchy satisfied by $\hat{D}_1$, $\hat{D}_2$, $\hat{W}_3^2 \ldots$:

$$\frac{\partial\hat{R}_1}{\partial\tau} + u^\mu \partial_\mu \hat{R}_1 + m\tau_0 \frac{\partial}{\partial u^\mu}\{\Delta^{\mu\nu}(u_\rho)\dot{\gamma}_\nu \hat{R}_1\} = -\frac{\partial}{\partial\dot{\gamma}^\mu}\{\dot{\gamma}^\mu \hat{R}_1\} + \frac{\partial}{\partial u^\mu}\left\{u_\nu \frac{e^2}{m}\int d\tau'\, d_4x'\, d_4u'\, d_4\dot{\gamma}' \times (u'^\nu \partial^\mu - u'^\mu \partial^\nu) \cdot D_{\text{ret}}(x_\rho - x'_\rho)\hat{R}_2\right\}. \quad (4.23)$$

[41] The remark concerning the increase of the phase-space volume element, effected in Sec. 2, is also valid in this many-particle case.

[42] The notation is slightly incorrect.

In Eq. (4.23), the term involving $\ddot{\gamma}^\mu \hat{R}_1$ may easily (but tediously) be obtained from Eq. (4.7). In fact, it leads to terms involving third- and second-order random distributions so that Eq. (4.23) is much more complicated than Eq. (4.17). Equation (4.23) allows the obtention of a hierarchy for D_1, etc., but its main interest lies in the possibilities it raises in looking for kinetic equations including radiation effects (exactly as in Sec. 2). Indeed, integrating both sides of Eq. (4.23) over the $\dot{\gamma}$ variables, we get the following (random) equation:

$$\frac{\partial}{\partial\tau} R_1(x_\nu, u_\nu; \tau) + u^\mu \partial_\mu R_1(x_\nu, u_\nu; \tau) + \frac{e^2}{m}\frac{\partial}{\partial u^\mu}\left\{u_\nu \int d\tau'\, d_4x'\, d_4u'(u'^\nu \partial^\mu - u'^\mu \partial^\nu) \cdot D_{\text{ret}}(x_\rho - x'_\rho) R_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau')\right\} = -\tau_0 \frac{\partial}{\partial u^\mu}\left\{\Delta^{\mu\nu}(u_\rho)\int d_4\dot{\gamma} \cdot \dot{\gamma}_\nu \hat{R}_1(x_\nu, u_\nu, \dot{\gamma}_\nu; \tau)\right\} \quad (4.24)$$

in the derivation of which we assumed a sufficiently vanishing behavior at infinity in the $\dot{\gamma}$ variables, of the density $\hat{R}_1$.

Equation (4.24) consists of two terms. The left-hand side of this equation represents nothing but the fundamental equation generating the renormalized Klimontovich hierarchy. The right-hand side is *proportional to* τ_0 (and in general will be "small") and couples the usual densities [depending on (x_ν, u_ν)] to the generalized densities [depending on $(x_\nu, u_\nu, \dot{\gamma}_\nu)$] and therefore is a term *including radiation effects*.

In another paper [R. Hakim and A. Mangeney, J. Math. Phys. (to be published)], we shall give an approximate hierarchy valid at order one in τ_0 and from which several kinetic equations (thus including radiation effects) will be derived.

D. Statistical Treatment of Fields and Particles

According to a large number of authors relativistic statistical mechanics should treat both fields and particles. In such a theory, bare particles plus the total field (including also the self-fields) are dealt with so that the theory should be renormalized at another stage.

Consequently we start with the equations of motion for the fields and particles, written as

$$m_0 \frac{du_i^\mu}{d\tau_i} = eF^{\mu\nu}(x_{\rho i})u_{\nu_i}, \quad i = 1 \cdots N, \quad (4.25)$$

$$\partial_\mu F^{\mu\nu *}(x_\rho) = 0, \quad (4.26)$$

$$\partial_\mu F^{\mu\nu}(x_\rho) = \sum_{i=1}^{i=N} e\int_{-\infty}^{+\infty} d\tau_i \delta[x_\rho - x_{\rho_i}(\tau_i)]u_i^\nu(\tau_i), \quad (4.27)$$

where m_0 is the mechanical *bare mass*. Equations (4.25) and (4.27) are equivalent to

$$\frac{\partial R_1}{\partial\tau} + u^\mu \partial_\mu R_1 + \frac{e}{m_0} F^{\mu\nu} u_\nu \frac{\partial}{\partial u^\mu} R_1 = 0, \quad (4.28)$$

$$\partial_\mu F^{\mu\nu}(x_\rho) = e\iint d_4u\, d\tau u^\nu R_1(x_\nu, u_\nu; \tau). \quad (4.29)$$

With the help of the notations

$$L_{\mu\nu} = \tfrac{1}{2}\{u_\mu(\partial/\partial u^\nu) - u_\nu(\partial/\partial u^\mu)\}, \quad \lambda = e/m_0, \quad (4.30)$$

Eq. (4.28) reads

$$\partial R_1/\partial\tau + u^\mu \partial_\mu R_1 + \lambda L_{\mu\nu} F^{\mu\nu} R_1 = 0. \quad (4.31)$$

Taking now the average value of this last equation over *both field and particle* "initial data," we obtain the first equation of a nonrenormalized hierarchy:

$$(\partial/\partial\tau)D_1 + u^\mu \partial_\mu D_1 + \lambda L_{\mu\nu}\langle F^{\mu\nu}(x_\rho) R_1(x_\rho, u_\rho; \tau)\rangle = 0. \quad (4.32)$$

Note also that from equations similar to Eq. (4.28) satisfied by the random densities R_k equations analogous to Eq. (4.32) are obtained for the densities D_k:

$$(\partial/\partial\tau)D_k + u^\mu \partial_\mu D_k + \lambda L_{\mu\nu}\langle F^{\mu\nu}(x_\rho) R_k(x_\rho, u_\rho, \tau; \cdots; x_{\rho_k}, u_{\rho_k}, \tau_k)\rangle = 0 \quad (4.33)$$

(and other similar equations referring to the other sets of variables). Setting now

$$\mathbf{\Lambda}^k \equiv \mathbf{\Lambda}^k(x_1^\rho, \cdots, x_k^\rho; x^\rho, u^\rho, \tau) = \|\langle F^{\mu_1\nu_1}(x_1^\rho) \otimes \cdots \otimes F^{\mu_k\nu_k}(x_k^\rho) \otimes R_1(x_\rho, u_\rho; \tau)\rangle\| \quad (4.34)$$

(with $\mathbf{\Lambda}^0 \equiv D_1$) we find [after multiplying Eq. (4.31) by a suitable number of factors $F^{\mu\nu}$ and taking the average value] the general equation satisfied by $\mathbf{\Lambda}^k$ to be

$$(\partial/\partial\tau)\mathbf{\Lambda}^k + u^\mu \partial_\mu \mathbf{\Lambda}^k + \lambda \mathbf{L}_k \mathbf{B}_k \mathbf{\Lambda}^{k+1} = 0, \quad k = 1, 2, \cdots, \infty, \quad (4.35)$$

where the operator $\mathbf{B}_k$ is defined by

$$(\mathbf{B}_k \mathbf{\Lambda}^{k+1})^{\mu_1\nu_1\cdots\mu_k\mu_k\mu\nu} = g^\mu_{\mu_{k+1}} g^\nu_{\nu_{k+1}} \int\cdots\int d_4x \cdots d_4x'_{k+1} \times \{\delta(x_1^\rho - x_1^{\rho'}) \otimes \cdots \otimes \delta(x_k^\rho - x_k^{\rho'}) \otimes \delta(x^\rho - x_{k+1}^{\rho'})\} \times (\Lambda^{k+1})^{\mu_1\nu_1\cdots\mu_{k+1}\nu_{k+1}}, \quad (4.36)$$

while the operator $\mathbf{L}_k$ is

$$(\mathbf{L}_k \mathbf{\Lambda}^{k+1})^{\mu_1\nu_1\cdots\mu_k\nu_k} = (\mathbf{L}\mathbf{\Lambda}^{k+1})^{\mu_1\nu_1\cdots\mu_k\nu_k}.$$

By introducing an infinite-vector $\mathbf{\Lambda}$ whose components

are the Λ^k's, Eq. (4.35) can be cast into a more compact form. Indeed setting

$$L = \begin{pmatrix} L_1 & 0 & 0 & 0 & \cdots \\ 0 & L_2 & 0 & 0 & \cdots \\ 0 & 0 & L_3 & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & 0 & L_k \\ & & & & \cdot \\ & & & & \cdot \\ & & & & \cdot \end{pmatrix}, \quad (4.37)$$

$$B = \begin{pmatrix} B_1 & 0 & 0 & 0 & \cdots \\ 0 & B_2 & 0 & 0 & \cdots \\ 0 & 0 & B_3 & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & 0 & B_k \\ & & & & \cdot \\ & & & & \cdot \\ & & & & \cdot \end{pmatrix}, \quad (4.38)$$

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & \\ 0 & 0 & 1 & 0 & \cdots & \\ 0 & 0 & 0 & 1 & 0 & \\ & & & & \cdot & \\ \cdot & \cdot & \cdot & 0 & 1 & \cdot \\ & & & & & \cdot \\ & & & & \cdot & \cdot \\ & & & & \cdot & \cdot \end{pmatrix}, \quad (4.39)$$

Eq. (4.35) can be rewritten as

$$(\partial/\partial\tau)\mathbf{\Lambda} + u^\mu\partial_\mu\mathbf{\Lambda} + \lambda\mathbf{LBA}\mathbf{\Lambda} = 0, \quad (4.40)$$

the *formal* solution of which is easily found to be

$$\mathbf{\Lambda}(\tau) = \exp\{-(u^\mu\partial_\mu + \lambda\mathbf{LBA})\tau\}\mathbf{\Lambda}(0). \quad (4.41)$$

[$\mathbf{\Lambda}(0)$ may be replaced by $\mathbf{\Lambda}(\tau_1)$, τ_1 being arbitrary.] In order to obtain an expansion of $\mathbf{\Lambda}(\tau)$ in powers of λ it is preferable to work in interaction representation by setting

$$L_0 = u^\mu\partial_\mu, \qquad L_1 = \mathbf{L}\cdot\mathbf{B}\cdot\mathbf{A}. \quad (4.42)$$

However, λ is not an interesting parameter because it contains the bare mass and not the observable mass.

The knowledge of $\mathbf{\Lambda}(\tau)$ is, of course, not sufficient to characterize completely the system under study.[43] In particular, the various moments of the field are needed. They satisfy the equations

$$\partial_\mu\langle F^{\mu_1\nu_1}(x_1^\rho)\otimes\cdots\otimes F^{\mu_k\nu_k}(x_k^\rho)\otimes F^{\mu\nu}(x^\rho)\rangle = \iint d\tau\cdot d_4u u^\nu(\mathbf{\Lambda}^k(\tau))^{\mu_1\nu_1\cdots\mu_k\nu_k}, \quad (4.43)$$

which can be rewritten symbolically

$$\partial_\mu\mathcal{F}^{\mu\nu} = e\iint d\tau\, d_4u\mathbf{\Lambda}(\tau)u^\nu, \quad (4.44)$$

$$\mathcal{F}^{\mu\nu} = \{\langle F^{\mu_1\nu_1}\otimes\cdots\otimes F^{\mu_k\nu_k}\otimes F^{\mu\nu}\rangle\}. \quad (4.45)$$

Equation (4.44) can also be solved formally and leads to

$$\mathcal{F}^{\mu\nu} = e\int d\tau'\, d_4x'\, d_4u' \times\{\mathbf{\Lambda}(\tau')[u'^\nu\partial^\mu - u'^\mu\partial^\nu]D_{\text{ret}}(x_\rho - x_\rho) + \mathcal{F}_0^{\mu\nu}, \quad (4.46)$$

where D is the appropriate elementary solution of $\Box D = \delta$ and where $\mathcal{F}_0^{\mu\nu}$ represents either the correlations of the initial field *or* those of the incident field. In the latter case the proper time integration [in Eqs. (4.43), (4.44), and (4.46)] goes from minus infinity to plus infinity. In the former case,[44] this integration goes from zero to infinity. Then $\mathcal{F}_0^{\mu\nu}$ refers to the initial correlation of the fields through

$$\mathcal{F}_0^{\mu\nu} = \int_\Sigma\{\partial D(x_\rho - x'_\rho)\mathcal{F}_\Sigma^{\mu\nu}(x'_\rho) - D(x_\rho - x'_\rho)\partial\mathcal{F}_\Sigma^{\mu\nu}\}\, d\Sigma, \quad (4.47)$$

where ∂ is the normal derivative to Σ, which is itself the "initial physical space." In Eq. (4.47), $\mathcal{F}_\Sigma^{\mu\nu}$ and $\partial\mathcal{F}_\Sigma^{\mu\nu}$ are not independent. $\partial\mathcal{F}_\Sigma^{\mu\nu}$ may be obtained (at least in principle) from $\mathcal{F}_\Sigma^{\mu\nu}$ and Maxwell equations.

E. Remarks and Discussion

(1) In the above developments we were mainly concerned with the statistical problem as set in Paper I: i.e., there is no average value over "initial conditions," the only random elements being R_1 in the action-at-a-distance viewpoint or R_1 *and* $F^{\mu\nu}$ (or possibly

[43] In particular, functions like

$$\left\langle\left\{\sum_i\delta[X - X_i(\tau)]\otimes\delta[X' - X_i(\tau')]\right\}\otimes F^{\mu_1\nu_1}(1)\cdots F^{\mu_k\nu_k}(k)\right\rangle$$

(with $X = \{x_\mu, u_\mu\}$) are also needed to specify *completely* the system. More generally the average values of products of fields by the random densities giving rise to various transition probabilities are equally needed.

[44] See the discussion below.

$F_{\text{ni}}^{\mu\nu}$) in the field case. However, in Eq. (4.46) we have also interpreted $\mathcal{F}_0^{\mu\nu}$ as resulting from correlation of an "initial field" $F_\Sigma^{\mu\nu}$ [Eq. (4.47)]. In fact, this departure from our general philosophy was just an illustration of a way of setting the statistical problem.[1] As indicated in Paper I, there is *a priori* no reason why an arbitrary $F_\Sigma^{\mu\nu}$ would result from the past of the system, so that the above interpretation and Eq. (4.47) are valid only provided one makes a further assumption. This supplementary assumption is that of the "switching on of the interaction on Σ."

(2) Again in the field point of view, the field $F^{\mu\nu}$ may always be split into an incident field and an interacting field; this latter contains also the self-fields and depends functionally on R_1. Therefore if we eliminate once again the fields between Eqs. (4.28) and (4.29), we are led to the fundamental equation generating the unrenormalized Klimontovich hierarchy *to which one must add* a supplementary term of the form

$$(e/m_0)F_{\text{in}}^{\mu\nu}u_\nu(\partial/\partial u^\mu)R_1. \tag{4.48}$$

Next, average values may again be taken and a hierarchy similar both to the unrenormalized Klimontovich one and to Eq. (4.35) is found.

(3) Another point is that in the field point of view the theory contains self-energy divergences and therefore demands to be renormalized. For instance, it should be renormalized at each order of an eventual perturbation expansion. Secondly, other solutions of the different equations for the moments can also be obtained by performing a cluster expansion—as Dupree[45] did in the nonrelativistic case. Here again the theory should be renormalized.

Unfortunately there is no general recipe for such a program of renormalization of a *classical* theory. The only possibilities that remain consist in considering the lowest-order terms either in a perturbation or in a cluster expansion and in getting rid of infinities in some way. However, in so doing we could perfectly keep *finite* terms which in fact should be included in the *observable* mass. For these reasons we prefer to start with an *a priori* renormalized theory.

(4) It should be noted that, as is well known, the field point of view also yields the Lorentz–Dirac equation [although with the supplementary term arising from $F_{\text{in}}^{\mu\nu}$, i.e., $(e/m)F_{\text{in}}^{\mu\nu}u_\nu$]. Therefore, we could also use a renormalized theory based on Eq. (4.16) to which a term including $F_{\text{in}}^{\mu\nu}$ should be added and apply again the Klimontovich method, etc. In this sense we should have a "renormalized field theory."

[45] T. H. Dupree, Phys. Fluids **6**, 1714 (1963).

(5) As a first conclusion we see that, whatever the viewpoint adopted, the treatment of the field aspect is much more involved than the action-at-a-distance one.

5. SIMPLE KINETIC EQUATIONS FOR AN ELECTRON GAS

In this section, we illustrate the above formalism by a *rederivation* of two well-known covariant kinetic equations, i.e., Vlasov and Landau kinetic equations.[46] To this end we use the *renormalized* Klimontovich hierarchy given in Sec. 4 at the order zero in τ_0 (i.e., radiation is neglected). In another paper, we give similar kinetic equations for scalar interactions.[47] In all that follows, the electron gas is assumed to be embedded in a uniform neutralizing positive background.

A. Covariant Vlasov Equation

The Vlasov equation is a kinetic equation valid at order (ne^2) ($n \simeq$ density) which is equally obtained by assuming the absence of binary correlations, i.e., (in the relativistic case):

$$D_2(x_\nu, u_\nu, \tau; x'_\nu, u'_\nu, \tau') = D_1(x_\nu, u_\nu; \tau) \otimes D_1(x'_\nu, u'_\nu; \tau'). \tag{5.1}$$

Note that the factorization of D_2 implies that of $\mathcal{N}_2$. Using now the first equation of the renormalized Klimontovich hierarchy [Eq. (4.3)] and taking Eq. (5.1) into account, we obtain the covariant Vlasov equation:

$$\frac{\partial D_1}{\partial \tau} + u^\mu \partial_\mu D_1 + \frac{Ne^2}{m}\int \{u'^\nu \partial^\mu - u'^\mu \partial^\nu\} \cdot D_{\text{ret}}(x_\rho - x'_\rho) \cdot D_1(x'_\rho, u'_\rho; \tau')\, d\tau'\, d_4x'\, d_4u' \cdot \frac{\partial}{\partial u^\mu} D_1(x_\rho, u_\rho; \tau) = 0, \tag{5.2}$$

which, of course, reduces to conventional forms after integrating over τ. Equation (5.2) may be generalized in several aspects and used in a similar manner as in the classical case. In particular, a dispersion relation for the propagation of a small disturbance may be obtained. In another paper we shall see that radiation phenomena imply a modification of Eq. (5.2).

[46] In fact, the covariant Vlasov equation has been derived by a large number of authors (see Paper I). However, the various derivations used are not completely correct. In the same way, there exist two derivations of the relativistic Landau equation. One has been given by A. Mangeney [Ann. Phys. **10**, 191 (1965)] and is rather involved, and not in a covariant way. The other one has been given by Yu. L. Klimontovich[38] and is incorrect on several points. In particular, this author used the unrenormalized hierarchy and got rid of the subsequent infinities because of a number of errors of calculation, etc. In the following we derive these equations "rigorously" in the sense that the derivation involves no more assumptions than in the nonrelativistic case (when using the BBGKY hierarchy).

[47] R. Hakim, Nuovo Cimento (to be published).

Let us now come back to the field point of view. From Eq. (4.32), by imposing the factorization

$$\langle R_1 \otimes F^{\mu\nu}\rangle = \langle R_1\rangle \otimes \langle F^{\mu\nu}\rangle, \tag{5.3}$$

we find

$$\frac{\partial D_1}{\partial \tau} + u\partial_\mu D_1 + \frac{e}{m_0}\langle F^{\mu\nu}\rangle u_\nu \frac{\partial}{\partial u^\mu} D_1 = 0 \tag{5.4}$$

and

$$\left.\begin{aligned} \partial_\mu \langle F^{\mu\nu *}\rangle &= 0, \\ \partial_\mu \langle F^{\mu\nu}\rangle &= \int Ne\, d\tau'\, d_4u' u'^\nu D_1 \end{aligned}\right\}. \tag{5.5}$$

Eliminating now $\langle F^{\mu\nu}\rangle$ between Eqs. (5.5) and (5.4) we obtain Eq. (5.2) with this difference: m_0 *occurs instead of* m. It follows that, strictly speaking, the equation obtained reduces to

$$(\partial D_1/\partial\tau) + u^\mu \partial_\mu D_1 = 0, \tag{5.6}$$

since the bare mass m_0 is infinite! In fact, the Vlasov equation might be obtained in the field point of view. However, it would be very difficult to justify (at the approximation considered) the replacement of m_0 by m.[48]

This slight difficulty exists as well in all non-renormalized hierarchies, as is the case in Klimontovich hierarchy.[38] This author imposes the condition

$$\langle R_1 \otimes R_1\rangle = \langle R_1\rangle \otimes \langle R_1\rangle, \tag{5.7}$$

which is similar to Eq. (5.3). In fact, we have already seen that

$$\langle R_1 \otimes R_1\rangle = N(N-1)D_2 + NP_2,$$

and comparing with condition (5.1) (which is the relativistic generalization of the classical condition), the term involving P_2 appears to be responsible for the change $m_0 \to m$, as expected.

B. Covariant Landau Equation

(1) Now we *rederive* the relativistic Landau equation in an improved way. The Landau approximation is characterized by several assumptions among which are found:

(a) Absence of three particle correlations (i.e., the third-order correlation function vanishes);

(b) Validity at the order $\chi^4 \sim e^4$ (where χ is the expansion parameter);

(c) Small energy-momentum transfers during collisions;

(d) Existence of two time scales (the times considered are long compared to the correlation time);

(e) Spatial homogeneity of the system.

Of course, exactly as in the classical case, these approximations can be justified rigorously. Furthermore, they are not completely independent.

(2) As usual,[49] we start from the first two equations of the (renormalized) hierarchy,[50] i.e., from Eqs. (4.32) and (4.33). Using the cluster expansion

$$\begin{aligned} D_1 &= g_1, \\ D_2 &= D_1 \otimes D_1 + g_2, \\ D_3 &= D_1 \otimes D_1 \otimes D_1 + D_1 \otimes g_2 + D_1 \otimes g_2 + D_1 \\ &\quad \otimes g_2 + g_3, \end{aligned} \tag{5.8}$$

these equations may be rewritten as

$$\frac{\partial}{\partial\tau} D_1 + u^\mu \partial_\mu D_1 + \frac{Ne^2}{m}\left\{\int [G(D_1 \otimes D_1) + Gg_2]\right\} = 0, \tag{5.9}$$

$$\frac{\partial}{\partial\tau} g_2 + u^\mu \partial_\mu g_2 + \frac{e^2}{m}\int GW_3^2 + \frac{Ne^2}{m}\left\{\int G[D_1 \otimes g_2 + D_1 \otimes g_2 + Gg_3]\right\} = 0. \tag{5.10}$$

In Eqs. (5.9) and (5.10) G is the operator defined at the beginning of Sec. 4. Of course, there exists another equation similar to Eq. (5.10).

(3) Let us now use the approximations considered at the beginning of the paragraph. Assumption (a) implies that the last term of Eq. (5.10) vanishes. Assumption (b) implies that g_2 must be calculated at order e^2 [in order that Eq. (5.9) be valid at order e^4]. Therefore, Eq. (5.10) is rewritten as

$$\frac{\partial}{\partial\tau} g_2 + u^\mu \partial_\mu g_2 = -\frac{e^2}{m}\int GW_3^{2[0]}, \tag{5.11}$$

which shows, as expected, that g_2 is of order e^2. At order zero W_3^2 is given by

$$\begin{aligned} W_3^{2[0]}(x''_\rho, u''_\rho, \tau''; x'_\rho, u'_\rho, \tau'; \{x_\rho, u_\rho, \tau\}) \\ = D_1(x_\rho, u_\rho; \tau) D_1(x'_\rho, u'_\rho; \tau') \\ \times \delta[x''_\rho - x'_\rho - u''_\rho(\tau'' - \tau')]\delta[u''_\rho - u'_\rho], \end{aligned} \tag{5.12}$$

and this is equivalent to assumption (c): particles move practically along straight world lines or, equivalently, the field acting on particle 1 is the field produced by particle 2 moving along a straight world line.

[48] It is also clear that the factorization (5.3) is incorrect.

[49] D. C. Montgomery and D. A. Tidman, *Plasma Kinetic Theory* (McGraw-Hill Book Company, Inc., New York, 1964).

[50] At the order considered ($\sim e^4$) it is possible to show that for a spatially homogeneous system the effects of radiation play no role, being in e^6 at the lowest order: I. Prigogine and Ph. de Gottal, Physica 31, 677 (1965). However, these authors use a perturbative treatment which involves only one expansion parameter e^2 so that $\tau_0 \sim e^2$. In fact there are two expansion parameters ($\sim e^2$ and $\sim \tau_0$) and radiation phenomena occur at the order $\sim e^4\tau_0$ for homogeneous systems (i.e., at order e^6), or even at order $e^2\tau_0$ for an inhomogeneous system.

Approximations (c) are used in solving the simple inhomogeneous Eq. (5.11). They amount to neglecting the arbitrary homogeneous solution of this equation. Furthermore, the densities D_1 occurring in Eq. (5.12) are to be "frozen" (adiabatic hypothesis[49]) in the calculation of g_2.

Equation (5.11) may be solved either with the use of Fourier transformation, or more simply by using the "causal" Green function

$$K(x_\rho - x'_\rho; u_\rho - u'_\rho; \tau - \tau') = \theta(\tau - \tau')\delta[x_\rho - x'_\rho - u_\rho(\tau - \tau')] \otimes \delta(u_\rho - u'_\rho) \tag{5.13}$$

and letting the "initial" proper time tend to minus infinity (this is legitimate because of the existence of two time-scales: "initial" correlations are destroyed). Finally the expression obtained for g_2 (after tedious calculations) is the one given by Klimontovich[51]; using the expression for g_2 in Eq. (5.9) and taking into account condition (e)[52] the covariant Landau equation is found[53]:

$$\frac{\partial}{\partial\tau} D_1 + u^\mu \partial_\mu D_1 = \frac{Ne^4}{m^2} \frac{\partial}{\partial u^\beta} \int \epsilon^{\alpha\beta}(u'_\rho, u_\rho) \times \left\{ D_1 \otimes \frac{\partial}{\partial u^\alpha} D_1 - D_1 \otimes \frac{\partial}{\partial u^\alpha} D_1 \right\}, \tag{5.14}$$

where the tensor $\epsilon^{\alpha\beta}$ is the one given by Klimontovich.

From Eq. (5.14), a relativistic Fokker–Planck equation may be obtained, etc.

[It is interesting to note that the preceding calculation furnishes the relativistic correlation function g_2 as a functional of D_1 at order e^2. Hence, when D_1 is chosen so as to represent an equilibrium state (i.e., when D_1 is the Jüttner–Synge distribution function), then we obtain the equilibrium correlation function at order e^2, $g_{2\text{eq}}$. $g_{2\text{eq}}$ is needed when we want to generalize in a covariant way the Guernsey kinetic equation.]

6. SUMMARY AND DISCUSSION

In Paper I we discussed the basic statistical problems. First, we showed that, if "initial data" (to be specified more precisely later) are to be actually related to the measures of an "observer," then *it seems* that they should not be sufficient to characterize the ulterior behavior of the system. Next passing to the mathematical initial data, we showed that *it seems* they cannot be given on a spacelike hypersurface since the knowledge of the entire past of the system *seems to be required.* Therefore we concluded that the basic relativistic statistics cannot be set into a form similar to the Newtonian one, at least without further assumptions. Finally, after analyzing the classical notion of a Gibbs ensemble we defined a relativistic Gibbs ensemble as being the data (a) of the manifold of solutions of the equations of motion and (b) the data of a probability over this manifold. This point of view led us to consider as basic random element $R_1(x_\nu, u_\nu; \tau)$ (and possibly the in-field).

At this point it seems to be worthwhile to discuss a slight mystification involved in the theory. Apparently, knowing the equations of motion governing the system and "randomizing," either the "initial data" or the manifold of solutions seems to lead to statistical mechanics. In fact, it is so only with a slight mystification. Indeed, we generally deal with *only one* physical system and *not* with an infinity of similar systems. In classical statistical mechanics this difficulty is avoided by the *assumptions* of ergodic properties.

[Let us consider for simplicity the question of equilibrium. Since we deal with only one system, the only possible average values which may be calculated are *temporal averages*; i.e.,

$$\int K(t, t') A[q(t'), p(t')]\, dt' = \bar{A}.$$

Strocchi[54] has shown that, under simple plausible assumptions, the averaging operation is the usual time average. We are therefore led to assume ergodic properties.]

Here we have not *proved* a theorem similar to Strocchi's one and we have not yet a precise idea of its relativistic form. Hence we cannot invoke some "covariant ergodic properties" and therefore our model rests on *the hope* (or the assumption) that it will be convenient in describing the properties of only one system.

Once the basic statistics are introduced, phase space is defined. Contrary to the Newtonian case where phase space is the set of initial data, the relativistic case phase space is only *suggested* by the form of the equations of motion and thus *is chosen for convenience.* Phase space is then an $8N$- or $12N$-dimensional space according to the choice of

[51] After an integration over τ and τ'.

[52] The spatial homogeneity of the system implies that there exists a timelike unit four-vector α^μ such that the x_ν dependence of D_1 occurs only through

$$D_1(x_\nu, u_\mu; \tau) = D_1(\alpha^\mu x_\mu, u_\nu; \tau).$$

Hence the "Vlasov term" in Eq. (5.9) gives rise to a term involving a constant electromagnetic field itself annihilated by the positive uniform background.

[53] After simple but rather tedious calculations. Note that, in obtaining the symmetrical form of the collision term, relations such

$$\partial_\mu \left\{ \int_{-\infty}^{+\infty} d\tau D_{\text{ret}}(x_\rho - x'_\rho - u_\rho\tau) u^\mu \right\} = 0$$

must be used.

[54] F. Strocchi, thesis (Pisa). See also, Orsay Report Th.118 (1965)

equations of motion without radiation reaction, nonrenormalized *or* with radiation reaction (in the electromagnetic case). The use of acceleration variables in the electromagnetic case (i.e., the use of a $12N$-dimensional phase space) is practically imposed by the form of the equations of motion on the first hand and by the need to deal with radiation phenomena (see below) on the other hand. For instance, let us assume we want to derive an equation for a random density depending only on $(\cdots x_i^\mu, u_i^\mu \cdots)$. It is easy to see that this is not possible since $\dot{\gamma}_i^\mu$ cannot be expressed in terms of *only* $(\cdots x_i^\mu, u_i^\mu \cdots)$ but also includes γ_i^μ. Therefore we are naturally led to γ_i^μ-dependent densities and hence to a $12N$-dimensional phase space. At this point, it seems to be worthwhile to emphasize strongly that the term "phase space" is not adequate since our "phase space" has nothing to do with the "initial data" of the system; it is only chosen for convenience. On these phase spaces densities are defined through the intermediary of currents. This intermediate step is *demanded* by the geometrical nature of the problems considered; in particular it is required because of invariance under changes of coordinates (preserving the $+ - - -$ character of the Minkowski metric). These invariance requirements lead to define average values as fluxes of generalized currents of properties considered. Of course, these average values reduce to the ordinary ones when choosing 3-planes $t = \text{const}$ to calculate them. In general these average values are by no means similar to the Newtonian ones especially because of their geometrical structure. In particular, *local averages* are not completely satisfactory.

An alternative way of defining densities on phase spaces is again suggested by the form of the equations of motion. It consists in defining proper time-(or any other parameter) dependent densities. These densities, which are naturally related to the above ones, are obtained by averaging over the possible paths of the particles (and possibly over the fields) a *random density describing one given realization* (i.e., one motion) *of the process*. The chief interest of these random densities arises from the ease it allows in deriving the equations they satisfy (i.e., the fundamental equations generating the relativistic hierarchies). In other words, they permit the use of the elegant methods of Klimontovich. We first applied these methods to the case of interactions via a scalar potential and obtained two hierarchies, a nonrenormalized and a renormalized one. In obtaining them we neglected "radiation" (i.e., mesons emission) arguing that "radiation" needs a quantal treatment. In fact this point should be elaborated further. Next we dealt with electromagnetic phenomena giving several possible hierarchies: field, with or without radiation reaction, etc. It was clear that the field point of view leads to complicated equations which involve the usual infinities. This is the reason why we preferred starting with the resulting equations (i.e., the Lorentz–Dirac equations) which occur as well from the action-at-a-distance point of view. Note that if we did not neglect classical meson emission, it would not have been possible to deal with scalar interactions in such a way. It has indeed been shown[55] that the field and action-at-a-distance viewpoints yield different equations of motion (nonlocal) for this scalar case.

Another interesting possibility of such an approach is that since radiation effects are completely taken into account, it is in principle possible to evaluate radiation quantities such as correlation functions for the radiation field. We say "in principle" because the averages considered above seem to lead to troubles. Indeed, let us consider the average radiated field at infinity (or more precisely the far field) at point x_ν. Its expression is given by Eq. (2.30). In order to obtain the average field $\langle F^{\mu\nu}_{\text{rad}\,\infty} \rangle$ we should first calculate the "far-field current"

$$J^{\rho\mu\nu}(x_\nu, x'_\nu) = \iint d_4u'\, d_4\gamma' u'^\rho F^{\mu\nu}_{\text{rad}\,\infty}(x_\nu; x'_\nu, u'_\nu \gamma'_\nu) \times \mathcal{N}(x'_\nu, u'_\nu, \gamma'_\nu),$$

whose physical meaning is (presently) completely obscure. Next we should calculate the flux of $J^{\rho\mu\nu}$ through an arbitrary spacelike surface Σ:

$$\langle F^{\mu\nu}_{\text{rad}\,\infty} \rangle_\Sigma(x_\nu) = \int_\Sigma J^{\rho\mu\nu}\, d\Sigma_\rho .$$

Unfortunately, the current $J^{\rho\mu\nu}$ is, in general, *not* conservative:

$$\partial_\rho J^{\rho\mu\nu} \neq 0$$

so that $\langle F^{\mu\nu}_{\text{rad}\,\infty} \rangle$ actually depends on Σ! In fact, this difficulty may be removed by remarking that the field at point x_ν comes from all events situated on the backward null cone $\Gamma^-(x_\nu)$. Therefore, Σ *must* be restricted to be $\Gamma^-(x_\nu)$ in problems involving radiation (although Γ^- is not spacelike).

Another problem is that of equilibrium. We strongly emphasized that definition of equilibrium states is yet unknown even in the Newtonian framework. Of course, it is possible *to define* equilibrium average values by taking time averages and next invoking ergodism. However, the problem remains open: how to select the equilibrium densities? (or the

[55] P. Havas, Phys. Rev. 87, 309 (1952).

ensemble averages). From a relativistic point of view the same problems are also unsolved. Furthermore, problems arising from the complicated nature of the equations of motion arise. Indeed we suggested in Paper I to define canonical distribution using information theoretical arguments, but here also we were led to rather involved functional expressions very difficult to solve. Another possibility would be the definition of microcanonical density through

$$\mathcal{N}_N = \left\langle \delta\left(P^\mu - \int_{\Sigma^{3N}} T^{\mu\rho_1 \cdots \rho_N} d\Sigma_{\rho_1 \cdots \rho_N} \right) \right\rangle$$

(this expression does not actually depend on Σ^{3N} because of conservation relations satisfied by the generalized random momentum-energy tensor $T^{\mu\rho_1 \cdots \rho_N}$ since we deal with a closed system). Unfortunately, very complicated expressions occur also in this case.

Throughout these papers (and also in Paper III) we have discussed both field and action-at-a-distance viewpoints. It is, however, clear that the action-at-a-distance point of view is much simpler to handle in a statistical framework than the field one. Furthermore, action-at-a-distance may be generalized in a straightforward way (in the statistical framework) so as to take into account more general kinds of interactions, spinning or extended particles. In both points of view general relativity may be taken into account, at least in principle, using in Einstein's equations the momentum-energy tensor of the system. However, some minor modifications are needed: (a) phase space is the tangent fibre bundle to the manifold $V_1^{4N} \times \cdots \times V_N^{4N}$; (b) densities are defined exactly as in Paper I but much more care is required in normalizing them; (c) equations for R_1 include one more term, of the form $(\partial/\partial u^\mu)\{\Gamma^\mu_{\alpha\beta} u^\alpha u^\beta R_1\}$, which couples the hierarchy to Einstein's equations, etc. ($\Gamma^\mu_{\alpha\beta}$ are the well-known Christoffel symbols.)

Finally we conclude these remarks on relativistic statistical mechanics by saying that the possibilities suggested in these papers are merely plausible and will remain so until the difficult subjacent dynamical problems be solved. In our opinion, a fully satisfactory theory should include quantum effects and, in view of astrophysical applications, gravitational effects.

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Time Behavior of a Reactor and Ergodic Theory of Semigroups

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The solution of the time-dependent neutron transport equation is a semigroup of linear transformations acting on a Banach space. There are some ergodic theorems that can be used to describe the asymptotic behavior of the solution under very general conditions on the semigroup. The results are compared with Wing's famous approach.

I. INTRODUCTION

THE solution of the initial-value problem in neutron transport theory (linear Boltzmann equation) leads in some important cases to a semigroup of bounded linear transformations in a certain Hilbert space.[1-6] A reactor R is defined on a bounded convex point set in the n_1-dimensional Euclidean space ($n_1 \leq 3$). The endpoints of the neutron velocity vectors are in the interior of an n_2-dimensional sphere S with radius $v_{\max}$ ($n_2 \leq 3$). All square integrable functions on the point set $R \times S$ of the $n_1 + n_2$-dimensional phase space (μ space of statistical mechanics) form the Hilbert space $L_2(R \times S)$. The solution of the time-dependent neutron transport equation is to be found in this space under the boundary condition that no neutrons enter R from outside for all $t > 0$. It turns out to be an Abelian semigroup of bounded linear transformations in L_2 with parameter $t \geq 0$. One possible representation of this semigroup is formed by a Neumann series.[4-6] It makes a classification to the number of collisions and can be used well during a time interval short compared to the mean collision time. Another representation that is apt for the asymptotic behavior in times large compared to the mean collision time is based on the spectral theory of the nonsymmetric transport operator. Without reference to the kind of representation of the semigroup it is already possible to state some theorems on the asymptotic behavior with the help of ergodic theory. As it is done often in statistical mechanics, $R \times S$ is divided into a finite number of cells labeled 1 to n. A special neutron distribution is an n-dimensional vector $\mathbf{h} = (h_1, \cdots h_n)$, $h_i \geq 0$, h_i meaning the number of neutrons in cell i. Naturally this is only an approximation; for an exact description we should have a function in $n_1 + n_2$ variables of the Hilbert space L_2. But it suffices to get some features on the asymptotic behavior under a few very general assumptions on the semigroup. Heavy use is made of Ref. 7.

II. THE DISCRETE μ SPACE

The bounded set $R \times S$ in μ space is divided into n number of cells. $\Omega = \{w_1, \cdots w_n\}$ is the set of all cells, the ith cell is labeled w_i. A special neutron distribution is an n-dimensional vector $\mathbf{h} = (h_1, \cdots h_n)$. The components h_i are the number of neutrons in cell w_i, $h_i \geq 0$. The set of all $\mathbf{h}$ (h_i real, not necessarily nonnegative) form an n-dimensional linear space $H(\Omega)$. The neutron distribution with only one neutron in cell w_i is written $e_i = (0, \cdots \overset{i}{1}, \cdots 0)$. A partial ordering can be introduced in $H(\Omega)$

$$h \leq g :\Leftrightarrow h_i \leq g_i \quad \text{for all} \quad i = 1, \cdots n.$$

$H(\Omega)$ turns out to be a vector lattice. Supremum, infimum, and absolute value of vectors are again vectors defined by

$$(g \vee h)_i = \max [g_i, h_i],$$
$$(g \wedge h)_i = \min [g_i, h_i],$$
$$|g|_i = |g_i|.$$

We have the decomposition of a vector $\mathbf{h}$

$$\mathbf{h} = h^+ - h^-, \quad h^+ = h \vee 0, \quad h^- = (-h) \vee 0.$$

If there is another decomposition

$$\mathbf{h} = h' - h'', \quad h' \vee 0, \quad h'' \vee 0,$$

we have

$$h' \geq h^+, \quad h'' \geq h^-.$$

A norm is defined in $H(\Omega)$.

Definition:

$$\|h\| = \sum_{i=1}^{n} |h_i|.$$

[1] G. M. Wing, *An Introduction to Transport Theory* (John Wiley & Sons, Inc., New York, 1962).
[2] S. Albertoni and B. Montagnini, in *Proceedings of a Symposium, Karlsruhe* (International Atomic Energy Agency, Vienna, 1965).
[3] R. Bednarz, in *Proceedings of a Symposium, Karlsruhe* (International Atomic Energy Agency, Vienna, 1965).
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Of course, this is not the only way to make $H(\Omega)$ a normed-space. Another possibility is

$$\|h\|_1 = \left(\sum_{i=1}^{n} h_i^2\right)^{\frac{1}{2}}$$

as Wing[1] has done. $\|h\|_1$ has no direct physical meaning, but $\|h\|$ has: it is the total number of neutrons in $R \times S$, if $h_i \geq 0$. Because of the equivalence of all norms, $\|h\|_1$ (times a constant) is an upper bound for the total number of neutrons. The norm $\|h\|_1$ comes from an inner product

$$(g_1 h) = \sum_{i=1}^{n} g_i \bar{h}_i,$$
$$\|h\|_1 = (h_1 h)^{\frac{1}{2}}.$$

This inner product has a physical meaning equaling the number of neutron counts of a certain array of neutron detectors, $g_i \geq 0$ is the neutron density, $h_i \geq 0$ the weight function for the location and sensitivity of the detectors.

The unit sphere $\|h\| \leq 1$ is an octahedron for $n = 3$. We have the triangle inequality for all norms:

$$\|g + h\| \leq \|g\| + \|h\|.$$

The following relations are true for this special norm:

$$\|g + h\| = \|g\| + \|h\|, \quad h \geq 0, \quad g \geq 0;$$
$$\|h\| = \|h^+\| + \|h^-\|.$$

The convex hull of the basis vectors $\mathbf{e}_i$, the set

$$V = \left\{h \mid h_2 \geq 0, \sum_{i=1}^{n} h_i = 1\right\},$$

is the set of all neutron distributions with total number 1. V is a simplex with vertices in $\mathbf{e}_i$.

III. THE NEUTRON TRANSPORT PROCESS

Our aim is to find the time behavior of a neutron distribution h given at time $t = 0$. The neutron transport process is linear, so is the neutron transport equation and the superposition principle is valid. We get a set of linear transformations $G = \{T_t \mid t \geq 0\}$. This set G has some general properties that are shared by the semigroup of the transport equation and that are physically evident. A list of these properties follows.

(a) G is a set of $n \times n$ matrices $T_t = (T_{ik}^{(t)})$.

(b) T_t is a linear transformation of $H(\Omega)$ into itself.

(c) $T_{ik}^{(t)}$ can be defined as the probability that a neutron from cell ω_i will reach cell ω_τ after time t. $T_{ik}^{(t)}$ is nonnegative.

(d) Because of the uniqueness of the solution of the initial-value problem we get

$$T_{t_1} T_{t_2} = T_{t_1 + t_2}. \tag{1}$$

In other words: T_t forms an Abelian semigroup with unit element T_0.

(e) After a neutron pulse has been started at time $t = 0$ in a cell, the whole reactor $R \times S$ will be filled with neutrons after a certain time, and in every cell there will be a positive number of neutrons. This time τ can be approximated by

$$\tau = d/v_{\max}, \tag{2}$$

with d the diameter of R. This fact can be seen easily from the Neumann representation.[4,5] Then the semigroup has the property

$$T_{ik}^{(t)} > 0 \quad \text{for all } t \geq \tau \quad \text{and all } i_1 k. \tag{3}$$

(f) $T_{ik}^{(t)}$ are continuous functions in $t \geq 0$ for all i, k.

We restrict ourselves to the continuous case with parameter $t \geq 0$. In the discontinuous case G would be the cyclic semigroup $\{T_0, T, T^2, \cdots\}$ of powers of one transform T. If

$$\sum_{k=1}^{n} T_{ik}^{(t)} = 1,$$

then T_t is called stochastic. Such matrices occur in diffusion processes of particles enclosed in a container. In the case of neutron transport this does not occur because of leakage, absorption, and fission.

In the linear n^2-dimensional space L of all linear transformations of $H(\Omega)$ into itself, a norm can be introduced—the operator norm.

Definition:

$$\|P\| = \sup_{\|h\| \leq 1} \|Ph\| \tag{4}$$

Geometrically $\|P\|$ can be found easily: the unit sphere is deformed by P linearly. Then we look for the least unit sphere containing this set. We only have to compute $Pe_1, Pe_2, \cdots, Pe_n$ and find the minimum of the norms. If this matrix has nonnegative elements, it suffices to find

$$\|P\| = \sup \|Ph\|, \quad \|h\| \leq 1, \quad h \geq 0. \tag{5}$$

For a stochastic matrix we have $\|P\| = 1$. If $\|P\| \leq 1$, P is called a contraction on $H(\Omega)$.

It is trivial that this norm is a continuous function in L, the product is jointly continuous in $P, Q \in L$, i.e., $L \times L$ is mapped in a continuous way onto L. Moreover

$$\|Ph\| \leq \|P\| \, \|h\|, \quad h \in H(\Omega); \qquad \|PQ\| \leq \|P\| \, \|Q\|. \tag{6}$$

IV. THE CRITICAL REACTOR

From now on, G is a semigroup of matrices satisfying (a)–(f). The following three cases are possible:

(1) $$\limsup_{t\to\infty} \|T_t e_1\| = \infty. \tag{7}$$

This is true then for all e_k, because

$$T_\tau e_k = \alpha_1 e_1 + \cdots + \alpha_n e_n, \quad \text{all} \quad \alpha_i > 0;$$
$$\|T_{t+\tau} e_k\| = \alpha_1 \|T_{t+\tau} e_1\| + \cdots + \alpha_n \|T_{t+\tau} e_n\|.$$

In addition

$$\limsup_{t\to\infty} \|T_t\| = \infty. \tag{8}$$

Otherwise, there would exist an upper bound K,

$$\|T_t\| \leq K \quad \text{for all} \quad t \geq 0,$$
$$\|T_t e_1\| \leq K \quad \text{for all} \quad t \geq 0,$$

contrary to (7). The total number of neutrons in the reactor increase infinitely for every initial distribution; this is the behavior of a supercritical reactor.

(2) $$\limsup_{t\to\infty} \|T_{te} l_k\| \leq K_2, \quad \liminf_{t\to\infty} \|T_t e_1\| = 0. \tag{9}$$

This is true then for all e_k, because

$$T_\tau e_1 = \alpha_1 e_1 + \cdots + \alpha_n e_n, \quad \text{all} \quad \alpha_i > 0,$$
$$\|T_{t+\tau} e_1\| = \alpha_1 \|T_{t+\tau} e_1\| + \cdots + \alpha_1 \|T_{t+\tau} e_n\|$$

lim inf of the left side disappears, so does every one on the right side. In addition

$$\liminf_{t\to\infty} \|T_t\| = 0. \tag{10}$$

Otherwise there would exist to every T_t, a $h_t \geq 0$ with $\|h_t\| = 1$;

$$\|T_t h_t\| = \|T_t\| \geq K > 0,$$

$$h_t = \alpha_1^{(t)} e_1 + \cdots + \alpha_n^{(t)} e_n, \quad \text{all} \quad \alpha_i^{(t)} \geq 0, \quad \sum_{i=1}^{n} \alpha_i^{(t)} = 1;$$

$$\|T_t\| = \sum_{i=1}^{n} \alpha_i^{(t)} \|T_t e_i\|,$$

lim inf of the right side disappears, and so does that on the left side. This is the behavior of a subcritical reactor.

(3) The critical reactor:

$$0 < K_1 \leq \liminf_{t\to\infty} \|T_t e_i\| \leq \limsup_{t\to\infty} \|T_t e_i\| \leq K_2, \tag{11}$$

or equivalently,

$$K_1 \leq \|T_t\| \leq K_2. \tag{12}$$

The semigroup $G \leq L$ is norm bounded (and conditionally compact[8]). We can form the closure $\bar{G}$ of it. It is compact, bounded with the same bound and Abelian, if G had these properties.

V. ASYMPTOTIC BEHAVIOR OF THE CRITICAL REACTOR

For every $h \in H(\Omega)$ the mapping $P \to Ph$ of L onto H is linear and continuous. The image of G is called G orbit,

$$Gh = \{Ph \mid P \in G\}.$$

This orbit is conditionally compact if G is. The closure $\bar{G}$ of a conditionally compact set $G \leq L$ yields $\bar{G}h$ as the closure of Gh

$$\bar{G}h = \overline{Gh}. \tag{13}$$

Definition: A set $M \leq H$ is called G invariant if it contains the G orbit of each of its points.

Definition: A set is called minimal G invariant, if M is closed, M is G invariant, and M is minimal with this property, i.e., for every closed G-invariant set $N \leq M$, it follows that $N = M$.

Definition: $r \in H$ is called G invariant if the orbit closure $\bar{G}r$ is minimal G invariant.

Lemma 1: If $r \in H$ is G-reversible, then for every pair $\bar{P}$, $\bar{Q} \in \bar{G}$, there exists a $\bar{R} \in \bar{G}$ such that

$$\bar{R}\bar{P}r = \bar{Q}r. \tag{14}$$

Proof. $\bar{G}\bar{P}r$ is closed, G invariant, and $\bar{G}\bar{P}r \leq \bar{G}r$. Because of the minimal property it follows $\bar{G}\bar{P}r = \bar{G}r$, so there must exist a $\bar{R}$ such that $\bar{R}\bar{P}r = \bar{Q}r$.

Take $\bar{Q} = I$; there exists a $\bar{R}$ such that $\bar{R}\bar{P}r = r$. This means that $\bar{G}$ acts like a group on r.

Definition: $f \in H$ is called a G-flight vector if $0 \leq \bar{G}f$.

Definition: R is the set of all G-reversible vectors, F the set of all G-flight vectors.

Lemma 2: There exists always a G-reversible vector in the orbit closure $\bar{G}h$ of an arbitrary $h \in H$.

Proof. See Appendix A.

The sets R and F are never empty, at least they contain the point zero. We want to prove more: that they are linear G-invariant subspaces and that H is their direct sum. First, F is a linear space: if $g, h \in F$, then $\bar{P}$, $\bar{Q} \in \bar{G}$ exist such that

$$\bar{P}g = 0, \quad \bar{Q}h = 0.$$

[8] *Definition:* A set is called conditionally compact, if its closure is compact. In a finite dimensional space the concepts bounded and conditionally compact are equivalent.

Then

$$\bar{P}\bar{Q}(f+g) = \bar{Q}\bar{P}f + \bar{P}\bar{Q}g = 0.$$

Second, H can be represented as the direct sum $H = R + F$; this means that every $h \in H$ can be written as a sum of $h = r + f, r \in R, f \in F$. In addition, $r \in \bar{G}h$. For if we choose a reversible $r_0 \in \bar{G}h$ (Lemma 2) and a $\bar{P} \in \bar{G}$ with $\bar{P}h = r_0$, we can find $\bar{R} \in \bar{G}$ such that $\bar{R}\bar{P}r_0 = r_0$, (Lemma 1) and put $\bar{R}r_0 = r$ and $f = h - r$. We get $r \in R$ (because r_0 was), $r \in Gh$ (because $r = \bar{R}\bar{P}h$) f is a flight vector

$$\bar{P}f = \bar{P}(h - r) = \bar{P}h - \bar{P}\bar{R}r_0 = r_0 - r_0 = 0.$$

To prove linearity of R is more difficult.

The Splitting Theorem: G is a norm-bounded Abelian semigroup of transformations acting on H. Then the set R and F are G-invariant linear subspaces of H, and H is their direct sum

$$H = R + F \quad R \cap F = \{0\}. \tag{15}$$

The mappings

$$P_R: h \to r, \quad P_F: h \to f \tag{16}$$

are orthogonal linear idempotents commuting with G and form a decomposition of I.

$$P_R^2 = P_R, \quad P_R P_F = P_F P_R = 0, \quad P_F^2 = P_F;$$
$$P_R + P_F = I, \tag{17}$$
$$P_R P = P P_R, \quad P_F P = P P_F \quad (P \leq G).$$

Moreover $P_R \in \bar{G}$. For proof, see Appendix B.

VI. UNIQUENESS OF THE EQUILIBRIUM

Corollary 1: R has dimension one. The equilibrium distribution r (a fixed point of G) is unique. Assume R has dimension at least two, then $P_R e_1 = r_1$, $P_R e_2 = r_2$, r_1, r_2 being linearly independent.

$$P_R T_t e_1 = r_1, \quad \text{for all} \quad t = 0;$$
$$P_R T_\tau e_1 = T_\tau P_R e_1 = a_1 P_R e_1 + a_2 P_R e_2 + \cdots$$
$$= a_1 r_1 + a_2 r_2 + \cdots \quad \text{all} \quad a_i > 0,$$

contrary to $a_2 = 0$.

Corollary 2: The approach to equilibrium goes with exponential speed. This can be shown by the following argument: There is a T_{t_0} that shrinks the intersection M of the unit sphere E and F by one half. The set $M = E \cap F$ is compact. Then for every $h \in M$ there exists a finite sequence $f_1, \cdots, f_m \in F$ such that h is in a $1/4K_2$-neighborhood of some f_i. Choose T_{t_i} such that

$$\|T_{t_i} f_i\| \leq \frac{1}{4K_2}$$

and put $T_{t_0} = T_{t_1} \cdots T_{t_m}$ $(t_0 = t_1 + \cdots + t_m)$. Then for an arbitrary $h \in M$

$$\|T_{t_0} h\| \leq \|T_{t_0}(h - f_i)\| + \|T_{t_0} f_i\|$$
$$\leq \|T_{t_0}(h - f_i)\| + \|T_{t_0 - t_i} T_t f_{i_i}\|$$
$$\leq K_2(-1/4K_2) + K_2(-1/4K_2) = \tfrac{1}{2}.$$

For $t = nt_0$ and all $h \in M$ we get

$$\|T_{nt_0} h\| \leq (\tfrac{1}{2})^n.$$

For an arbitrary $t = t' + nt_0$, $0 \leq t' < t_0$ and all $h \in M$

$$\|T_{nt_0} T_{t'} h\| \leq (\tfrac{1}{2})^n \|T_{t'} h\| \leq (\tfrac{1}{2})^n \cdot K_2 \leq K_3 e^{-\kappa t}$$

for a suitably chosen K_3 and κ. Finally if h is arbitrary (by the splitting theorem)

$$h = r + f,$$
$$\|T_t h - r\| \leq K_3 \|f\| e^{-\kappa t}.$$

VII. THE SLAB REACTOR

As an example let us consider the simple case of a slab reactor $R = \{x \mid -a \leq x \leq +a\}$ with monoenergetic neutrons $S = \{\mu \mid -1 \leq \mu \leq +1\}$. $R \times S$ is a rectangle in the two-dimensional phase space. It is divided by lines parallel to the axes into cells (Fig. 1). The cells are numbered 1–n. Figure 2 shows the space $H(\Omega)$ for $n = 2$. The simplex V is a part of a straight line; also the one-dimensional subspace R is drawn. The orbits of Ge_1, resp. Ge_2 approach r_1, resp. r_2 on R. r_1 has a total number of neutrons less than r_2. The reason is in the special choice of e_1 and e_2. The pulse started in e_1 at time $t = 0$ will loose many neutrons through the boundary $x = +a$ before it builds up a critical distribution, in contrast to a pulse started in e_2 that will first increase the number of neutrons before loosing neutrons by leakage through the boundary.

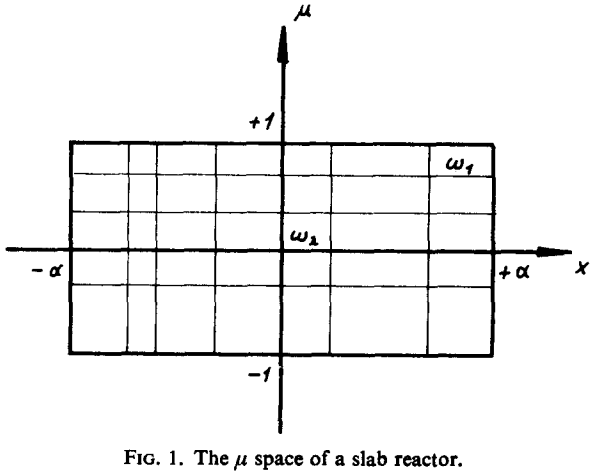

FIG. 1. The μ space of a slab reactor.

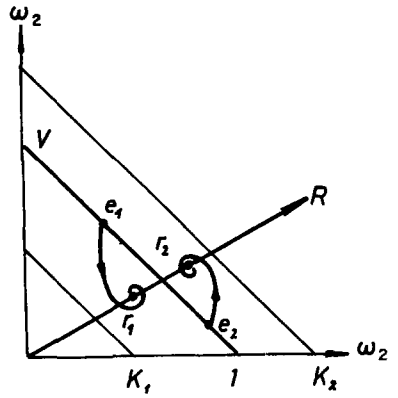

FIG. 2. The orbits in the space H for $n = 2$.

VIII. COMPARISON TO WING'S METHOD

The generalization to the semigroup that represents the solution of the linear Boltzmann equation is obvious. [Assumptions (a)–(f) are clearly satisfied.] The question as to whether the splitting theorem remains true in this general case can be answered in the affirmative.[9] H can be chosen as the Banach space of $L_1(R \times S)$ integrable functions or the Hilbert space of $L_2(R \times S)$ integrable ones. Because of the equivalence of all norms we get

$$K_1 \leq \|T_t\| \leq K_2,$$
$$K_5 \leq \|T_t\|_1 \leq K_6$$

and vice versa. Wing[1] has given a representation of the semigroup that contains explicitly the decomposition into $H = R + F$.

$$h(x, \mu, t) = \sum_{i=1}^{N} e^{(\beta i - 1)t}(h_1 \psi_i^*)\psi_i + B_t f,$$

$$\beta_1 > \beta_2 \geq \cdots \geq \beta_N.$$

In the case of the critical reactor $\beta_1 = 1$,

$$h = r + f,$$
$$r = (h_1 \psi_1^*)\psi_1, \quad f = h - r;$$
$$\|T_t h - r\| \leq K_3 e^{-\beta 2 t} \|f\|.$$

APPENDIX A

If the orbit closure of $h\bar{G}h$ is closed, $\bar{G}$ invariant, and $\bar{G}h$ is minimal, then we are ready. If it is not, then there exists a proper subset $N_1 \leq \bar{G}h$ that is closed and $\bar{G}$ invariant. For every such chain $Gh \geq N_1 \geq N_2 \geq \cdots$, there exists a lower bound $N = \bigcap_{i=1}^{\infty} N_i$ that is closed (because of compactness) and $\bar{G}$ invariant. By Zorns Lemma there exists a minimal $\bar{G}$-invariant set in $\bar{G}h$.

APPENDIX B

Every $\bar{P} \in \bar{G}$ induces a continuous mapping of $\bar{G}$ onto itself by multiplication $\bar{Q} \to \bar{P}\bar{Q}$. So $\bar{G}$ may be considered as an Abelian semigroup of continuous mappings of the compact set $\bar{G}$ onto itself. Again we get the existence of at least one minimal $\bar{G}$-invariant subset $\bar{G}_0 \leq \bar{G}$ (Lemma 2). $\bar{G}_0$ is uniquely determined. If $\bar{G}_1$ is of the same kind, $\bar{G}_0\bar{G}_1 = \{\bar{P}\bar{Q} \mid \bar{P} \in \bar{G}_0, \bar{Q} \in G_1\}$, which is compact as the continuous image of the compactum $\bar{G}_0 \times \bar{G}_1$, would turn out to be a $\bar{G}$-invariant subset of $\bar{G}_0 \cap \bar{G}_1$ and thus $\bar{G}_0 = \bar{G}_1$. If $\bar{P} \in \bar{G}$ is arbitrary. $\bar{P}\bar{G}_0$ is compact and $\bar{G}$-invariant and thus $\bar{P}\bar{G}_0 = \bar{G}_0$ ($\bar{P} \in \bar{G}$). Thus we see there is division in $\bar{G}_0$. Even for every $\bar{P} \in \bar{G}$, $\bar{Q} \in \bar{G}_0$, there exists an $\bar{R} \in \bar{G}_0$ with $\bar{P}\bar{R} = \bar{Q}$. Applying this to $\bar{P} = \bar{Q}^2$ and putting $\bar{E}_0 = \bar{Q}\bar{R}$, we obtain the existence of an idempotent $\bar{E}_0 \in \bar{G}_0$, $\bar{E}_0^2 = \bar{Q}^2\bar{R}\bar{R} = \bar{Q}\bar{R} = \bar{E}_0$. We see that the space of flight vectors is annulated by each $\bar{Q} \in \bar{G}_0$. Indeed if we choose $f \in F$, and then $\bar{P} \in \bar{G}$ with $\bar{P}f = 0$, there exists a $\bar{R} \in \bar{G}_0$ with $\bar{P}\bar{R} = \bar{Q}$ and we obtain $\bar{Q}f = \bar{P}\bar{R}f = 0$. As a consequence $F = \bar{Q}^{-1}0$, $\bar{Q} \in \bar{G}_0$, and F is a linear space.

Next we show $\bar{Q}H$ consists of reversible vectors for any $\bar{Q} \in \bar{G}_0$. Again if we choose $h \in H$ and $\bar{P} \in \bar{G}$, and then $\bar{R} \in \bar{G}_0$ with $\bar{Q}\bar{P}\bar{R} = \bar{Q}$, we obtain for $r = \bar{Q}h$, $\bar{R}\bar{P}r = \bar{R}\bar{P}\bar{Q}h = \bar{Q}h = r$.

Finally we show that each $\bar{Q} \in \bar{G}_0$ maps the set R of all reversible vectors onto itself. Now if we choose $r \in R$ and $\bar{P} \in \bar{G}$ such that $\bar{P}\bar{Q}r = r$, then we have $\bar{Q}\bar{P}r = r$ and $\bar{P}r \in R$. Combining our last two results we obtain $\bar{Q}H = R$, $\bar{Q} \in \bar{G}_0$. As a consequence R turns out to be a linear space. It follows: if $\bar{E}_0 \in \bar{G}_0$ is idempotent, then

$$R = \bar{E}_0 H, F = \bar{E}_0^{-1}O = (I - \bar{E}_0)H,$$

and all elements of R remain fixed under $\bar{E}_0$. As $H = R + F$, $\bar{E}_0$ is uniquely determined, it also follows that $R \cap F = \{0\}$. Consequently for any $h \in H$, $h = \bar{E}_0 h + (I - \bar{E}_0)h = r + f$ is the unique decomposition of h and we obtain $P_R = \bar{E}_0$, $P_F = I - \bar{E}_0$.

[9] K. Jacobs, *Neuere Methoden und Ergebnisse der Ergodentheorie* (Springer-Verlag, Berlin, 1960).

Upper Bounds to Eigenvalues of the One-Dimensional Sturm-Liouville Equation

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This work develops a straightforward technique for giving an upper bound to any eigenvalue of the one dimensional Sturm–Liouville problem. It is shown that *any trial function* that fulfills the proper boundary condition of the problem and possesses the same number of nodes as an exact eigenfunction of the problem can provide an upper bound to that eigenfunction's eigenvalue. Application of the above technique is made to provide a one-sided bound to quantum mechanical scattering phase shifts.

I. INTRODUCTION

CONSIDER the differential equation

$$(d/dx)(p\,dy/dx) - (q - \lambda r)y = 0 \qquad (1)$$

in a region R, $a \leq x \leq b$, in which $p(x)$ and $r(x)$ are both positive in the interior of R, with homogeneous boundary conditions prescribed at the end points (a, b);

$$(\alpha y + \beta\, dy/dx)_{x=a} = (\alpha y + \beta\, dy/dx)_{x=b} = 0, \qquad (2)$$

or if $p(x) = 0$ on a boundary, y and dy/dx must only be finite, or if $p(a) = p(b)$ the periodic boundary conditions $y(a) = y(b)$ and $dy(a)d/x = dy(b)/dx$ are sufficient.[1]

Then (1) has solutions $y_i(x)$ for only certain values of $\lambda = \lambda_i$. The spectrum of eigenvalues with a finite smallest member λ_0 and extending to $+\infty$ are extremals of the expression

$$\lambda = \frac{\int_R [p(dy/dx)^2 + qy^2]\,dx}{\int_R ry^2\,dx}, \qquad (3)$$

and consequently any trial function $y_T^{(x)}$ inserted into (3) provides an upper bound to λ_0, the smallest eigenvalue[2];

$$\lambda_0 \leq \frac{\int_R [p(dy_T/dx)^2 + qy_T^2]\,dx}{\int_R ry_T^2\,dx}. \qquad (4)$$

Similarly if a trial function can be guaranteed to be orthogonal to the first n eigenfunctions in the sense

$$\int_R ry_T y_i\,dx, \qquad (5)$$

then it can be shown that $y_T^{(x)}$ provides an upper bound to the $n + 1$ eigenvalue using (4) (Ref. 2).

However, in general no eigenfunctions are known exactly in a problem where variational methods are employed, so estimates to higher eigenvalues made with trial functions orthogonal to the *trial functions* for the lower eigenvalues will not be upper bounds to the true eigenvalues.

It is the purpose of this note to present a straightforward method for providing upper bounds to any of the eigenvalues of (1).

II. UPPER BOUNDS FOR ANY EIGENVALUE

Consider the problem specified by (1) subject to the appropriate boundary conditions. The true solutions of (1) have the properties[3]

$$(d/dx)(p\,dy_i/dx) - (q - r\lambda_i)y_i = 0, \qquad (6)$$

$$\int_R ry_i y_j\,dx = \delta_{ij}, \qquad (7)$$

$$\int_R \left[p\frac{dy_i}{dx}\frac{dy_j}{dx} + qy_i y_j\right] dx = \lambda_i \delta_{ij} \qquad (8)$$

and are extremals of (3).

In one dimension each eigenvalue is uniquely specified by the number of separate regions R_α into which R is broken, each region separated from its neighbors by the nodes (zeros) of the eigenfunction.[4] The lowest eigenvalue of (1) has an eigenfunction with no nodes.

For each region R_α the eigenfunction is a nodeless eigenfunction satisfying the same Sturm–Liouville differential equation with homogeneous boundary conditions. The nth eigenvalue λ_n with eigenfunction $y_n(x)$ is then the lowest eigenvalue of the same problem for each region R_α.

If the nodes of $y_n(x)$ were known, an upper bound to λ_n could be obtained by picking any region R_α and using the usual variational technique to find an upper bound for the region's lowest eigenvalue. However, in the general case the nodes of $y_n(x)$ are not known.

[1] F. B. Hildebrand, *Methods of Applied Mathematics* (Prentice-Hall, Englewood Cliffs, New Jersey, 1965), 2nd ed., p. 90.
[2] Reference 1, p. 205.
[3] Reference 1, p. 89.
[4] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1937), 1st English ed., p. 454.

Assume that a trial function $y_t(x)$ with the same number of nodes as the desired $y_n(x)$ is being used to estimate λ_n. In general the nodes of $y_t(x)$ do not coincide with the nodes of $y_n(x)$. The following theorem is now proved:

Given a region R divided into $n \geq 2$ regions R_α, if the Sturm–Liouville equation is solved in each region R_α for its lowest eigenvalue $\lambda_0^{(\alpha)}$ with the boundary conditions $y(x) = 0$ on all interior boundaries and the original homogenous boundary conditions on the exterior boundaries, then

$$\max \{\lambda_0^{(\alpha)}\} \geq \lambda_n, \tag{9}$$

where λ_n is the nth eigenvalue of the same Sturm–Liouville equation on the whole region R.

Proof: Let p_i be the interior boundary points of the regions R_α. Let q_i be the nodes of the exact eigenfunction $y_n(x)$. Using the known result[5] that the eigenvalues of the Sturm–Liouville problem monotonically decrease with enlarging a region, we have the following:

The necessary condition that $\lambda_0^{(1)} \leq \lambda_n$ is that the first boundary point of the divided region be greater than the first node of $y_n(x)$; i.e.,

$$p_1 \geq q_1. \tag{10}$$

Similarly, the necessary condition that $\lambda_0^{(2)}$ and $\lambda_0^{(1)} \leq \lambda_n$ is that

$$p_1 \geq q_1 \quad \text{and} \quad p_2 \geq q_2. \tag{11}$$

These conditions can be restated until we have the necessary condition that $\lambda_0^{(1)}, \lambda_0^{(2)}, \cdots, \lambda_0^{(n-1)} \leq \lambda_n$ which is that

$$\begin{aligned} p_1 &\geq q_1, \\ p_2 &\geq q_2, \\ &\cdots \\ p_{n-1} &\geq q_{n-1}. \end{aligned} \tag{12}$$

But the nth region has the exterior boundary $x = a$, and the condition $p_{n-1} \geq q_{n-1}$ demands by the monotonicity of the eigenvalues with region size that

$$\lambda_0^{(n)} \geq \lambda_n. \tag{13}$$

Therefore at least one $\lambda_0^{(\alpha)}$ must be greater than or equal to λ_n.

With this theorem it is now straightforward to obtain upper bounds to any eigenvalue of the Sturm–Liouville equation over the whole region R. Pick a trial $y_t(x)$ with the same number of nodes as the desired $y_n(x)$. Take $y_t(x)$ in each nodeless region R and calculate an upper bound to that region's lowest eigenvalue;

$$\lambda_T^{(\alpha)} = \frac{\int_{R_\alpha} [p(dy_T/dx)^2 + qy_T^2]\, dx}{\int_{R_\alpha} ry_T^2\, dx}. \tag{14}$$

Using (4) we have

$$\lambda_T^{(\alpha)} \geq \lambda_0^{(\alpha)} \tag{15}$$

and consequently

$$\max \{\lambda_T^{(\alpha)}\} \geq \max \{\lambda_0^{(\alpha)}\}. \tag{16}$$

But by use of the theorem proved above, (9), we have

$$\max \{\lambda_T^{(\alpha)}\} \geq \lambda_n, \tag{17}$$

the desired result and a computable upper bound to λ_n.

To get the best possible upper bound to λ_n the trial function $y_t(x)$ can be adjusted until all the $\lambda_T^{(\alpha)}$ are equal.

To make more clear what has been shown in this work, a comparison with the work of MacDonald[6] is made. MacDonald showed that a trial function $y_t(x)$ made up of n or more independent functions will provide an upper bound to λ_n by means of diagonalization of an $n' \times n'$ ($n' \geq n$) matrix in the Rayleigh–Ritz procedure.

In this work it has been shown *that any trial function possessing exactly $n - 1$ nodes* will give an upper bound to λ_n. For large n the procedure developed here will involve substantially less labor than the method of MacDonald.

III. GENERALIZATION TO THE N-DIMENSIONAL CASE

The technique can be generalized to the N-dimensional Sturm–Liouville equation. There is an important qualification which arises, however. In two or more dimensions the eigenfunctions of the Sturm–Liouville equation are not uniquely specified by their node topology.[7] Consequently, in an N-dimensional generalization of the proof given above, there is no guarantee that an upper bound to any specific eigenfunction of that given node topology will be obtained.

All that can be proven in the N-dimensional case is that the procedure presented in Sec. II of this work will yield an eigenvalue estimate which is an upper bound to the lowest eigenvalue of the family of eigenvalues belonging to the given node topology of the trial eigenfunction.

[5] Reference 4, p. 421.

[6] J. K. L. MacDonald, Phys. Rev. 43, 830 (1933).

[7] Reference 4, p. 455.

IV. BOUNDS ON SCATTERING PHASE SHIFTS

In the quantum-mechanical central potential scattering problem the radial wave equation for the Lth partial wave is

$$(d^2u_L/dr^2) - [L(L+1)/r^2]u_L + 2M(E-V)u_L = 0, \tag{18}$$

where $u = r\psi$. It is assumed that the potential vanishes outside some range $r = a$.

If the radial wavefunction is solved in a large spherical volume of radius R with the boundary condition

$$U(R) = 0, \tag{19}$$

then the exterior solution for $u(r)$, $r > a$, is a phase-shifted free-particle solution with the phase shift approaching the true scattering phase shift as $R \to \infty$.

A method for obtaining a one-sided bound to the scattering phase shift δ_L is now presented which is analogous to that of Percival.[8]

Let $r = r_0$ be an estimate of the first wavefunction node outside of the potential region ($r_0 > a$). A trial wavefunction is now shown to provide a bound on δ_L. For the region $r_0 \leq r \leq R$, the proper phase-shifted free-particle solution of

$$(d^2u_L/dr^2) - [L(L+1)/r^2]u_L + k^2u_L = 0 \tag{20}$$

is assumed where $k^2 = 2ME$. For finite R the k's which fulfill the boundary conditions

$$u(r_0) = u(R) = 0 \tag{21}$$

form a discrete spectrum, but when we take the limit $R \to \infty$ this spectrum becomes dense.

For the region $r < r_0$ a trial function with any chosen number of nodes can be used. The proper boundary conditions on the trial function are

$$\lim_{r \to 0} u_T(r) \text{ is finite}, \tag{22}$$

and

$$u_T(r_0) = 0. \tag{23}$$

The energy estimate

$$E_T^{(\alpha)} = \frac{\int_{R_\alpha} \left[\frac{1}{2M}\left(\frac{du_T}{dr}\right)^2 + \left(\frac{L(L+1)}{r^2} + V\right)u_T^2\right] dr}{\int_{R_\alpha} u_T^2\, dr} \tag{24}$$

is then calculated for each nodeless region R_α of the interior interval $0 \leq r \leq r_0$. For the exterior trial function the free-particle phase-shifted wavefunction appropriate to the energy and wavenumber given by

$$\max\{E_T^{(\alpha)}\} \equiv k^2/2M \tag{25}$$

is selected. [In the limit $R \to \infty$ a wavenumber k can be found arbitrarily close to fulfilling (25).]

[8] I. C. Percival, Proc. Phys. Soc. (London) A70, 494 (1957).

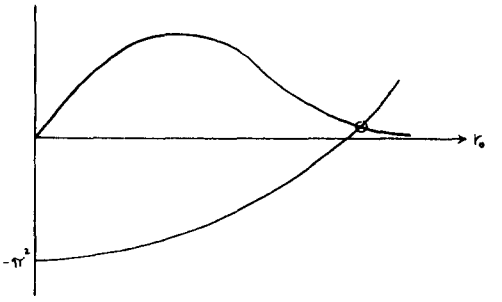

FIG. 1. The graphical solution of (31) for a repulsive potential. The movement of the curve intercept from the x-axis intercept indicates the negative phase shift of the potential.

By the theorem proved in this work, (9), (25) gives an upper bound to the energy for a state of the total number of nodes in the trial function constructed above. Since the energy of the state is a monotonically increasing function of the selected node location r_0, while for large R the energy is changing infinitesimally with changing r_0, r_0 is an upper bound to the node location for the exact scattering function at the energy given by (25).

To translate the bound on r_0 into a bound on the phase shift of the scattering wavefunction, consider the most general exterior free-particle wavefunction,[9]

$$\psi_L(r) \sim [\cos\delta_L j_L(kr) - \sin\delta_L \eta_L(kr)]. \tag{26}$$

Requiring (26) to have a node at r_0 gives

$$\tan\delta_L = j_L(kr_0)/\eta_L(kr_0), \tag{27}$$

where $j_L(x)$ and $\eta_L(x)$ are the spherical Bessel functions and spherical Neumann functions of order L. Equation (27) then gives a one-sided bound on the phase shifts δ_L by expressing δ_L in terms of r_0 and the wavenumber k.

To summarize the procedure consider the following steps.

(1) Pick an $r_0 > a$.

(2) Pick an *arbitrary* trial function on the interval $0 \leq r \leq r_0$ which fulfills the boundary conditions (22) and (23).

(3) An energy and wavenumber is determined by (25).

(4) (27) then gives a bound to the phase shift at wavenumber k.

The procedure developed above is somewhat more general than the similar work of Percival.[8] Percival, following the work of MacDonald,[6] employs the Rayleigh–Ritz procedure and the diagonalization of an $n \times n$ matrix to obtain his trial functions. It has been shown here that any trial function provides a phase-shift bound.

[9] L. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., p. 104.

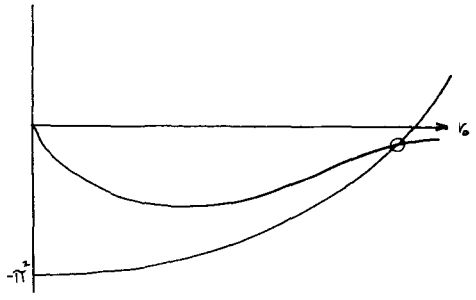

FIG. 2. The graphical solution of (31) for a weakly attractive potential. The movement of the curve intercept from the x-axis intercept indicates the positive phase shift of the potential.

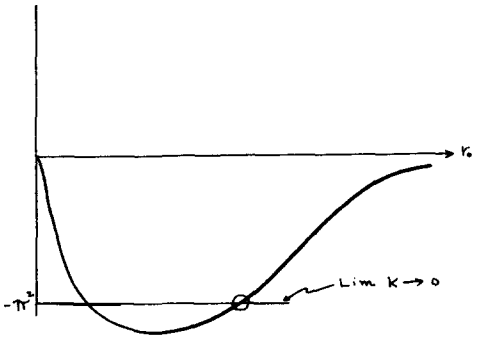

FIG. 3. The graphical solution of (31) for a strongly attractive potential. An intercept remains at finite r_0 for the limit $k = 0$, indicating a bound state of the potential exists.

V. APPLICATION TO AN S-WAVE PHASE-SHIFT CASE

For S waves, (24) gives the relation between r_0 and k for a trial function $y_t(x)$,

$$k^2 = \frac{\int_0^{r_0}\left[\left(\frac{du_T}{dr}\right)^2 + 2MVu_T^2\right] dr}{\int_0^{r_0} u_T^2\, dr}. \tag{28}$$

A simple trial function to use is

$$u_T(r) = \sin(\pi r/r_0), \tag{29}$$

which, when used in (28), gives

$$k^2 - \frac{\pi^2}{r_0^2} = \frac{4M}{r_0}\int V(r)\sin^2\left(\frac{\pi r}{r_0}\right) dr \tag{30}$$

or

$$(kr_0)^2 - \pi^2 = 4Mr_0\int V(r)\sin^2\left(\frac{\pi r}{r_0}\right) dr. \tag{31}$$

Figures 1–3 plot the solution of (31) for the three cases of a repulsive potential, weak attractive potential, and strong attractive potential. Figure 3 gives a solution of (31) for r_0 finite and $k = 0$ indicating a phase shift in excess of $\frac{1}{2}\pi$, or a bound state.

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Logarithmic Density Behavior of a Nonequilibrium Boltzmann Gas

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We consider the temporal evolution of the BBGKY hierarchy in the Boltzmann approximation for spatially homogeneous nonequilibrium situations, in the absence of initial correlations. For times of the order of the mean free time or greater, the single particle function f_1 is found to be of the form

$$f_1 = f_1^0 + \epsilon f_1^1 + \epsilon^2 |\ln \epsilon| \tilde{f}_1^1 + O(\epsilon^2)$$

with $\epsilon = nr_0^3$ (n is the density, r_0 the range of binary interaction) and f_1^0, f_1^1, and $\tilde{f}_1^1$ of order unity. For times less than the mean free time, with t in units of the duration of a binary interaction, f_1 is of the form

$$f_1 = f_1^0 + \epsilon f_1^1 + \epsilon^2 (\ln t) \tilde{f}_1^1 + O(\epsilon^2).$$

In both cases the same formally higher-order binary correlation functions are neglected.

I. INTRODUCTION

IN a previous paper,[1] the usual low-density expansion applicable to a Boltzmann gas was carried out, using a multiple time and space scale technique, to yield an expression for the lowest-order two-particle correlation function on the scale of the collision time and the mean free path. In the present paper this technique has been extended by introducing streaming operators which are generalizations of the operators first used by Bogoliubov[2] and which allow higher-order corrections in ϵ to the correlation functions to be obtained. (Here we note that $\epsilon = nr_0^3$, where n is the density and r_0 is the range of the binary potential.)

The new result which this technique yields is the appearance of correction terms which are logarithmic in the density. It was pointed out earlier[1] that terms which varied as t^{-1} on the interaction time scale appeared in the correlation functions. Clearly, on going to higher order in the expansion, such terms have to be integrated and yield $\ln t$ behavior.[3] In the present paper the apparent divergence from this source (among others) is removed by the introduction of generalized streaming operators which allow us to carry out the expansion for times on the collisional time scale. An $\epsilon \ln \epsilon$ behavior is obtained with correction terms of order ϵ.

A further result which appears naturally in the course of this work is that the complete Choh–Uhlenbeck collision operator is derived. In Ref. 1 we established this result with two caveats: (a) that

$$\lim_{t-t_0 \to \infty} e^{-H_2^0(t-t_0)} g_2^1(t_0, \epsilon t, \cdots)$$

vanished, and (b) that

$$\lim_{t-t_0 \to \infty} A(t - t_0)$$

vanished.

In fact we show (by using the generalized streaming operator technique) that the appropriate modifications of conditions (a) and (b) are satisfied to order ϵ.

In Sec. II the usual hierarchy is given, but higher-order terms are included with the usual lower-order terms, so that more convenient forms for the solution are obtained. In Sec. III higher-order corrections for the two- and three-particle correlations are obtained and the Choh–Uhlenbeck collision operator derived. In Sec. IV the $\ln \epsilon$ terms are obtained and shown to be convergent, and in Sec. V the contributions to the kinetic equation are obtained. A number of appendixes with details for the formal manipulations and estimates are also given.

II. EQUATIONS OF THE HIERARCHY UP TO $s = 4$

In this section we write the equations of the BBGKY hierarchy for a spatially homogeneous system in a form which is particularly suited for carrying out the higher-order calculations we need to

* A preliminary account of this work was reported at Washington, D.C.: Bull. Am. Phys. Soc. **10**, 531 (1965).

[1] E. Frieman and R. Goldman, J. Math. Phys. **7**, 2153 (1966).

[2] N. N. Bogoliubov, in *Studies in Statistical Mechanics*, J. De Boer and G. E. Uhlenbeck, Eds. (Interscience Publishers, Inc., New York, 1962), Vol. 1, p. 5.

[3] For further discussions of the $\ln t$ behavior see: J. Weinstock, Phys. Rev. **132**, 454 (1963); J. R. Dorfman and E. G. D. Cohen, Phys. Letters **16**, 124 (1965); J. V. Sengers, Phys. Rev. Letters **15**, 515 (1965); K. Kawasaki and I. Openheim, Phys. Rev. **139A**, 1763 (1965); J. Weinstock, *ibid.* **140A**, 40 (1965); L. K. Haines, J. R. Dorfman, and M. H. Ernst, *ibid.* **144**, 207 (1966).

do. The notation and units are identical to those used in Ref. 1. The hierarchy is written as

$$\frac{\partial f_s}{\partial \tilde{t}} + H_s f_s = \epsilon \sum_{i=1}^{s} \int d\Omega_{s+1} \theta_{i,s+1} f_{s+1}, \tag{2.1}$$

where

$$d\Omega_{s+1} = d\mathbf{x}_{s+1}\, d\mathbf{v}_{s+1}. \tag{2.2}$$

As usual we introduce

$$\begin{aligned} g_1 &= f_1, \\ g_2 &= f_2 - f_1 f_1, \end{aligned} \tag{2.3}$$

etc., and find

$$\begin{aligned} \frac{\partial g_s}{\partial \tilde{t}} + H_s g_s - \sum_{j=1}^{s} \sum_{i<j} \sum_{\alpha=1}^{s-1} \theta_{ij} g_\alpha(i, \cdots) g_{s-\alpha}(j, \cdots) \\ = \sum_{i=1}^{s} \int \theta_{i,s+1} \Big[\sum_{\alpha=1}^{s} g_\alpha(i, \cdots) \\ \times g_{s+1-\alpha}(s+1, \cdots) + g_{s+1} \Big] d\Omega_{s+1}. \end{aligned} \tag{2.4}$$

To proceed with the expansion we write

$$g_s = \sum_{m=0}^{\infty} \epsilon^m g_s^m(\mathbf{x}_1 \cdots \mathbf{x}_s, \mathbf{v}_1 \cdots \mathbf{v}_s, t, \epsilon \mathbf{x}_1 \cdots \epsilon \mathbf{x}_s, \epsilon t, \cdots), \tag{2.5}$$

$$H_s = \sum_{m=0}^{\infty} \epsilon^m H_s^m, \tag{2.6}$$

and

$$\frac{\partial}{\partial \tilde{t}} = \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial \epsilon t} + \epsilon^2 \frac{\partial}{\partial \epsilon^2 t} + \cdots. \tag{2.7}$$

Here

$$H_s^0 = \sum_{i=1}^{s} v_i \cdot \frac{\partial}{\partial x_i} - \sum_{j=1}^{s} \sum_{i<j} \theta_{ij} \tag{2.8}$$

with

$$\theta_{ij} = \frac{\partial \phi(x_{ij})}{\partial x_i} \cdot \left(\frac{\partial}{\partial v_i} - \frac{\partial}{\partial v_j} \right) \tag{2.9}$$

and

$$H_s^m = \sum_{i=1}^{s} \epsilon^m v_i \cdot \frac{\partial}{\partial \epsilon^m x_i}, \quad m \geq 1. \tag{2.10}$$

The expansion of (2.4) which follows upon using (2.5)–(2.10) is not unique since terms which are formally of higher order in ϵ can be kept in the lower order equations. We exploit this freedom in the following to enable us to get bounded solutions more easily.

It is convenient to write

$$g_s^1 = (g_s^1)_\alpha + \epsilon (g_s^1)_\beta, \quad s = 1, 2, 3 \tag{2.11}$$

since we expect that ln ϵ behavior will appear. Thus in (2.11) we allow for $(g_s^1)_\beta$ being of order ln ϵ while $(g_s^1)_\alpha$ is of order unity.

The expanded equations of the hierarchy can now be written as:

$s = 1$:

$$\partial g_1^0 / \partial t = 0, \tag{2.12}$$

$$\frac{\partial (g_1^1)_\alpha}{\partial t} + \frac{\partial g_1^0}{\partial \epsilon t} = \int d\Omega_2 \theta_{12} g_2^0, \tag{2.13}$$

$$\begin{aligned} \frac{\partial g_1^2}{\partial t} + \frac{\partial (g_1^1)_\alpha}{\partial \epsilon t} + \frac{\partial (g_1^1)_\beta}{\partial t} + \epsilon \frac{\partial g_1^2}{\partial \epsilon t} \\ + \epsilon \frac{\partial (g_1^1)_\beta}{\partial \epsilon t} + \epsilon \frac{\partial g_1^3}{\partial t} + \epsilon^2 \frac{\partial g_1^3}{\partial \epsilon t} + \cdots \\ = \int d\Omega_2 \theta_{12} (g_2^1 + \epsilon g_2^2 + \epsilon^2 g_2^3 + \cdots). \end{aligned} \tag{2.14}$$

$s = 2$:

$$(\partial g_2^0 / \partial t) + H_2^0 g_2^0 - \theta_{12} g_1^0 g_1^0 = 0, \tag{2.15}$$

$$\begin{aligned} \frac{\partial (g_2^1)_\alpha}{\partial t} + H_2^0 (g_2^1)_\alpha + \frac{\partial g_2^0}{\partial \epsilon t} + H_2^1 g_2^0 + \epsilon \frac{\partial}{\partial (\epsilon t)} (g_2^1)_\alpha \\ + \epsilon H_2^1 (g_2^1)_\alpha - \theta_{12} [g_1^0 (g_1^1)_\alpha + (g_1^1)_\alpha g_1^0] \\ = \sum_{i=1}^{2} \int \theta_{i3} [g_3^0 + g_1^0(i) g_2^0 + g_1^0(3) g_2^0]\, d\Omega_3, \end{aligned} \tag{2.16}$$

$$\frac{\partial (g_2^1)_\beta}{\partial t} + H_2^0 (g_2^1)_\beta - \theta_{12} [g_1^0 (g_1^1)_\beta + (g_1^1)_\beta g_1^0] = 0, \tag{2.17}$$

$$\begin{aligned} \frac{\partial g_2^2}{\partial t} + H_2^0 g_2^2 + \epsilon \frac{\partial (g_2^1)_\beta}{\partial \epsilon t} + \epsilon H_2^1 (g_2^1)_\beta + \epsilon \frac{\partial g_2^2}{\partial \epsilon t} \\ + \epsilon H_2^1 g_2^2 - \theta_{12} (g_1^0 g_1^2 + g_1^2 g_1^0 + g_1^1 g_1^1) \\ = \sum_{i=1}^{2} \int \theta_{i3} [(g_3^1)_{\alpha s} + (g_3^1)_{\alpha n s} + g_1^0(3) [(g_2^1)_{\alpha s}(i) + (g_2^0)_{\alpha n s}(i)] \\ + (g_1^1)_\alpha(i) g_2^0(3) + g_1^0(i) [(g_2^1)_{\alpha s}(3) + (g_2^1)_{\alpha n s}(3)] \\ + (g_1^1)_\alpha(3) g_2^0(i)]\, d\Omega_3. \end{aligned} \tag{2.18}$$

$s = 3$:

$$\begin{aligned} \frac{\partial g_3^0}{\partial t} + H_3^0 g_3^0 - \theta_{12} [g_1^0(1) g_2^0 + g_1^0(2) g_2^0] \\ - \theta_{13} [g_1^0(1) g_2^0 + g_1^0(3) g_2^0] \\ - \theta_{23} [g_1^0(2) g_2^0(2, 3) + g_1^0(3) g_2^0(1, 2)] = 0, \end{aligned} \tag{2.19}$$

$$\begin{aligned} \frac{\partial (g_3^1)_\alpha}{\partial t} + H_3^0 (g_3^1)_\alpha + \frac{\partial g_3^0}{\partial (\epsilon t)} + H_3^1 g_3^0 + \epsilon \frac{\partial}{\partial \epsilon t} (g_3^1)_\alpha + \epsilon H_3^1 (g_3^1)_\alpha \\ - \theta_{12} [g_1^0(1) (g_2^1)_\alpha + (g_1^1)_\alpha(1) g_2^0 + g_1^0(2) (g_2^1)_\alpha + (g_1^1)_\alpha(2) g_2^0] \\ - \theta_{13} [g_1^0(1) (g_2^1)_\alpha + (g_1^1)_\alpha(1) g_2^0 + (g_1^1)_\alpha(3) g_2^0 + g_1^0(3) (g_2^1)_\alpha] \\ - \theta_{23} [g_1^0(2) (g_2^1)_\alpha + (g_1^1)_\alpha(2) g_2^0 + (g_1^1)_\alpha(3) g_2^0 + g_1^0(3) (g_2^1)_\alpha] \\ = \sum_{i=1}^{3} \int \theta_{i4} [g_4^0 + g_3^0(i) g_1^0(4) + g_3^0(4) g_1^0(i) \\ + \sum_{\substack{j \neq i,4 \\ k \neq i,j,4}} g_2^0(j, 4) g_2^0(i, k)]\, d\Omega_4. \end{aligned} \tag{2.20}$$

$s = 4$:

$$\begin{aligned} \frac{\partial g_4^0}{\partial t} + H_4^0 g_4^0 - \sum_{i=1}^{4} \sum_{j=1}^{i-1} \sum_{\substack{\alpha \neq i,j \\ \beta \neq i,j,\alpha}} \theta_{ij} [g_1^0(i) g_3^0(j, \alpha, \beta) \\ + g_1^0(j) g_3^0(i, \alpha, \beta) + g_2^0(i, \alpha) g_2^0(j, \beta)] = 0. \end{aligned} \tag{2.21}$$

Note that in writing (2.12)–(2.21) we have not introduced $\epsilon^n t$ and $\epsilon^n H_s^n$, $n \geq 2$ variations since we have shown in Ref. 1 that the asymptotic solution appears to have no such long-time, long-space variation. Further, we have used the decomposition

$$(g_3^1)_\alpha = (g_3^1)_{\alpha s} + (g_3^1)_{\alpha ns}. \tag{2.22}$$

We show that $(g_3^1)_{\alpha s}$ contributes secular terms while $(g_3^1)_{\alpha ns}$ does not.

III. FORMAL SOLUTION OF "REVISED" HIERARCHY

The philosophy of the calculation is, of course, to solve the above equations order by order. However, as we continue the expansion we wish it to hold for longer and longer times. Thus we must be prepared to remove secular terms by balancing them against functions which are undetermined, and we must estimate the error terms to show that the various functions are bounded.

In Ref. 1 we determined g_3^0 fully. However, the determination of g_s^1 was only valid for times $t \ll 1/\epsilon$. Our first task, therefore, is to construct an expression for g_2^1 valid on the time scale $t \sim 1/\epsilon$. g_s^1 has been decomposed into $(g_2^1)_\alpha$ and $(g_2^1)_\beta$. A formal solution for $(g_2^1)_\alpha$ can easily be obtained but $(g_2^1)_\beta$ must be determined by removing secular behavior from g_2^2. g_2^2 in turn depends on known functions and $(g_3^1)_\alpha$. Thus $(g_3^1)_\alpha$ must be determined. In fact it is shown that it is sufficient for our purposes to determine g_3^1 as a functional of $(g_2^1)_\alpha$.

A. Determination of $(g_2^1)_\alpha$

We now go on to calculate $[g_2^1(t, \epsilon t)]_\alpha$ subject to the initial condition

$$[g_2^1(0, 0)]_\alpha = 0 \tag{3.1}$$

and then seek to write

$$[g_2^1(t, \epsilon t)]_\alpha = [g_2^1(t, \epsilon t)]_{\alpha s} + [g_2^1(t, \epsilon t)]_{\alpha ns}, \tag{3.2}$$

where $[g_2^1(t, \epsilon t)]_{\alpha s}$ produced a secular contribution to (2.18).

From Eq. (2.16) for $|x_{12}| < r_0$ we have

$$(g_2^1)_\alpha = \int_0^t e^{-[H_2^0 + \epsilon H_2^1 + \epsilon(\partial/\partial\epsilon t)](t-t')} \times \left\{ -\frac{\partial g_2^0}{\partial \epsilon t} + \theta_{12}[g_1^0(g_1^1)_\alpha + (g_1^1)_\alpha g_1^0] + \sum_{i=1}^{2} \int d\Omega_3 \theta_{i3}[g_3^0 + g_1^0(i)g_2^0 + g_1^0(3)g_2^0] \right\} dt'. \tag{3.3}$$

It is apparent that this is the same as the Choh–Uhlenbeck triple collision term on neglect of the terms $(\epsilon H_2^1 + \epsilon(\partial/\partial\epsilon t))$ within the exponential factor, and in the limit $t \to \infty$.

For $|x_{12}| > r_0$, x_{12} not almost $\| v_{12}$ (i.e., trajectories such that Particles 1 and 2 have not interacted in the past), we have

$$(g_2^1)_\alpha = \int_0^t e^{-[H_2^0 + \epsilon H_2^1 + \epsilon(\partial/\partial\epsilon t)](t-t')} \times \left\{ \sum_{i=1}^{2} \int \theta_{i3}[g_3^0 + g_1^0(i)g_2^0 + g_1^0(3)g_2^0]\, d\Omega_3 \right\} dt'. \tag{3.4}$$

For $|x_{12}| > r_0$, x_{12} almost $\| v_{12}$ (i.e., trajectories such that Particles 1 and 2 have interacted in the past):

$$(g_2^1)_\alpha = \int_0^t e^{-[H_2^0 + \epsilon H_2^1 + \epsilon(\partial/\partial\epsilon t)](t-t')} \times \left\{ -\frac{\partial g_2^0}{\partial t_1} - H_2^1 g_2^0 S(t' - t^*) + \theta_{12}(g_1^0 g_1^1 + g_1^1 g_1^0) + \sum_{i=1}^{2} \int \theta_{i3}[g_3^0 + g_1^0(i)g_2^0 + g_1^0(3)g_2^0]\, d\Omega_3 \right\} dt' \tag{3.5}$$

with t^* the maximum value of t' such that

$$e^{-H_2^0(t-t')}\theta_{12} \neq 0.$$

[We have $S(x) = 1$, $x > 0$; $S(x) = 0$, $x < 0$.]

We now seek to divide (3.4) and (3.5) into parts which contribute to secularities in g_2^2 and parts which do not. To this end we note for $|x_{12}| > 2r_0$:

$$g_3^0(t') = e^{-[H_2^0(i,3) + v_j \cdot (\partial/\partial x_j)]\tau}[g_3^0(t - \tau) + g_1^0(i)g_2^0(t' - \tau) + g_1^0(3)g_2^0(t' - \tau)] - [g_1^0(i)g_2^0(t') + g_1^0(3)g_2^0(t')]. \tag{3.6}$$

(Throughout this paper we consider only binary potentials such that there exists an upper bound τ of order unity to the duration of all binary interactions.)

Also for $|x_{12}| > r_0$, on using (2.19), the integral within (3.4) and (3.5) may be rewritten:

$$\sum_{\substack{i=1 \\ (j=3-i)}}^{2} \int_{|x_{i3}| < r_0} \left[\frac{\partial g_3^0}{\partial t'} + \sum_{j=1}^{3} v_j \cdot \frac{\partial}{\partial x_j} g_3^0 \right] d\Omega_3 = \left(\frac{\partial}{\partial t'} + v_1 \cdot \frac{\partial}{\partial x_1} + v_2 \cdot \frac{\partial}{\partial x_2} \right) \sum_{i=1}^{2} \int_{|x_{i3}| < r_0} g_3^0\, d\Omega_3 + \sum_{i=1}^{2} \int_{|x_{i3}| < r_0} v_{3i} \cdot \frac{\partial}{\partial x_3} g_3^0\, d\Omega_3. \tag{3.7}$$

On using (3.6) and (3.7) in (3.4) we have

$$(g_2^1)_\alpha = (g_2^1)_{\alpha s} + (g_2^1)_{\alpha ns}, \tag{3.8}$$

where we define

$$(g_2^1)_{\alpha s} = \int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\Bigg\{\sum_{\substack{i=1\\(j=3-i)}}^{2}\int_{|x_{i3'}|=r_0} v_{3'i} \times [\epsilon^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]r}(g_1^0 g_2^0(t'-\tau) + g_1^0(3')g_2^0(t'-\tau)) - g_1^0(i)g_2^0(t')](x_{i3'} \parallel v_{i3'})\, d\sigma_{3'}\, dv_{3'}\Bigg\} dt' \tag{3.9}$$

and

$$\begin{aligned}(g_2^1)_{\alpha n s} &= \int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)]t} \times \frac{\partial}{\partial t'}\Bigg[e^{[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial(\epsilon t))]t'}\sum_{\substack{i=1\\(j=3-i)}}^{2}\int_{|x_{i3}|<r_0} g_3^0\, dx_3\, dv_3\Bigg] dt' \\ &+ \int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\sum_{\substack{i=1\\(j=3-i)}}^{2}\int_{|x_{i3'}|=r_0} v_{3'i} \times [e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]r} g_3^0(t'-\tau)(x_{i3'} \parallel v_{i3'}) - g_3^0(t')(x_{i3'} - \parallel v_{i3'})] \times d\sigma_{3'}\, dv_{3'}\, dt' \\ &- \int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\left(\epsilon H_2^1 + \epsilon\frac{\partial}{\partial\epsilon t}\right) \times \sum_{i=1}^{2}\int_{|x_{i3}|<r_0} g_3^0\, d\Omega_3\, dt'.\end{aligned} \tag{3.10}$$

[At this point we note that throughout this paper the combination $|x_{\alpha\beta}| = r_0$; $x_{\alpha\beta} \parallel v_{\alpha\beta}$ denotes that particles α and β are at the distance r_0 beyond which the binary force between particles vanishes, and that α and β are moving apart; the combination $|x_{\alpha\beta}| = r_0$, $x_{\alpha\beta} - \parallel v_{\alpha\beta}$ (i.e., $x_{\alpha\beta} \parallel -v_{\alpha\beta}$) denotes the same separation, but that α and β are approaching each other.]

For (3.5), on using

$$\frac{\partial g_2^0}{\partial\epsilon t} + H_2^1 g_2^0 = -\sum_{i=1}^{2}\int_{|x_{i3'}|=r_0;x_{i3'}\parallel v_{i3'}} |v_{i3'}|\, g_1^0(3')g_2^0\, d\sigma_{3'}\, dv_{3'}, \tag{3.11}$$

we note

$$(g_2^1)_\alpha(x_{12}\ \text{almost} \parallel v_{12}) = O(1). \tag{3.12}$$

B. Determination of $(\epsilon g_2^1)_\beta$

Now, we first determine the form of $(g_3^1)_\alpha$ for $|x_{i3}| < r_0$, $|x_{12}| > r_0$. Parts of this function determine the secular behavior of (2.18) which, in turn, is used in the definition of $(\epsilon g_2^1)_\beta$.

From (2.20) one obtains on using (2.12), (2.13), (2.15), (2.16), and (2.21), and neglecting terms of order ϵ:

$$\begin{aligned}(g_3^1)_\alpha(t,\epsilon t) &= e^{-H_3^0\tau}\{(g_3^1)_\alpha(t-\tau,\epsilon t) + g_1^0(i)(g_2^1)_\alpha(t-\tau,\epsilon t) + [g_1^1(i)]_\alpha g_2^0 + g_1^0(3)(g_2^1)_\alpha + [g_1^1(3)]_\alpha g_2^0\} \\ &\quad - \{g_1^0(i)(g_2^1)_\alpha(t,\epsilon t) + [g_1^1(i)]_\alpha g_2^0 + g_1^0(3)(g_2^1)_\alpha + [g_1^1(3)]_\alpha g_2^0\} + 0.\end{aligned} \tag{3.13}$$

Specifically we note

$$0 = \int_{t-\tau}^{t} e^{-H_3^0(t-t')}(I + l)\, dt' \tag{3.14}$$

with I given by the integral term of (2.18) and l a linear function of the integral terms within (2.10) and (2.13). We note that in (3.13) and (3.14) we have

$$\tau = O(1). \tag{3.15}$$

On substituting (3.13) in (2.18) one may verify that the only terms within (2.18) which yield secular contributions to g_2^2 for $|x_{12}| < r_0$ are those terms linear in $(g_2^1)_{\alpha s}$. (See Appendix A for details.)

On removing secular behavior from (2.18) we obtain as a sufficient condition for the finiteness of g_2^2 for $|x_{12}| < r_0$

$$\frac{\partial(\epsilon g_2^1)_\beta}{\partial\epsilon t} + H_2^1(\epsilon g_2^1)_\beta = \sum_{i=1}^{2}\int\theta_{i3}e^{-H_3^0\tau} \times [g_1^0(i)(g_2^1)_{\alpha s}(t-\tau) + g_1^0(3)(g_2^1)_{\alpha s}(t-\tau)]\, d\Omega_3. \tag{3.16}$$

On combining (3.16) and (2.17) we have

$$\begin{aligned}\frac{\partial(\epsilon g_2^1)_\beta}{\partial t} + H_2^0(\epsilon g_2^1)_\beta + \epsilon\frac{\partial(\epsilon g_2^1)_\beta}{\partial\epsilon t} + \epsilon H_2^1(\epsilon g_2^1)_\beta &= \epsilon\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0] + \epsilon\sum_{i=1}^{2}\int\theta_{i3}e^{-H_3^0\tau} \\ &\quad \times [g_1^0(i)(g_2^1)_{\alpha s}(t-\tau) + g_1^0(3)(g_2^1)_{\alpha s}(t-\tau)]\, d\Omega_3.\end{aligned} \tag{3.17}$$

From (3.17) we obtain directly

$$\begin{aligned}(\epsilon g_2^1)_\beta = \int_0^t e^{-[H_2^0+\epsilon(\partial/\partial\epsilon t)+\epsilon H_2^1](t-t')} &\times \Big\{\epsilon\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0] + \epsilon\sum_{i=1}\int\theta_{i3}e^{-H_3^0\tau} \\ &\times [g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau) + g_1^0(3)(g_2^1)_{\alpha s}(t'-\tau)]\Big\}\, d\Omega_3\, dt'.\end{aligned} \tag{3.18}$$

On using

$$\theta_{i3} = \left(H_2^0 + \epsilon\frac{\partial}{\partial\epsilon t} + \epsilon H_2^1\right) + v_3\cdot\frac{\partial}{\partial x_3} - H_3^0 - \left(\epsilon\frac{\partial}{\partial\epsilon t} + \epsilon H_2^1\right) \tag{3.19}$$

and neglecting terms of relative size $(\ln\epsilon)^{-1}$, (3.18) becomes (see Appendix B for details)

$$\begin{aligned}(\epsilon g_2^1)_\beta = \int_0^t e^{-[H_2^0+\epsilon(\partial/\partial\epsilon t)+\epsilon H_2^1](t-t')} &\times \Bigg\{\epsilon\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^1] + \epsilon\sum_{\substack{i=1\\(j=3-i)}}^{2}\int_{|x_{i3}|<r_0} v_{3i} \\ &\cdot\frac{\partial}{\partial x_3}e^{-H_3^0\tau}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau) + g_1^0(3)(g_2^1)_{\alpha s}(t'-\tau)]\, d\Omega_3\Bigg\} dt'.\end{aligned} \tag{3.20}$$

From (3.12), (3.20) is not affected to order ϵ by using the form (3.9) for x_{12} almost $\| v_{12}$.

IV. ASYMPTOTIC FORM FOR $(g_2^1)_\alpha + \epsilon(g_2^1)_\beta$ FOR $|x_{12}| < r_0$

From (3.3), after some algebra (see Appendix C for details), we can write to order ϵ:

$$(g_2^1)_\alpha = I(x_{12}, \epsilon x_{12} = 0, t, \epsilon t) + J(x_{12}, \epsilon x_{12} = 0, t, \epsilon t) \tag{4.1}$$

with

$$\begin{aligned} I = &\int_{\max(t-1/\epsilon,0)}^{t} e^{-H_2^0(t-t')} \\ &\times \left\{ -\frac{\partial g_2^0}{\partial \epsilon t} + \theta_{12}[g_1^0(g_1^1)_\alpha + (g_1^1)_\alpha g_1^0] \right. \\ &\left. + \sum_{i=1}^{2} \int \theta_{i3}[g_3^0 + g_1^0(i)g_2^0 + g_1^0(3)g_2^0]\, d\Omega_3 \right\} dt' \\ &+ \int_0^{t-1/\epsilon} e^{-[H_2^0 + \epsilon H_2^1 + \epsilon(\partial/\partial \epsilon t)](t-t')} \\ &\times \left\{ \sum_{i=1}^{2} \int \theta_{i3}[g_3^0 + g_1^0(i)g_2^0 + g_1^0(3)g_2^0]\, d\Omega_3 \right\} dt' \end{aligned} \tag{4.2}$$

and

$$J = -\int_{\max(t-1/\epsilon,0)}^{t} \epsilon e^{-H_2^0(t-t')} \left(H_2^1 + \frac{\partial}{\partial \epsilon t} \right) (\tilde{g}_2^1)_{\alpha s}\, dt' \tag{4.3}$$

with $\max(t - 1/\epsilon, 0)$ denoting the larger of $t - 1/\epsilon$ and 0, and

$$\begin{aligned} &(\tilde{g}_2^1)_{\alpha s}(x_{12}, \epsilon x_{12} = 0, \epsilon t, v_1, v_2) \\ &\equiv \int_0^\infty e^{-H_2^0 \tau'} \sum_{\substack{i=1 \\ (j=3-1)}}^{2} \int_{|x_{i3'}|=r_0} v_{3'i} \left\{ e^{-[H_3^0(i,3') + v_{j'} \cdot (\partial/\partial x_j)]\tau} \right. \\ &\quad \times [g_1^0(i)g_2^0(t \to \infty) + g_1^0(3')g_2^0(t \to \infty)] \\ &\quad \left. - g_1^0(i)g_2^0(t \to \infty) \right\} (x_{i3'} \| v_{i3'})\, d\sigma_{3'}\, dv_{3'}\, d\tau'. \end{aligned} \tag{4.4}$$

From (3.20), after some algebra, we can write (see Appendix D for details):

$$\epsilon(g_2^1)_\beta = K(x_{12}, \epsilon x_{12} = 0, t, \epsilon t) \tag{4.5}$$

with

$$\begin{aligned} K = &\int_{\max(t-1/\epsilon,0)}^{t} e^{-H_2^0(t-t')} \\ &\times \left\{ \epsilon\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0] + \epsilon \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} d\Omega_3 v_{3i} \right. \\ &\left. \cdot \frac{\partial}{\partial x_3} e^{-H_3^0 \tau} [g_1^0(i)(\tilde{g}_2^1)_{\alpha s} + g_1^0(3)(\tilde{g}_2^1)_{\alpha s}] \right\} dt'. \end{aligned} \tag{4.6}$$

On combining (4.1) and (4.5) and specifying only the t dependence of I, J, and K, we have for (x_{12}, $\epsilon x_{12} = 0$, ϵt):

$$\begin{aligned} (g_2^1)_\alpha + \epsilon(g_2^1)_\beta = &\lim_{t\to\infty} I(t) + \lim_{t\to\infty} [J(t) + K(t)] \\ &+ \left\{ [I(t) - \lim_{t\to\infty} I(t)] \right\} + \left\{ [J(t) + K(t)] \right. \\ &\left. - \lim_{t\to\infty} [J(t) + K(t)] \right\}. \end{aligned} \tag{4.7}$$

The term

$$\lim_{t\to\infty} I(t),$$

which is evaluated at $\epsilon x_{12} = 0$, determines the standard Choh–Uhlenbeck triple collision integral within an error of order ϵ.

The term

$$\lim_{t\to\infty} [J(t) + K(t)]$$

on the neglect of contributions of order ϵ may be written (see Appendix E for details):

$$\begin{aligned} &\lim_{t\to\infty} [J(t) + K(t)] \\ &\quad = \epsilon \lim_{t\to\infty} \int_{t-1/\epsilon}^{t} e^{-H_2^0(t-t')} \{\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0]\} \\ &\qquad + \epsilon\, |\ln \epsilon|\, G(x_{12}, v_1, v_2, \epsilon t) \end{aligned} \tag{4.8}$$

with

$$\begin{aligned} &G(x_{12}, v_1, v_2, \epsilon t) \\ &\equiv e^{-H_2^0 \tau} \frac{1}{|v_{12}|} \left\{ \sum_{\substack{i=1 \\ (j=3-i)}}^{2} \int v_{3i} [e^{-H_2^0(i,3)\tau} - 1] \right. \\ &\quad \times [g_1^0\{[\tilde{g}_2^1(\mathbf{x}_{12}, \epsilon \mathbf{x}_{12}, \epsilon t, v_1, v_2)]_{\alpha s} |x_{12}|\} \\ &\quad (\epsilon x_{12} = 0, |x_{12}| = 1/\epsilon, \mathbf{x}_{12} \| -\mathbf{v}_{12})] \\ &\quad + g_1^0\{[\tilde{g}_2^1(\mathbf{x}_{3j}, \epsilon \mathbf{x}_{3j}, \epsilon t, v_3, v_j)]_{\alpha s} |x_{3j}|\} \\ &\quad \times [\epsilon x_{3j} = 0, |x_{3j}| = 1/\epsilon, \mathbf{x}_{3j} \| -\mathbf{v}_{ij}(-)^j] \times d\sigma_3\, d_3 v_3 \\ &\quad - \left(\frac{\partial}{\partial \epsilon t} + H_2^1 \right) \{[\tilde{g}_2^1(\mathbf{x}_{12}, \epsilon \mathbf{x}_{12}, \epsilon t, v_1, v_2)]_{\alpha s} |x_{12}|\} \\ &\quad \left. (\epsilon x_{12} = 0, |x_{12}| = 1/\epsilon, x_{12} \| -v_{12}) \right\}. \end{aligned} \tag{4.8a}$$

Within (4.8) we note $t_0 = O(1)$, $\tau = O(1)$ and

$$\mathbf{v}_{12} = \mathbf{v}_{12}, \tag{4.9a}$$

$$e^{-H_2^0(1,2)t_0} \bar{\mathbf{v}}_{12} = e^{-H_2^0(1,2)t_0} \mathbf{v}_{12}, \tag{4.9b}$$

$$e^{-H_2^0(i,3)\tau} \bar{\mathbf{v}}_{12} = \bar{\mathbf{v}}_{12}. \tag{4.9c}$$

Moreover, to evaluate terms of the form

$$v_{12} \cdot (\partial/\partial \epsilon x_{12}) g_2^0(t \to \infty, j, 3) \tag{4.10}$$

which occur within (4.8) on using (4.4) we note

$$\epsilon x_{j3} = \epsilon x_{i3} - \epsilon x_{ij}, \tag{4.11}$$

from which

$$v_{12} \cdot \frac{\partial}{\partial \epsilon x_{12}} g_2^0(t \to \infty, j, 3) = (-)^j v_{12} \cdot \frac{\partial g_2^0(t \to \infty, j, 3)}{\partial \epsilon x_{j3}}. \tag{4.12}$$

Further, since we may choose

$$(\partial g_2^0/\partial \epsilon x_{\alpha\beta}) \times \mathbf{v}_{ab} = 0, \tag{4.13}$$

we note that for an arbitrary vector α

$$\alpha \cdot \frac{\partial g_2^0}{\partial \epsilon x_{ij}} = \alpha \cdot \frac{v_{ij}}{|v_{ij}|^2} v_{ij} \cdot \frac{\partial g_2^0}{\partial \epsilon x_{ij}}. \tag{4.14}$$

The term

$$I(t) - \lim_{t\to\infty} I(t) \tag{4.15a}$$

for $t < \epsilon - 1$ may be written in the form

$$I(t) - \lim_{t\to\infty} I(t) = (\tilde{g}_2^1)_{\alpha s}(t, \epsilon t = 0, \epsilon x_{12} = 0) - (\tilde{g}_2^1)_{\alpha s}(\epsilon t = 0, \epsilon x_{12} = 0) + \gamma, \tag{4.15b}$$

where

$$\begin{aligned}(\tilde{g}_2^1)_{\alpha s}&(t, \epsilon t, \epsilon x_{12} = 0)\\ &= \int_0^t e^{-H_2^0(t-t')} \sum_{\substack{i=1\\(j=3-i)}}^{2} \int_{|x_{13'}|=r_0} v_{3'i}\{e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]\tau}\\ &\quad\times [g_1^0(i)g_2^0(t'-\tau, \epsilon x_{3'j} = 0)\\ &\quad + g_1^0(3')g_2^0(t'-\tau, \epsilon x_{ij} = 0)]\\ &\quad - g_1^0(i)g_2^0(t', \epsilon x_{3'j} = 0)\}\,(x_{i3'} \parallel v_{i3'})\, d\sigma_{3'}\, dv_{3'}\, dt'\\ &\equiv \int_0^t e^{-H_2^0(t-t')}\tilde{O} g_2^0(t')\, d\sigma_{3'}\, dv_{3'}\, dt'\end{aligned} \tag{4.16}$$

and

$$(\tilde{g}_2^1)_{\alpha s}(\epsilon t, \epsilon x_{12} = 0) \equiv \int_{-\infty}^t e^{-H_2^0(t-t')}\tilde{O} g_2^0(t' \to \infty)\, d\sigma_{3'}\, dv_{3'}\, dt' \tag{4.17}$$

and

$$\begin{aligned}\gamma &= (\tilde{g}_2^1)_{\alpha s}(t, \epsilon t) - (\tilde{g}_2^1)_{\alpha s}(t \to \infty, \epsilon t)\\ &\quad - [(\tilde{g}_2^1)_{\alpha s}(t, \epsilon t = 0) - (\tilde{g}_2^1)_{\alpha s}(t \to \infty, \epsilon t = 0)]\\ &\quad + I(t, \epsilon t) - (\tilde{g}_2^1)_{\alpha s}(t, \epsilon t) - [I(t \to \infty, \epsilon t)\\ &\quad - (\tilde{g}_2^1)_{\alpha s}(t \to \infty, \epsilon t)] + (\tilde{g}_2^1)_{\alpha s}(\epsilon t = 0)\\ &\quad - (\tilde{g}_2^1)_{\alpha s}(t \to \infty, \epsilon t = 0)\end{aligned} \tag{4.18}$$

with all functions in (4.18) evaluated for $\epsilon x_{12} = 0$.

Within (4.15b) we write for $\epsilon^{-1} > t > 1$ (see Appendix F for details)

$$\begin{aligned}(\tilde{g}_2^1)_{\alpha s}&(t, \epsilon t = 0, \epsilon x_{12} = 0) - (\tilde{g}_2^1)_{\alpha s}(\epsilon t = 0, \epsilon x_{12} = 0)\\ &= \frac{1}{t}\{t'[(\tilde{g}_2^1)_{\alpha s}(t', \epsilon t = 0, \epsilon x_{12} = 0)\\ &\quad - (\tilde{g}_2^1)_{\alpha s}(\epsilon t = 0, \epsilon x_{12} = 0)]\}(t' = \epsilon^{-1}).\end{aligned} \tag{4.19}$$

In doing this we have neglected contributions due to the nonzero range of the binary potential. It may be shown that these neglected contributions as well as the terms in γ do not affect g_1 to lower order than ϵ^2. Hence they are not considered in the determination of the $\epsilon^2 \ln \epsilon$ behavior of g_1.

For $t \gg \epsilon^{-1}$ the term

$$I(t) - \lim_{t\to\infty} I(t)$$

from (4.2) may be estimated to be

$$\frac{O\epsilon}{(\epsilon t)^2} + O\int_{t'=\epsilon^{-1}}^t e^{-\epsilon v_{12}t' - \epsilon(t-t')}(v_{12}^2 t'^2)^{-1}\, dt'. \tag{4.20}$$

For $v_{12} > \frac{1}{2}$, this becomes

$$= \frac{O\epsilon}{(\epsilon t)^2} + O\epsilon e^{-\epsilon v_{12}t}[(\epsilon v_{12}t)^{-1} + (\epsilon v_{12}t)^{-2}]. \tag{4.21}$$

For $v_{12} > \frac{1}{2}$, this becomes

$$= \frac{O\epsilon}{(\epsilon t)^2} + O\epsilon e^{-\epsilon t/2}. \tag{4.22}$$

The term

$$\left\{[J(t) + K(t)] - \lim_{t\to\infty}[J(t) + K(t)]\right\}$$

within (4.7) does not contribute to g_1 in order lower than ϵ^2. This is discussed later.

V. DETERMINATION OF g_1 TO ORDER LOWER THAN ϵ^2

We now study the effect of our analysis on g_1. From (2.13) we have

$$\frac{\partial g_1^0}{\partial \epsilon t} = \lim_{t\to\infty} \int \theta_{12} g_2^0(t, \epsilon t)\, d\Omega_2 \tag{5.1}$$

and

$$\frac{\partial (g_1^1)_\alpha}{\partial t} = \int \theta_{12}\left[g_2^0(t, \epsilon t) - \lim_{t\to\infty} g_2^0(t, \epsilon t)\right] d\Omega_2. \tag{5.2}$$

On substituting (4.7) in (2.14), from the logarithmic finiteness of $(g_1^1)_\beta$ we obtain

$$\lim_{t\to\infty} \frac{\partial (g_1^1)_\alpha}{\partial \epsilon t} = \lim_{t\to\infty} \int \theta_{12} I(x_{12}, \epsilon x_{12} = 0, \epsilon t, t, v_1, v_2)\, d\Omega_2. \tag{5.3}$$

On noting that the contribution from (4.19) is of the form

$$A(x_{12}, v_1, v_2) S(\epsilon^{-1} - t)/t \tag{5.4}$$

[with $S(x) = 0$, $x < 0$; $S(x) = 1$, $x > 0$] and the right-hand side of (4.8) is of the form

$$\epsilon \lim_{t\to\infty} \int_{t-1/\epsilon}^t e^{-H_2^0(t-t')}\{\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0]\}\, dt' + \epsilon\,|\ln \epsilon|\, G(x_{12}, v_1, v_2, \epsilon t) \tag{5.5}$$

and combining (2.14) with (5.3) we obtain

$$\frac{\partial(g_1^1)_\beta}{\partial t}+\epsilon\frac{\partial(g_1^1)_\beta}{\partial\epsilon t}+\frac{\partial g_1^2}{\partial t}+\epsilon\frac{\partial g_1^2}{\partial\epsilon t}+\epsilon\left(\frac{\partial g_1^3}{\partial t}+\epsilon\frac{\partial g_1^3}{\partial\epsilon t}\right)+\cdots$$
$$=\int\theta_{12}\Bigg\{\frac{A(x_{12},v_1,v_2)S(\epsilon^{-1}-t)}{t}+\epsilon\lim_{t\to\infty}\int_{t-1/\epsilon}\times e^{-H_2{}^0(t-t')}\{\theta_{12}[g_1^0(g_1^1)_\beta+(g_1^1)_\beta g_1^0]\}\,dt'$$
$$+\epsilon\,|\ln\epsilon|\,G(x_{12},v_1,v_2,\epsilon t)+\epsilon B+\{J(t)+K(t)-\lim_{t\to\infty}[J(t)+K(t)]\}$$
$$+\epsilon g_2^2+\epsilon^2 g_2^3+\cdots\Bigg\}\,d\Omega_2-\frac{\partial}{\partial\epsilon t}\Big[(g_1^1)_\alpha(t,\epsilon t)-\lim_{t\to\infty}(g_1^1)_\alpha(t,\epsilon t)\Big]. \quad (5.6)$$

Within (5.6) the term B is $O(1)$ and is derived from contributions of $O(\epsilon)$ to

$$\Big[I(t)-\lim_{t\to\infty}I(t)\Big] \quad \text{and} \quad \lim_{t\to\infty}[J(t)+K(t)],$$

as well as earlier contributions to g_2^1 which were deemed to be of order ϵ.

From (5.6) we are free to define

$$\frac{\partial(g_1^1)_\beta}{\partial t}=\int\theta_{12}\frac{A(x_{12},v_1,v_2)}{t}, \quad t<\epsilon^{-1}, \quad (5.7a)$$
$$\partial(g_1^1)_\beta/\partial t=0, \quad t>\epsilon^{-1}. \quad (5.7b)$$

Then on subtracting (5.7) from (5.6) we obtain

$$\epsilon\frac{\partial(g_1^1)_\beta}{\partial\epsilon t}+\frac{\partial g_1^2}{\partial t}+\epsilon\frac{\partial g_1^2}{\partial\epsilon t}+\epsilon\left(\frac{\partial g_1^3}{\partial t}+\epsilon\frac{\partial g_1^3}{\partial\epsilon t}\right)+\cdots$$
$$=\int\theta_{12}\Bigg\{\epsilon\lim_{t\to\infty}\int_{t-1/\epsilon}^{t}e^{-H_2{}^0(t-t')}\{\theta_{12}[g_1^0(g_1^1)_\beta+(g_1^1)_\beta g_1^0]\}\,dt'$$
$$+\epsilon\,|\ln\epsilon|\,G(x_{12},v_1,v_2,\epsilon t)+\epsilon B'+\{J(t)+K(t)\}-\lim_{t\to\infty}[J(t)+K(t)]$$
$$+\epsilon g_2^2+\epsilon^2 g_2^3+\cdots\Bigg\}\,d\Omega_2-\frac{\partial}{\partial(\epsilon t)}\Big[(g_1^1)_\alpha(t,\epsilon t)-\lim_{t\to\infty}(g_1^1)_\alpha\cdot(t,\epsilon t)\Big] \quad (5.8)$$

with B' of order unity.[4]

From (5.7a) and (5.7b) for $t>\epsilon^{-1}$ we can write

$$(g_1^1)_\beta=|\ln\epsilon|\lim_{t\to\infty}(\tilde g_1^1)_\beta(t,\epsilon t) \quad (5.9)$$

with

$$\lim_{t\to\infty}(\tilde g_1^1)_\beta(t,\epsilon t)=O(1).$$

[4] In this connection we note from (4.21) and (4.22) that within (5.8) the contribution from

$$\int d\Omega_2\Big[1-\lim_{t\to\infty}I(t)\Big]$$

or $t\gg\epsilon^{-1}$ is of order $\epsilon(\epsilon t)^{-2}$. Therefore the t^{-1} behavior of (5.6) or $t<\epsilon^{-1}$ does not persist for $t\ll\epsilon^{-1}$.

On integrating (5.8) for a range in t specified by $\tau_1<t<\tau_2$, $\tau_2-\tau_1=\epsilon^{-1}$, $\tau_1>\epsilon^{-1}$, and simplifying (5.5) with (5.7b), we have as a condition for g_1^2 to be finite:

$$\frac{\partial}{\partial\epsilon t}\Big[\lim_{t\to\infty}(\tilde g_1^1)_\beta\Big]$$
$$=\int\theta_{12}\Big\{e^{-H_2{}^0\tau}\Big[g_1^0(1)\lim_{t\to\infty}(\tilde g_1^1)_\beta+\lim_{t\to\infty}(\tilde g_1^1)_\beta g_1^0(2)\Big]+G(x_{12},v_1,v_2,\epsilon t)\Big\}\,d\Omega_2. \quad (5.10)$$

Here $\tau=O(1)$.

One may use (5.7a) to get

$$\lim_{t\to\infty}(g_1^1)_\beta(t,\epsilon t=0)$$

from $(g_1^1)_\beta$ $(t=0,\ \epsilon t=0)$. One may then use (5.10) to get

$$\lim_{t\to\infty}(g_1^1)_\beta(t,\epsilon t)$$

from

$$\lim_{t\to\infty}(g_1^1)_\beta(t,\epsilon t=0).$$

For $t>\epsilon^{-1}$ and physical combinations of t and ϵt $(\epsilon t/\epsilon=t)$, these two operations determine $(g_1^1)_\beta$. For $t<\epsilon^{-1}$ after using (5.10) one must use (5.7a) again.

To within one part in $|\ln\epsilon|$ we obtain:

$$(g_1^1)_\beta(t,\epsilon t)=\ln t\lim_{t\to\infty}(\tilde g_1^1)_\beta(t,\epsilon t). \quad (5.11)$$

On combining (5.7), (5.8), and (5.10) we have

$$\frac{\partial g_1^2}{\partial t}+\epsilon\frac{\partial g_1^2}{\partial\epsilon t}+\epsilon\left(\frac{\partial g_1^3}{\partial t}+\epsilon\frac{\partial g_1^3}{\partial\epsilon t}\right)+\cdots$$
$$=\int\theta_{12}\Big\{\Big(1-\lim_{t\to\infty}\Big)[J(t)+K(t)]+\epsilon B'+\epsilon g_2^2+\epsilon^2 g_2^3+\cdots\Big\}\,d\Omega_2$$
$$-\frac{\partial}{\partial\epsilon t}\Big[(g_1^1)_\alpha(t,\epsilon t)-\lim_{t\to\infty}(g_1^1)_\alpha(t,\epsilon t)\Big].$$

It is possible to verify (see Appendix G for details) that the contribution to g_1 from the terms in

$$\Big(1-\lim_{t\to\infty}\Big)[J(t)+K(t)]$$

and

$$-\partial/\partial\epsilon t\Big[(g_1^1)_\alpha(t,\epsilon t)-\lim_{t\to\infty}(g_1^1)_\alpha(t,\epsilon t)\Big]$$

is of order ϵ^2. Further we note that the contributions to g_1 from the terms in $\epsilon g_2^2+\epsilon^2 g_2^3+\cdots$ will be discussed in a subsequent paper.

VI. CONCLUSIONS

We obtain to order $\epsilon^2 \ln \epsilon$, $\epsilon = nr_0^3$, the single-particle function solution to the BBGKY hierarchy in the Boltzmann approximation, subject to the initial condition: $g_s(t=0) = 0$, $s > 1$. A necessary part of these results has been the introduction and extensive usage of a generalization of the Bogoliubov streaming operator. This operator, acting on the zero-order correlation functions determined in Ref. 1, ultimately produces a kinetic evolution equation for the one-particle function of the general form:

$$\partial f_1/\partial \epsilon t \sim \text{(Boltzmann function)} + \epsilon\,\text{(Choh–Uhlenbeck function)} + \epsilon\,|\ln \epsilon|\, G + \epsilon^2 H. \quad (6.1)$$

The function G is given by Eq. (4.8a). In thermal equilibrium, G vanishes as it should. On the neglect of terms of order unity, H is given by

$$\int \theta_{12}(g_2^2 + \epsilon g_2^3 + \cdots)\, d\Omega_2. \quad (6.2)$$

The terms in (6.2) are formally of order unity, but they are as yet unevaluated in detail.

It is interesting to note that the t^{-1} dependence of

$$\left(1 - \lim_{t\to\infty}\right) g_2^1(t, \epsilon t)$$

produces a contribution to $f(1)$ of order $\epsilon^2 \ln \epsilon$, although the term

$$\left(1 - \lim_{t\to\infty}\right) g_2^1(t, \epsilon t)$$

does not enter into the kinetic equation directly. This apparent discrepancy is resolved by noting that within the framework of the kinetic theory the contribution to $f(1)$ from

$$\left(1 - \lim_{t\to\infty}\right) g_2^1(t, \epsilon t)$$

serves as part of the initial condition on $f(1)$. Hence the behavior of the single-particle function is Markoffian to order $\epsilon^2 \ln \epsilon$. From Appendixes C and D it is almost certainly non-Markoffian in order ϵ^2.

ACKNOWLEDGMENTS

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APPENDIX A. ON THE CONTRIBUTION OF VARIOUS TERMS IN (3.13) TO THE SECULAR BEHAVIOR OF (2.18)

1. Justification of Neglect of the Contribution of I in (3.13) to Eq. (2.18)

We now demonstrate for x_{12} almost $\parallel -v_{12}$ that the contribution of I to Eq. (2.18) is of order $|x_{12}|^{-2}$. To establish this it is necessary to examine I in some detail since $\theta_{i4}[g_4^0 + \cdots + g_3^0(4, \cdots)g_1^0(i)]$ is in general unbounded in terms of $[g_4^0 + \cdots + g_3^0(4)g_1^0(i)]$ with increasing $|x_{12}|$.

To see this we note from Ref. 1, Eq. (4.19):

$$\nabla_{v_i} g_2^0(x_{ij}, v_i, v_j) \approx \exp\left\{-\int_{\epsilon t^*}^{\epsilon t} \nu(\epsilon t', v_1, v_2)\, d\epsilon t'\right\} \times \nabla_{v_i} e^{-H_2^0(t-\tau)}(e^{-H_2^0\tau} - 1) f_1^0(\epsilon t^*) f_1^0(\epsilon t^*).$$

Since

$$e^{-H_2^0(t-\tau)} = e^{-v_{ij}\cdot(\partial/\partial x_{ij})(t-\tau)},$$

a simple expansion and differentiation results in

$$\nabla_{v_i} e^{-H_2^0(t-\tau)} = (-)(t-\tau)e^{-H_2^0(t-\tau)}\nabla_i + e^{-H_2^0(t-\tau)}\nabla_{v_i}.$$

Since ∇_i is of order unity, this operator is of order $t - \tau \approx x_{12}/v_{12}$.

We note that for an operator A such that

$$A\mathfrak{L} \equiv A[g_4^0 + g_1^0(i)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0] = \text{order of } [g_4^0 + g_1^0(i)g_3^0 + \cdots + g_2^0(14)g_2^0] \quad (A1)$$

the size of

$$\int_{\Omega\sim 1} A\mathfrak{L}\, d\Omega_4 \quad (A2)$$

or

$$\int_{\Sigma\sim 1} A\mathfrak{L}\, d\sigma_4\, dv_4 \quad (A3)$$

(whichever the case may be) can be determined by phase space considerations. (Here $d\sigma_4$ is a surface element of Particle 4 coordinate space.) If x_{12} almost $\parallel v_{12}$ or x_{23} almost $\parallel v_{23}$, (A2) and (A3) are at most of order unity since A does not change the order. Otherwise (x_{12} almost $\parallel v_{12}$) it is required that a particle located in the volume around Particle 1 had an interaction in the past with a particle located in the volume around Particle 2 in order to yield a contribution from a region of phase space. By the standard geometric considerations the phase space for this is of order $|x_{12}|^{-2}$. Therefore, in this case (A2) or (A3) is at most of order $|x_{12}|^{-2}$.

We show that I is composed of terms which are either directly of the form of Eqs. (A2) and (A3) or are of the form of terms which on a fast-time, fast-space scale are total derivatives of terms of the form of Eqs. (A2) and (A3). In either case the contribution to

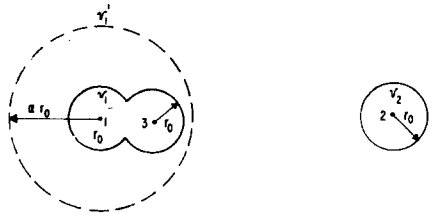

FIG. 1. Volumes of integration for (A5) and (A6).

$(g_3^1)_\alpha$ in (2.15) is of order $|x_{12}|^{-2}$ for x_{12} not almost $\| v_{12}$.

From (2.21) for $x_{13} < r_0$ in particular:

$$\sum_{i=1}^{3} \theta_{i4}[g_4^0 + \cdots + g_3^0(4, \cdots)g_1^0(i)]$$
$$= + \frac{\partial g_4^0}{\partial t} + \sum_{i=1}^{4} v_i \cdot \frac{\partial}{\partial x_i} g_4^0$$
$$- \theta_{13}[g_4^0 + g_1^0(1)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0]. \tag{A4}$$

Therefore

$$I = \int_{\mathfrak{V}_1+\mathfrak{V}_2} \Big[\frac{\partial g_4^0}{\partial t} + H_3^0 g_4^0 + v_4 \cdot \frac{\partial}{\partial x_4} g_4^0 + \Big(H_3^0 - \sum_{i=1}^{3} v_i \cdot \frac{\partial}{\partial x_i} \Big)(g_1^0(1)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0) \Big] d\Omega_4. \tag{A5}$$

The integration volumes $\mathfrak{V}_1$ and $\mathfrak{V}_2$ in x_4 space are such that: for $\mathfrak{V}_1$, we have $|x_{14}|, |x_{34}| < r_0$; for $\mathfrak{V}_2$, we have $|x_{24}| < r_0$. $\mathfrak{V}_1'$ is such that $|x_{14}| < \alpha r_0$, $\alpha = O(1)$. Moreover, $\mathfrak{V}_1'$ is chosen to include $\mathfrak{V}_1$ uniformly over the entire duration of a (1, 3) interaction (see Fig. 1).

We note

$$I = \int_{\mathfrak{V}_1+\mathfrak{V}_2} = \int_{\mathfrak{V}_1'} + \int_{\mathfrak{V}_2}. \tag{A6}$$

Moreover, since

$$H_3^0 \Big(\int_{\mathfrak{V}_1'} dx_4\, dv_4 \Big) = \int_{\mathfrak{V}_1'} v_1 \cdot d\sigma_4\, dv_4 = \int_{\mathfrak{V}_1'} v_1 \cdot \frac{\partial}{\partial x_4} d\Omega_4$$

we have

$$\Big(H_3^0 \int_{\mathfrak{V}_1'} \Big) - \int_{\mathfrak{V}_1'} v_1 \cdot \frac{\partial}{\partial x_4} = 0, \tag{A7}$$

$$\Big(H_3^0 \int_{\mathfrak{V}_2} \Big) - \int_{\mathfrak{V}_2} v_2 \cdot \frac{\partial}{\partial x_4} = 0. \tag{A8}$$

[Here

$$\Big(H_3^0 \int_{\mathfrak{V}_1'} \Big)$$

denotes that H_3^0 just acts on the limits of integration.]

Therefore we obtain

$$I = \Big(\frac{\partial}{\partial t} + H_3^0 \Big) \int_{\mathfrak{V}_1'} g_4^0 + \int_{\mathfrak{V}_1'} v_{41} \cdot \frac{\partial}{\partial x_4} g_4^0$$
$$+ \Big(\frac{\partial}{\partial t} + H_3^0 \Big) \int_{\mathfrak{V}_2'} g_4^0 + \int_{\mathfrak{V}_2'} v_{42} \cdot \frac{\partial}{\partial x_4} g_4^0 + H_3^0$$
$$\times \int_{\mathfrak{V}_1'} [g_1^0(1)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0]\, d\Omega_4$$
$$- \int_{\mathfrak{V}_1'} v_1 \cdot \frac{\partial}{\partial x_4} [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]\, d\Omega_4$$
$$- \int_{\mathfrak{V}_1'} \Big(v_1 \cdot \frac{\partial}{\partial x_1} + v_2 \cdot \frac{\partial}{\partial x_2} + v_3 \cdot \frac{\partial}{\partial x_3} \Big)$$
$$\times [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]\, d\Omega_4$$
$$+ H_3^0 \int_{\mathfrak{V}_2'} [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]\, d\Omega_4$$
$$- \int_{\mathfrak{V}_2'} v_2 \cdot \frac{\partial}{\partial x_4} [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]\, d\Omega_4$$
$$- \int \Big(v_1 \cdot \frac{\partial}{\partial x_1} + v_2 \cdot \frac{\partial}{\partial x_2} + v_3 \cdot \frac{\partial}{\partial x_3} \Big)$$
$$\times [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]\, d\Omega_4. \tag{A9}$$

Since $\partial/\partial t$ does not change the order of

$$[g_1^0(1)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0],$$

terms of the form

$$\frac{\partial}{\partial t} [g_1^0(1)g_3^0 + \cdots + g_2^0(14)g_2^0]$$

may be added to (A9) without affecting the order of the contribution from (A9). We thus see that the only possibly troublesome terms in (A9) are

$$\int_{\mathfrak{V}_1'} + \int_{\mathfrak{V}_2} \Big(v_1 \cdot \frac{\partial}{\partial x_1} + v_2 \cdot \frac{\partial}{\partial x_2} + v_3 \cdot \frac{\partial}{\partial x_3} \Big)$$
$$\times [g_1^0(1)g_3^0 + g_1^0(3)g_3^0 + g_2^0(12)g_2^0 + g_2^0(14)g_2^0]\, d\Omega_4$$
$$(\equiv I_{\mathfrak{V}_1'} + I_{\mathfrak{V}_2}), \tag{A10}$$

since all other terms are of the form of Eqs. (A2) and (A3) or are total derivatives of the form of Eqs. (A2) and (A3).

In the following discussion we neglect contributions involving $\partial/\partial t$ since this operator does not affect the order of the terms following it. Moreover, we observe:

(1) In $\mathfrak{V}_1'$, $\theta_{24} = 0, \theta_{14}, \theta_{34} \neq 0$.

(2) In $\mathfrak{V}_2$, $\theta_{14} = \theta_{34} = 0, \theta_{24} \neq 0$.

Also $|x_{12}|$ is such that $\theta_{12} = 0, \theta_{23} = 0$.

We consider

$$I_{\mathfrak{V}_1'} = \int_{\mathfrak{V}_1'}\Big[g_1^0(1)\Big(v_2\cdot\frac{\partial}{\partial x_2} + v_3\cdot\frac{\partial}{\partial x_3}\Big) g_3^0(2,3,4) + g_1^0(3)\Big(v_1\cdot\frac{\partial}{\partial x_1} + v_2\cdot\frac{\partial}{\partial x_2}\Big) g_3^0(1,2,4) + g_2^0(1,2)v_3\cdot\frac{\partial}{\partial x_3} g_2^0(3,4) + g_2^0(2,3)v_1\cdot\frac{\partial}{\partial x_1} g_2^0(1,4)\Big] d\Omega_4 \tag{A11}$$

and

$$I_{\mathfrak{V}_2} = \int_{\mathfrak{V}_2}\Big[g_1^0(1)\Big(v_2\cdot\frac{\partial}{\partial x_2} + v_3\cdot\frac{\partial}{\partial x_3}\Big) g_3^0(2,3,4) + g_1^0(3)\Big(v_1\cdot\frac{\partial}{\partial x_1} + v_2\cdot\frac{\partial}{\partial x_2}\Big) g_3^0(1,2,4) + g_2^0(1,2)v_3\cdot\frac{\partial}{\partial x_3} g_2^0(3,4) + g_2^0(2,3)v_1\cdot\frac{\partial}{\partial x_1} g_2^0(1,4)\Big] d\Omega_4 . \tag{A12}$$

On adding and subtracting $v_4\cdot\partial/\partial x_4$ in all terms in (A11) and (A12) we see that only terms in g_3^0 are possibly not of the form of Eqs. (A2) and (A3). A sample one of the g_3^0 terms is

$$I_1 = \Big(v_2\cdot\frac{\partial}{\partial x_2} + v_3\cdot\frac{\partial}{\partial x_3} + v_4\cdot\frac{\partial}{\partial x_4}\Big) g_3^0(2,3,4) \tag{A13}$$

defined for Particle 4 in the region $\mathfrak{V}_1'$. On using (2.19), (A13) becomes

$$\Big(v_2\cdot\frac{\partial}{\partial x_2} + v_3\cdot\frac{\partial}{\partial x_3} + v_4\cdot\frac{\partial}{\partial x_4}\Big) \times \{(e^{-H_3^0 r})[g_3^0 + g_1^0 g_2^0(2,4) + g_1^0 g_2^0(2,3)] - g_1^0 g_2^0(2,4) - g_1^0 g_2^0(2,3)\}. \tag{A14}$$

Since only $\theta_{34} \neq 0$,

$$I_1 = \Big(v_2\cdot\frac{\partial}{\partial x_2} + v_3\cdot\frac{\partial}{\partial x_3} + v_4\cdot\frac{\partial}{\partial x_4}\Big) \times (e^{-H_3^0 r})[g_3^0 + g_1^0 g_2^0(2,4) + g_1^0 g_2^0(2,3] = \Big(v_3\cdot\frac{\partial}{\partial x_3'} + v_{23}\cdot\frac{\partial}{\partial x_{23}} + v_{43}\cdot\frac{\partial}{\partial x_{43}}\Big) \times (e^{-H_3^0 r})[g_3^0 + g_1^0 g_2^0(2,4) + g_1^0 g_2^0(2,3)].$$

There is no contribution from $v_3\cdot\partial/\partial x_3'$. The contribution from $v_{43}\cdot\partial/\partial x_{43}$ can be evaluated as a surface integral and is therefore either the order of unity or $1/|x_{12}|^2$. If there is only one interaction in (2, 3, 4) space prior to the (3, 4) interaction, $v_{23}\cdot\partial/\partial x_{23}$ does not change the order of the function to the right of it. If there is more than one interaction prior to the (2, 4) interaction then the term

$$v_{23}\cdot(\partial/\partial x_{23})e^{-H_3^0 r} g_3^0$$

may be of the order $|x_{12}|$. Since the corresponding phase space volume is of order $1/|x_{12}|^2$ compared to the volume with only one interaction prior to the (3, 4) interaction, the contribution from multiple interactions in the past may be neglected. The phase space from single interactions in the past is of order $1/|x_{12}|^2$. Since

$$\int d\Omega_4 v_{23}\cdot\frac{\partial}{\partial x_{23}} e^{-H_3^0 r}[g_3^0 + \cdots + g_1^0 g_2^0(2,3)] = 0\int\{e^{-H_3^0 r}[g_3^0 + \cdots + g_1^0 g_2^0(2,3)]\, d\Omega_4\}$$

we conclude the contribution from $v_{23}\cdot\partial/\partial x_{23}$ to $I_{\mathfrak{V}_1'}$ is of order $1/|x_{12}|^2$. The remaining contributions in g_3^0 within $I_{\mathfrak{V}_1'}$ and $I_{\mathfrak{V}_2}$ can be treated in the same manner with similar conclusions. The treatment of (A4) for $x_{23} < r_0$ is the same.

2. Proof That the Contribution from $e^{-H_3^0 r}(g_3^1)_\alpha(t-\tau, \epsilon t)$ in (3.13) to (2.18) Is Nonsecular

By previous discussion within this section and in Ref. 1 the contribution of the term linear in 0 to Eq. (2.18) is of order $1/|x_{12}|^2$ for x_{12} almost $\| -v_{12}$. We now seek to show that the contribution from

$$e^{-H_3^0 r}(g_3^1)_\alpha(t-\tau, \epsilon t)$$

to Eq. (2.18) is also of order $1/|x_{12}|^2$ for x_{12} almost $\| -v_{12}$. Our procedure is to evaluate $\{g_3^1[t-\tau, \epsilon(t-\tau)]\}_\alpha$ subject to the initial condition:

$$[g_3^1(t=0, \epsilon t=0)]_\alpha = 0.$$

The contribution from $(g_3^1)_\alpha(t-\tau, \epsilon t) - (g_3^1)_\alpha[t-\tau, \epsilon(t-\tau)]$ is of higher order.

For regions of three-particle phase space with streaming motion such that there are interactions for $0 < t' < t-\tau$ one has, since there are no secularities in f_3^1 and hence in $(g_3^1)_\alpha$, that $(g_3^1)_\alpha$ is at most of order unity.

For x_{12} almost $\| -v_{12}$ the corresponding contribution to (2.18) is of order $1/|x_{12}|^2$. For a greater number of preceding interactions the contribution decreases at least as rapidly with increasing $|x_{12}|$.

Similarly the contribution to (2.18) for x_{12} almost $\| -v_{12}$ from regions of phase space with $|x_{i4}| < r_0$, $|x_{i'4}| < r_0$, $|x_{ii'}| > r_0$ is of order $|x_{12}|^{-2}$.

For the remaining trajectories one has for $|x_{i4}| < r_0$

$$g_4^0(t) = e^{-H_4^0 r}[g_4^0(t-\tau) + g_3^0(i)g_1^0(4) + g_3^0(4)g_1^0(i) + g_2^0(i,j)g_2^0 + g_2^0(i,k)g_2^0] - [g_3^0(i)g_1^0(4) + g_3^0(4)g_1^0(i) + g_2^0(i,j)g_2^0 + g_2^0(i,k)g_2^0] \tag{A15}$$

and

$$\theta_{i4} = -H_4^0 + H_3^0 + v_4 \cdot \frac{\partial}{\partial x_4}. \tag{A16}$$

Then (2.20) may be written

$$\left(\frac{\partial}{\partial t} + H_3^0 + \epsilon\frac{\partial}{\partial \epsilon t} + \epsilon H_3^1\right)(g_3^1)_\alpha$$
$$= \left\{\left[\left(\frac{\partial}{\partial t} + H_3^0 + \epsilon\frac{\partial}{\partial \epsilon t} + \epsilon H_3^1\right) - \left(\epsilon H_3^1 + \epsilon\frac{\partial}{\partial \epsilon t}\right)\right]\sum_{i=1}^{3}\int_{|x_{i4}|<r_0} + \sum_{i=1}^{3}\int_{|x_{i4}|<r_0} v_{4i}\cdot\frac{\partial}{\partial x_4}\right\}$$
$$\times e^{-H_4^0\tau}[g_4^0(t-\tau) + \cdots + g_2^0(i,k)g_2^0]\, d\Omega_4. \tag{A17}$$

On using the initial conditions on $(g_3^1)_\alpha$ and $g_s^0 (s > 1)$ we obtain to order ϵ:

$$(g_3^1)_\alpha[t-\tau, \epsilon(t-\tau)]$$
$$= \sum_{i=1}^{3}\int_{|x_{i4}|=r_0} e^{-H_4^0\tau}\{g_4^0[t-2\tau, \epsilon(t-\tau)]$$
$$+ g_1^0(i)g_3^0(4) + \cdots\}\, d\Omega_4$$
$$+ \int_0^{t-\tau} e^{-(H_3^0+\epsilon H_3^1+\epsilon[\partial/\partial(\epsilon t)])(t-\tau-t')}$$
$$\times \sum_{i=1}^{3}\int_{|x_{i4}|<r_0} v_{4i}\cdot\frac{\partial}{\partial x_4}\{e^{-H_4^0\tau}[g_4^0(t'-\tau) + \cdots]\}\, d\Omega_4\, dt'$$
$$- \int_0^t e^{-(H_3^0+\epsilon H_3^1+\epsilon[\partial/\partial(\epsilon t)])(t-\tau-t')}\epsilon\left(\frac{\partial}{\partial(\epsilon t)} + H_3^1\right)$$
$$\times \sum_{i=1}^{3}\int_{|x_{i4}|<r_0} e^{-H_4^0\tau}[g_4^0(t'-\tau) + \cdots]\, d\Omega_4\, dt'. \tag{A18}$$

We first consider $(g_3^1)_\alpha$ for $e^{-H_3^0(t-\tau)}|x_{13}|$ of order unity such that for some t' with $t - \tau \geq t' \geq 0$,

$$\alpha r_0 \geq e^{-H_3^0(t-\tau-t')}|x_{12}| \geq r_0 \tag{A19}$$

with α of order unity. The considerations for $e^{-H_3^0(t-\tau)}|x_{13}|$ of order unity are the same if one replaces $|x_{12}|$ by $|x_{23}|$ in (A19). Also, the considerations are unchanged if $e^{-H_3^0(t-\tau)}|x_{23}|$ (in place of $e^{-H_3^0(t-\tau)}|x_{13}|$) is of order unity.

For the term in (A18) of the form

$$\int_{|x_{i4}|<r_0} e^{-H_4^0\tau} \tag{A20}$$

we restrict our considerations to four-body trajectories with two interactions in the past. This implies g_4^0 can be ignored. The correlations (with the order of their contributions) which are "possibly favored" since they involve a (1, 2) interaction in the past are

$i = 1$: $g_1^0(4)g_3^0(1,2,3)$ $\dfrac{1}{|x_{13}|^2|x_{12}|_-^2} + \dfrac{1}{\theta|x_{12}|^2|x_{13}|_-^2}$

$g_2^0(1,2)g_2^0(3,4)$ $\dfrac{1}{\theta|x_{12}|^2|x_{13}|^2}$;

$i = 2$: $g_1^0(4)g_3^0(1,2,3)$ $\dfrac{1}{\theta|x_{12}|^2|x_{13}|_-^2}$

$g_2^0(1,2)g_2^0(3,4)$ $\dfrac{1}{\theta|x_{12}|^2|\bar{x}_{12}|^2}$;

$i = 3$: $g_1^0(4)g_3^0(1,2,3)$ $\dfrac{1}{|x_{13}|^2|x_{12}|_-^2} + \dfrac{1}{|x_{23}|^2|x_{12}|_-^2}$.

Here and below $\bar{x}_{12} = e^{-H_3^0(t-\tau)}|x_{12}|$. The $-$ subscript denotes evaluation at $t_- < t - \tau$. θ is the angle between x_{12} and v_{12}.

The correlations which are not favored are

$i = 1$: $g_1^0(1)g_3^0(2,3,4)$ $\dfrac{1}{|x_{13}|^2|x_{12}|_-^2} + \dfrac{1}{|x_{12}|^2|x_{13}|_-^2}$

$g_2^0(1,3)g_2^0(2,4)$ $\dfrac{1}{|x_{13}|^2|x_{12}|^2}$;

$i = 2$: $g_1^0(2)g_3^0(1,3,4)$ $\dfrac{1}{|x_{12}|^2|x_{13}|_-^2} + \dfrac{1}{|x_{23}|^2|x_{13}|_-^2}$

$g_2^0(2,3)g_2^0(1,4)$ $\dfrac{1}{|x_{12}|^2|x_{23}|^2}$;

$i = 3$: $g_1^0(3)g_3^0(1,2,4)$ $\dfrac{1}{|x_{13}|^2|x_{12}|_-^2} + \dfrac{1}{|x_{23}|^2|x_{12}|_-^2}$

$g_2^0(1,3)g_2^0(2,4)$ $\dfrac{1}{|x_{13}|^2|x_{12}|^2}$

$g_2^0(2,3)g_2^0(1,4)$ $\dfrac{1}{|x_{12}|^2|x_{13}|^2}$.

The dominant contribution from (A20) is of order $|x_{12}|^{-2}|x_{13}|^{-2}\theta^{-1}$, but on integrating over θ for the contribution to (2.18) there is a $\sin\theta$ weighting factor which makes the contribution of order $|x_{12}|^{-2}|x_{13}|^{-2}$. Integrated contributions of this order also occur from other terms above.

The estimate of the dominant term in the above comes from considering that the change in v_{12} perpendicular to x_{12} for $e^{-H_4^0\tau}g_2^0(1,2)$ to be nonzero is of order $|x_{12}|^{-1}$ for 1 and 2 almost intersecting in the past, and that for $\partial\phi/\partial x$ of order unity the corresponding volume in real space is of order $|x_{12}|^{-2}\theta^{-1}$. The other possibly favored terms are estimated in a similar manner.

Next, within (A18) we consider the terms in

$$\int_{|x|_{i4}<r_0} v_{4i}\cdot\frac{\partial}{\partial x_4}. \tag{A21}$$

As before, we neglect contributions from $e^{-H_4^0\tau}g_4^0$.

The orders of the correlation contributions as functions of t' (with variables evaluated at t') are

$$i = 1: \quad g_1^0(1)g_3^0(3,4,2)\ \frac{1}{|x_{13}|^2\,|x_{23}|^2_{--}} + \frac{1}{|x_{12}|^2\,|x_{23}|^2_{--}}$$

$$g_1^0(4)g_3^0(1,2,3)\ \frac{1}{|x_{13}|^2\,|x_{23}|^2_{--}} + \frac{1}{|x_{12}|^2\,|x_{23}|^2_{--}}$$

$$g_2^0(1,2)g_2^0(3,4)\ \frac{1}{|x_{12}|^2\,|x_{13}|^2}$$

$$g_2^0(1,3)g_2^0(2,4)\ \frac{1}{|x_{12}|^2\,|x_{13}|^2}.$$

For $i = 2$, the contributions are the same in form on interchange of 1 and 2 and similarly for $i = 3$. Here the $--$ subscript denotes evaluation at $t_{--} < t'$.

The contribution from the terms immediately above to $[g_3^1(x_{12}, \cdots)]_x$ is seen to be of order $|x_{12}|^{-2}$. Thus from the evaluations of (A20) and (A21) we find that the contribution of $e^{-H_3{}^0\tau}(g_3^1)_\alpha$ to (2.18) is of order $|x_{12}|^{-2}$

Further, we note that on combining features of the two preceding estimates, one obtains that the contribution to (2.18) from the term in $(\epsilon H_3^1 + \epsilon\partial/\partial\epsilon t)$ within (A18) is of order $\epsilon\,|x_{12}|^{-2}$.

3. Consideration of Remaining Terms in (3.13)

The contribution from the terms in (3.13) linear in g_2^0 is of order $|x_{12}|^{-2}$.

For the terms linear in $(g_2^1)_{\alpha ns}$ [as given by (3.10)] we note that the first term on the right-hand side of (3.10) can be written as

$$[1 - e^{-[H_2{}^0 + \epsilon H_2{}^1 + \epsilon(\partial/\partial\epsilon t)](t-\tau)}] \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} g_3^0\, d\Omega_3. \quad \text{(A22)}$$

On noting that

$$\sum_{i=1}^{2} \int_{|x_{i3}|<r_0} g_3^0\, d\Omega_3$$

decreases with increasing $|x_{12}|$ as $|x_{12}|^{-2}$ due to phase space considerations since

$$e^{-[H_2{}^0 + \epsilon H_2{}^1 + \epsilon(\partial/\partial\epsilon t)](t-\tau)} \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} g_3^0\, d\Omega_3$$

vanishes if there are no correlations at $t = 0$, $\epsilon t = 0$, we estimate that the contribution of (A22) to (2.18) through (3.13) is of order $|x_{12}|^{-2}$.

The second group of terms on the right-hand side of (3.10) is linear in g_3^0 with arguments corresponding to particle locations prior to the $(i, 3')$ interaction. From phase space consideration this contribution, which involves two interactions prior to the $(i, 3')$ interaction, is of order $|\mathbf{x}_{12} - \mathbf{v}_{12}(t - t')|^{-4}$. Therefore for these terms we have an estimate:

$$\int_{\theta=1/|x_{12}|}^{\pi} \frac{\sin\theta\, d\theta}{|v_{12}|} \times \int_0^{|v_{12}|t} \frac{ds}{[(s - |x_{12}|\cos\theta)^2 + |x_{12}|^2 \sin^2\theta]^2}. \quad \text{(A23)}$$

This expression is

$$O\int_{\theta=1/|x_{12}|}^{\pi} \frac{d\theta}{|x_{12}|^3 \sin^2\theta\,|v_{12}|} = O\,\frac{1}{|x_{12}|^2\,|v_{12}|}.$$

Since the operators H_2^1 and $\partial/\partial\epsilon t$ acting on g_3^0 are nonsingular, one may verify that the contribution from the third group of terms in (3.10) is at most of order ϵ.

For the terms linear in $(g_2^1)_{\alpha s}$ we assume for convenience that the velocity of particle i is isotropically distributed with respect to the velocity of particle j as a result of the i, 3 interaction in (2.18). Then, on performing first the integration in (3.9) over t' and next an integration over velocity directions, on letting $\tau = t - t'$ we obtain as an estimate of the contribution to the integral term of (2.18) from the terms comprising $(g_2^1)_{\alpha s}$:

$$\int_{\theta=1/|x_{12}|}^{\pi} \sin\theta\, d\theta \int_{\tau=0}^{t} |x_{12} - v_{12}\tau|^{-2}\, d\tau$$

$$\approx \int_{\theta=1/|x_{12}|}^{\theta=\pi} \sin\theta\, d\theta \int_{\tau=0}^{\infty} |x_{12} - v_{12}\tau|^{-2}\, d\tau$$

$$= \int_{\theta=1/|x_{12}|}^{\theta=\pi} \sin\frac{\theta\, d\theta}{|v_{12}|} \int_{s=1}^{\infty} \frac{ds}{(s - |x_{12}|\cos\theta)^2 + |x_{12}|^2 \sin^2\theta}. \quad \text{(A24)}$$

This expression is approximately $\pi^2(2\,|x_{12}|\,|v_{12}|)^{-1}$ and hence is $O(|x_{12}|^{-1})$ on taking v_{12}^{-1} to be of order unity. Hence the terms linear in $(g_2^1)_{\alpha s}$ lead to secular behavior in (2.18).

APPENDIX B. ON THE CONNECTION BETWEEN (3.20) AND (3.18)

One notes that (3.20) is obtained from (3.18) in the following manner:

To within order ϵ in place of (3.18) we have

$$\epsilon \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} \left(-H_3^0 + v_3 \cdot \frac{\partial}{\partial x_3} + H_2^0\right) \times e^{-H_3{}^0\tau}[g_1^0(i)(g_2^1)_{\alpha s}(t' - \tau) + \cdots]\, d\Omega_3, \quad \text{(B1)}$$

which is the same as

$$\epsilon H_2^0 \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3$$
$$+\epsilon^2\left(H_2^1+\frac{\partial}{\partial\epsilon t}\right)\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3$$
$$+\epsilon\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{3i}\frac{\partial}{\partial x_3}\{e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\}\,d\Omega_3$$
$$-\epsilon\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} e^{-H_3^0 r}H_3^0[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3$$
$$-\epsilon^2\left(H_2^1+\frac{\partial}{\partial\epsilon t}\right)\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3. \quad \text{(B2)}$$

The next to last line of (B2) to order $\epsilon/|x_{12}|^2$ can be written

$$\epsilon\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} e^{-H_3^0 r}\frac{\partial}{\partial t'}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3. \quad \text{(B3)}$$

The contribution to $(g_2^1)_\beta$ corresponding to (3.18) is

$$\int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\epsilon\left(\frac{\partial}{\partial t'}+H_2^0+\epsilon H_2^1+\epsilon\frac{\partial}{\partial\epsilon t}\right)\sum_{i=1}^{2}\int e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3\,dt'$$
$$+\int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}(-\epsilon^2)\left(H_2^1+\frac{\partial}{\partial\epsilon t}\right)\sum_{i=1}^{2}\int e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\,d\Omega_3\,dt'$$
$$+\epsilon\int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{3i}\cdot\frac{\partial}{\partial x_3}\{e^{-H_3^0 r}[g_1^0(i)(g_2^1)_{\alpha s}(t'-\tau)+\cdots]\}\,d\Omega_3\,dt'. \quad \text{(B4)}$$

The first time integral of (B4) is the integral of a total derivative and is therefore seen to be $O(\epsilon)$. The second time integral is of order $\epsilon^2 \ln \epsilon$. On neglecting terms of order ϵ only the third integral of (B4) remains.

APPENDIX C. ASYMPTOTIC FORM FOR $(g_2^1)_\alpha$: $|x_{12}| < r_0$

We have

$$(g_2^1)_\alpha=\int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}\Big\{\theta_{12}[g_1^0(g_1^1)_\alpha+(g_1^1)_\alpha g_1^0]$$
$$-\frac{\partial g_2^0}{\partial(\epsilon t)}+\sum_{i=1}^{2}\int\theta_{i3}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\Big\}\,dt'. \quad \text{(C1)}$$

We note

$$\int_0^t=\int_0^{\max(t-1/\epsilon,0)}+\int_{\max(t-1/\epsilon,0)}^{t-\tau}+\int_{t-\tau}^{t}. \quad \text{(C2)}$$

In $\int_{t-\tau}^{t}$ we can substitute $e^{-[H_2^0+\epsilon(H_2^1+\epsilon(\partial/\partial\epsilon t))](t-t')}$ for $e^{-H_2^0(t-t')}$ to order ϵ.

For

$$\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}$$
$$\times\sum_{i=1}^{2}\int\theta_{i3}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\,dt' \quad \text{(C3)}$$

we note

$$g_3^0+g_1^0g_2^0+g_2^0g_1^0=e^{-H_3^0 r}(g_3^0+g_1^0g_2^0+g_2^0g_1^0) \quad \text{(C4)}$$

and

$$\theta_{i3}=-H_3^0+\left(H_2^0+\epsilon H_2^1+\epsilon\frac{\partial}{\partial\epsilon t}\right)$$
$$+v_3\cdot\frac{\partial}{\partial x_3}-\left(\epsilon H_2^1+\epsilon\frac{\partial}{\partial\epsilon t}\right). \quad \text{(C5)}$$

Therefore (C3) may be written

$$\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)]t}\Big[\frac{\partial}{\partial t'}e^{[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)]t'}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} e^{-H_3^0 r}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3$$
$$+e^{[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)]t'}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{3i}\cdot\frac{\partial}{\partial x_3}e^{-H_3^0 r}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\Big]\,dt'+\epsilon h. \quad \text{(C6)}$$

Here h is of order unity as are h' and h'' in the equations which follows.

On expanding the operator $e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}$ for the term in v_{3i} in (C6) we have for (C6):

$$\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-H_2^0 t}\frac{\partial}{\partial t'}\left[e^{H_2^0 t'}\sum_{i=1}^{2}\int e^{-H_3^0\tau}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\right]dt'$$
$$+\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-H_2^0(t-t')}\left[\sum_{i=1}^{2}\int v_{3i}\cdot\frac{\partial}{\partial x_3}\,e^{-H_3^0\tau}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\right]dt'$$
$$+\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-H_2^0(t-t')}\sum_{n=1}^{\infty}\frac{(-)^n}{n!}\left(\epsilon H_2^1+\epsilon\frac{\partial}{\partial\epsilon t}\right)^n(t-t')^n$$
$$\times\left[\sum_{i=1}^{2}\int v_{3i}\cdot\frac{\partial}{\partial x_3}\,e^{-H_3^0\tau}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\right]dt'+\epsilon h'. \qquad \text{(C7)}$$

This may be rewritten as

$$\int_{\max(t-1/\epsilon,0)}^{t-\tau} e^{-H_2^0(t-t')}\sum_{i=1}^{2}\int\theta_{i3}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\,dt$$
$$+\int_{\max(t-1/\epsilon,0)}^{t} e^{-H_2^0(t-t')}\sum_{n=1}^{\infty}\frac{(-)^n}{n!}\left(\epsilon H_2^1+\epsilon\frac{\partial}{\partial\epsilon t}\right)^n(t-t')^n$$
$$\times\sum_{i=1}^{2}\int v_{3i}\cdot\frac{\partial}{\partial x_3}\,e^{-H_3^0\tau}(g_3^0+g_1^0g_2^0+g_2^0g_1^0)\,d\Omega_3\,dt'+\epsilon h''. \qquad \text{(C8)}$$

The terms in θ_{i3} combine with the contributions from $\int_{t-\tau}^{t}$ and $\int_0^{\max(t-1/\epsilon,0)}$ to give the term $I(t)$.

The contributions within (C8) from the summation $\sum_{n=1}^{\infty}$ which are linear in $e^{-H_3^0\tau}g_3^0$ are of order ϵ from phase space considerations.

For the contribution from the $n=1$ term from terms linear in $e^{-H_3^0\tau}g_3^0$ we replace $g_2^0(t'-\tau)$ and $g_2^0(t')$ by $g_2^0(t\to\infty)$. To find the corresponding error we note that independently of t' the phase space for interactions prior to $t=0$ is of order $(v_{12})^{-2}t^{-2}$. [Here and in succeeding appendixes we indicate the v_{12} dependence of the contributions for $v_{12}<v_{av}$. Since this dependence is always of the form $(v_{12})^{\beta}$, $\beta\geq -2$, there are no resulting singularities in the single-particle distribution function.] The corresponding contribution to $(g_2^1)_\alpha$ is

$$O(v_{12})^{-2}\int_{\max(t-1/\epsilon,0)}^{t-\tau}\epsilon(t-t')t^{-2}\,dt'$$
$$=\begin{cases}O[\epsilon(v_{12})^{-2}], & t<\epsilon^{-1}\\ O\{\epsilon[\epsilon(v_{12})t]^{-2}\}, & t\gg\epsilon^{-1}.\end{cases}$$

The remaining part of the $n=1$ contribution to $(g_2^1)_\alpha$ is

$$-\int_{\max(t-1/\epsilon,0)}^{t-\tau}\epsilon(t-t')e^{-H_2^0(t-t')}\left(H_2^1+\frac{\partial}{\partial\epsilon t}\right)$$
$$\times\sum_{\substack{i=1\\ j=3-i}}^{2}\int_{|x_{i3'}|=r_0}v_{3'i}\{e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]\tau}\cdot$$
$$\times[g_1^0(i)g_2^0(t\to\infty)+g_1^0(3')g_2^0(t\to\infty)]$$
$$-g_1^0(i)g_2^0(t\to\infty)(x_{i3'}\parallel v_{i3'})\}\,d\sigma_{3'}\,dv_{3'}\,dt'. \qquad \text{(C9)}$$

Since

$$\sum_{\substack{i=1\\ (j=3-i)}}^{2}\int_{|x_{i3'}|=r_0}v_{3'i}\{e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]\tau}$$
$$\times[g_1^0(i)g_2^0(t\to\infty)+g_1^0(3')g_2^0(t\to\infty)]$$
$$-g_1^0(i)g_2^0(t\to\infty)(x_{i3'}\parallel v_{i3'})\}\,d\sigma_{3'}\,dv_{3'}$$
$$=\frac{C(\epsilon x_{12},\epsilon t)}{|x_{12}|^2}+O\left(\frac{1}{|x_{12}|^3}\right) \qquad \text{(C10)}$$

to within order ϵ, (C9) becomes

$$\int_{\max(t-1/\epsilon,0)}^{t}\epsilon e^{-H_2^0(t-t')}\left(H_2^1+\frac{\partial}{\partial\epsilon t}\right)(\tilde{g}_2^1)_{\alpha s}\,dt'. \qquad \text{(C11)}$$

The contribution from each term linear in $e^{-H_3^0\tau}g_2^0$ in $\sum_{n=2}^{\infty}$ of (C8) may be verified to be of order $\epsilon(v_{12})^{-2}$ for $t<\epsilon^{-1}$ and of order $\epsilon(\epsilon v_{12}t)^{-2}$ for $t\gg\epsilon^{-1}$. Since $(\epsilon H_2^1+\epsilon\partial/\partial\epsilon t)$ is of order unity the sum converges in either case and its order is unchanged.

APPENDIX D. ASYMPTOTIC FORM FOR $\epsilon(g_2^1)_\beta$

From (3.20) and (3.9) we obtain

$$(\epsilon g_2^1)_\beta=\int_0^t e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')}$$
$$\times\left\{\epsilon\theta_{12}[g_1^0(g_1^1)_\beta+(g_1^1)_\beta g_1^0]+\epsilon\sum_{i=1}^{2}\int_{|x_{i3}|<r_0}v_{3i}\cdot\frac{\partial}{\partial x_3}\right.$$
$$\times e^{-H_3^0\tau}\left[\left(g_1^0(3)\int_0^{t'-\tau}e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t'-\tau-t'')}\right.\right.$$
$$\times\sum_{\substack{i=1\\ (j=3-i)}}^{2}\int_{|x_{i3'}|=r_0}v_{3'i}[e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]\tau}$$
$$\times[g_1^0(i)g_2^0(j,3',t''-\tau)+g_1^0(3')g_2^0(t''-\tau)]$$
$$\left.\left.-g_1^0(i)g_2^0(t'')]\,d\sigma_{3'}\,dv_{3'}\,dt''\right)+[3\to i,\,i\to 3]\right]\Bigg\}\,dt'. \qquad \text{(D1)}$$

We first note that within (D1)

$$\int_0^t=\int_{t-1/\epsilon}^{t}+\int_0^{t-1/\epsilon}. \qquad \text{(D2)}$$

Due to the exponential damping of the g_2^0 terms the

contribution from $\int_0^{t-1/\epsilon}$ to $(\epsilon g_2^1)_\beta$ is of order

$$\epsilon \int_{1/\epsilon}^{\infty} dt \int_{\theta=0}^{\pi/2} \frac{e^{-\epsilon t\,|v_{12}|\,\sin\theta}}{t\,|v_{12}|\,\sin\theta} \sin\theta\, d\theta.$$

On using the form for $\epsilon t \gg 1$, this is of order

$$\int_{1/\epsilon}^{\infty} \frac{1}{|v_{12}|^2 t^2}\, dt$$

which is of order $\epsilon/|v_{12}|^2$. Since the velocity is three dimensional, this term only contributes to g_1 in order ϵ^2.

Also within (D1) we have

$$\int_0^{t'-\tau} dt'' = \int_0^{t-1/\epsilon} dt'' + \int_{t-1/\epsilon}^{t'-\tau} dt''. \tag{D3}$$

The contribution involving the combination

$$\int_{t-1/\epsilon}^{t} dt' \int_0^{t-1/\epsilon} dt''$$

within (D1) is of order

$$\epsilon \int_{t-1/\epsilon}^{t} dt' \int_0^{t-1/\epsilon} \frac{dt''}{d^2(t'')}. \tag{D4}$$

Here $d(t'')$ denotes the separation between the two particles in g_2^0 at time t''; therefore, by phase space considerations, $d^{-2}(t'')$ orders the size of the integrand as a function of t''. Since $d^{-2}(t'')$ is nonsingular in three-dimensional space, and since Particles 1 and 2 are together at time t, $d^{-2}(t'')$ is of order

$$\{[v_{12}(t-t')]^2 + v_{av}^2(t'-t'')^2\}^{-1}.$$

Hence (D4) is of order $\epsilon/(v_{12})$.

For $|x_{12}| < r_0$ we have

$$e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')} = e^{-H_2^0(t-t')} e^{-[\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t-t')} \tag{D5}$$

and

$$e^{-[H_2^0+\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t'-\tau-t'')} = e^{-H_2^0(t'-\tau-t'')} e^{-[\epsilon H_2^1+\epsilon(\partial/\partial\epsilon t)](t'-\tau-t'')} \tag{D6}$$

with an error of order ϵ. On inserting (D5) and (D6) in (D1) and expanding the exponential operators involving $(\epsilon H_2^1 + \epsilon\partial/\partial\epsilon t)$ we obtain, on keeping the leading correction terms,

$$\begin{aligned}(\epsilon g_2^1)_\beta = {} & \int_{t-1/\epsilon}^{t} e^{-H_2^0(t-t')} \Big\{ \epsilon\theta_{12}[g_1^0(g_1^1)_\beta + (g_1^1)_\beta g_1^0] \\ & + \epsilon \sum_{i=1}^{2} \int_{|x_{i3}|<r_0} v_{3i}\cdot\frac{\partial}{\partial x_3} e^{-H_3^0 \tau} \Big[\Big(g_1^0(3) \int_{t-1/\epsilon}^{t'-\tau} e^{-H_2^0(t'-\tau-t'')} \\ & \times \sum_{\substack{i=1 \\ (j=3-i)}}^{2} \int_{|x_{i3'}|=r} v_{3'i} \{ e^{-[H_2^0(i,3')+v_j\cdot(\partial/\partial x_j)]\tau} \\ & \times [g_1^0(i) g_2^0(t''-\tau) + g_1^0(3') g_2^0(t''-\tau)] - g_1^0(i) g_2^0(t'')\} \\ & \times dx_{3'i\perp}\, dv_{3'}\, dt'' \Big) + (3 \to i,\ i \to 3) \Big] \Big\} dt' \\ & + O \int_{t-1/\epsilon}^{t} \int_{t-1/\epsilon}^{t'} \frac{\epsilon^2 (t-t'')\, dt''\, dt'}{d^2(t'')}. \end{aligned} \tag{D7}$$

The error term of (D7) is $O\epsilon^2(\ln\epsilon) v_{12}^{-1}$.

By repeating the argument for (D4) to within $O(\epsilon)$ we can extend the integration range over t'' in (D7) from 0 to $t - 1/\epsilon$. Furthermore, since $g_2^0(t'')$ and $g_2^0(t''-\tau)$ vanish for $t'' \le 0$ we may write the lower limit of t' integration as the maximum of $t - 1/\epsilon$ and 0.

Therefore on neglecting the difference between $t''-\tau$ and t'' within (D7) we write for the contributions linear in g_2^0

$$\epsilon \int_{\max(t-1/\epsilon,0)}^{t} dt' \int_0^{t'-\tau} dt'' \mathfrak{L}[g_2^0(\infty) + g_2^0(t'') - g_2^0(\infty)] \tag{D8}$$

with the operator $\mathfrak{L}$ a linear operator of order unity. For a given t'' and t' the contribution in $g_2^0(t'') - g_2^0(\infty)$ is of the order ϵ multiplied by the phase space for interactions prior to time $t'' = 0$. The phase space is estimated by the expression $\epsilon(v_{12}t)^{-2}$. Hence we have

$$\epsilon \int_{\max(t-1/\epsilon,0)}^{t} dt' \int_0^{t'-\tau} dt'' \mathfrak{L}[g_2^0(t'') - g_2^0(\infty)] = O[\epsilon(v_{12})^{-2}]. \tag{D9}$$

The phase space for interactions earlier than $(t + t'')$ before t is similarly of order $[(v_{12})(t + t'')]^{-2}$. Hence we have

$$\epsilon \int_{\max(t-1/\epsilon,0)}^{t} dt' \int_{-\infty}^{0} dt'' \mathfrak{L} g_2^0(\infty) = \epsilon \int_{\max(t-1/\epsilon,0)}^{t} dt' \int_0^{\infty} \frac{dt''}{[v_{12}(t+t'')]^2}, \tag{D10}$$

which is also of order $\epsilon(v_{12})^{-2}$.

On combining (D8) to (D10) in (D7), (4.6) is obtained.

APPENDIX E. ON THE DERIVATION OF THE ASYMPTOTIC FORM OF $\lim_{t\to\infty}[J(t) + K(t)]$

First we note that $e^{-H_3^0 \tau}[(x_{i3})_\parallel = \infty]$ denotes that i and 3 are projected backwards in time through an interaction, and that $e^{-H_3^0 \tau}[(x_{i3})_\parallel = -\infty]$ denotes that i and 3 are projected backwards in time prior to an interaction. Within (4.6) we take $e^{-H_3^0 \tau}[(x_{i3})_\parallel = \infty] = e^{-H_2^0(i,3)\tau}[(x_{i3})_\parallel = \infty]$ and $e^{-H_3^0 \tau}[(x_{i3})_\parallel = -\infty] = 1$, and we assume

$$\{g_2^1(j,3)[(x_{i3})_\parallel = \infty]\}_\alpha = \{g_2^1(j,3)[(x_{i3})_\parallel = -\infty]\}_\alpha.$$

These assumptions introduce errors within the integrand of order $e^{-H_2^0(t-t')}|x_{12}|^{-2}$, which result in errors in

$$\lim_{t\to\infty}[J(t) + K(t)]$$

of order ϵ. Hence they are valid for obtaining the $\ln\epsilon$ behavior of

$$\lim_{t\to\infty}[J(t) + K(t)].$$

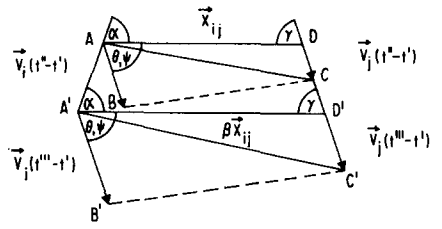

FIG. 2. Geometric picture for integrals within (E4).

We now seek to simplify,

$$\epsilon\int_{\max(t-1/\epsilon,0)}^{t} e^{-H_2^0(t-t')}\Big[\sum_{i=1}^{2}\int v_{3i}[e^{-H_2^0(i,3)\tau}-1]\times\{g_1^0(3)[\tilde{g}_2^1(i,j)]_{\alpha s}+g_1^0[\tilde{g}_2^1(3,j)]_{\alpha s}\}-\Big(\frac{\partial}{\partial\epsilon t}+H_2^1\Big)[\tilde{g}_2^1(i,j)]_{\alpha s}\Big]\,dt'\,d\sigma_3\,dv_3. \quad \text{(E1)}$$

We note

$$[\tilde{g}_2^1(x_{ij},v_i,v_j)]_{\alpha s}=\int_{-\infty}^{t'} e^{-H_2^0(t'-t'')}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{i3}\times\{[e^{-H_2^0(i,3)\tau}-1]g_1^0g_2^0(j,3)+e^{-H_2^0(i,3)\tau}g_1^0g_2^0(i,j)\}\,d\sigma_3\,dv_3\,dt'' \quad \text{(E2)}$$

and

$$[\tilde{g}_2^1(\beta x_{ij},v_i,v_j)]_{\alpha s}=\int_{-\infty}^{t'} e^{-H_2^0(t'-t''')}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{i3}\{\ \}\,d\sigma_3\,dv_3\,dt'''. \quad \text{(E3)}$$

For specificity we may let $|\beta x_{ij}|=1/\epsilon$. From (E2) and (E3):

$$[\tilde{g}_2^1(x_{ij},v_i,v_j)]_{\alpha s}=[\tilde{g}_2^1(\beta x_{ij},v_i,v_j)]_{\alpha s}\times\frac{\displaystyle\int_{-\infty}^{t'} e^{-H_2^0(t'-t'')}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{i3}\{\ \}\,d\sigma_3\,dv_3\,dt''}{\displaystyle\int_{-\infty}^{t'} e^{-H_2^0(t'-t''')}\sum_{i=1}^{2}\int_{|x_{i3}|<r_0} v_{i3}\{\ \}\,d\sigma_3\,dv_3\,dt'''}. \quad \text{(E4)}$$

If

$$(t'''-t')=\beta(t''-t'), \quad \text{(E5)}$$

then $ABCD$ and $A'B'C'D'$ in Fig. 2 are geometrically similar and similarly oriented. Moreover, for Fig. 3 at a *given impact parameter* with respect to C or C' the velocities of particles of the same speed traveling from i backwards to j differ in direction at most by an angle of order $r_0/|x_{ij}|$. Since this difference produces a variation in $[\tilde{g}_2^1(x_{ij})]_{\alpha s}$ of order $(1/|x_{ij}|)[\tilde{g}_2^1(x_{ij})]_{\alpha s}$ it provides a contribution of order ϵ to

$$\lim_{t\to\infty}[J(t)+K(t)]$$

which may be neglected.

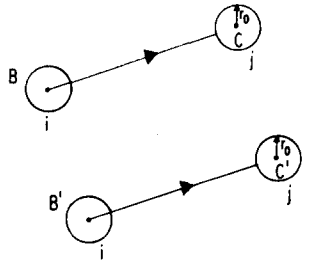

FIG. 3. Detail for the parallelness of velocities with the same impact parameter with respect to C or C' of Fig. 2.

Since $(B'C')=\beta(BC)$ (again with the neglect of corrections of the order of $1/|x_{ij}|$ relative to the dominant contribution):

$$\frac{[\text{phase space covered by } d\sigma_3\,dv_3 \text{ in (E2)}]}{[\text{phase space covered by } d\sigma_3\,dv_3 \text{ in (E3)}]}=\beta^2. \quad \text{(E6)}$$

Furthermore, from (E5) we have

$$dt'''=\beta\,dt''. \quad \text{(E7)}$$

On inserting (E6) and (E7) in (E4) we obtain

$$[\tilde{g}_2^1(x_{ij},v_i,v_j)]_{\alpha s}=\{[\tilde{g}_2^1(\beta x_{ij},v_i,v_j)]_{\alpha s}/|x_{ij}|\}\beta\,|x_{ij}|, \quad \text{(E8)}$$

which is the same as

$$\big(\{[\tilde{g}_2^1((x_{ij})',v_i,v_j)]_{\alpha s}\,|(x_{ij})'|\}/|x_{ij}|\big)\qquad(|(x_{ij})'|=1/\epsilon,\,(\mathbf{x}_{ij})'\parallel\mathbf{x}_{ij}). \quad \text{(E9)}$$

On using (4.9) and neglecting the difference in direction between $\mathbf{x}_{ij}$ and $-\mathbf{v}_{ij}$ which by reasoning analogous to that following Fig. 2 produces a variation of order $1/|x_{ij}|^2$ in $(g_2^1)_{\alpha s}$ and hence a variation of ϵ in

$$\lim_{t\to\infty}[J(t)+K(t)],$$

(E1) becomes to order ϵ [with $\tau=O(1)$]:

$$\epsilon\int_{t=t-1/\epsilon}^{t-\tau} e^{-H_2^0(t-t')}\frac{1}{|x_{ij}|}\Big[\sum_{\substack{i=1\\(j=3-i)}}^{2}\int v_{3i}(e^{-H_2^0(i,3)\tau}-1)\times g_1^0\{[\tilde{g}_2^1((x_{ij})',v_i,v_j)]_{\alpha s}\,|(x_{ij})'|\}(|(x_{ij})'|=1/\epsilon,\,(\mathbf{x}_{ij})'\parallel-(\bar{\mathbf{v}}_{ij}))+g_1^0\{[\tilde{g}_2^1((x_{3j})',v_3,v_j)]_{\alpha s}\,|(x_{3j})'|\}[|(x_{3j})'|=1/\epsilon,\,(\mathbf{x}_{3j})'\parallel(-\bar{\mathbf{v}}_{ij})]\Big]\,d\sigma_3\,dv_3-\Big(\frac{\partial}{\partial\epsilon t}+H_2^1\Big)\{[\tilde{g}_2^1((x_{ij})',v_i,v_j)]_{\alpha s}\,|(x_{ij})'|\}[|(x_{ij})'|=1/\epsilon,\,(\mathbf{x}_{ij})'\parallel(-\bar{\mathbf{v}}_{ij})]\,dt'. \quad \text{(E10)}$$

On neglecting terms of order $1/|x_{ij}|^{-2}$ in (E10) we have

$$e^{-H_2^0(t-t')}\frac{1}{|x_{ij}|}=\frac{1}{|v_{ij}|\,(t-t')}.$$

APPENDIX F. ON THE EVALUATION OF (5.15)

We now seek to evaluate for $|x_{12}| < r_0$:

$$A(t) = [\bar{g}_2^1(t, \epsilon t = 0, \epsilon x_{12} = 0)]_{\alpha s} - [\bar{g}_2^1(\epsilon t = 0, \epsilon x_{12} = 0)]_{\alpha s}. \quad \text{(F1)}$$

The remaining part of

$$\left(1 - \lim_{t\to\infty}\right) I(t)$$

depends on source terms which are either of order ϵ or are more sharply localized in space around $|x_{12}| < r_0$ than the source terms for $A(t)$, and hence should decrease more rapidly with increasing t. With $\tilde{O}$ defined in (4.16) we have

$$A(t) = -\int_{-\infty}^{0} e^{-H_2^0(t-t'')}\tilde{O}g_2^0(\infty)\, dt''\, d\sigma_{3'}\, dv_{3'} + \int_0^t e^{-H_2^0(t-t'')}\tilde{O}[g_2^0(t'') - g_2^0(\infty)]\, d\sigma_{3'}\, dv_{3'}\, dt'', \quad \text{(F2)}$$

$$A(t') = -\int_{-\infty}^{0} e^{-H_2^0(t'-t''')}\tilde{O}g_2^0(\infty)\, dt'''\, d\sigma_{3'}\, dv_{3'} + \int_0^{t'} e^{-H_2^0(t'-t''')}\tilde{O}[g_2^0(t''') - g_2^0(\infty)\, dt'''\, d\sigma_{3'}\, dv_{3'}. \quad \text{(F3)}$$

From Eqs. (F2) and (F3) we have

$$A(t) = A(t')\left[-\int_{-\infty}^{0} e^{-H_2^0(t-t'')}\tilde{O}g_2^0(\infty)\, d\sigma_{3'}\, dv_{3'}\, dt'' + \int_0^t e^{-H_2^0(t-t'')}\tilde{O}[g_2^0(t'') - g_2^0(\infty)]\, d\sigma_{3'}\, dv_{3'}\, dt''\right] \times \left[-\int_{-\infty}^{0} e^{-H_2^0(t'-t''')}\tilde{O}g_2^0(\infty)\, d\sigma_{3'}\, dv_{3'}\, dt''' + \int_0^{t'} e^{-H_2^0(t'-t''')}\tilde{O}[g_2^0(t''') - g_2^0(\infty)]\, d\sigma_{3'}\, dv_{3'}\, dt'''\right]^{-1}. \quad \text{(F4)}$$

On writing

$$t''' = t'\alpha, \quad \text{(F5)}$$

$$t'' = t\alpha, \quad \text{(F6)}$$

and following the arguments within Appendix E we obtain in analogy to (E6):

$$\frac{[\text{phase space covered by } d\sigma_3\, dv_3 \text{ in numerator of (F4) at } t\alpha]}{[\text{phase space covered by } d\sigma_3\, dv_3 \text{ in denominator of (F4) at } t'\alpha]} = \frac{t^{-2}}{(t')^{-2}}. \quad \text{(F7)}$$

Moreover [in analogy to (E7)] we have from (F5) and (F6):

$$dt''' = t'\, d\alpha, \quad \text{(F8)}$$

$$dt'' = t\, d\alpha. \quad \text{(F9)}$$

On combining (F7) to (F9) we have

$$\{[\bar{g}_2^1(t, \epsilon t = 0, \epsilon x_{12} = 0)]_{\alpha s} - [\bar{g}_2^1(t \to \infty, \epsilon t = 0, \epsilon x_{12} = 0)]_{\alpha s}\} = A(t, \epsilon t = 0, \epsilon x_{12} = 0) = \frac{1}{t}[t'A(t', \epsilon t = 0, \epsilon x_{12} = 0)]\left(t' = \frac{1}{\epsilon}\right). \quad \text{(F10)}$$

Since all events contributing to (F4) through the terms in g_2^0 occur prior to $t = 0$ or $t' = 0$ (as the case may be), the distance between the $(i, 3')$ interaction and the earlier interaction involving j is either of order $t\delta$ or $t'\delta$ for $|v_{12}|$ of order δ. Consequently in (F10) the errors due to the nonzero range of the binary potential are of order

$$t^{-1}\delta^{-1}[t^{-1} + (t')^{-1}]. \quad \text{(F11)}$$

The contribution of (F11) to g_1 relative to the contribution of (F10) to g_1 is of order one part in $\ln \epsilon$.

APPENDIX G. CONTRIBUTION OF $\left(1 - \lim_{t\to\infty}\right)[J(t) + K(t)]$ TO g_1

From Appendix E and Eqs. (5.7) we have for $t < \epsilon^{-1}$

$$\left(1 - \lim_{t\to\infty}\right)[J(t) + K(t)] = \epsilon\left(1 - \lim_{t\to\infty}\right)e^{-H_2^0\tau}[g_1^0(1)(g_1^1)_\beta + g_1^0(2)(g_1^1)_\beta] + \epsilon \ln \epsilon t B(x_{12}, v_1, v_2, \epsilon t) + \epsilon G'' \quad \text{(G1)}$$

with G'' of order unity. On neglecting the terms in $\epsilon G''$ which may be incorporated with the term $\epsilon G'$ of Eq. (5.8), Eq. (G1) is found to be of the form

$$\left(1 - \lim_{t\to\infty}\right)[J(t) + K(t)] = \epsilon \ln(\epsilon t) C(x_{12}, v_1, v_2, \epsilon t) \quad \text{(G2)}$$

with C of order $(v_{12})^{-1}$.

Thus on integrating (5.8) for a range in t specified by $0 < t < \epsilon^{-1}$, the contribution to g_1^2 is seen to be of order unity.

From (5.2) the contribution from

$$\left(1 - \lim_{t\to\infty}\right)\partial/\partial\epsilon t(g_1^1)_\alpha$$

is of order ϵ^2.

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New Approach to the Ising Model. II

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Onsager's results for the partition and correlation functions for the Ising model on a two-dimensional rectangular lattice are rederived using a Green's function technique. The definition of the Green's function is based on a recently published casting of the Ising model into a many-body fermion problem. The relation between this approach and other methods used for solving the Ising problem are indicated.

1. INTRODUCTION

RECENTLY the two-dimensional Ising model has been solved using descriptions which have been similar to the theory of many-fermion problems. Schultz, Mattis, and Lieb,[1] starting from the algebraic expression of Onsager,[2] have given a proof which is very similar to, and uses the techniques of, the theory of noninteracting fermions. In a previous paper[3] a proof was given in which the partition function was expressed as a vacuum-to-vacuum expectation value of an expression which is analogous to e^{-iHt} in many fermion theory. However, there the starting point was the combinatorial expression of Kac and Ward.[4] It is interesting that the algebraic and the combinatorial methods should both be able to be expressed as problems in many fermion-theory, or quantum statistical mechanics.

Both these reformulations of the Ising problem are important, because one would now hope to be able to use the techniques of the quantum theory of many particles to obtain approximations to the unsolved Ising problems. One of the most powerful techniques in this field is the method of Green's functions. Many people[5] have used Green's function techniques to obtain approximations to the Ising model but generally their methods have not yielded good results. This may be because their approaches do not even give Onsager's exact result when applied to the soluble Ising lattices. In this paper we show that, starting with the approach of I, we can define and evaluate Green's functions, which give the exact results for the partition and correlation functions for the soluble cases. It is hoped in later work to use this formalism to obtain perturbation expansions about the exact solutions obtained here for the unsolved problems. It is interesting to note that Kadanoff[6] has also developed a Green's function technique which gives exact results, and that his approach is based on the many fermion formalism of Schultz, Mattis, and Lieb.

In I it was shown how the partition functions of the soluble Ising lattices could be reduced to the vacuum expectation value of an operator $\exp(-H)$, where H is a quadratic expression of fermion creation and annihilation operators. Hence H resembles the Hamiltonian of a noninteracting fermion system and the "time" is the lattice coordinate. In Sec. 2 we generalize this method to express the correlation functions as the vacuum expectation value of $\exp(-H')$, where H' can be regarded as a perturbed Hamiltonian. This can be expanded as a series in analogy with Dyson's perturbation expansion in field theory. In Sec. 3 we define and evaluate the Green's function which is then used in Sec. 4 to calculate the terms of the perturbation series. The series can be summed to give the exact result because H' is quadratic. In Sec. 5 we use the Green's function to evaluate the partition function.

2. CORRELATION FUNCTION AS AN EXPECTATION VALUE

The correlation function $\langle s_1 s_{k+1}\rangle$ for a pair of spins located at the sites 1 and $k+1$ is defined as

$$\langle s_1 s_{k+1}\rangle = Z^{-1}(\cosh K_1 \cosh K_2)^N \sum_{s=\pm 1} s_1 s_{k+1} \times \prod_{j=1}^{N}(1 + x s_j s_{j+1})(1 + y s_j s_{j+m}), \quad (1)$$

where Z is the partition function, $s_j = \pm 1$ represents the state of the spins at the lattice site j, $\pm K_1 kT$ and $\pm K_2 kT$ are the interaction energies between horizontal and vertical pairs of spins, respectively, and

$$x = \tanh K_1, \quad y = \tanh K_2.$$

We only consider correlations where the $(k+1)$th

[1] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).
[2] L. Onsager, Phys. Rev. **65**, 117 (1944).
[3] C. A. Hurst, J. Math. Phys. **7**, 305 (1966), hereafter referred to as I.
[4] M. Kac and J. C. Ward, Phys. Rev. **88**, 1332 (1952).
[5] See, for example, R. L. Bell, Phys. Rev. **143**, 215 (1966).
[6] L. P. Kadanoff, Nuovo Cimento **44**, 276 (1966).

spin is on the same horizontal row as the first spin. The generalization to other cases is straightforward. Using the identity

$$s_1 s_{k+1} = (s_1 s_2)(s_2 s_3) \cdots (s_k s_{k+1}),$$

Eq. (1) can be written as

$$\langle s_1 s_{k+1} \rangle = Z_1^{-1} x^k \sum_{s=\pm 1} \prod_{j=1}^{N} (1 + x_j s_j s_{j+1})(1 + y s_j s_{j+m}), \tag{2}$$

where

$$x_j = x^{-1} \quad \text{if} \quad j \leq k$$
$$= x \quad \text{if} \quad j > k,$$

and $Z_1 = Z(\cosh K_1)^{-N} (\cosh K_2)^{-N}$.

Apart from the j dependence of x_j, Eq. (2) is identical with the expression for the partition function. Thus, using the same technique that was used in I to express the partition function in an S-matrix form, we obtain a similar S-matrix expression. It has been shown[7] that an expression such as in Eq. (2) can alternatively be written in terms of fermion creation and annihilation operators, $a_j^{(1)*}$, $a_j^{(2)*}$, $a_j^{(1)}$, $a_j^{(2)}$. We have

$$\begin{aligned}\langle s_1 s_{k+1} \rangle &= Z_1^{-1} x^k \langle 0| \prod_{j=1}^{N} (1 + a_{j-m}^{(2)} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-1}^{(1)} \\ &\quad + y a_j^{(2)*} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-m}^{(2)} + y a_j^{(2)*} a_{j-m}^{(2)} \\ &\quad + x_j y a_j^{(2)*} a_j^{(1)*} + x_j y a_j^{(2)*} a_j^{(1)*} a_{j-m}^{(2)} a_{j-1}^{(1)}) |0\rangle \\ &= Z_1^{-1} x^k \langle 0| \prod_{j=1}^{N} \exp (a_{j-m}^{(2)} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-1}^{(1)} \\ &\quad + y a_j^{(2)*} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-m}^{(2)} \\ &\quad + y a_j^{(2)*} a_{j-m}^{(2)} + x_j y a_j^{(2)*} a_j^{(1)*}) |0\rangle. \end{aligned} \tag{3}$$

The product in Eq. (3) is to be taken in order of increasing j from right to left. If we define an ordering operator T which puts the products in this order we can combine the exponentials to give

$$\begin{aligned}\langle s_1 s_{k+1} \rangle = Z_1^{-1} x^k \langle 0| T \exp \Big(&\sum_{j=1}^{N} a_{j-m}^{(2)} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-1}^{(1)} \\ &+ y a_j^{(2)*} a_{j-1}^{(1)} + x_j a_j^{(1)*} a_{j-m}^{(2)} \\ &+ y a_j^{(2)*} a_{j-m}^{(2)} + x_j y a_j^{(2)*} a_j^{(1)*} \Big) |0\rangle. \end{aligned} \tag{4}$$

Now, defining the operators

$$A^{(1)}(j) = a_{j-1}^{(1)}, \quad A^{2}(j) = a_{j-m}^{(2)},$$
$$A^{(3)}(j) = x a_j^{(1)*}, \quad A^{4}(j) = y a_j^{(2)*},$$

the exponent in Eq. (4) can be written as

$$\sum_{j=1}^{N} \sum_{p,q=1}^{4} \tfrac{1}{2} k_{pq} A^p(j) A^q(j) + \sum_{j=1}^{k} \sum_{p,q=1}^{4} \tfrac{1}{2} k'_{pq} A^p(j) A^q(j) \left(\frac{1}{x^2} - 1 \right), \tag{5}$$

where the (4×4) matrices k and k' are defined as

$$k = \begin{pmatrix} 0 & -1 & -1 & -1 \\ 1 & 0 & -1 & -1 \\ 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$

$$k' = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

The first summation of Eq. (5) is just the term obtained in I for the partition function. The second summation can be regarded as the perturbation which takes care of the j dependence of x_j.

Defining

$$S(N) = \exp \left(\sum_{j=1}^{N} \sum_{p,q=1}^{4} \tfrac{1}{2} k_{pq} A^p(j) A^q(j) \right)$$

as the unperturbed S matrix we have

$$\begin{aligned}\langle s_1 s_{k+1} \rangle = Z_1^{-1} x^k \langle 0| T \exp \Bigg[&\sum_{j=1}^{k} \sum_{p,q=1}^{4} \tfrac{1}{2} k'_{pq} A^p(j) A^q(j) \\ &\times \left(\frac{1}{x^2} - 1 \right) \Bigg] S(N) |0\rangle. \end{aligned}$$

If we expand the exponential we obtain the series

$$\begin{aligned}&\langle s_1 s_{k+1} \rangle \\ &= Z_1^{-1} x^k \langle 0| T \Bigg[1 + \sum_{n=1}^{\infty} \frac{1}{n!} \Bigg[\sum_{j=1}^{k} \sum_{p,q=1}^{4} \tfrac{1}{2} k'_{pq} A^p(j) A^q(j) \\ &\qquad \times \left(\frac{1}{x^2} - 1 \right) \Bigg]^n \Bigg] S(N) |0\rangle. \end{aligned} \tag{6}$$

3. EVALUATION OF THE GREEN'S FUNCTION

In order to sum the perturbation series in Eq. (6) we first have to evaluate the Green's function defined by

$$\begin{aligned}G^{s,t}(u, v) &= \langle 0| T A^s(u) A^t(v) S(N) |0\rangle / \langle 0| T S(N) |0\rangle \\ &= Z_1^{-1} \langle 0| T A^s(u) A^t(v) \\ &\quad \times \sum_{n=0}^{\infty} \frac{1}{n!} \left[\sum_{j=1}^{N} \sum_{p,q=1}^{4} \tfrac{1}{2} k_{pq} A^p(j) A^{(q)}(j) \right]^n |0\rangle. \end{aligned} \tag{7}$$

The vacuum-to-vacuum expectation value of a product of creation and annihilation operators is evaluated by means of Wick's theorem. This means summing over time contractions between all possible pairs of operators which appear in the product. The time contraction of two operators $A^p(j)$ and $A^q(k)$ is written

[7] H. S. Green and C. A. Hurst, *Order–Disorder Phenomena* (Interscience Publishers, Inc., New York, 1964).

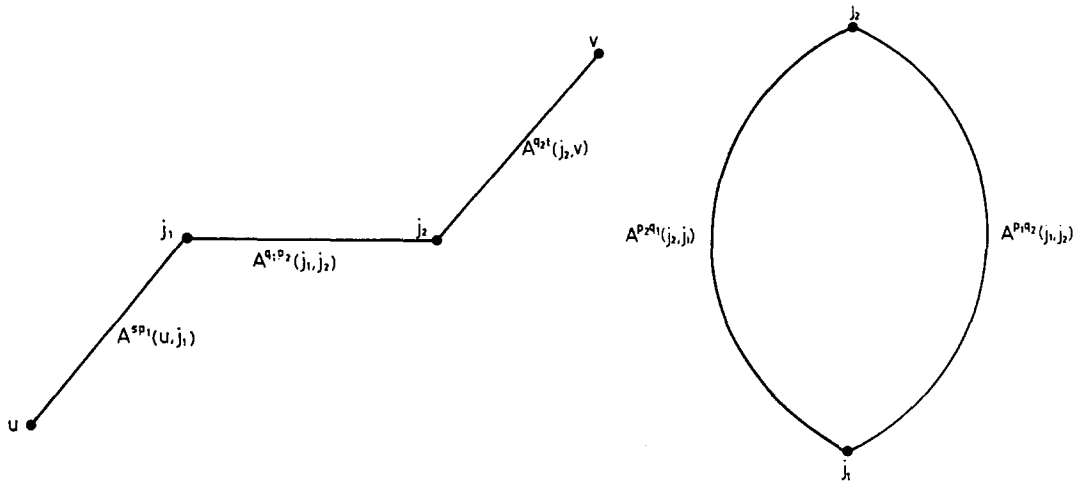


FIG. 1. Examples of graphs corresponding to contractions.

as $A^{pq}(j,k)$ and defined by

$$T\{A^p(j)A^q(k)\} = N\{A^p(j)A^q(k)\} + A^{pq}(j,k).$$

Calculating all the time contractions, we can express the results in the following way.

$$A(j,k) = \begin{pmatrix} 0 & 0 & x\delta_{j-1,k} & 0 \\ 0 & 0 & 0 & y\delta_{j-m,k} \\ -x\delta_{j+1,k} & 0 & 0 & 0 \\ 0 & -y\delta_{j+m,k} & 0 & 0 \end{pmatrix}$$

$$= \frac{1}{N}\sum_{r=1}^{N}\omega^{r(j-k)}\begin{pmatrix} 0 & 0 & x\omega^{-r} & 0 \\ 0 & 0 & 0 & y\omega^{-mr} \\ -x\omega^{r} & 0 & 0 & 0 \\ 0 & -y\omega^{mr} & 0 & 0 \end{pmatrix}$$

$$\equiv \frac{1}{N}\sum_{r=1}^{N}\omega^{r(j-k)}A(r), \tag{8}$$

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

A possible set of time contractions on a product of operators can be represented by a diagram so that summing over all the contractions is equivalent to summing over all the diagrams. The diagrams that result from Eq. (7) will be closed loops, together with a line starting and ending with the operators $A^s(u)$, $A^t(r)$. For example, the diagrams in Fig. 1 represent a possible contraction on the products

$$A^s(u)\,A^t(v)\,A^{p_1}(j_1)\,A^{q_1}(j_1)\,A^{p_2}(j_2)\,A^{q_2}(j_2)$$

and

$$A^{p_1}(j_1)\,A^{q_1}(j_1)\,A^{p_2}(j_2)\,A^{q_2}(j_2),$$

respectively. There is a factor $(-1)^p$ appearing in Wick's theorem, but this is easily accounted for since p is even for a line graph and odd for a single closed loop graph.

Now a diagram with n vertices (excluding the vertices u and v) in which all of the vertices have different values of j_i will occur $2^n n!$ times, since there are $n!$ ways of choosing these vertices from the products in Eq. (7) and the 2^n arises from the fact that each vertex can be either

$$A^p(k)\,A^q(k) \quad \text{or} \quad -A^q(k)\,A^p(k).$$

If all the vertices do not have different values of j, and if ν_1 have the same value k_1, ν_2 the value k_2 etc., a given diagram will occur $n!\,2^n/\nu_1!\,\nu_2!\cdots\nu_i!$ times. However, if these vertices are identical, in drawing all the graphs joining the n points we get $\nu_1!\,\nu_2!\cdots\nu_i!$ graphs topologically the same. Thus, in summing over all graphs of n vertices, each one appears $n!\,2^n$ times, which means we need only sum topologically different diagrams and multiply the contribution of these by $n!\,2^n$. This factor cancels the $1/n!\,2^n$ factor appearing in Eq. (7). This means that in summing over topologically different diagrams the contribution from a given diagram depends only on the time contractions represented by the diagram. Hence the contribution from a disconnected diagram is the product of the contributions from its connected components. Thus we can factorize out the summation over all closed loop diagrams.

$$\begin{matrix}\text{Summation}\\ \text{over all}\\ \text{graphs}\end{matrix} = \begin{bmatrix}\text{summation over}\\ \text{line graphs}\end{bmatrix}\begin{bmatrix}\text{summation over}\\ \text{loop graphs}\end{bmatrix}.$$

But the summation over all loop graphs is equivalent to evaluating

$$\langle 0|\,TS(N)\,|0\rangle = Z_1.$$

Hence to evaluate the Green's function we need to sum only over all line graphs. The contribution from a line of $n+1$ points is

$$k_{p_1q_1}\cdots k_{p_{n-1}q_{n-1}}\,A^{sq_1}(u,j_1)\,A^{p_1q_2}(j_1,j_2)\cdots \times A^{p_{n-2}q_{n-1}}(j_{n-2},j_{n-1})\,A^{p_{n-1}t}(j_{n-1},v).$$

Let L_n be the contribution from summing over all topologically different graphs of $(n+1)$ vertices, starting at u and ending on v. Then

$$L_n=\sum_{j_i=1}^{N}\sum_{p_i,q_i=1}^{4}k_{p_1q_1}\cdots k_{p_{n-1}q_{n-1}} \times A^{sq_1}(u,j_1)\cdots A^{p_{n-1}t}(j_{n-1},v),$$

which when written in terms of the matrices $A(j,k)$ is

$$L_n=\sum_{j_i=1}^{N}A^{s\dagger}(u,j_1)kA(j_1,j_2)\cdots kA^t(j_{n-1},v),$$

where $A^{s\dagger}$ is the sth row of the matrix A. Substituting in Eq. (8) we get

$$L_n=N^{-n}\sum_{j_i,r_i}\omega^{r_1(u-j_1)+\cdots+r_n(j_{n-1}-v)}A^{s\dagger}(r_1)k\cdots kA^t(r_n)$$
$$=N^{-1}\sum_{r=1}^{N}\omega^{r(u-v)}A^{s\dagger}(r)(kA(r))^{n-2}kA^t(r).$$

Summing over all L_n we have

$$G^{s,t}(u,v)=N^{-1}\sum_{n=1}^{\infty}\sum_{r=1}^{N}\omega^{r(u-v)}A^{s\dagger}(r)[kA(r)]^{n-2}kA^t(r)$$
$$=N^{-1}\sum_{r=1}^{N}\omega^{r(u-v)}A^{s\dagger}(r)\times\frac{1}{1-kA(r)}A^{-1}(r)k^{-1}kA^t(r).$$

Writing the Green's function as a 4×4 matrix gives

$$G(u,v)=N^{-1}\sum_{r=1}^{N}\omega^{r(u-v)}A(r)\frac{1}{1-kA(r)}. \qquad (9)$$

The elements of the matrix $A(r)(1-kA(r))^{-1}$ are

$$\Delta(r)(1,1)=x^2y(\omega^{-mr}-\omega^{mr}),$$
$$\Delta(r)(1,2)=xy\omega^{(1-m)r}-x^2y\omega^{-mr}-xy^2\omega^r-x^2y^2,$$
$$\Delta(r)(1,3)=x\omega^r-xy\omega^r(\omega^{-mr}+\omega^{mr})-x^2(1-y^2)+xy^2\omega^r,$$
$$\Delta(r)(1,4)=-xy^2\omega^r-x^2y^2+xy\omega^{(m+1)r}-x^2y\omega^{mr},$$
$$\Delta(r)(2,1)=-xy\omega^{(m-1)r}+xy^2\omega^{-r}+x^2y\omega^{mr}+x^2y^2,$$
$$\Delta(r)(2,2)=xy^2(\omega^r-\omega^{-r}),$$
$$\Delta(r)(2,3)=-x^2y\omega^{mr}-x^2y^2+xy\omega^{(m+1)r}-xy^2\omega^r,$$
$$\Delta(r)(2,4)=y\omega^{mr}-xy\omega^{mr}(\omega^r+\omega^{-r})-y^2(1-x^2)+x^2y\omega^{mr},$$
$$\Delta(r)(3,1)=-x\omega^{-r}+xy\omega^{-r}(\omega^{mr}+\omega^{-mr})+x^2(1-y^2)-xy^2\omega^{-r},$$
$$\Delta(r)(3,2)=-xy\omega^{-(m+1)r}+x^2y\omega^{-mr}+xy^2\omega^{-r}+x^2y^2,$$
$$\Delta(r)(3,3)=x^2y(\omega^{mr}-\omega^{-mr}),$$
$$\Delta(r)(3,4)=-xy^2\omega^{-r}-x^2y^2+xy\omega^{(m-1)r}-x^2y\omega^{mr},$$
$$\Delta(r)(4,1)=-xy\omega^{-(m+1)r}+xy^2\omega^{-r}+x^2y\omega^{-mr}+x^2y^2,$$
$$\Delta(r)(4,2)=-y\omega^{-mr}+xy\omega^{-mr}(\omega^r+\omega^{-r})+y^2(1-x^2)-yx^2\omega^{-mr},$$
$$\Delta(r)(4,3)=-xy\omega^{(-m+1)r}+xy^2\omega^r+yx^2\omega^{-mr}+x^2y^2,$$
$$\Delta(r)(4,4)=-xy^2(\omega^r-\omega^{-r}),$$
$$\Delta(r)=(1+x^2)(1+y^2)-x(1-y^2)(\omega^r+\omega^{-r})-y(1-x^2)(\omega^{mr}+\omega^{-mr}). \qquad (10)$$

This completes the definition and evaluation of our Green's function.

4. EVALUATION OF CORRELATION FUNCTION

We have expressed the correlation function as

$$\langle s_1s_{k+1}\rangle=x^kZ_1^{-1}\langle0|\,T\left[1+\sum_{n=1}^{\infty}\frac{1}{n!}\left[\sum_{j=1}^{k}\tfrac{1}{2}k'_{pq}A^p(j)A^q(j)\right]^n\times\left(\frac{1}{x^2}-1\right)^nS(N)\,|0\rangle. \qquad (11)$$

To evaluate this we again use Wick's theorem, which means summing all diagrams in the above products. Now, if the factor $S(N)$ were not present in Eq. (11) we would sum over all diagrams, whose contributions would be given by the time contractions $A^{pq}(j,k)$. These diagrams that arise from the series part of Eq. (11) and not from the factor $S(N)$ we call skeleton diagrams. It is clear that since the operators appear in pairs the skeleton diagrams are going to be closed loops. Now, by a familiar technique used in field theory, when we include the contributions from $S(N)$, we sum all possible skeleton diagrams, but instead of using the propagator $A^{pq}(j,k)$ we must now use the Green's function $G^{pq}(j,k)$ to determine the contribution from a diagram. For, as we have already seen, the Green's function is a summation over all diagrams between two points and so the above technique is equivalent to summing over all skeleton diagrams where now each line in the skeleton diagram represents a partial summation over all possible diagrams between two points. The contribution from the sum over skeleton diagrams will have to be multiplied by Z_1, which takes account of all the closed loops arising from the factor $S(N)$.

To sum all the skeleton diagrams which arise from

$$\left[1+\sum_{n=1}^{\infty}\frac{1}{n!}\left[\sum_{j=1}^{k}\tfrac{1}{2}k'_{pq}A^p(j)A^q(j)\left(\frac{1}{x^2}-1\right)\right]^n\right],$$

we first notice that the factor $1/2^n n!$ can be removed by summing only topologically different diagrams. This means that the contribution of a disconnected graph is the product of its connected parts. This fact enables us to use the linked cluster expansion

sum over all diagrams =

exp [sum over connected diagrams].

Thus we have to sum over topologically different connected loops. The contribution from a single n-point loop is

$$k'_{p_1q_1}\cdots k'_{p_nq_n}G^{q_1p_2}(j_1,j_2)G^{q_2p_3}(j_2,j_3)\cdots G^{q_np_1}(j_n,j_1)\times\left(\frac{1}{x^2}-1\right)^n.$$

Let L_n be the contribution from the sum of topologically different loops with n vertices. Then

$$L_n=\sum_{j_i=1}^{k}\sum_{p_i,q_i=1}^{4}\frac{-1}{2n}k'_{p_1q_1}\cdots k'_{p_nq_n}\times G^{q_1p_2}(j_1,j_2)\cdots G^{q_np_1}(j_n,j_1)\left(\frac{1}{x^2}-1\right)^n,$$

where the factor $1/2n$ comes from the fact that in summing over p_1q_1j we get each graph repeated $2n$ times since it is a cyclic graph. The minus sign comes from the factor $(-1)^p$ which occurs in the definition of Wick's theorem. Hence

$$\begin{aligned}L_n&=\sum_{j_i=1}^{k}-\frac{1}{2n}\operatorname{Tr}\left(k'G(j_1,j_2)\cdots k'G(j_n,j_1)\right)\left(\frac{1}{x^2}-1\right)^n\\&=\sum_{j_i=1}^{k}-\frac{1}{n}\sum_{r_i=1}^{N}N^{-n}\omega^{r_1(j_1-j_2)+\cdots r_n(j_n-j_1)}\times[c(r_1)c(r_2)\cdots c(r_n)]\left(\frac{1}{x^2}-1\right)^n,\end{aligned}\tag{12}$$

where

$$c(r)=[-x^2-x^2y^2-x^2y(\omega^{mr}+\omega^{-mr})+x\omega^{-r}(1-y^2)]/\Delta(r).$$

The last step in Eq. (12) is given in the Appendix.

When the size of the lattice is very large, we can convert the summations in Eq. (12) to integrals. If we write

$$r=s+(t-1)n$$

and set

$$\phi=2\pi ms/N;\quad\theta=[2\pi(t-1)/m]+(\phi/m),$$

we obtain

$$\omega^r=\exp(i\theta);\quad\omega^{mr}=\exp(i\phi).$$

The summation $\sum_{r=1}^{N}$ is equivalent to $\sum_{s=1}^{n}\sum_{t=1}^{m}$, and in the limit of large n, m this can be written as

$$\frac{mn}{(2\pi)^2}\int_0^{2\pi}\int_0^{2\pi}d\theta\,d\phi.$$

Then Eq. (12) becomes

$$\begin{aligned}L_n=\sum_{j_i=1}^{k}-\frac{1}{n}\frac{1}{(2\pi)^{2n}}\int_0^{2\pi}d\theta_1\cdots d\theta_n\,d\phi_1\cdots d\phi_n\\\times e^{i\theta_1(j_1-j_2)+\cdots+i\theta_n(j_n-j_1)}\\\times[c(\theta_1,\phi_1)c(\theta_2,\phi_2)\cdots c(\theta_n,\phi_n)]\left(\frac{1}{x^2}-1\right)^n,\end{aligned}$$

where

$$c(\theta,\phi)=[-x^2-x^2y^2-2x^2y\cos\phi+xe^{-i\theta}(1-y^2)]/\Delta(\theta,\phi)$$

with

$$\Delta(\theta,\phi)=(1+x^2)(1+y^2)-2x(1-y^2)\times\cos\theta-2y(1-x^2)\cos\phi.$$

The integrals over the ϕ_i can be evaluated immediately since the following relation holds[8]:

$$\frac{1}{2\pi}\int_0^{2\pi}d\phi c(\theta,\phi)\left(\frac{1}{x^2}-1\right)=1-\frac{f(\theta)}{x},$$

where $f(\theta)=u(e^{i\theta})/u(e^{-i\theta})$,

$$u(e^{i\theta})=(1-Be^{i\theta})^{\frac{1}{2}}(1-Ae^{i\theta})^{-\frac{1}{2}},$$

$A=(1-y)/x(1+y)$, and $B=x(1-y)/(1+y)$.

Thus,

$$\begin{aligned}L_n=-\frac{1}{n}\sum_{j_i=1}^{k}\frac{1}{(2\pi)^n}\int_0^{2\pi}d\theta_1\cdots d\theta_n\\\times e^{i\theta_1(j_1-j_2)+\cdots+i\theta_n(j_n-j_1)}\\\times\left[1-\frac{f(\theta_1)}{x}\right]\cdots\left[1-\frac{f(\theta_n)}{x}\right].\end{aligned}\tag{13}$$

We can simplify this multiple integral by defining the operator P_k by

$$P_kh(\phi)=\sum_{j=1}^{k}\frac{1}{2\pi}\int_0^{2\pi}d\theta e^{ij(\phi-\theta)}h(\theta).$$

P_k is a projection operator which projects out the frequencies 1 to k of the Fourier series of $h(\phi)$. We also define P_kf as an operator which acts on a function $h(\phi)$ as follows:

$$(P_kf)h(\phi)=\sum_{j=1}^{k}\frac{1}{2\pi}\int_0^{2\pi}d\theta e^{ij(\phi-\theta)}f(\theta)h(\theta).$$

If we now introduce an extra integral and delta function

$$\int_0^{2\pi}d\phi\delta(\phi-\theta_n)=\int_0^{2\pi}d\phi\sum_{l=-\infty}^{\infty}e^{il(\phi-\theta_n)}$$

into the multiple integral expression in Eq. (13), we

[8] Reference 7, p. 139.

obtain

$$L_n = -\frac{1}{n}\sum_{l=-\infty}^{\infty}\sum_{j_i=1}^{k}\frac{1}{(2\pi)^{n+1}}\int_0^{2\pi}d\phi \times\int_0^{2\pi}d\theta_i e^{il(\phi-\theta_n)}e^{ij_1(\theta_1-\theta_n)}\cdots e^{ij_n(\phi-\theta_{n-1})} \times\left[1-\frac{f(\theta_1)}{x}\right]\cdots\left[1-\frac{f(\theta_n)}{x}\right].$$

We can then use the above definition of the operator $P_k f$ to write this as

$$L_n = -\frac{1}{n}\sum_{l=-\infty}^{\infty}\frac{1}{2\pi}\int_0^{2\pi}d\phi e^{il\phi}P_k\left(1-\frac{f}{x}\right) \times P_k\left(1-\frac{f}{x}\right)\cdots P_k\left(1-\frac{f}{x}\right)e^{-il\phi}$$

$$= -\frac{1}{n}\sum_{l=-\infty}^{\infty}\frac{1}{2\pi}\int_0^{2\pi}d\phi e^{il\phi}\left[P_k\left(1-\frac{f}{x}\right)\right]^n e^{-il\phi}$$

$$= -(1/n)\,\mathrm{Tr}\left[P_k\left(1-\frac{f}{x}\right)\right]^n. \tag{14}$$

Thus we have the result that

$$\sum_{n=1}^{\infty}L_n = \mathrm{Tr}\log\left[1-P_k\left(1-\frac{f}{x}\right)\right] = \log\left(\langle s_1 s_{k+1}\rangle x^{-k}\right). \tag{15}$$

This expression is the same as that obtained by Kadanoff,[6] although the derivations are seemingly unrelated. Also, this expression is simply related to the integral equations used by Green[9] and by Hartwig,[10] and the Toeplitz determinant of Montroll, Potts, and Ward[11] to evaluate the correlation functions. The integral equations can be obtained from Eq. (15) by writing

$$\mathrm{Tr}\log\{1-P_k[1-f(\theta)/x]\} = \log\prod_{i=1}^{k}\lambda_i,$$

where λ_i are the eigenvalues of the equation

$$[1-P_k+P_k f(\theta)/x]u_i(\theta) = \lambda_i u_i(\theta). \tag{16}$$

Multiplying by $(1-P_k)$ gives

$$(1-P_k)u_i(\theta) = (1-P_k)\lambda_i u_i(\theta)$$

and hence $u_i(\theta) = P_k u_i(\theta)$ for $\lambda_i \neq 1$. Multiplying Eq. (16) by P_k we get

$$P_k x^{-1}f(\theta)u_i(\theta) = \lambda_i P_k u_i(\theta) = \lambda_i u_i(\theta), \quad \lambda_i \neq 1.$$

This is the integral equation which was derived by different methods by Green and Hartwig.

The Toeplitz determinant of MPW can also be written in the form of Eq. (15). We regard $f(e^{i\theta})$ as a Toeplitz matrix with elements f_{i-j} given by the $(i-j)$th Fourier coefficient of $f(e^{i\theta})$. The projection operators P_k when written in matrix notation have zero elements everywhere except the diagonal elements (1, 1) to (k, k), which are unity. Then Eq. (15) can be written $\log(\langle s_1 s_{k+1}\rangle x^{-k}) = \log\det(1-P_k+P_k x^{-1}f)$, which gives the same result as MPW.

The evaluation of Eq. (15) can be carried out in a variety of ways. The generalization of Szego's theorem enables us to evaluate the Toeplitz determinant form of Eq. (15). This is the method used by MPW. Green was able to solve the integral equation form exactly because $f(e^{i\theta})$ can be factorized and then its inverse can be found. The method presented here was first given by Kadanoff.[6] It also relies on the fact that we can find the inverse of the operator $P_k f(\theta)$ as $k \to \infty$, and hence is related to Green's method. The technique when applied to the matrix representation of $P_k f(\theta)$ gives us an alternative proof of Szego's theorem, which is given later. Thus it appears that all the approaches are closely connected.

To evaluate Eq. (15) we take the perfect differential of the equation with respect to the variables A and B.

$$d\log\langle s_1 s_{k+1}\rangle = \sum_{n=1}^{\infty}dL_n + k\frac{dx}{x}. \tag{17}$$

Using Eq. (14) we obtain

$$dL_n = +\mathrm{Tr}\{P_k[1-x^{-1}f(\theta)]P_k\}^{n-1}P_k d[x^{-1}f(\theta)].$$

The extra operator P_k which is inserted simplifies the future work and makes no difference to the expression since $P_k^2 = P_k$.

$$\sum_{n=1}^{\infty}dL_n = \mathrm{Tr}\left(1-P_k+P_k x^{-1}f(\theta)P_k\right)^{-1}P_k\, d[x^{-1}f(\theta)]. \tag{18}$$

To evaluate the inverse of $[1-P_k+P_k x^{-1}f(\theta)P_k]$ we use some properties of $u(e^{i\theta})$. Now, $u(z) = (1-Bz)^{\frac{1}{2}} \times (1-Az)^{-\frac{1}{2}}$ has a single singularity at the point $z = A^{-1}$, and $u^{-1}(z)$ has a singularity at $z = B^{-1}$. If the low-temperature case $T < T_c$ is considered, it can be shown[11] that $B < A < 1$. Thus, the singularities of $u(z)$ and $u^{-1}(z)$ lie outside the unit circle. Hence $u^{\pm 1}(z)$ are analytic and can be expanded as a Taylor series inside the unit circle.

$$u(z) = \sum_{n=0}^{\infty}u_n z^n, \quad u^{-1}(z) = \sum_{n=0}^{\infty}u'_n z^n.$$

If we define

$$P = \lim_{k\to\infty}P_k,$$

we see that P projects out all positive frequencies of the Fourier series, and $(1-P)$ the negative frequencies.

[9] H. S. Green, Z. Physik 171, 129 (1963).
[10] R. E. Hartwig (to be published).
[11] E. W. Montroll, R. B. Potts, and J. C. Ward, J. Math. Phys. 4, 308 (1963), to be referred to as MPW.

Since $u^{\pm 1}(e^{i\theta})P$ consists of only positive frequencies the following equations are true.

$$\begin{aligned}(1-P)u^{\pm 1}(e^{i\theta})P &= 0,\\ u^{\pm 1}(e^{i\theta})P &= Pu^{\pm 1}(e^{i\theta})P,\\ Pu^{\pm 1}(e^{-i\theta})(1-P) &= 0,\\ Pu^{\pm 1}(e^{i\theta}) - u^{\pm 1}(e^{i\theta})P &= Pu^{\pm 1}(e^{i\theta})(1-P).\end{aligned} \tag{19}$$

Using these equations we can see by multiplication that $[1 - P + u^{-1}(e^{i\theta})Pxu(e^{-i\theta})]$ is the right and the left inverse of $[1 - P + Pf(\theta)x^{-1}P]$. Substituting this into Eqs. (17) and (18) we get

$$d\log M = \mathrm{Tr}\{u^{-1}(e^{i\theta})Pxu(e^{-i\theta})\, d[f(e^{i\theta})x^{-1}]\} + \lim_{k\to\infty} kx^{-1}\,dx, \tag{20}$$

where

$$M = \lim_{k\to\infty}\langle s_1 s_{k+1}\rangle$$

is the magnetization.

$$d[f(e^{i\theta})x^{-1}] = f(e^{i\theta})\,d(x^{-1}) + u^{-1}(e^{-i\theta})x^{-1}\,du(e^{i\theta}) + u(e^{i\theta})x^{-1}\,d[u^{-1}(e^{-i\theta})]. \tag{21}$$

Substituting Eq. (21) in Eq. (20) means we have three traces to evaluate. The first one can be evaluated to give

$$-\lim_{k\to\infty} kx^{-1}\,dx,$$

which cancels the last term in Eq. (20). The trace involving the third term in Eq. (21) gives the interesting contribution and we evaluate this explicitly. Using the last equation in (19) we have to evaluate

$$\mathrm{Tr}\,\big(Pu(e^{-i\theta})\,d(u^{-1}(e^{-i\theta}))\big) - \mathrm{Tr}\,\big(Pu^{-1}(e^{i\theta})(1-P)u(e^{i\theta})\,d\log u(e^{-i\theta})\big). \tag{22}$$

The first term here is similar to the trace obtained from the second term in Eq. (21) and when written out in full is

$$\int_0^{2\pi}\frac{d\phi}{2\pi}\sum_{l=-\infty}^{\infty}e^{il\phi}\int_0^{2\pi}\frac{d\theta}{2\pi}\sum_{j=1}^{\infty}e^{ij(\phi-\theta)}\,d\log u(e^{-i\theta})e^{-il\theta} = \sum_{j=1}^{\infty}\int\frac{d\theta}{2\pi}\,d\log u(e^{i\theta}) = 0$$

since the integral is zero. The second term of Eq. (22) is

$$\begin{aligned}&-\int_0^{2\pi}\frac{d\phi}{2\pi}\sum_{l=-\infty}^{\infty}e^{il\phi}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\sum_{j_1=1}^{\infty}e^{ij_1(\phi-\theta_1)}u^{-1}(e^{i\theta_1})\\ &\quad\times\int_0^{2\pi}\frac{d\theta_2}{2\pi}\sum_{j_2=0}^{\infty}e^{-ij_2(\theta_1-\theta_2)}u(e^{i\theta_2})\,d\log u(e^{-i\theta_2})e^{-il\theta_2}\\ &= -\int_0^{2\pi}\frac{d\theta_1}{2\pi}\sum_{j_1=1}^{\infty}e^{ij_1(\theta_2-\theta_1)}u^{-1}(e^{i\theta_1})\int_0^{2\pi}\frac{d\theta_2}{2\pi}\sum_{j_2=0}^{\infty}\\ &\quad\times e^{-ij_2(\theta_1-\theta_2)}u(e^{i\theta_2})\,d\log u(e^{-i\theta_2})\\ &= -\sum_{j_1=1}^{\infty}\sum_{j_2=0}^{\infty}\int_0^{2\pi}\frac{d\theta_2}{2\pi}e^{i\theta_2(j_1+j_2)}u'_{j_1+j_2}u(e^{i\theta_2})\,d\log u(e^{-i\theta_2}).\end{aligned}$$

Now the summation over j_1 and j_2 is such that $j_1 + j_2 = i$ occurs i times. Hence the above can be written

$$\begin{aligned}&-\sum_{j=1}^{\infty}\int_0^{2\pi}\frac{d\theta}{2\pi}je^{ij\theta}u'_j u(e^{i\theta})\,d\log u(e^{-i\theta})\\ &\quad= i\int\frac{d\theta}{2\pi}\frac{d}{d\theta}[u^{-1}(e^{i\theta})]u(e^{i\theta})\,d\log u(e^{-i\theta})\\ &\quad= i\int\frac{d\theta}{2\pi}\frac{d}{d\theta}\log u(e^{i\theta})\,d\log u(e^{-i\theta}).\end{aligned}$$

Substituting the explicit expressions for $u(e^{i\theta})$ we obtain

$$\begin{aligned}&d\log M\\ &= i\int_0^{2\pi}\frac{d\theta}{2\pi}\left[\frac{1}{4}\left(\frac{-iBe^{i\theta}}{1-Be^{i\theta}}+\frac{iAe^{i\theta}}{1-Ae^{i\theta}}\right)\right.\\ &\quad\left.\times\left(\frac{-dBe^{-i\theta}}{1-Be^{-i\theta}}+\frac{dAe^{-i\theta}}{1-Ae^{-i\theta}}\right)\right]\\ &= -\oint\frac{dz}{2\pi iz}\left[\frac{1}{4}\left(\frac{-Bz}{1-Bz}+\frac{Az}{1-Az}\right)\right.\\ &\quad\left.\times\left(\frac{-dBz^{-1}}{1-Bz^{-1}}+\frac{dAz^{-1}}{1-Az^{-1}}\right)\right]\\ &= -\frac{1}{4}\left(\frac{dB\cdot B}{1-B^2}-\frac{A\,dB}{1-AB}-\frac{dAB}{1-BA}+\frac{A\,dA}{1-A^2}\right)\\ &= \tfrac{1}{8}d\log[(1-B^2)(1-A^2)/(1-AB)^2].\end{aligned}$$

Integrating we obtain

$$M^8 = (1-B^2)(1-A^2)/(1-AB)^2.$$

The constant of integration is zero, since $M = 1$ at zero temperature.

This is the exact result for the magnetization of a square lattice for temperatures below the critical temperature. For temperatures above the critical temperature we can show that $B < 1$ but $A > 1$. Hence our expansions for $u^{\pm 1}(z)$ do not hold for the high-temperature case. However, we can obtain some similarity between the high- and low-temperature cases if we consider $f(z)$ as given by

$$f(z) = v(z)[zv(z^{-1})]^{-1},$$

where

$$v(z) = (1-Bz)^{\frac{1}{2}}(1-A^{-1}z)^{\frac{1}{2}}.$$

Now $v(z)^{\pm 1}$ are analytic inside the unit circle and hence have expansions which only have positive powers of z. However, the extra factor z in the definition of $f(z)$ now prevents us from finding an inverse to the operator $[1 - P + Pf(e^{i\theta})P]$. In fact, the presence of this extra factor z means that this operator has a zero eigenvalue with an eigenfunction $e^{i\theta}v^{-1}(e^{i\theta})$. We have already shown that $M = \prod_{i=1}^{\infty}\lambda_i$

and hence $M = 0$ provided the product of the remaining eigenvalues is finite.

Some justification of the last statement can be provided in the following way. We notice that the operator can be factorized into

$$(1 - P + Pe^{-i\theta}P) \times [1 - P + Pv(e^{i\theta})v^{-1}(e^{-i\theta})P].$$

Using the relation

$$\text{Tr ln}\,(AB) = \text{Tr ln}\,A + \text{Tr ln}\,B,$$

we get

$$\ln M = \text{Tr ln}\,(1 - P + Pv(e^{i\theta})v^{-1}(e^{-i\theta})P) + \text{Tr ln}\,(1 - P + Pe^{-i\theta}P). \quad (23)$$

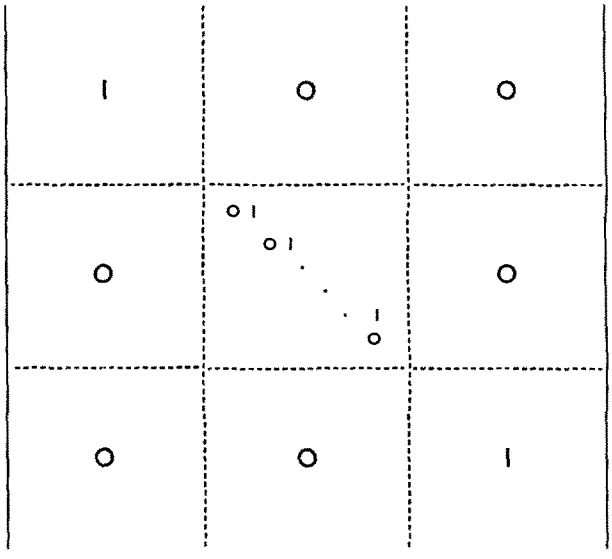
If the first term on the right-hand side of Eq. (23) is evaluated by the same method as was used in the low-temperature case we obtain

$$\ln (1 - A^{-2})(1 - B^2)(1 - A^{-1}B)^2.$$

The second term in Eq. (23) can be evaluated by writing

$$\text{Tr ln}\,(1 - P + Pe^{-i\theta}P) = \lim_{k\to\infty} \text{Tr ln}\,(1 - P_k + P_k e^{-i\theta}P_k) = \lim_{k\to\infty} \ln \det (1 - P_k + P_k e^{-i\theta}P_k).$$

This determinant has ones on the diagonal elements except for the elements (1, 1) to (k, k) where there are ones on an off-diagonal. It has the form



This determinant is obviously zero. In the limit as $k \to \infty$ the determinant remains zero. This definition of the value of the infinite determinant is in accordance with the physical representation of an infinite lattice as a limiting case of a sequence of finite lattices, and so is the most natural one to choose. If instead the infinite determinant were evaluated by just calculating its eigenvalues an ambiguity would arise because the operator $Pe^{-i\theta}P$ is non-Hermitian and possesses a continuous infinity of eigenvalues in the region of the complex plane $|\lambda| < 1$. In a certain sense this approach still leads to the conclusion $M = 0$, but it is more difficult to justify. Substituting these results into Eq. (23) we see that the magnetization is zero for all temperatures above the critical point.

5. PARTITION FUNCTION

In this section we show how the partition function can be calculated using the expressions we have already obtained for the Green's function. Starting with the expression obtained in I for the partition function we have

$$Z_1 = \langle 0|\, T \exp\left[\sum_{j=1}^{N}\sum_{p,q=1}^{4} \tfrac{1}{2}k_{pq}A^p(j)A^q(j)\right]|0\rangle.$$

Taking the differential with respect to x and y of this expression gives us

$$dZ_1 = \langle 0|\, T\left[\sum_{j=1}^{N}\sum_{p,q=1}^{4} k'_{pq}A^p(j)A^q(j)\frac{1}{x}\,dx + \tfrac{1}{2}k''_{pq}A^p(j)A^q(j)\frac{1}{y}\,dy\right]S(N)\,|0\rangle,$$

where

$$k' = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 1 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$k'' = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 \\ 1 & 1 & 1 & 0 \end{pmatrix}.$$

Using the definition for Green's functions, we obtain

$$\frac{dZ_1}{Z_1} = \sum_{j=1}^{N}\sum_{p,q=1}^{4}\left[\tfrac{1}{2}k'_{pq}G^{pq}(j,j)\frac{dx}{x} + \tfrac{1}{2}k''_{pq}G^{pq}(j,j)\frac{dy}{y}\right] = \sum_{j=1}^{N}\sum_{p,q=1}^{4}\frac{1}{2}\left(k'_{pq}\frac{dx}{x} + k''_{pq}\frac{dy}{y}\right)G^{pq}(j,j) = \sum_{j=1}^{N}\text{Tr}\,\frac{1}{2}\left(k'\frac{dx}{x} + k''\frac{dy}{y}\right)G(j,j).$$

Now

$$G(j,j) = \frac{1}{N}\sum_{r=1}^{N}A(r)\frac{1}{1 - kA(r)}$$

and it can be seen that

$$\left(k'\frac{dx}{x} + k''\frac{dy}{y}\right)A(r) = dA(r).$$

Thus,

$$\frac{dZ_1}{Z_1} = \sum_{r=1}^{N} \mathrm{Tr}\, dA(r) \frac{1}{1 - kA(r)},$$

$$d \log Z_1 = \sum_{r=1}^{N} d\, \mathrm{Tr} \log [1 - kA(r)].$$

Integrating gives

$$\log Z_1 = \sum_{r=1}^{N} \log \det [1 - kA(r)],$$

which is the usual expression. Kadanoff[6] has calculated an expression for the partition function in a similar manner to the above using a Green's function which is based on the algebraic approach.

APPENDIX

We give here an outline of the proof of Eq. (12). Using Eq. (9), we see that $k'G$ has the structure

$$\begin{pmatrix} a_1 & a_2 & 0 & a_4 \\ a_1 & a_2 & 0 & a_4 \\ 0 & b_2 & b_3 & b_4 \\ -a_1 & -a_2 & 0 & -a_4 \end{pmatrix},$$

where $a_1 = -G^{31}$, $a_2 = -G^{32}$, $a_4 = -G^{34}$, and $b_3 = G^{13} + G^{23} - G^{34}$. The zero entries arise since

$$\sum_{r=1}^{N} (\omega^r - \omega^{-r}) = 0.$$

Thus the trace of $k'G$ is $(a_1 + a_2 - a_4) + b_3$, which on substitution of the values from Eq. (10) gives

$$\mathrm{Tr}\,(k'G) = b_3 + b_3^*,$$

where

$$b_3(j_1, j_2) = \sum_{r=1}^{N} \omega^{(j_1 - j_2)} \times [-x^2y^2 - x^2 - x^2y(\omega^{mr} + \omega^{-mr}) + x\omega^{-r}(1 - y^2)]\Delta(r)^{-1}.$$

Similarly $k'G_1\, k'G_2$ can be written

$$\begin{pmatrix} a_1 & a_2 & 0 & a_4 \\ a_1 & a_2 & 0 & a_4 \\ 0 & b_2 & b_3 & b_4 \\ -a_1 & -a_2 & 0 & -a_4 \end{pmatrix} \times \begin{pmatrix} A_1 & A_2 & 0 & A_4 \\ A_1 & A_2 & 0 & A_4 \\ 0 & B_2 & B_3 & B_4 \\ -A_1 & -A_2 & 0 & -A_4 \end{pmatrix}$$

from which we obtain

$$\mathrm{Tr}\,(k'G_1\, k'G_2) = b_3^* B_3^* + b_3 B_3.$$

We can repeat this procedure obtaining

$$\mathrm{Tr}\,(k'G_1\, k'G_2 \cdots k'G_n) = b_3(1)\, b_3(2) \cdots b_3(n) + b_3^*(1)\, b_3^*(2) \cdots b_3^*(n).$$

The summation over r_i means that the contribution from the complex conjugate b^* is the same as that from b. Hence we obtain Eq. (12).

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Relation Between "Outer" and "Inner" Multiplicity for $SU(2)$ and $SU(3)$

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The Clebsch–Gordan series for $SU(3)$ is given in terms of irreducible representations of $SU(3)$ such that the "outer" multiplicity of the Clebsch–Gordan series is related to the "inner" multiplicity of irreducible representations.

1. INTRODUCTION

IN the direct product $D(m) \otimes D(m')$ of two irreducible representations with highest weights m and m', respectively, the $D(m)\otimes$ may be considered as an operator acting on the state vectors of the irreducible representation $D(m')$. It has been shown that this operator can always be classified as a *tensor operator* [transforming under $SU(n)$ as states of the irreducible representation $D(m)$] and, moreover, that this operator has precisely dim $[(m)]$ independent matrix elements.[1] The advantage of this operator point of view lies in the fact the Clebsch–Gordan series itself, $D(m) \otimes D(m')$ from which we started, may contain fewer than dim $[(m)]$ terms. (This corresponds to symmetry vanishings of the reduced matrix elements of the operator.) Both points of view have intrinsic advantage, the operator view for general relationships, and the "representation view" for practical applications.

The present paper is concerned with the latter view and the Clebsch–Gordan series for $SU(2)$ and $SU(3)$ is examined. It is shown how the "outer multiplicity" of the Clebsch–Gordan series can easily be related to the "inner multiplicity" of irreducible representations. (The terms stem from Ref. 2.) As an example, $SU(2)$ is first treated in some detail.

2. "OUTER–INNER" MULTIPLICITY FOR $SU(2)$

The weight space of $SU(2)$ is a straight line, as is well known. As for all $SU(n)$ groups this space can be embedded in a Euclidean space with one more dimension, the straight line being given by $(x, -x)$. The weights $m = (m_1, m_2)$ lie on that line, and thus $m_1 = -m_2$. The two roots of $SU(2)$ are $(1, -1)$ and $(-1, 1)$. R_0, half the sum over the positive roots, is then given as $R_0 = \frac{1}{2}(1, -1)$.[3] Any weight of $SU(2)$ is an integer multiple of R_0 (see Fig. 1).

From the relation[4]

$$\chi(m')X(m + R_0) = \sum_{m'''} X(m''' + R_0), \qquad (1)$$

where the exponents of the character $\chi(m')$ contain the weights of the irreducible representation $D(m')$ and where $X(m + R_0)$ is the elementary alternating sum[5] of $m + R_0$, it can immediately be seen that if $D(m')$ is chosen to be smaller or equal to $D(m)$, i.e., $m_1' \leq m_1$, there corresponds to each weight $\bar{m}' \in D(m')$ one and only one term on the right-hand side of (1) and thus one irreducible representation $D(m''')$. This is true, since if $m_1' \leq m_1$, so $m_1' < m_1 + \frac{1}{2}$ and thus the sum of the lowest weight of $D(m')$, namely $-m'$, and $m + R_0$,

$$(m + R_0) - m', \qquad (2)$$

can never reach the origin and therefore also not the negative part of the weight space, see Fig. 1. This is Biedenharn's lemma applied to $SU(2)$.[6]

However, if $D(m')$ is now admitted to be larger than $D(m)$, some part of the weight diagram of $D(m')$ may cover the zero (the singular hyperplane) and, in general, also negative values. This domain is responsible for the deviation of the outer multiplicity from the inner multiplicity. From the definition of the elementary alternating sum it can be seen that the elementary alternating sum of the zero weight is zero, while the elementary alternating sum of the negative

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[2] A. J. Macfarlane, L. O'Raifeartaigh, and P. S. Rao, J. Math. Phys. 8, 536 (1967).
[3] This embedding, trivial for $SU(2)$, becomes of advantage for $n \geq 3$ (for instance with respect to the properties of the weights under the Weyl group).
[4] D. Speiser, *Group Theoretical Concepts and Methods in Elementary Particle Physics*, F. Gürsey, Ed. (Gordon and Breach, New York, 1965), p. 201; J. P. Antoine and D. Speiser, J. Math. Phys. 5, 1226, 1560 (1964).
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[6] F. Zaccaria, J. Math. Phys. 7, 1548 (1966); B. Vitale, Nuovo Cimento 44, 291 (1966).

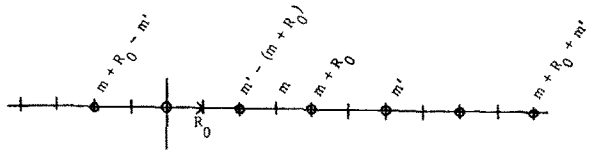

FIG. 1. $D(m') \otimes D(m)$: the encircled points are the ones obtained if $D(m')$ is superimposed to the point $m + R_0$.

weight of (2) is equal to the elementary alternating sum of that weight reflected on the zero point, apart from a change of sign. Thus the elementary alternating sums of the negative weights cancel pairwise with their reflected counterparts. However, all the elementary alternating sums that cancel (and possibly the one equal to zero) just form the weight diagram of the irreducible representation $D(m' - (m + R_0))$. Therefore, the Clebsch–Gordan series for $SU(2)$ can be written in terms of irreducible representations as

$$D(m') \otimes D(m) = \sum_{\bar{m}' \in D(m')} D(m + \bar{m}') - \sum_{\bar{m}' \in D(m' - (m + R_0))} D(-R_0 + \bar{m}'), \quad (3)$$

where the two sums go over all weights $\bar{m}'$ of $D(m')$ and $D(m' - (m + R_0))$, respectively. It should be noted that in the sum $D(m)$ with negative m can occur, i.e., $m_1 < 0$. These terms $D(m)$ do not correspond to irreducible representations and always cancel out in (3). Also, the second term of (3) does not contribute when $m' - (m + R_0)$ is a negative weight, since then $D(m' - (m + R_0))$ is not an irreducible representation.

3. "OUTER-INNER" MULTIPLICITY FOR $SU(3)$

The consideration of Sec. 2 suggests that also in the case of $SU(3)$ it might be possible to relate the highest weights of the irreducible representations which cause the deviation of the outer multiplicity from the inner multiplicity to irreducible representations of $SU(3)$, as happens to be the case for $SU(2)$. Thus, again forming

$$\sum_{\bar{m}' \in D(m')} D(m + \bar{m}'),$$

which is the Clebsch–Gordan series of $D(m') \otimes D(m)$ for the case when inner and outer multiplicity are the same, irreducible representations have to be subtracted from this expression in order to account for the deviation from the inner multiplicity.

As in the case of $SU(2)$ the two-dimensional weight space is embedded in a three-dimensional weight space in the usual manner (Fig. 2). For any weight $m = (m_1, m_2, m_3)$ of $SU(3)$ then $m_1 + m_2 + m_3 = 0$ holds. For convenience, the (p, q), $p = m_1 - m_2$, $q = m_2 - m_3$, notations are used.

In order to simplify the situation the direct product $D(p, q) \otimes D(p', q')$ is always taken such that

$$p + q \leq p' + q' + 1. \quad (4)$$

Condition (4) ensures that only the fundamental domain and the two neighboring domains can contribute to the multiplicity structure of

$$D(p, q) \otimes D(p', q').$$

Moreover, the direct product $D(p, q) \otimes D(p', q')$ is limited at first to direct products of the form

$$D(m, r) \otimes D(p + n - 1, n - 1), n \geq 1, \quad (5)$$

such that one half of the fundamental domain is covered by these direct products. The rest,

$$D(m, r) \otimes D(n - 1, p + n - 1), n \geq 1, \quad (6)$$

can be easily obtained afterwards from symmetry arguments. The integer n can be thought of as the distance of the point $(p + n, n)$ from the point $(p, 0)$ in terms of the vector R_0. Then, if the direct product (5) is formed, the following observations are made (Figs. 2–5).

(a) If the domain of the irreducible representation $D(m, r)$ overlapping into the two neighboring domains is reflected on the singular hyperplanes [as in the case of $SU(2)$] the (two) regions thus obtained in general do not correspond to single irreducible representations. But these regions can always be covered by several overlapping irreducible representations, overlapping in such a way that care is taken to the multiplicities of the points contained in the part leaking out of the fundamental domain.

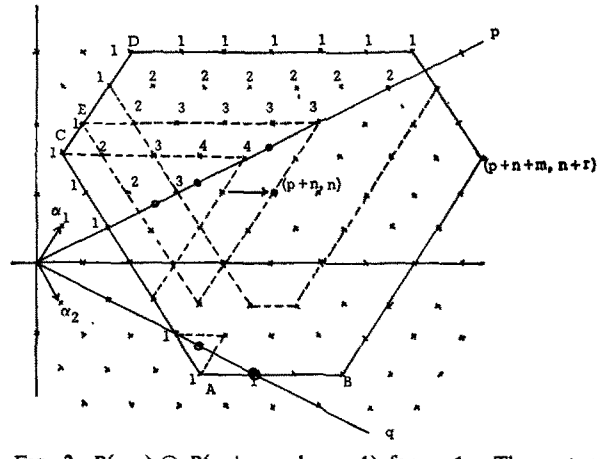

FIG. 2. $D(m,r) \otimes D(p + n - 1, n - 1)$ for $n < r$. The vectors A, B, C, D, E, indicated above are for the general case, thus ignoring the particular values of the diagram ($m = 6, r = 3, p = 6, n = 2$). These points are then given by A: $(p + n - m - r, n + m)$; B: $(p + n - m, m + n + r)$; C: $(p + n - r, n - m)$; D: $(p + n + r, n - m - r)$; E: $(p + 3n - r - 2, -m + 1)$, as can be seen easily by using the Weyl group, $\alpha_1 = (1, -1, 0)$, $\alpha_2 = (0, 1, -1)$. With the help of these points and Figs. 3–5, the statements made in Sec. 3 can be verified. The dots (circles) indicate the centers of the irreducible representations.

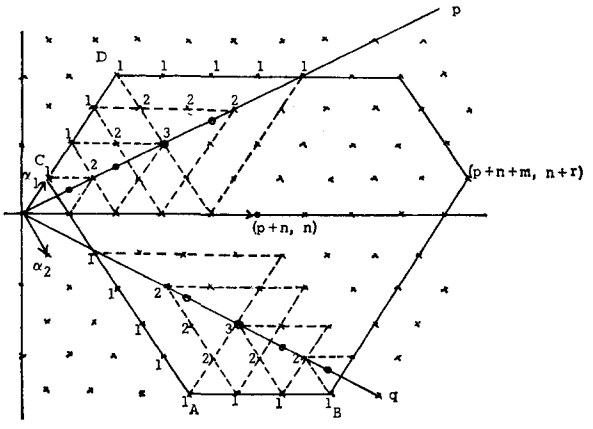

FIG. 3. The case $n \geq r$. (See caption for Fig. 2.) In this example: $p = 0$, $n = 5$.

(b) The centers of these irreducible representations all lie on the singular hyperplanes [as they do for $SU(2)$].

(c) At most one nontriangular irreducible representation can occur. This is the case for $m \neq 0$, $r - n > 0$. It is the irreducible representation

$$D(m, r - n). \tag{7}$$

(d) The point, $(p + n, n)$, its reflected image $(p + 2n, -n)$, and the point $(p + 3n, 0)$ form a triangle in whose center the center of a nontriangular irreducible representation lies. Thus, its center lies on the point

$$(p + 2n, 0). \tag{8}$$

(e) The centers of the triangular irreducible representations lie equidistant from each other, the distance between two neighbors being $(2, 0)$ or $(0, 2)$. The dimensionality of the irreducible representations is increased by going along the positive p axes, decreased by going along the positive q axes.

(f) The series of triangular representations along the q coordinate starts at the point $(0, 2n + p - r)$, giving the series

$$(0, 2n + p - r), \cdots, \quad (0, 2n + p - r + 2k), \cdots, \quad (0, 2n + p + r). \tag{9}$$

The corresponding irreducible representations are

$$\begin{gathered} D(m + r - p - n, 0), \cdots, \\ D(m + r - p - n - k, 0), \cdots, \\ D(m - n - p, 0). \end{gathered} \tag{10}$$

Thus the series terminates either for $k = r$ or when $D(m + r - p - n - k, 0)$ becomes $D(0, 0)$. This implies that $D(p, q)$ with a negative p and/or q are omitted, they do not correspond to irreducible representations.

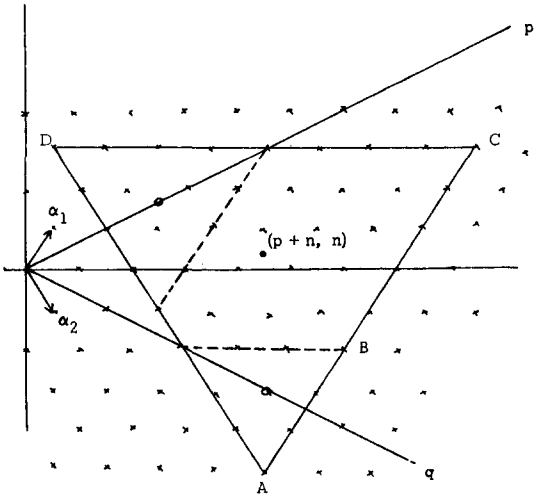

FIG. 4. A: $(p + n - m, n + m)$; B: $(m - n - p, 2n + p)$; C: $(p + n + m, n)$; D: $(p + n, n - m)$.

(g) The series of triangles along the p axes begins for $n < r$ at the point $(p + 2n - (r - n) - 2, 0)$ giving the series

$$\begin{gathered} (p + 3n - r - 2, 0), \cdots, \\ (p + 3n - r - 2 - 2k, 0), \cdots, \\ (p + n - r, 0), \end{gathered} \tag{11}$$

and the corresponding irreducible representations

$$\begin{gathered} D(m - 1, 0), \cdots, D(m - 1 - k, 0), \cdots, \\ D(m - n, 0), \end{gathered} \tag{12}$$

where again this series terminates for $k = n - 1$ or if $D(m - 1 - k, 0)$ becomes $D(0, 0)$.

For $n \geq r$ a series of triangles occurs with centers at the points

$$\begin{gathered} (p + n + r, 0), \cdots, (p + n + r - 2k, 0), \cdots, \\ (p + n - r, 0) \end{gathered} \tag{13}$$

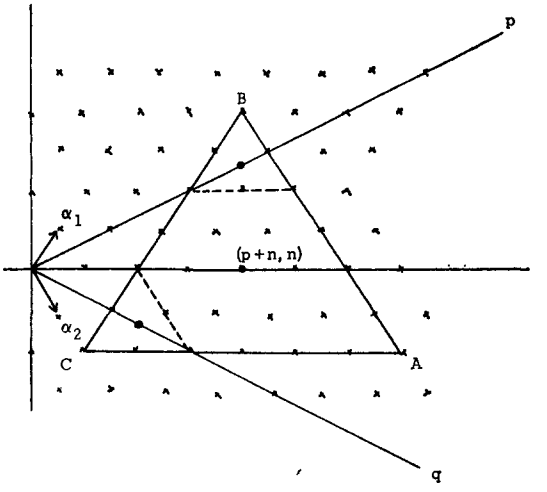

FIG. 5. A: $(p + n, n + r)$; B: $(p + n + r, n - r)$; C: $(p + n - r, n)$.

with the corresponding irreducible representations

$$D(m+r-n,0),\cdots,\quad D(m+r-n-k,0),\cdots,D(m-n,0). \tag{14}$$

Again this series terminates like the ones above.

(h) For irreducible representations of the form $D(m,0)$ it can be deduced from Fig. 4 that at most the two irreducible representations

$$D(m-n,0),\quad D(m-n-p,0) \tag{15}$$

with their centers at the points

$$(p+n,0),\quad (0,2n-p) \tag{16}$$

have to be subtracted.

(i) For irreducible representations of the form $D(0,r)$, Fig. 5 shows that at most the two irreducible representations

$$D(0,r-n),\quad D(0,r-n-p) \tag{17}$$

with centers at

$$(p+2n,0),\quad (0,n) \tag{18}$$

have to be taken into account.

Knowing these facts it is now easy to write down the Clebsch–Gordan series for

$$D(m,r)\otimes D(p+n-1,n-1).$$

However, it has to be done in four pieces.

$$\begin{aligned}
&D(m,r)\otimes D(p+n-1,n-1)\\
&=\sum_{(p'',q'')\in D(m,r)} D((p+n-1,n-1)+(p'',q''))\\
&\quad-\sum_{i=0}^{r}\sum_{(p'',q'')\in D(m+r-n-i,0)} D((p+n+r-1-2i,-1)\\
&\quad+(p'',q''))\\
&\quad-\sum_{i=0}^{r}\sum_{(p'',q'')\in D(m+r-p-n-i,0)} D((-1,p+2n-r\\
&\quad-1+2i)+(p'',q''))\\
&\qquad\qquad\text{for}\quad n\geq r;\ m,r\neq 0,\quad (19a)\\
&=\sum_{(p'',q'')\in D(m,r)} D((p+n-1,n-1)+(p'',q''))\\
&\quad-\sum_{(p'',q'')\in D(m,r-n)} D((p+2n-1,-1)+(p'',q''))\\
&\quad-\sum_{i=0}^{n-1}\sum_{(p'',q'')\in D(m-1-i,0)} D((p+3n-r-3-2i,-1)\\
&\quad+(p'',q''))\\
&\quad-\sum_{i=0}^{r}\sum_{(p'',q'')\in D(m+r-p-n-i,0)} D((-1,p+2n-r\\
&\quad-1+2i)+(p'',q''))\\
&\qquad\qquad\text{for}\quad n<r;\ m,r\neq 0,\quad (19b)\\
&=\sum_{(p'',q'')\in D(m,0)} D((p+n-1,n-1)+(p'',q''))\\
&\quad-\sum_{(p'',q'')\in D(m-n,0)} D((p+n-1,-1)+(p'',q''))\\
&\quad-\sum_{(p'',q'')\in D(m-n-p,0)} D((-1,2n+p-1)+(p'',q''))\\
&\qquad\qquad\text{for}\quad r=0,\quad (19c)\\
&=\sum_{(p'',q'')\in D(0,r)} D((p+n-1,n-1)+(p'',q''))\\
&\quad-\sum_{(p'',q'')\in D(0,r-n)} D((p+2n-1,-1)+(p'',q''))\\
&\quad-\sum_{(p'',q'')\in D(0,r-n-p)} D((-1,n-1)+(p'',q'')),\\
&\qquad\qquad\text{for}\quad m=0,\quad (19d)
\end{aligned}$$

where $m+r\leq p+2n-1$. The sums $\sum_{(p'',q'')\in D(p,q)}$ always have to be extended over *all* weights (p'',q'') of the irreducible representation $D(p,q)$, i.e., multiple weights are to be taken as many times as their multiplicity is. Again, as for $SU(2)$, $D(p,q)$ with negative p and/or q can occur in the sum. However, all these $D(p,q)$ cancel out. If such a $D(p,q)$ occurs as $\sum_{(p'',q'')\in D(p,q)}$ this sum is to be deleted, since $D(p,q)$ is not an irreducible representation.

The Clebsch–Gordan series for

$$D(r,m)\otimes D(n-1,p+n-1),\quad m+r\leq p+2n-1$$

is obtained simply by interchanging the p and q components on the right-hand side of (19).

4. REMARKS

The connection between the inner and outer multiplicity in terms of irreducible representations as given above seems to be unique in spite of the fact that there exist examples where the irreducible representations to be subtracted can be chosen differently. So, for instance, in Fig. 2 the two irreducible representations on the lower hyperplane could be chosen to be $D(0,0)$ and $D(0,1)$ (at different points) instead of $D(1,0)$ and $D(0,0)$. However, as soon as one goes to the general case (Fig. 3), it turns out that the latter choice has to be taken.

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Unitary Representations of the Lorentz Group and Particle Dynamics*

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We examine the quantum dynamics of particles with arbitrary spin implied by explicit use of the infinite dimensional unitary representation of the Lorentz group, introduced by Majorana. Comparison with the classical theory of spinning particles shows that this unitary representation leads to a quantum mechanical analog of the relativistic pure gyroscope.

I. INTRODUCTION

RECENTLY there has been much interest in the possible application of the infinite dimensional unitary representations of the Lorentz group to the elementary particles. To enhance this point of view it is the purpose of this paper to study the dynamics derived from the first-order wave equation for a point particle of arbitrary spin when the matrices involved are Majorana's infinite dimensional unitary representation of the Lorentz group.[1]

Fradkin[2] has recently called attention to Majorana's original paper on the subject of the unitary representations. We make explicit use of the properties of Majorana's representation to display the quantum mechanical counterpart of the classical pure gyroscope.

The classical relativistic point particle, with spin which satisfies the criteria for a pure gyroscope,[3] is first presented in its Hamiltonian formulation. We then develop the quantum dynamics associated with the Majorana representation and by a comparison based on the traditional Poisson bracket, commutator bracket correspondence, infer that the quantum description of the pure gyroscope must utilize the properties of this unitary representation if the correspondence is to be valid for arbitrary spin.

II. CLASSICAL DESCRIPTION

The classical relativistic pure gyroscope is a charged point particle with spin. The magnetic properties of such a particle are described by the antisymmetric spin tensor $s_{\mu\nu}$, which satisfies the supplementary condition

$$s_{\mu\nu}v_\nu = 0, \tag{1}$$

where $x_\mu = (\mathbf{x}, ict)$, and $v_\nu = \dot{x}_\nu = dx_\nu/d\tau$ is the four velocity when τ is the proper time, and $v_\mu v_\mu = -c^2$. The supplementary condition (1) is the covariant statement of the vanishing of the electric dipole moment in the rest frame.[4] If π_μ denotes the kinetic four momentum $P_\mu - e/cA_\mu$, then the description of the pure gyroscope motions is given by

$$\pi_\mu = mv_\mu - \dot{s}_{\mu\nu}v_\nu, \tag{2}$$

$$\dot{\pi}_\mu = e/cF_{\mu\nu}v_\nu, \tag{3}$$

$$\dot{s}_{\mu\nu} = \pi_\mu v_\nu - \pi_\nu v_\mu. \tag{4}$$

In order to obtain a Hamiltonian formulation it is necessary to know the functional relation between velocity and momentum. This is readily obtained by multiplying (2) by $s_{\rho\sigma}s_{\sigma\mu}$, making use of (1), and the identity[5]

$$-2s_{\rho\sigma}s_{\sigma\mu}s_{\mu\nu} = (s_{\alpha\beta}s_{\alpha\beta})s_{\rho\nu}. \tag{5}$$

The necessary relation is then seen to be

$$mv_\mu = \pi_\mu + 2(s_{\mu\rho}s_{\rho\nu}\pi_\nu/s_{\alpha\beta}s_{\alpha\beta}), \tag{6}$$

where in virtue of the equations of motion, $s_{\alpha\beta}s_{\alpha\beta}$ is a constant of the motion. Writing $v_\mu\pi_\mu = -mc^2$ in the form

$$\tfrac{1}{2}(v_\mu\pi_\mu + mc^2) = 0, \tag{7}$$

Equation (6) permits the form (7) to be identified as the covariant Hamiltonian

$$H = \frac{\pi_\mu\pi_\mu}{2m} + \frac{mc^2}{2} + \frac{s_{\mu\sigma}s_{\rho\nu}\pi_\mu\pi_\nu}{ms_{\alpha\beta}s_{\alpha\beta}} = 0. \tag{8}$$

We are justified in calling (8) the Hamiltonian for the pure gyroscope for when use is made of the Poisson bracket angular momentum properties of the $s_{\mu\nu}$,[5,6] i.e.,

$$(s_{\mu\nu}, s_{\rho\sigma}) = s_{\mu\rho}\delta_{\nu\sigma} + s_{\nu\sigma}\delta_{\mu\rho} - s_{\mu\sigma}\delta_{\nu\rho} - s_{\nu\rho}\delta_{\mu\sigma}, \tag{9}$$

the Poisson bracket equations of motion: $\dot{x}_\mu = (x_\mu, H)$; $\dot{\pi}_\mu = (\pi_\mu, H)$; and $\dot{s}_{\mu\nu} = (s_{\mu\nu}, H)$, are Eqs.

* This work was sponsored in part by the TRW Independent Research program and the Office of Naval Research.

[1] E. Majorana, Nuovo Cimento 9, 335 (1932).

[2] D. M. Fradkin, Am. J. Phys. 34, 314 (1966).

[3] Many authors have discussed this subject. The most concise statement of the theory, together with a most complete reference list, is to be found in the book by H. C. Corben, *Classical and Quantum Theories of Spinning Particles* (to be published), Sec. 8.

[4] J. Frenkel, Z. Physik 37, 243 (1926).

[5] S. Shanmugadashan, Can. J. Phys. 31, 1 (1953).

[6] H. A. Kramers, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1957), Sec. 57.

(2), (3), and (4), respectively. Further, (6) and (9) yield the additional Poisson bracket relation

$$(v_\mu, s_{\rho\sigma}) = v_\rho\delta_{\mu\sigma} - v_\sigma\delta_{\mu\sigma} - \pi_\rho(x_\sigma, v_\mu) + \pi_\sigma(x_\rho, v_\mu). \tag{10}$$

In the next section we see the remarkable extent to which the classical expressions (1)–(10) find their operator analog in the quantum theory.

Anticipating the ensuing quantum mechanical analysis it is of interest to note Corben's relation between the rest energy and spin of the classical free particle. For the case $\mathbf{P} = 0$, Eqs. (3) and (4) have the solutions[7]

$$\mathbf{s} = \text{const}, \quad \mathbf{v} = \boldsymbol{\Omega} \times \mathbf{r},$$

where $s_i = \frac{1}{2}\epsilon_{ijk}s_{jk}$, and $\boldsymbol{\Omega} = -(\mu c^2/s^2)\mathbf{s}$, and μ is a constant for given $|\mathbf{v}|$. Thus the particle moves, in a plane normal to $\mathbf{s}$, in a circle of radius

$$r = (v/c)s/\mu c,$$

with energy

$$E = \mu c^2 = mc^2/\gamma = -\mathbf{s}\cdot\boldsymbol{\Omega}.$$

For this motion, the invariant, intrinsic spin s_0 is related to the observable spin s by

$$s_0 = [\tfrac{1}{2}(s_{\alpha\beta}s_{\alpha\beta})]^{\frac{1}{2}} = s/\gamma,$$

and therefore the energy is given by

$$E = mc^2(s_0/s). \tag{11}$$

Thus the energy in the momentum rest frame, properly called the rest energy, varies inversely with the magnitude of the observable spin. Classically then, a continuum of states with increasing spin and decreasing rest energy is predicted, a consequence which finds its counterpart in the quantum theory presented in the next section.

III. THE MAJORANA REPRESENTATION

The basis of this relativistic quantum description of a charged, spinning, point particle is the first-order wave equation

$$(ic\gamma_\mu\pi_\mu + mc^2)\psi = 0, \tag{12}$$

where $\pi_\mu = -i\hbar\partial_\mu - e/cA_\mu$, and the γ_μ are the infinite dimensional matrices specified by Majorana.[1] The spin operators

$$\gamma_{\mu\nu} = (\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu) \tag{13}$$

are the generators of the homogeneous Lorentz group and therefore satisfy the general, representation-invariant, commutation relations

$$[\gamma_{\mu\nu}, \gamma_{\rho\sigma}] = \gamma_{\mu\rho}\delta_{\nu\sigma} + \gamma_{\nu\sigma}\delta_{\mu\rho} - \gamma_{\mu\sigma}\delta_{\nu\rho} - \gamma_{\nu\rho}\delta_{\mu\sigma}, \tag{14}$$

$$[\gamma_\sigma, \gamma_{\mu\nu}] = -\gamma_\mu\delta_{\nu\sigma} + \gamma_\nu\delta_{\mu\sigma}. \tag{15}$$

[7] A. Papapetrou, Praktika Acad. d'Thenes **14**, 540 (1939).

While (14) is the operator counterpart of (9), (15) differs from (10), since the operators for position and velocity in the first-order quantum theory necessarily commute.

As a consequence of (13), (14), and (15) it can be seen that

$$[\gamma_\sigma, \gamma_{\mu\nu}\gamma_{\mu\nu} - 2\gamma_\mu\gamma_\mu] = 0, \tag{16}$$

therefore the combination $\gamma_{\mu\nu}\gamma_{\mu\nu} - 2\gamma_\mu\gamma_\mu$ must be treated as a c number, a result which is also representation invariant and is true of finite as well as infinite dimensional representations. The Majorana representation implies the further restriction that $\gamma_{\mu\nu}\gamma_{\mu\nu}$ is separately a c number, i.e.,

$$[\gamma_\sigma, \gamma_{\mu\nu}\gamma_{\mu\nu}] = 0, \tag{17}$$

as a consequence of which

$$\gamma_\mu\gamma_{\mu\rho} + \gamma_{\mu\rho}\gamma_\mu = 0, \tag{18}$$

$$[\gamma_\rho, \gamma_\mu\gamma_\mu] = 0. \tag{19}$$

Equation (18) represents the operator analog of the supplementary condition (1), and (19) implies that in this representation $\gamma_\mu\gamma_\mu$ is also to be treated as a c number. Thus we begin to see the reflection of the classical theory of the pure gyroscope in the quantum theory through the Majorana representation. Relation (17) implies the constancy of $\gamma_{\mu\nu}\gamma_{\mu\nu}$ which, as we saw, has as its classical counterpart the constancy of $s_{\mu\nu}s_{\mu\nu}$. Likewise the c number character of $\gamma_\mu\gamma_\mu$ is necessary if we expect to reflect the classical relativistic definition, $v_\mu v_\mu = -c^2$. In the case of the finite dimensional representations, only the Dirac matrices for spin $\frac{1}{2}$ display these characteristics, whereas turning to the Majorana representation provides a correspondence valid for arbitrary spin.

Further instructive properties of the Majorana representation are derivable from the relation

$$\gamma_{\mu\rho}\gamma_{\rho\nu} + \gamma_{\nu\rho}\gamma_{\rho\mu} = -(\gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu) + 2\gamma_\rho\gamma_\rho\delta_{\mu\nu}, \tag{20}$$

which is itself a consequence of (18). Let us introduce the particular c numbers, $\gamma_\rho\gamma_\rho = -a$, and $\gamma_{\rho\sigma}\gamma_{\rho\sigma} = b$. If we multiply (20) once on the left and once on the right by $\gamma_{\nu\sigma}$, add the two expressions, and again use (18), we obtain

$$\gamma_{\nu\sigma}(\gamma_{\mu\rho}\gamma_{\rho\nu} + \gamma_{\nu\rho}\gamma_{\rho\mu}) + (\gamma_{\mu\rho}\gamma_{\rho\nu} + \gamma_{\nu\rho}\gamma_{\rho\mu})\gamma_{\nu\sigma} = -1/b(4a + 1)(\gamma_{\alpha\beta}\gamma_{\alpha\beta})\gamma_{\mu\sigma}, \tag{21}$$

which, modulo numerical coefficients, is the operator analog of the classical identity (5). The explicit relation between the c numbers a and b may be obtained by multiplying (20) by $\delta_{\mu\nu}$, giving $b = 3a$.

To illustrate the dynamical correspondence between the classical theory of Sec. II and the quantum theory

in the Majorana representation, we consider $H = ic\gamma_\mu\pi_\mu + mc^2$ to be the proper time Hamiltonian. The operator dynamics are then given by

$$\dot{\pi}_\mu = i/\hbar[\pi_\mu, H] = e/cF_{\mu\nu}(ic\gamma_\nu), \tag{22}$$

$$(\hbar/i)\dot{\gamma}_{\mu\nu} = [\gamma_{\mu\nu}, H] = \pi_\mu(ic\gamma_\nu) - \pi_\nu(ic\gamma_\mu), \tag{23}$$

which clearly represent the operator counterparts of the classical equations (3) and (4). Once again Eqs. (22) and (23) are a consequence of the general group properties (14) and (15), and are therefore representation-invariant. When the bilinear associations[9]

$$ic\langle\gamma_\mu\rangle = v_\mu, \quad h/i\langle\gamma_{\mu\nu}\rangle = s_{\mu\nu}, \tag{24}$$

are made, the Eqs. (22) and (23) yield (3) and (4).

If we now seek the quantum counterpart of (6) we are again forced to the Majorana representation. In order to separate the orbital and spin contributions to the current, we express the current as[10]

$$\langle\gamma_\mu\rangle = \frac{-i}{2mc}\int\bar{\psi}(\gamma_\mu\gamma_\rho + \gamma_\rho\gamma_\mu)\pi_\rho\psi\, d^4x, \tag{25}$$

where surface terms have been neglected. Using (20) we have

$$ic\langle\gamma_\mu\rangle = \frac{1}{2m}\int\bar{\psi}[2\gamma_\sigma\gamma_\sigma\pi_\mu - (\gamma_{\mu\sigma}\gamma_{\sigma\rho} + \gamma_{\rho\sigma}\gamma_{\sigma\mu})\pi_\rho]\psi\, d^4x. \tag{26}$$

Making use of (24) we may write (26) in terms of the classical variables as

$$-mv_\mu = (a\pi_\mu/m) + (bs_{\mu\rho}s_{\rho\nu}\pi_\nu/2ms_{\alpha\beta}s_{\alpha\beta}), \tag{27}$$

which, modulo the coefficients a and b, is the same as (6). This relation (27) implies that the classical Hamiltonian constructed from the quantum theory, in the Majorana representation, is

$$H = \frac{a\pi_\mu\pi_\mu}{2m} - \frac{mc^2}{2} + \frac{bs_{\mu\rho}s_{\rho\nu}\pi_\mu\pi_\nu}{4ms_{\alpha\beta}s_{\alpha\beta}} = 0. \tag{28}$$

[8] M. E. Rose, *Relativistic Electron Theory* (John Wiley & Sons, Inc., New York), Sec. 11.
[9] K. Rafanelli and R. Schiller, Phys. Rev. **135**, B279 (1964).
[10] W. Gordon, Z. Physik **50**, 5630 (1927).

The Hamiltonian (28) and the associated relation (27) yield the Poisson bracket equations of motion (3) and (4) independent of the values of a and b.

Further, with regard to the discussion on the dependence of classical rest energy on spin, the wave equation (12), for the free particle in the frame defined by $P_\mu = (0, iE/c)$ becomes

$$\gamma_4 E\psi = mc^2\psi. \tag{29}$$

As shown by Majorana, γ_4 is diagonal and has the eigenvalue $(j + \frac{1}{2})$, where j is the spin of the state considered. Therefore the rest energy of the given state is

$$E = mc^2/(j + \tfrac{1}{2}). \tag{30}$$

Thus, to mirror the classical result (11), the quantum theory predicts a discrete set of states whose rest energy decreases with increasing spin.

IV. CONCLUSION

The preceding analysis shows a striking correspondence between the classical and quantum theories of spinning particles when the classical theory describes a pure gyroscope and the quantum theory is couched in the language of Majorana's infinite dimensional unitary representation of the Lorentz group.

The operator properties, essential to a meaningful reflection of the properties of the classical variables, find expression only for spin $\frac{1}{2}$ when the finite dimensional representations are considered. Only when we turn to the infinite dimensional matrices of Majorana can the correspondence be extended to the case of arbitrary spin.

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Electromagnetic Behavior of Superconductors with Impurity Scattering

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A general equation for the electromagnetic current **J** of a superconductor responding to a frequency-dependent external electromagnetic field and under the influence of impurity scattering and temperature has been derived in momentum space using the Green's function method. This general equation can be regarded in two ways. (a) It is the Fourier transform, from coordinate space to momentum space, of the equation of Mattis and Bardeen [D. C. Mattis and J. Bardeen, Phys. Rev. **111**, 412 (1958), Eq. (3.3)]. (b) It summarizes, in one equation, the previous works of Abrikosov *et al.* on the electromagnetic behavior of superconductors. In addition to these general properties, this equation also shows, in particular, that for a superconducting alloy with a few percent of impurity concentration, the kernel for the current is the same as that of a Pippard pure superconductor, with $\frac{3}{4}vk$, where v is the Fermi velocity and k is the momentum exchange during collision replaced by τ_{tr}, the transport collision time, valid for all temperatures up to T_c, the transition temperature. Expressions of the current in closed form for both superconducting alloys and normal metal with impurity are also given for $vk \sim 1/\tau$.

I. INTRODUCTION

WE discuss here the derivation of a general formula for the electromagnetic current **J** of a metal including the following five parameters: gap Δ, collision time τ, temperature T, frequency of external field w, and vk, where v is the Fermi velocity of the electrons in the metal and k is the momentum exchange during collision. A superconductor is known as the London type if vk is small, and is known as the Pippard type if vk is large. In a normal metal, for vk small, the phenomenon is known as the normal skin effect, while for vk large, it is known as the anomalous skin effect. Already a good number of results have been derived by Abrikosov *et al.*[1–4] using the Green's function method. However, all their results include four or less of the five parameters mentioned above, while we would like to derive an equation which includes all the five parameters, thus summarizing all their previous work in one equation.

From another point of view, the equation that we wish to derive can also be regarded as the Fourier transform, from coordinate space to momentum space, of the equation of Mattis and Bardeen.[5] Needless to say, because of the complexity of the parameters involved and the problem of analyticity of the equation, it is impossible to obtain the Fourier transform directly from the equation of Mattis and Bardeen. We must therefore look for a solution to the problem at a much earlier stage, and we start with the derivation of the current **J** from the well-known "Kubo formula."[6]

As far as the problem of analyticity is concerned, the method we are going to use resembles closely that of Ambegaokar and Langer,[7] and is almost the same as indicated by Evans and Rickayzen[8] in another context, in the discussion of the Meissner effect. It is the following. We notice that the Green's function used by Abrikosov is actually $G(w + i\delta)$, which has singularities in the upper half-plane, with complicated analyticity problems when impurity scattering is present. If, however, one works with $G(w)$, without $i\delta$, then one finds that in the complex w plane it has only cuts on the real axis, but is analytic everywhere else. Then using a theorem by Baym and Mermin,[9] we are able to obtain the spectral weight function $A(w)$ by analytic continuation. In most cases, the final expression for current that we obtain can be integrated analytically, without having to have recourse to numerical computation, as is necessary in the case of Mattis and Bardeen's expression, calculated by Miller.[10]

[1] A. A. Abrikosov and L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **35**, 1558 (1958); **36**, 319 (1959) [English transl.: Soviet Phys.—JETP **8**, 1090 (1959); **9**, 220 (1959)].

[2] A. A. Akrikosov, L. P. Gorkov, and I. M. Khalatnikov, Zh. Eksperim. i Teor. Fiz. **35**, 265 (1958); **37**, 187 (1959) [English transl.: Soviet Phys.—JETP **8**, 182 (1959); **10**, 132 (1960)].

[3] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1963).

[4] I. M. Khalatnikov and A. A. Abrikosov, Advan. Phys. **8**, 45 (1959).

[5] D. C. Mattis and J. Bardeen, Phys. Rev. **111**, 412 (1958).

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[7] V. Ambegaokar, *Brandeis Lectures*, Vol. 2, *Astrophysics and the Many-Body Problem* (W. A. Benjamin, Inc., New York, 1962), pp. 323–438.

[8] A. B. Evans and G. Rickayzen, Ann. Phys. (New York) **33**, 275 (1965).

[9] G. Baym and M. Mermin, J. Math. Phys. **2**, 232 (1961).

[10] P. B. Miller, Phys. Rev. **118**, 928 (1960).

2. DERIVATION OF THE GENERAL FORMULA

We start with the current–current correlation function. Following Rickayzen[11] and Ambegaokar,[7] we have

$$\mathbf{j} = \mathbf{j}_p + \mathbf{j}_D,$$

where $\mathbf{j}_D = -Ne^2\mathbf{A}/m$, and

$$\mathbf{j}_p(\mathbf{x}, t_x) = \int_{-\infty}^{t_x} dt_y\, d^3\mathbf{y} i[\mathbf{j}(\mathbf{x}, t_x), \mathbf{j}(\mathbf{y}, t_y)]\, \mathbf{A}(\mathbf{y}, t_y) \quad (1)$$

and

$$[\mathbf{j}(\mathbf{x}, t_x), \mathbf{j}(\mathbf{y}, t_y)] \equiv f_>(\mathbf{x}, \mathbf{y}, t_x - t_y) - f_<(\mathbf{x}, \mathbf{y}, t_y - t_x). \quad (2)$$

Since the current $\mathbf{j}$ is a physical quantity, it is absolutely convergent, and can be continued into the complex t plane;

	$i\beta$	
II		I
III	0	IV
	$-i\beta$	

t plane, $\beta = 1/k_BT$.

We continue $f_>$ into the lower regions III and IV, $f_<$ into the upper regions I and II. The periodicity condition for $f_>$ and $f_<$ is

$$f_<(w) = e^{-w\beta} f_>(w).$$

Define

$$\phi(w) = f_>(w)(1 - e^{-\beta w}). \quad (3)$$

We have

$$f_>(\mathbf{x}, \mathbf{y}, t_x - t_y) = (-ie/2m)^2(\nabla_x - \nabla_{x'})(\nabla_y - \nabla_{y'}) \times T[\psi^\dagger(\mathbf{x}', t_{x'})\psi(\mathbf{x}, t_x)\psi^\dagger(\mathbf{y}', t_{y'})\psi(\mathbf{y}, t_y)].$$

The inequality in time ordering here depends on how t is extended from real to complex values. If one uses the "restricted time region" as done by Ambegaokar, the inequality refers to the negative imaginary part of t. If one uses the regions in II and IV (e.g., Baym), the inequality refers to the real part of t. In any case,

$$f_>(\mathbf{x}, \mathbf{y}, t_x - t_y) = (-ie/2m)^2(\nabla_x - \nabla_{x'})(\nabla_y - \nabla_{y'}) \times [-\mathcal{G}(x - y')\mathcal{G}(y - x') + \mathcal{F}^\dagger(x' - y')\mathcal{F}(y - x)], \quad (4)$$

where $\mathcal{G}$ and $\mathcal{F}$ are the well-known Green's functions of a superconductor originally defined by Gorkov.[12] We now take the Fourier series components, and write

$$f_>(\mathbf{x}, \mathbf{y}, t_x - t_y) = \frac{i}{\beta}\sum_m e^{-i\nu_m(t_x - t_y)} F_>(\nu_m, \mathbf{x}, \mathbf{y}),$$

where

$$\nu_m = 2\pi m/(-i\beta), \quad m = 0, \pm 1, \pm 2, \cdots.$$

Thus,

$$F_>(\nu_m, \mathbf{x}, \mathbf{y}) = \int_0^{-i\beta} f_>(\mathbf{x}, \mathbf{y}, t_x - t_y) \times e^{i\nu_m(t_x - t_y)}\, d(t_x - t_y). \quad (5)$$

Similarly, writing out only the time components, we define

$$\mathcal{G}(t_x - t_y) = \frac{i}{\beta}\sum_l \mathcal{G}(\zeta_l) e^{-i\zeta_l(t_x - t_y)},$$

where

$$l = 0, \pm 1, \pm 2, \cdots, \quad \zeta_l = \mu + (2l + 1)\pi/(-i\beta),$$

$$\mathcal{G}(\zeta_l) = \int_0^{i\beta} e^{i\zeta_l(t_x - t_y)}\mathcal{G}(t_x - t_y)\, d(t_x - t_y).$$

From (4) and (5),

$$F_>(\nu_m, \mathbf{x}, \mathbf{y}) = \left(-\frac{ie}{2m}\right)^2(\nabla_x - \nabla_{x'})(\nabla_y - \nabla_{y'})\frac{1}{-i\beta} \times \left[-\sum_l \mathcal{G}(\mathbf{x}, \mathbf{y}', \zeta_l)\mathcal{G}(\mathbf{y}, \mathbf{x}', \zeta_l + \nu_m) + \sum_l \mathcal{F}^\dagger(\mathbf{x}', \mathbf{y}', \zeta_l)\mathcal{F}(\mathbf{y}, \mathbf{x}, \zeta_l + \nu_m)\right]. \quad (6)$$

Next we define the spectral weight function A such that

$$\mathcal{G}(\mathbf{x}, \mathbf{y}', \zeta_l) = \int \frac{dw}{2\pi}\frac{A_g(\mathbf{x}, \mathbf{y}', w)}{\zeta_l - w}. \quad (7)$$

If we continue from discrete ζ_l to continuous ζ, we have

$$G(\mathbf{x}, \mathbf{y}', \zeta) = \int \frac{dw}{2\pi}\frac{A_g(\mathbf{x}, \mathbf{y}', w)}{\zeta - w}. \quad (8)$$

It has been shown by Baym and Mermin[9] that the continuation from (7) to (8) is unique if $G(\mathbf{x}, \mathbf{y}', \zeta)$ has only cuts on the real ζ axis, but is analytic elsewhere. Then from (8) we obtain

$$A(w) = i[G(w + i\delta) - G(w - i\delta)]. \quad (9)$$

Since the $F^\dagger F$ term is entirely similar to the GG term, we write $A(w)$ to include both A_g and A_f. [cf. Eq. (16).]

We now transform the summation in (6) into a contour integral, and then deform the contour on the

[11] G. Rickayzen, *Lecture Notes on the Many-Body Problem, from the First Bergen International School of Physics* (W. A. Benjamin, Inc., New York, 1962); *Theory of Superconductivity* (John Wiley & Sons, Inc., New York, 1965).

[12] L. P. Gorkov, Zh. Eksperim. i Teor. Fiz. **34**, 735 (1958) [English transl.: Soviet Phys.—JETP **7**, 505 (1958)].

two sides in the negative sense. Thus,

$$F_>(\nu_m, \mathbf{x}, \mathbf{y}) = \left(-\frac{ie}{2m}\right)^2 \tfrac{1}{2}i(\nabla_x - \nabla_{x'})(\nabla_y - \nabla_{y'}) \times \int \frac{dw_1\, dw_2}{(2\pi)^2} A(\mathbf{x} - \mathbf{y}', w_1)A(\mathbf{y} - \mathbf{x}', w_2) \times \frac{[\tanh(w_1/2T) - \tanh(w_2/2T)]}{w_1 - w_2 + \nu_m}. \quad (10)$$

From (3) and (5) we have, omitting $\mathbf{x}$ and $\mathbf{y}$,

$$F_>(\nu_m) = i\int_{-\infty}^{\infty} \frac{\phi(w)}{\nu_m - w}\frac{dw}{2\pi}. \quad (11)$$

Combining (10) and (11), we have

$$\phi(\mathbf{x}, \mathbf{y}, w) = \left(-\frac{ie}{2m}\right)^2 \tfrac{1}{2}(\nabla_x - \nabla_{x'}) \times (\nabla_y - \nabla_{y'}) \int \frac{dw_1\, dw_2}{(2\pi)^2}, A(\mathbf{x} - \mathbf{y}', w_1)A(\mathbf{y} - \mathbf{x}', w_2)2\pi\delta(w + w_1 - w_2) \times [\tanh(w_1/2T) - \tanh(w_2/2T)]. \quad (12)$$

We now take the Fourier transform of (5) in t and $\mathbf{x}$, and get

$$\mathbf{j}_x(\mathbf{k}, w_0) = -\frac{e^2}{m^2}\int \mathbf{p}\cdot\mathbf{p}\cdot\mathbf{A}(\mathbf{k}, w_0)\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{dw_1\, dw_2}{(2\pi)^2}\frac{A_g(\mathbf{p} + \tfrac{1}{2}\mathbf{k}, w_1)A_g(\mathbf{p} - \tfrac{1}{2}\mathbf{k}, w_2) - A_f(\mathbf{p} + \tfrac{1}{2}\mathbf{k}, w_1)A_f(\mathbf{p} - \tfrac{1}{2}\mathbf{k}, w_2)}{w_0 - w_2 + w_1 + i\delta} \times [\tanh(w_1/2T) - \tanh(w_2/2T)], \quad (13)$$

where a factor 2 has come from summing over spin, and A_g and A_f are to be obtained from (7), (8), and (9). The thermal Green's functions $\mathfrak{G}$ and $\mathfrak{F}$ are the same as Abrikosov and Gorkov's, where we have changed the sign of our $\mathfrak{G}$ to agree with their $\mathfrak{G}$. Since the current depends only on the product of two $\mathfrak{G}$'s, it does not change (13). $\mathfrak{F}$ is a matrix proportional to

$$\hat{I} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Since $\hat{I}\hat{I} = -1$, we can treat $\hat{I}$ as i, thus obtaining the time-dependent G and F in complete agreement with Gorkov's G and F.

Equation (13) is the starting point for the calculation of current. Following Abrikosov and Gorkov, we have

$$\mathfrak{G}_0 = \frac{-(iw_n + E)}{w_n^2 + E^2 + \Delta^2}, \quad \mathfrak{F}_0^\dagger = \frac{\Delta}{w_n^2 + E^2 + \Delta^2}. \quad (14)$$

Putting $iw_n \to w$, we have

$$G_0 = \frac{w + E}{w^2 - E^2 - \Delta^2}, \qquad F_0^\dagger = \frac{-\Delta\hat{I}}{w^2 - E^2 - \Delta^2} = \frac{-i\Delta}{w^2 - E^2 - \Delta^2}. \quad (15)$$

Or, writing in Nambu's form,

$$G_{0,n} = \begin{pmatrix} G_0 \\ F_0^\dagger \end{pmatrix} = (w - E\sigma_3 + \Delta\sigma_2)^{-1}U,$$

where

$$U = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

At this stage the effect of impurity scattering must be taken into consideration. The problem was first solved by Edwards[13] for normal metals, and has been well presented by Rickayzen[11] in the case of superconductors. We refer to his article for further details. The Green's function $\tilde{G}_n$ of a superconductor with impurities is obtained from the Green's function of a pure superconductor $G_{0,n}$ through the Dyson equation.

The Dyson equation is

$$\tilde{G}_n = (G_{0,n}^{-1} - \Sigma)^{-1}U, \quad \tilde{G}_n = \begin{pmatrix} \tilde{G} \\ \tilde{F}^\dagger \end{pmatrix},$$

where

$$\Sigma(\mathbf{k}) = n\int \frac{d^3\mathbf{k}'}{(2\pi)^3}\sigma_3 G_{0,n}(\mathbf{k}', w)\sigma_3 |u(\mathbf{k} - \mathbf{k}')|^2 = (w + \Delta\sigma_2)\chi + \sigma_3\chi';$$

χ' is the renormalization of energy, and can be absorbed in E;

$$\chi = -\frac{1}{2\pi\tau}\int dE \frac{1}{E^2 - w^2 + \Delta^2} = 0 \quad \text{for} \quad w^2 > \Delta^2 = \frac{-1}{2\tau(\Delta^2 - w^2)^{\frac{1}{2}}} \quad \text{for} \quad \Delta^2 > w^2.$$

Thus,

$$\tilde{G}_n = \frac{(w - \Delta\sigma_2)(1 - \chi) + E\sigma_3}{w^2(1 - \chi)^2 - \Delta^2(1 - \chi)^2 - E^2}U.$$

For $w^2 > \Delta^2$, the denominator is $w^2 - (\Delta^2 + E^2)$. For $w^2 < \Delta^2$, the denominator is $w^2\eta^2 - (\Delta^2\eta^2 + E^2)$, where

$$\eta = 1 + \frac{1}{2\tau(\Delta^2 - w^2)^{\frac{1}{2}}} = \text{real}.$$

[13] S. F. Edwards, Phil. Mag. 3, 1020 (1958).

In both cases, $\tilde{G}_n(w)$ has only a cut on the real axis. Thus by the theorem of Baym and Mermin, the continuation is unique, and $\tilde{G}_n(w)$ is the required Green's function.

From $\tilde{G}_n(w)$, we obtain $A(w)$;

$$A(w) = \begin{pmatrix} A_g \\ A_f \end{pmatrix} = [\tilde{G}_n(w + i\delta) - \tilde{G}_n(w - i\delta)]i$$

$$= \begin{pmatrix} \tilde{G}(w + i\delta) - \tilde{G}(w - i\delta) \\ \tilde{F}^\dagger(w + i\delta) - \tilde{F}^\dagger(w - i\delta) \end{pmatrix} i, \tag{16}$$

$$\tilde{G}(w + i\delta) = \frac{w\eta_+ + E}{w^2\eta_+^2 - E^2 - \Delta^2\eta_+^2},$$
$$\tilde{F}^\dagger(w + i\delta) = \frac{-i\Delta\eta_+}{w^2\eta_+^2 - E^2 + \Delta^2\eta_+^2}, \tag{17}$$

where

$$\eta_+ = 1 + i/2\tau(w^2 - \Delta^2)^{\frac{1}{2}} \quad \text{for } w^2 > \Delta^2,$$
$$= 1 + 1/2\tau(\Delta^2 - w^2)^{\frac{1}{2}} \quad \text{for } \Delta^2 > w^2,$$

$$\tilde{G}(w - i\delta) = \frac{w\eta_- + E}{w\eta_-^2 - E^2 - \Delta^2\eta_-^2},$$
$$\tilde{F}^\dagger(w - i\delta) = \frac{-i\Delta\eta_-}{w^2\eta_-^2 - E^2 - \Delta^2\eta_-^2}, \tag{18}$$

where

$$\eta_- = 1 - i/2\tau(w^2 - \Delta^2)^{\frac{1}{2}}, \quad \text{for } w^2 > \Delta^2,$$
$$= 1 + 1/2\tau(\Delta^2 - w^2)^{\frac{1}{2}}, \quad \text{for } \Delta^2 > w^2.$$

Two cases can now be distinguished.

(1) The extreme anomalous skin effect region, where k is very large. In this case $1/\tau \ll vk$, and we can neglect $1/\tau$. Then the effect of impurity disappears and we can treat the superconductor as a pure metal. Obviously one should then get the results of Abrikosov and of Mattis and Bardeen. We show this explicitly afterwards.

(2) The normal skin effect region, where $vk \ll 1/\tau$. We can then neglect k. This is the result we are immediately interested in. Substituting (17) and (18) in (16), and averaging over the Green's function lines by summing over the ladder diagrams, we obtain after some calculation

$$\mathbf{j}(w_0) = -\frac{Ne^2}{mc}\tfrac{1}{4}\mathbf{A}(w_0)\int_{\Delta+\frac{1}{2}w_0}^{\infty} d\omega\left(\tanh\frac{w_+}{2T} - \tanh\frac{w_-}{2T}\right)\left\{\left[1 - \frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(w_-^2 - \Delta^2)^{\frac{1}{2}}}\right]\right.$$
$$\times \frac{-2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} + (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}} - \left[1 + \frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(w_-^2 - \Delta^2)^{\frac{1}{2}}}\right]$$
$$\left.\times \frac{-2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} - (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}^2}\right\} + \int_{\Delta-\frac{1}{2}w_0}^{\Delta+\frac{1}{2}w_0} d\omega \tanh\frac{w_+}{2T}\frac{(w_+w_- + \Delta^2)}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(\Delta^2 - w_-^2)^{\frac{1}{2}}i}$$
$$\times \left\{\frac{-2i[(1/\tau_{tr}) + (\Delta^2 - w_-^2)^{\frac{1}{2}}]}{(w_+^2 - \Delta^2) + [(\Delta^2 - w_-^2)^{\frac{1}{2}} + 1/\tau_{tr}]^2} + \frac{2i[(\Delta^2 - w_-^2)^{\frac{1}{2}}(1/\tau_{tr})]}{(w_+^2 - \Delta^2) + [(\Delta^2 - w_-^2)^{\frac{1}{2}} - 1/\tau_{tr}]^2}\right., \tag{19}$$

where $W_0 < 2\Delta$, $W_+ = W + \frac{1}{2}W_0$, $W_- = W - \frac{1}{2}W_0$,

$$\frac{1}{\tau_{tr}} = \frac{nmp_0}{(2\pi)^2}\int |u(\theta)|^2(1 - \cos\theta)\, d\Omega, \quad \frac{1}{\tau} = \frac{nmp_0}{(2\pi)^2}\int |u(\theta)|^2\, d\Omega,$$

and

$$\mathbf{j}(w_0) = -\frac{Ne^2}{mc}\tfrac{1}{4}\mathbf{A}(w_0)\int_{\Delta+\frac{1}{2}w_0}^{\infty} dw\left(\tanh\frac{w_+}{2T} - \tanh\frac{w_-}{2T}\right)$$
$$\times \left[1 - \frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(w_-^2 - \Delta^2)^{\frac{1}{2}}}\right]\frac{-2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} + (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}} - \left[1 + \frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(w_-^2 - \Delta^2)^{\frac{1}{2}}}\right]$$
$$\times \frac{-2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} - (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}^2} + \int_{\Delta-\frac{1}{2}w_0}^{\frac{1}{2}w_0-\Delta} -dw \tanh\frac{w_+}{2T}\left[\frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(w_-^2 - \Delta^2)^{\frac{1}{2}}}\right]$$
$$\times \left\{\frac{2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} + (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}^2} + \frac{2i/\tau_{tr}}{[(w_+^2 - \Delta^2)^{\frac{1}{2}} - (w_-^2 - \Delta^2)^{\frac{1}{2}}]^2 + 1/\tau_{tr}^2}\right\} + \int_{\frac{1}{2}w_0-\Delta}^{\frac{1}{2}w_0+\Delta} -dw \tanh\frac{w_+}{2T}$$
$$\times \left\{\frac{-2i[(1/\tau_{tr}) + (\Delta^2 - w_-^2)^{\frac{1}{2}}]}{w_+^2 - \Delta^2 + [(\Delta^2 - w_-^2)^{\frac{1}{2}} + 1/\tau_{tr}]^2} + \frac{2i[(\Delta^2 - w_-^2)^{\frac{1}{2}} - (1/\tau_{tr})]}{w_+^2 - \Delta^2 + [(\Delta^2 - w_-^2)^{\frac{1}{2}} - 1/\tau_{tr}]^2}\right\}\left[\frac{w_+w_- + \Delta^2}{-(w_+^2 - \Delta^2)^{\frac{1}{2}}(w^2 - \Delta^2)^{\frac{1}{2}}i}\right] \tag{20}$$

(for $w_0 > 2\Delta$).

From (19) and (20) we obtain, for $1/\tau_{tr} > \Delta$,

$$\mathbf{j}(w_0) = (Ne^2\Delta/mc\pi)\tau_{tr}\mathbf{A}(w_0)Q(w_0), \qquad (21)$$

where $Q(w_0)$ is the same as Eq. (6.11) of Khalatnikov and Abrikosov,[4] i.e., the kernel of a Pippard pure metal. The only change, apart from a numerical factor of $\frac{3}{16}$, is to replace $1/vk$ in the Pippard limit by τ_{tr}, in the alloy case (where v is the Fermi velocity and k is the momentum exchange).

The interpretation of this result is quite obvious. Since $1/vk \sim \xi/v$, where ξ is the coherence length, while $\tau_{tr} \sim l/v$, where l is the mean free path, the result means that in a superconducting alloy, the mean free path takes over the role of coherence distance. The present result is valid for all temperatures up to T_c, while the same conclusion was already contained in Abrikosov's work at zero temperature.

We have so far mentioned two extreme regions, the anomalous skin effect region and the normal skin effect region. There is yet a third region which is the intermediate region, where $vk \sim 1/\tau$. Starting from (13), we have obtained the current in this region for both superconductors and normal metal. The final results are

Superconductors:

For $w_0 < 2\Delta$,

$$vk \sim 1/\tau, \quad w_0 \quad \text{and} \quad T \ll vk; \quad (2\Delta w_0)^{\frac{1}{2}} < vk.$$

$$\mathbf{j}(\mathbf{k}, w_0) = \int_{\Delta-\frac{1}{2}w_0}^{\Delta+\frac{1}{2}w_0} d\omega \tanh\frac{w_+}{2T}\left[\frac{3Ne^2}{2mc}\mathbf{A}(\mathbf{k}, w_0)\right] \times \frac{-w_+w_- - \Delta^2}{2(w_+^2 - \Delta^2)^{\frac{1}{2}}(\Delta^2 - w_-^2)^{\frac{1}{2}}} \times \left[\frac{-1}{v^2k^2\tau} + \left(\frac{1}{vk} + \frac{1}{v^3k^3\tau}\right)\arctan vk\tau\right]. \qquad (22)$$

Normal metal:

$$vk \sim 1/\tau.$$

$$\mathbf{j}(\mathbf{k}, w_0) = -\frac{3Ne^2}{mc}\ln\cosh\frac{w_0}{2T} \times \left\{\frac{1}{vk}\ln\left[\frac{1 + (w_0 + vk)^2\tau^2}{1 + (w_0 - vk)^2\tau^2}\right]^{\frac{1}{2}} - \frac{i}{vk} \times [\arctan(w_0\tau + vk\tau) - \arctan(w_0\tau - vk\tau)]\right\}\mathbf{A}(\mathbf{k}, w_0). \qquad (23)$$

We have not averaged over the Green's function lines to change τ into τ_{tr}. However, as long as $vk < F_f$, the Fermi energy, it seems that τ_{tr} should take the place of τ. At any rate, it is safe to leave τ as a parameter. Equations (22) and (23) then give the current as a function of the other parameters Δ, w_0, T, and vk.

Finally, we show that our formula reproduces all the previous results of Abrikosov *et al.* when one or more of the parameters is put to the limit.

(a) $T = 0$.

From (19), we have, for $w_0 < 2\Delta$, $1/\tau_{tr} > \Delta$,

$$\mathbf{j}(w_0) = -\frac{Ne^2}{mc}\mathbf{A}(w_0)\tau_{tr}\int_{\Delta-\frac{1}{2}w_0}^{\Delta+\frac{1}{2}w_0} d\omega \times \frac{w_+w_- + \Delta^2}{(w_+^2 - \Delta^2)^{\frac{1}{2}}(\Delta^2 - w_-^2)^{\frac{1}{2}}}. \qquad (24)$$

This is the equation from which Abrikosov *et al.*[1] calculated the current for superconducting alloys at zero temperature.

(b) Pure metal. $\tau = \infty$. We have

$$\iint [A_g(w_1)A_g(w_2) - A_f(w_1)A_f(w_2)]\, d\omega_1\, d\omega_2 \times \frac{1}{w_0 - w_2 - w_1 + i\delta}\left(\tanh\frac{\omega_1}{2T} - \tanh\frac{\omega_2}{2T}\right) = -\pi^2\left(1 - \frac{E_+E_- + \Delta^2}{\epsilon_-\epsilon_+}\right)\left(\tanh\frac{\epsilon_+}{2T} + \tanh\frac{\epsilon_-}{2T}\right) \times \left(\frac{1}{\epsilon_+ + \epsilon_- + w_0 + i\delta} + \frac{1}{\epsilon_+ - \epsilon_- + w_0 - i\delta}\right) + \left(1 + \frac{E_-E_+ + \Delta^2}{\epsilon_-\epsilon_+}\right)\left(\tanh\frac{\epsilon_+}{2T} - \tanh\frac{\epsilon_-}{2T}\right) \times \left(\frac{1}{\epsilon_+ - \epsilon_- + w_0 + i\delta} + \frac{1}{\epsilon_+ - \epsilon_- - w_0 - i\delta}\right), \qquad (25)$$

where

$$\epsilon_+ = (E_-^2 + \Delta^2)^{\frac{1}{2}}, \quad \epsilon_- = (E_-^2 + \Delta^2)^{\frac{1}{2}}.$$

From (25) we obtain a current which is the same as Eq. (11) of Ref. 2(a) or Eq. (6.5) of Ref. 4. This equation can be used for both Pippard and London regions.

(c) Static field. $w = 0$.

From (19) we get, for $1/\tau_{tr} > \Delta$,

$$\mathbf{j} = -\frac{Ne^2}{mc}\mathbf{A}\tau_{tr}\int_{\Delta}^{\Delta+w_0} d\omega \tanh\frac{w}{2T} \times \frac{w(w - w_0) + \Delta^2}{(w^2 - \Delta^2)^{\frac{1}{2}}[\Delta^2 - (w - w_0)^2]^{\frac{1}{2}}}$$

for $w_0 \to 0$. Write $w' = w - \Delta$,

$$\mathbf{j} = -\frac{Ne^2}{mc}\mathbf{A}\tau_{tr}\int_0^{w_0} dw' \tanh\frac{\Delta + w'}{2T} \times \frac{2\Delta^2}{(2\Delta w')^{\frac{1}{2}}[2\Delta(w_0 - w')]^{\frac{1}{2}}}$$

$$= -\frac{Ne^2}{mc}\mathbf{A}\tau_{tr}\int_0^1 dt \tanh\frac{\Delta}{2T}\Delta\frac{1}{[t(1-t)]^{\frac{1}{2}}} \quad (\text{where } t = w'/w_0)$$

$$= -\sigma\mathbf{A}\Delta\tanh\frac{\Delta}{2T}\int_0^{\frac{1}{2}\pi}\frac{2\sin\theta\cos\theta\, d\theta}{\sin\theta\cos\theta} \quad (\text{where } t = \sin^2\theta)$$

$$= -\sigma\mathbf{A}[(\tanh(\Delta/2T)]\pi\Delta.$$

This agrees with the result of Abrikosov *et al.*[3]

SUMMARY

(1) We have obtained the general expression for the electromagnetic current **j** of a superconductor with impurity scattering at any temperature up to T_c, i.e., Eq. (13), as a function of input frequency w of the external electromagnetic field **A** and momentum exchange during collision **k**.

(2) This equation is the Fourier transform of Mattis and Bardeen's[4] Eq. (3.3), and summarizes in one equation all the previous work of Abrikosov and his co-workers on the electromagnetic behavior of superconductors. An explicit derivation of all their results from Eq. (13) has been given.

(3) We have found, in particular, a quantitative result in Eq. (21), which can be clearly interpreted as meaning that for most of superconducting alloys, as long as the impurity concentration is over a few percent, the mean free path l takes over the role of coherence distance ξ, regardless of temperature. In addition, we have also given expressions for the current in closed form for $vk \sim 1/\tau$ [Eqs. (22) and (23)].

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A Unifying Principle in Statistical Mechanics*

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A fundamental problem of statistical mechanics is to obtain simplified descriptions of complex systems. A general principle is presented for obtaining equations of motion for such descriptions. The principle involves maximizing an appropriate entropy functional. It also involves the particle dynamics through the Liouville equation. Various special cases are presented in which the principle yields the Vlasov equation, the Boltzmann equation, Euler's hydrodynamic equations, a generalization of Grad's ten-moment approximation, the Gibbs distribution (i.e., equilibrium statistical mechanics), and Onsager's equations of irreversible thermodynamics. The principle also yields, trivially, the Liouville equation and Hamilton's equations of classical mechanics. Some of these results have been derived elsewhere by very similar procedures, but apparently the generality of the principle has been unrecognized. In terms of the general principle, the origin of irreversibility in the various equations of motion is easily seen, and the relation between the numerous definitions of entropy is clarified. No *a priori* justification of the principle itself is given.

1. INTRODUCTION

A FUNDAMENTAL problem of statistical physics is to obtain simplified descriptions of complex systems. The formulas of equilibrium statistical mechanics and the equations of nonequilibrium theory have proven remarkably successful in practice, but when one examines their derivations one is confronted by a bewildering multitude of poorly justified methods. In a discipline which has a long tradition of paradoxes and controversies, the real question is why does it work so well? A great deal of research has been directed towards understanding the foundations of equilibrium theory. It is here that ergodic theory had its origin. But without additional unjustified assumptions, ergodic theory fails to explain the basic formulas. The state of affairs in nonequilibrium theory is even worse.

Confronted by the absence of any satisfactory derivation of fundamental formulas, one might be prepared, tentatively, to accept an approach which at least has the virtue of simplicity. For equilibrium theory, one such approach is the derivation of the canonical distribution formula by maximizing an appropriate entropy functional subject to prescribed average energy. This method was described very early by Gibbs[1] and has more recently been discussed

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[1] J. W. Gibbs, *Elementary Principles in Statistical Mechanics* (Yale University Press, New Haven, Connecticut, 1902; Dover Publications, Inc., New York, 1960).

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by Jaynes[2-4] who has emphasized its interesting connections with information theory. It is natural to ask if this method can be extended to nonequilibrium statistical mechanics.

Any such extension must obviously involve the dynamics of the system underlying the statistical description. We have found that it is possible to combine the process of maximizing an appropriate entropy functional with the "solution operator" of the Liouville equation to obtain a "general principle" which yields many of the equations of statistical mechanics, both equilibrium and nonequilibrium. The idea is a fairly obvious one and this principle, or a very similar principle, has been employed in special cases by other authors.[5-8] But apparently the generality of the principle has not been recognized earlier. Our main object in this paper is to demonstrate its generality—and its simplicity—by deriving a variety of basic results. It seems likely that other well-known results can be, or perhaps already have been, derived by this method. We emphasize that no *a priori* justification of the general principle is given.

No new equations are derived here, but it is clear that for almost any function or set of functions one wishes to choose to describe a many-body system, the principle will yield equations of motion for these functions. Thus, for example, there are no "closure" problems. Of course, it is not guaranteed that these equations will be sufficiently simple to be useful and it remains to be seen whether they will yield predictions that agree with experiment.

Before stating the principle, we must explain what we mean by a "simplified description." A good example is the "one-particle distribution function" of a many-body system. We call such a function a "state function." With each state function, we associate a "complete description," consisting of an equation of motion and an entropy functional. Then for any simpler state function (related by a linear transformation to the original one), we present (Sec. 3) a simple rule which yields a complete description (equation of motion plus entropy functional) for the new state function. The process can then be repeated. Thus, beginning with Liouville's equation of motion for the n-particle function, one can derive a wide variety of descriptions at various levels of complexity. (Because of this possibility of multiple levels of description, we avoid the terms "microscopic" and "macroscopic.") For each description the principle yields a new entropy functional. This explains the appearance of many definitions of entropy in physics and clarifies the relations among them. The origin of "irreversibility" in the equations as derived by the principle is also very easily seen. All of the work presented here is based on classical statistical mechanics, but it seems likely that there would be no serious obstacle to extending it to the quantum mechanical case.

In Sec. 4, we apply the principle which is stated in Sec. 3 to the one-particle distribution function. The resulting equation of motion is the Vlasov equation. In order to obtain the Boltzmann equation (Sec. 6), it is necessary to generalize the principle slightly. This is done in Sec. 5. Then the principle of Sec. 3 appears as a special case. In Secs. 7 and 8 we use the principle to derive hydrodynamic equations from the Boltzmann equation. The equations of Sec. 8 generalize those of Grad's "thirteen moment approximation." They reduce to Grad's equations when the pressure tensor is nearly scalar. For completeness, we repeat Gibbs' derivation of the canonical distribution function in Sec. 9, and in Sec. 10 we derive the equations of irreversible statistical mechanics and the Onsager relations by means of the general principle. Section 2 contains a brief discussion of the Liouville equation and related matters. By including this section, we facilitate the later derivations and provide a treatment which is almost self-contained.

2. CLASSICAL STATISTICAL MECHANICS: PRELIMINARIES

A conservative classical mechanical system with r degrees of freedom is characterized by its Hamiltonian $H(z)$, where $z = (q,p) = (q_1, \cdots, q_r, p_1, \cdots, p_r)$, the q_j are generalized coordinates, and the p_j the conjugate momenta. The state of the system at time t is determined by the point $z(t)$ in $2r$-dimensional "phase space" which moves on a trajectory determined by solving Hamilton's equations

$$\dot{q}_i = \partial H/\partial p_i, \quad \dot{p}_i = -\partial H/\partial q_i; \qquad i = 1, \cdots, r; \quad \dot{} = d/dt. \tag{2.1}$$

Under suitable conditions on H, the solution $z(t) = [q(t), p(t)]$, corresponding to given initial conditions $z(0)$, is uniquely determined. Therefore, in principle, there exists a one-parameter family of "solution

[2] E. T. Jaynes, Phys. Rev. **106**, 620 (1957).
[3] E. T. Jaynes, Phys. Rev. **108**, 171 (1957).
[4] E. T. Jaynes, *Probability Theory in Science and Engineering*, Colloquium Lectures in Pure and Applied Science, No. 4, Socony Mobil Oil Company (1958).
[5] L. S. Hall, Lawrence Radiation Laboratory, University of California, Report UCRL-6751 (1962).
[6] A. M. Kogan, J. Appl. Math. Mech. **29**, 130 (1965).
[7] R. Kubo, *Lectures in Theoretical Physics*, W. E. Brittin and L. G. Dunham, Eds. (Interscience Publishers, Inc., New York, 1959), Vol. I, pp. 120–203.
[8] J. L. Lebowitz, H. L. Frisch, and E. Helfand, Phys. Fluids **3**, 1 (1960).

operators" S_t such that

$$z(t) = S_t z(0), \quad S_0 = 1, \quad S_t S_{t'} = S_{t+t'}. \tag{2.2}$$

In practice the solution, and hence the solution operator, cannot be computed for any but the simplest systems. Any physical observable corresponds to a "phase function" $\psi(t, z) = \psi(t, q, p)$. The value $\psi[t, z(t)]$ of ψ corresponding to a state $z(t)$ clearly satisfies

$$\frac{d}{dt}\psi = \frac{\partial \psi}{\partial t} + (\psi; H) = \frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial \psi}{\partial p_i}\frac{\partial H}{\partial q_i}. \tag{2.3}$$

In particular,

$$(d/dt)H[z(t)] = 0, \tag{2.4}$$

i.e., $H(s_t z)$ is independent of t.

It is convenient to introduce a *momentum reversal operator* $\mathcal{R}$ defined simply by

$$\mathcal{R}z = \mathcal{R}(q, p) = (q, -p). \tag{2.5}$$

For any solution $q(t)$, $p(t)$ of (1), it is easy to see that $q^*(t) = q(-t)$, $p^*(t) = -p(-t)$ is also a solution of (2.1) provided the Hamiltonian is an even function of the momenta, i.e.,

$$H(\mathcal{R}z) = H(z). \tag{2.6}$$

It follows that

$$\begin{aligned}\mathcal{R}S_{-t}[q(0), p(0)] &= [q(-t), -p(-t)] \\ &= [q^*(t), p^*(t)] = S_t[q^*(0), p^*(0)] \\ &= S_t[q(0), -p(0)] = S_t\mathcal{R}[q(0), p(0)].\end{aligned} \tag{2.7}$$

Since the initial conditions $[q(0), p(0)]$ in (2.7) are arbitrary, we see from (2.7) and (2.5) that

$$\mathcal{R}S_{-t} = S_t\mathcal{R}, \quad \mathcal{R}^2 = 1. \tag{2.8}$$

This equation expresses the time-reversibility of Hamilton's equations and hence of the Liouville equation which we shall introduce shortly.

In statistical mechanics, we introduce a probability distribution P_t in phase space and a corresponding probability density $w(t, z)$ such that for every subset A,

$$P_t(A) = \int_A w(t, z)\, dz \tag{2.9}$$

is the probability that at time t, z is in A. The expected value of the observable corresponding to the phase function φ is now

$$\langle \varphi \rangle_t = \int \varphi w\, dz; \tag{2.10}$$

P_t must satisfy the obvious requirement of "conservation of probability,"

$$P_t(S_t A) = P_0(A). \tag{2.11}$$

It can easily be shown[9,10] that the volume element dz in phase space is preserved by the solution operators S_t, i.e.,

$$d(S_t z) = dz. \tag{2.12}$$

We see from (2.11) and (2.12) that for any set A

$$\int_{S_t A} w(t, z)\, dz = \int_A w(0, z)\, dz = \int_{S_t A} w(0, S_{-t}z)\, dz. \tag{2.13}$$

If we define the solution operator applied to a function by

$$S_t g(z) = g(S_t z), \tag{2.14}$$

it follows from (2.13) that

$$w(t, z) = S_{-t}w(0, z). \tag{2.15}$$

Since $w(t, z) = w(0, S_{-t}z)$, we see from (2.3) that

$$\partial w/\partial t = (H; w). \tag{2.16}$$

This is the Liouville equation and (2.15) is its formal solution.

From (2.12) we find that for any function $f(z)$

$$\int f(S_t z)\, dz = \int f(z)\, dz. \tag{2.17}$$

In particular, if we introduce the *basic entropy functional*

$$S[w] = -k\int w(t, z) \log w(t, z)\, dz, \tag{2.18}$$

we see from Eqs. (2.15), (2.14), and (2.17) that S is independent of t, i.e.,

$$(d/dt)S[w] = 0. \tag{2.19}$$

In (2.18) k is Boltzmann's constant.

For the most part we restrict our considerations to a system of n identical monatomic particles of mass m. If the jth particle has Cartesian coordinates $\mathbf{q}_j = (q_j^1, q_j^2, q_j^3)$ and momentum $\mathbf{p}_j = (p_j^1, p_j^2, p_j^3)$, we set $z_j = \mathbf{q}_j, \mathbf{p}_j$ and take the Hamiltonian to be of the form

$$\begin{aligned}H_n(z) &= H_n(z_1, \cdots, z_n) \\ &= \sum_{j=1}^{n} \frac{1}{2m}\mathbf{p}_j^2 + \sum_{1 \le i < j \le n} \varphi(|\mathbf{q}_i - \mathbf{q}_j|).\end{aligned} \tag{2.20}$$

Here $\varphi(r)$ is the interparticle potential function. The solution operator corresponding to (2.20) is denoted by $S_t^{(n)}$. We consider particles confined to a region $\mathfrak{D}$ of volume V. Then (2.20) should include an additional term $\sum_{j=1}^{n} u_{\mathfrak{D}}(\mathbf{q}_j)$, where $u_{\mathfrak{D}}(\mathbf{q})$ is zero inside $\mathfrak{D}$ and rapidly approaches infinity at the boundary. Since we

[9] H. Grad, *Kinetic Theory and Statistical Mechanics*, New York University, lecture notes (1950).

[10] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, Inc., New York, 1962).

let n and $\mathfrak{D}$ become infinite in such a way that the specific volume $v = V/n$ has a finite limit, we omit the additional terms in (2.20).

In an attempt to obtain a simplified description, one frequently introduces the "s-particle functions"

$$f_s(t, z_1, \cdots, z_s) = \int w(t, z_1, \cdots, z_n)\, dz_{s+1} \cdots dz_n, \qquad s = 1, 2, \cdots. \quad (2.21)$$

Then $f_n = w$. For identical particles, w is a symmetric function of $z_1, \cdots, z_n$ and is normalized by

$$\int w\, dz_1 \cdots dz_n = 1. \quad (2.22)$$

It follows that f_s is a symmetric function of $z_1, \cdots, z_s$ and

$$\int f_s\, dz_1 \cdots dz_s = 1. \quad (2.23)$$

For some purposes, it is more convenient to use the s-particle functions

$$F_s(t, z_1, \cdots, z_s) = V^s f_s. \quad (2.24)$$

In the limit, $n \to \infty$, $V \to \infty$, $V/n = v$, it is possible to obtain an expansion for $F_s(t, z_1, \cdots, z_s)$ in inverse powers of v in terms of the initial values $F_m(0, z_1, \cdots, z_m)$ of the m-particle functions and the solution operators $S_t^{(m)}$ for small values of $m \geq s$. In the simplest case, $s = 1$ and the leading terms of the expansion are given by[11]

$$F_1(t, z_1) = S_{-t}^{(1)} F_1(0, z_1) + \frac{1}{v} \int [S_{-t}^{(2)} F_2(0, z_1, z_2) - F_2(0, S_{-t}^{(1)} z_1, S_{-t}^{(1)} z_2)]\, dz_2 + O\left(\frac{1}{v^2}\right). \quad (2.25)$$

Since initial data can be specified at an arbitrary time, a more general form of the expansion is

$$F_1(t + \tau, z_1) = S_{-\tau}^{(1)} F_1(t, z_1) + \frac{1}{v} \int [S_{-\tau}^{(2)} F_2(t, z_1, z_2) - F_2(t, S_{-\tau}^{(1)} z_1, S_{-\tau}^{(1)} z_2)]\, dz_2 + O\left(\frac{1}{v^2}\right). \quad (2.26)$$

The remainder term includes the solution operators for three and more particles. Since the first two terms involve at most two particle interactions, it is clear that for given v the remainder cannot be neglected for all τ. Rather, one must impose the restriction [see Ref. 11(b)]

$$\tau \ll t_1 = v/r_0^2 \xi_0. \quad (2.27)$$

Here r_0 is the effective range of the interparticle potential, ξ_0 is the average particle speed, and t_1 is the average time between collisions. The expansion (2.26) is useful in our derivation of the Boltzmann equation in Sec. 6.

3. THE SPECIAL PRINCIPLE

A major goal of statistical mechanics is to obtain simplified descriptions of a complex system. An important example is given by

$$f_1(t, z_1) = \int w(t, z)\, dz_2 \cdots dz_n \quad (3.1)$$

which is a function of seven variables whereas w is a function of $6n + 1$ variables. The problem is to obtain an equation of motion for f_1 from the Liouville equation for w. In this case we proceed as follows: For given $f_1(t, z_1)$, many nonnegative symmetric normalized functions $w(t, z_1)$ can be found which satisfy (3.1). Of these functions, we choose the unique w which maximizes the basic entropy functional (2.18). We denote this function by $w(f_1; z)$ or simply $w[f_1]$ since it depends on the function f_1. (Thus $w[f_1]$ is a functional of f_1 and a function of z.) By construction it satisfies (3.1), i.e.,

$$f_1(t, z_1) = \int w[f_1]\, dz_2 \cdots dz_n. \quad (3.2)$$

We now assume that

$$\frac{\partial}{\partial t} f_1 = \int w_t[f_1]\, dz_2 \cdots dz_n, \quad (3.3)$$

where w_t is given by the Liouville equation (2.16). Thus,

$$\frac{\partial f_1}{\partial t} = \int (H; w[f_1])\, dz_2 \cdots dz_n, \quad (3.4)$$

which is the required equation of motion for f_1. It is important to note that $w[f_1]$ provides us not only with the equation of motion (3.4) but also a new entropy functional $S_1[f_1]$ defined by

$$S_1[f_1] = \max_{(3.1)} S[w] = S[w[f_1]]. \quad (3.5)$$

In Sec. 4 we actually compute $w[f_1]$ and analyze the resulting Eq. (3.4). Before doing so let us abstract from what we have done in order to obtain a principle.

We call a function such as $w(t, z)$ or $f_1(t, z_1)$, which describes the state of a statistical mechanical system, a *state function*. For a given state function u, we assume that we have a *complete description* consisting of an equation of motion

$$\partial u/\partial t = Mu \quad (3.6)$$

and an entropy functional,

$$S = S[u]. \quad (3.7)$$

[11] See (a) R. M. Lewis, J. Math. Phys. **2**, 222 (1961), Eqs. (41), (39), (42). Equation (8.5) of (b) N. N. Bogoliubov, *Studies in Statistical Mechanics*, J. DeBoer and G. E. Uhlenbeck, Eds. (North-Holland Publishing Company, Amsterdam, 1962), Vol. I, pp. 5–118 can also be transformed to yield (25).

Here u is a function of the time t and, in general, of other variables. In some cases (see Secs. 7, 8, and 10) u is a vector, i.e., a set of functions. M is an operator, in general, nonlinear, and S is real valued.

Given the description (3.6 and 3.7) in terms of u, we introduce a new state function derived from u,

$$f = Lu. \tag{3.8}$$

Here, L is a linear operator, in general not invertible.[12] In order to obtain a complete description in terms of f, we employ the following *special principle: For given f, let $u[f]$ be the unique*[13] *state function that maximizes* (3.7) *subject to* (3.8), *and possibly other side conditions such as normalization or symmetry conditions. Then the equation of motion for f is*

$$\partial f/\partial t = LMu[f], \tag{3.9}$$

and its entropy functional is

$$S_1[f] = S[u[f]]. \tag{3.10}$$

Beginning with the *basic description* in terms of w, i.e., the Liouville equation and the basic entropy functional, we may obtain descriptions for a great variety of derived state functions. Some of these are examined in succeeding sections. We see that the resulting equations of motion agree with or generalize well-known equations that have been obtained earlier by quite different methods. The established usefulness of these equations is the main source of confidence in the validity of our principle. For each description, an entropy functional arises naturally, defined by (3.10). This explains the appearance of many different definitions of entropy in different physical descriptions, and the relations between them.[14]

In our statement of the principle, we began with a complete description (3.6), (3.7) for a state function u. Since the derived description (3.9), (3.10) for f is complete we can, of course, repeat the process. If we introduce a new state function

$$g = \mathfrak{L}f, \tag{3.11}$$

we obtain from (3.9) and (3.10) the complete description for g,

$$\partial g/\partial t = \mathfrak{L}LMu[f[g]], \tag{3.12}$$

$$S_2[g] = S_1[f[g]] = S[u[f[g]]]. \tag{3.13}$$

Here $f[g]$ maximizes (3.10) subject to (3.11). It is quite natural to require that any principle, such as the one we have introduced, should be *transitive*. This means that the description (3.12), (3.13) which we have obtained in two steps should be the same as the description we would obtain for

$$g = \mathfrak{L}Lu \tag{3.14}$$

in one step by applying the principle to the original description (3.6), (3.7) for u. In fact if we do that the result is easily seen to be

$$\partial g/\partial t = \mathfrak{L}LM\hat{u}[g], \tag{3.15}$$

$$S_2[g] = S[\hat{u}[g]], \tag{3.16}$$

where $\hat{u}[g]$ maximizes (3.7) subject to (3.14). By comparing (3.12), (3.13) with (3.15), (3.16) we see that they agree if and only if

$$\hat{u}[g] = u[f[g]]. \tag{3.17}$$

But

$$\max_{g=\mathfrak{L}Lu} S[u] = \max_{g=\mathfrak{L}f} \{\max_{f=Lu} S[u]\} = \max_{g=\mathfrak{L}f} S[u[f]]$$
$$= S[u[f[g]]]. \tag{3.18}$$

Therefore $u[f[g]]$ maximizes (3.7) subject to (3.14), hence (3.17) is satisfied. This establishes the transitivity of the principle.

In closing this section, we observe a trivial consequence of our principle. Starting with w, we take $L = 1$. Then the "derived description" is again given by the Liouville equation and the basic entropy functional. In particular, if w is given initially by

$$w(0, z) = \delta(z - z_0), \tag{3.19}$$

then (2.15) yields

$$w(t, z) = \delta(S_{-t}z - z_0) \tag{3.20}$$

and (2.10) becomes

$$\langle \varphi \rangle_t = \varphi(S_t z_0). \tag{3.21}$$

Thus classical statistical mechanics, in terms of the Liouville equation and classical mechanics, appear trivially as special cases of our principle.

4. THE VLASOV EQUATION

We apply the principle stated in Sec. 3 to

$$f_1(z_1) = \int w(z)\, dz_2 \cdots dz_n. \tag{4.1}$$

We first maximize the basic entropy functional (2.18) subject to (2.22), (4.1) and the condition that w be a symmetric function of $z = (z_1, \cdots, z_n)$. This can be done conveniently by using the method of Lagrange multipliers. We introduce the functional

$$J(w, \lambda, \beta) = S[w] - \beta\left(\int w\, dz - 1\right) - Q(w, \lambda), \tag{4.2}$$

[12] If L were invertible, the description in terms of f would be equivalent to that in terms of u and no simplification would be accomplished.

[13] We assume that a unique maximum exists.

[14] See H. Grad, Commun. Pure Appl. Math. **14**, 323 (1961).

where $S[w]$ is given by (2.18) and

$$Q = \int \lambda(z_1)\left\{\int w(z)\, dz_2 \cdots dz_n - f_1(z_1)\right\} dz_1. \quad (4.3)$$

The conditions $\partial J/\partial\beta = 0$ and $\delta J/\delta\lambda(z_1) = 0$ yield (2.22) and (4.1). Since w is symmetric, (4.3) can be rewritten as

$$Q = \frac{1}{n}\sum_{i=1}^{n}\int \lambda(z_i) w\, dz - \int \lambda f_1\, dz_1. \quad (4.4)$$

Therefore the condition $\delta J/\delta w(z) = 0$ yields

$$-k(1 + \log w) - \beta - \frac{1}{n}\sum_{i=1}^{n}\lambda(z_i) = 0. \quad (4.5)$$

It follows that

$$w(z) = c\prod_{i=1}^{n}\exp\left\{-\frac{1}{n}\lambda(z_i)\right\}, \quad (4.6)$$

where c is a constant, and from (4.1) we see that the maximizing w is

$$w(z) = w[f_1] = \prod_{i=1}^{n} f_1(z_i). \quad (4.7)$$

The equation of motion for f_1 is now given by (3.9) or equivalently (3.4). Thus,

$$\frac{\partial f_1}{\partial t}(t, z_1) = \int\left\{H(z); \prod_{i=1}^{n} f_1(z_i)\right\} dz_2 \cdots dz_n. \quad (4.8)$$

If we now insert the Hamiltonian (4.20), then a straightforward calculation yields the equation

$$D_t f_1 = C[f_1], \quad (4.9)$$

where

$$D_t f_1 = \frac{\partial f_1}{\partial t} - \left\{\frac{1}{2m}\mathbf{p}_1^2; f_1(z_1)\right\} = \frac{\partial f_1}{\partial t} + \frac{1}{m}\sum_{\alpha=1}^{3} p_1^\alpha \frac{\partial f_1}{\partial q_1^\alpha}, \quad (4.10)$$

$$C[f_1] = (n-1)\int\{\varphi_{12}; f_1(z_1) f_1(z_2)\}\, dz_2$$

$$= (n-1)\sum_{\alpha=1}^{3}\int \frac{\partial\varphi_{12}}{\partial q_1^\alpha} f_1(z_2)\, dz_2 \frac{\partial f_1(z_1)}{\partial p_1^\alpha}. \quad (4.11)$$

Here $\varphi_{12} = \varphi(|\mathbf{q}_1 - \mathbf{q}_2|)$. The physical interpretation of Eq. (4.9) becomes more evident if we introduce the velocity vector $\boldsymbol{\xi}_1 = (1/m)\mathbf{p}_1$. Then

$$C[f_1] = -\sum_\alpha a_1^\alpha \frac{\partial f_1}{\partial \xi_1^\alpha}, \quad (4.12)$$

where

$$ma_1^\alpha = -\int \frac{\partial\varphi_{12}}{\partial q_1^\alpha} N(\mathbf{q}_2)\, d\mathbf{q}_2, \quad (4.13)$$

$$N(\mathbf{q}_2) = (n-1)\int f_1(\mathbf{q}_2, \mathbf{p}_2)\, d\mathbf{p}_2. \quad (4.14)$$

Now (4.9) becomes

$$\frac{\partial f_1}{\partial t}(t, \mathbf{q}_1, \mathbf{p}_1) + \sum_\alpha \xi_1^\alpha \frac{\partial f_1}{\partial q_1^\alpha} + \sum_\alpha a_1^\alpha \frac{\partial f_1}{\partial \xi_1^\alpha} = 0. \quad (4.15)$$

We see from (4.14) that $N(\mathbf{q}_2)$ is the number density of all but one of the particles, and from (4.13) that $\mathbf{F} = m\mathbf{a}_1 = m(a_1^1, a_1^2, a_1^3)$ is the average intermolecular force on the particle at the point $\mathbf{q}_1$ due to the remaining particles.

5. THE GENERAL PRINCIPLE

The principle introduced in Sec. 3 involves two steps. First we maximize the entropy $S[u]$, and then we use the equation of motion (3.6) for u. Insofar as (3.6) correctly describes the time evolution of u, the second step of the principle appears to be well justified. The first step is the questionable one. Surely it is here that, in order to obtain a simplified description, we pay the price of approximation. In the principle as stated in Sec. 3, the first step is made continuously, i.e., at every instant of time. If instead we could actually solve (3.6), perhaps approximately, at least for a short time τ, and maximize the entropy only after this time, we might obtain a better description for f. In some important cases this can actually be done.

In order to describe this process, we introduce the solution operator T_t of (3.6). Thus,

$$u(t) = T_t u(0), \quad T_0 = 1, \quad T_{t+t'} = T_t T_{t'}. \quad (5.1)$$

As in Sec. 3 we introduce the function $u[f]$ (which is also a functional of f) that maximizes (3.7) subject to (3.8) and hence satisfies

$$f(t) = Lu[f(t)]. \quad (5.2)$$

We now assume that

$$f(t + \tau) = LT_\tau u[f(t)]. \quad (5.3)$$

Since

$$\frac{\partial f(t)}{\partial t} = \frac{f(t+\tau) - f(t)}{\tau} + O(\tau), \quad (5.4)$$

we can, by neglecting a term of order τ, obtain the equation of motion for f,

$$\partial f/\partial t \approx (1/\tau)L\{T_\tau u[f(t)] - u[f(t)]\}. \quad (5.5)$$

The precise form of this equation of motion depends on the choice of τ, and how we make the approximation. (See Secs. 6, 10.) Thus we have been led to the following:

General principle: For given f, let $u[f]$ be the unique state function u that maximizes (3.7) subject to (3.8), and possibly other side conditions such as normalization or symmetry conditions. Then the equation of motion for f is given by (5.5) and its entropy functional by (3.10).

It is easily seen that for $\tau \to 0$, the general principle reduces to the special principle of Sec. 3.

An important feature of the equations of statistical mechanics is their "irreversibility." A great deal of work and considerable controversy has been concerned with the question of how irreversible equations can arise from the Liouville equation which is reversible. In our formulation the origin of the irreversibility is quite clear. If we assume that the description in terms of u has the property

$$S[u(t+\tau)] = S[T_\tau u(t)] \geq S[u(t)] \quad \text{for} \quad \tau > 0, \tag{5.6}$$

i.e., that the entropy is nondecreasing with time, then we can easily show that the derived description in terms of f has the same property. Since we have shown [see (2.19)] that the basic description in terms of w satisfies (5.6) (with strict equality), it will follow that every description derived (directly or indirectly) from it satisfies (5.6). In general (5.6) will not be a strict equality and the corresponding description may be called *irreversible.*

To demonstrate (5.6) for f, we recall that

$$S_1[f(t)] = S[u[f(t)]] = \max_{Lu=f(t)} S[u]. \tag{5.7}$$

Hence, from (5.3)

$$\begin{aligned} S_1[f(t+\tau)] &= \max_{Lu=f(t+\tau)} S[u] \\ &= \max_{Lu=LT_\tau u[f(t)]} S[u] \geq S[T_\tau u[f(t)]]. \end{aligned} \tag{5.8}$$

(Here the inequality would be an equality if L were invertible, i.e., if $Lu = Lu'$ would imply that $u = u'$.) Now from (5.6) and (5.8) we see that

$$S_1[f(t+\tau)] \geq S[u[f(t)]] = S_1[f(t)], \tag{5.9}$$

which is the property (5.6) in terms of f.

6. THE BOLTZMANN EQUATION

In this section we show that, after suitable approximations, the general principle, when applied to the Liouville equation, yields the Boltzmann equation for the one-particle function. Our derivation is similar to one we have given earlier[11a] for the Boltzmann equation, the main difference being that the "molecular chaos assumption" is now not required. Instead it is a consequence of the general principle. The essential tool in our derivation is the expansion (2.26) for F_1.

The assumptions we require are similar to those which are always made (explicitly or implicitly) in derivations of the Boltzmann equation: We again introduce the average particle speed ξ_0 and the effective range r_0 of the interparticle potential. [Then $\varphi(r) \approx 0$ for $r > r_0$.] We also introduce the average duration of a collision, $t_0 = r_0/\xi_0$, and the average time between collisions (mean free time), $t_1 = v/(r_0^2\xi_0)$. Here $v = V/n$ is the volume per particle. We now assume that

$$r_0/\xi_0 = t_0 \ll \tau \ll t_1 = v/r_0^2\xi_0, \tag{6.1}$$

$$F_1(t+\Delta t, \mathbf{q}_1 + \Delta\mathbf{q}_1, \mathbf{p}_1) \approx F_1(t, \mathbf{q}_1, \mathbf{p}_1) \quad \text{for} \quad |\Delta t| \leq \tau, \quad |\Delta\mathbf{q}_1| \leq \tau\xi_0. \tag{6.2}$$

The first condition simply requires that v be much larger than the "effective particle volume" $\frac{4}{3}\pi r_0^3$. It also defines the range of the parameter τ which appears in the statement of the general principle. The second condition requires that F_1 be slowly varying in the space and time coordinates (but not the momentum). The condition on the time variation is sometimes replaced by a "coarse-graining" or time-averaging of F_1.

We now apply the general principle to the one-particle function

$$F_1(t, z_1) = Vf_1 = V\int w(t, z)\, dz_2 \cdots dz_n. \tag{6.3}$$

As in Sec. 4 we maximize the basic entropy functional (2.18) subject to the normalization (2.22), the symmetry condition, and (6.3). The result is [see (4.7)]

$$w = w[F_1] = \tilde{w}(t, z) = \prod_{i=1}^{n} [V^{-1}F_1(t, z_i)]. \tag{6.4}$$

Now in (5.3)[15] we take f to be F_1 and u to be w. Then T_τ becomes the n-particle solution operator $S_{-\tau}^{(n)}$. Thus, (5.3) yields

$$\begin{aligned} F_1(t+\tau, z_1) &= V\int dz_2 \cdots dz_n S_{-\tau}^{(n)}\tilde{w}(t, z) \\ &= V\int dz_2 \cdots dz_n \tilde{w}(t+\tau, z) \\ &= \tilde{F}_1(t+\tau, z_1). \end{aligned} \tag{6.5}$$

Here $\tilde{w}(t+\tau, z) = S_{-\tau}^{(n)}\tilde{w}(t, z)$, i.e., $\tilde{w}(t', z)$ is the solution of the Liouville equation with initial conditions (6.4) specified at time t, and $\tilde{F}_1$ is the one-particle function corresponding to $\tilde{w}$. In fact, in general, we define

$$\tilde{F}_s(t', z_1, \cdots, z_s) = V^s\int \tilde{w}(t', z)\, dz_{s+1} \cdots dz_n, \quad s = 1, 2, \cdots. \tag{6.6}$$

It follows from (6.4) that at the initial time

$$\tilde{F}_s(t, z_1, \cdots, z_s) = \prod_{i=1}^{s} F_1(t, z_i), \quad s = 1, 2, \cdots. \tag{6.7}$$

[15] We proceed from (5.3), because we wish to be more explicit about the form of the approximation made in (5.5).

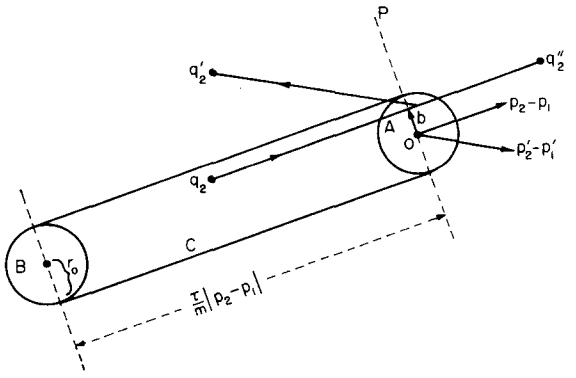

FIG. 1. Configuration space for a binary collision.

We now use (2.26) for $\tilde{F}_1$. Then (6.5) yields

$$F_1(t+\tau, z_1) = \tilde{F}_1(t+\tau, z_1) = S_{-\tau}^{(1)}\tilde{F}_1(t, z_1) + \frac{1}{v}\int [S_{-\tau}^{(2)}\tilde{F}_2(t, z_1, z_2) - \tilde{F}_2(t, S_{-\tau}^{(1)}z_1, S_{-\tau}^{(1)}z_2)]\, dz_2 + O\left(\frac{1}{v^2}\right). \quad (6.8)$$

Since (6.8) is an identity in z_1 we may replace z_1 by $S_\tau^{(1)}z_1$. We also transform the integration variable by replacing z_2 with $S_\tau^{(1)}z_2$, and use (6.7) and (2.12). The result is

$$\frac{1}{\tau}[F_1(t+\tau, S_\tau^{(1)}z_1) - F_1(t, z_1)] = \frac{1}{\tau v}\int [S_{-\tau}^{(2)}F_1(t, S_\tau^{(1)}z_1)F_1(t, S_\tau^{(1)}z_2) - F_1(t, z_1)F_1(t, z_2)]\, d\mathbf{q}_2\, d\mathbf{p}_2 + O\left(\frac{1}{v^2}\right). \quad (6.9)$$

The one-particle solution operator is given trivially by

$$S_\tau^{(1)}z_1 = S_\tau^{(1)}(\mathbf{q}_1, \mathbf{p}_1) = [\mathbf{q}_1 + (\tau/m)\mathbf{p}_1, \mathbf{p}_1]. \quad (6.10)$$

Hence, if we set $g(\tau) = F_1(t+\tau, S_\tau^{(1)}z_1)$ we see that $\dot{g}(\tau) = D_tF_1[t+\tau, \mathbf{q}_1 + (\tau/m)\mathbf{p}_1, \mathbf{p}_1]$, where

$$D_t = \frac{\partial}{\partial t} + \frac{1}{m}\sum_{\alpha=1}^{3} p_1^\alpha \frac{\partial}{\partial q_1^\alpha}. \quad (6.11)$$

Thus, if we apply the mean value theorem, the left side of (6.9) becomes

$$\frac{1}{\tau}[F_1(t+\tau, S_\tau^{(1)}z_1) - F_1(t, z_1)] = \frac{1}{\tau}[g(\tau) - g(0)] = \dot{g}(\tau^*) = D_tF_1\left(t+\tau^*, \mathbf{q}_1 + \frac{\tau^*}{m}\mathbf{p}_1, \mathbf{p}_1\right). \quad (6.12)$$

Here $0 < \tau^* < \tau$.

To evaluate the right side of (6.9), we choose fixed values of $z_1 = (\mathbf{q}_1, \mathbf{p}_1)$ and $\mathbf{p}_2$, and examine the integration with respect to $\mathbf{q}_2$ with the help of Fig. 1. In that figure, the coordinates are so chosen that the particle which is originally at the point $\mathbf{q}_1$ remains at the origin. In the figure, the regions A, B, and C together form a cylindrical region with spherical end surfaces. Outside of this region the particles do not interact, i.e., $S_{-\tau}^{(2)}[S_\tau^{(1)}z_1, S_\tau^{(1)}z_2] = [z_1, z_2]$ and the integrand in (6.9) vanishes. For points $\mathbf{q}_2$ in C, the operator $S_\tau^{(1)}$ maps $\mathbf{q}_2$ to $\mathbf{q}_2''$. Then $S_{-\tau}^{(2)}$ maps $\mathbf{q}_2''$ to $\mathbf{q}_2'$. For all points in C having the same orthogonal projection (given by the vector $\mathbf{b}$) onto the plane P, the momenta are the same, i.e., the final momenta $\mathbf{p}_1'$, $\mathbf{p}_2'$ are functions of $\mathbf{p}_1$, $\mathbf{p}_2$ and the "impact vector" $\mathbf{b}$.

We now insert (6.12) into (6.9) and use (6.2) to obtain

$$D_tF_1(t, \mathbf{q}_1, \mathbf{p}_1) = \frac{1}{\tau v}\int d\mathbf{p}_2 \int d\mathbf{q}_2 [F_1(t, \mathbf{q}_1, \mathbf{p}_1')F_1(t, \mathbf{q}_1, \mathbf{p}_2') - F_1(t, \mathbf{q}_1, \mathbf{p}_1)F_1(t, \mathbf{q}_1, \mathbf{p}_2)] + \cdots. \quad (6.13)$$

Here the remainder includes not only the remainder in (6.9), but an error due to the fact that the spherical regions A and B (regions of incomplete collisions) have been omitted and the ends of the cylinder C are not planes but spherical segments. Both remainders may be neglected by virtue of (6.1) which guarantees that C is large compared to A and B and that (2.27) is satisfied. In the integral with respect to $\mathbf{q}_2$ in (6.13) the integrand depends on $\mathbf{q}_2$ only through $\mathbf{p}_1'$ and $\mathbf{p}_2'$ which are functions of $\mathbf{b}$. Hence,

$$d\mathbf{q}_2 = (\tau/m)\,|\mathbf{p}_2 - \mathbf{p}_1|\, dA,$$

where dA is the area element on the plane P. Thus, neglecting the remainder term, we obtain the Boltzmann equation,

$$D_tF_1(t, \mathbf{q}_1, \mathbf{p}_1) = \frac{1}{mv}\int d\mathbf{p}_2 \int_P dA\, |\mathbf{p}_2 - \mathbf{p}_1| \times [F_1(t, \mathbf{q}_1, \mathbf{p}_1')F_1(t, \mathbf{q}_1, \mathbf{p}_2') - F_1(t, \mathbf{q}_1, \mathbf{p}_1)F_1(t, \mathbf{q}_1, \mathbf{p}_2)]. \quad (6.14)$$

In this section, we have used a notation similar to that of Refs. 11(a) and 11(b). In the next two sections we wish to compare our results with Refs. 9, 16, and 17. Therefore, we change the notation. We replace $\mathbf{q} = (q^1, q^2, q^3)$ by $\mathbf{x} = (x_1, x_2, x_3)$ and introduce the velocity vector $\boldsymbol{\xi} = (1/m)\mathbf{p} = (\xi_1, \xi_2, \xi_3)$. We replace the subscript 2 by 1 and omit the old subscript 1. We also set

$$F_1(t, \mathbf{q}_1, \mathbf{p}_1) = (v/m^4)f(t, \mathbf{x}, \boldsymbol{\xi}). \quad (6.15)$$

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[16] H. Grad, Commun. Pure Appl. Math. **2**, 331 (1949).

[17] H. Grad, in *Handbuch der Physik* (Springer-Verlag, Berlin, 1958), Vol. XII, pp. 205–294.

Then the Boltzmann equation (6.14) becomes

$$D_t f(t, \mathbf{x}, \boldsymbol{\xi}) = \frac{\partial f}{\partial t} + \sum_{i=1}^{3} \xi_i \frac{\partial f}{\partial x_i} = J[f], \quad (6.16)$$

where

$$J[f] = \frac{1}{m} \int d\boldsymbol{\xi}_1 \int_P dA\, |\boldsymbol{\xi}_1 - \boldsymbol{\xi}| \times [f(t, \mathbf{x}, \boldsymbol{\xi}') f(t, \mathbf{x}, \boldsymbol{\xi}_1') - f(t, \mathbf{x}, \boldsymbol{\xi}) f(t, \mathbf{x}, \boldsymbol{\xi}_1)]. \quad (6.17)$$

The Vlasov equation of Sec. 4 may also be written in the same notation. We note that

$$f_1 = \frac{1}{V} F_1 = \frac{v}{Vm^4} f = \frac{1}{nm^4} f. \quad (6.18)$$

If we replace $(n-1)/n$ by 1, (4.9) becomes (6.16) with

$$J[f] = -\frac{1}{m} \sum_{i=1}^{3} \mathcal{F}_i(t, \mathbf{x}) \frac{\partial f}{\partial \xi_i}(t, \mathbf{x}, \boldsymbol{\xi}), \quad (6.19)$$

$$\mathcal{F}_i(t, \mathbf{x}) = -\frac{1}{m} \int \frac{\partial}{\partial x_i} \varphi(|\mathbf{x} - \mathbf{x}_1|) \rho(t, \mathbf{x}_1)\, d\mathbf{x}_1, \quad (6.20)$$

and

$$\rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \boldsymbol{\xi})\, d\boldsymbol{\xi}. \quad (6.21)$$

Physically, ρ is the mass density and $\mathcal{F}$ is the average interparticle force vector.

Summarizing our results thus far, we see that, starting with a complete description in terms of the Liouville equation and the basic entropy functional, the special principle of Sec. 3 yields the Vlasov equation for the one-particle function and the general principle (with appropriate τ) yields the Boltzmann equation. In order to use either of these equations as a starting point for a further simplification, we need a complete description, i.e., in addition to the equation of motion (6.16), we require the entropy functional for f. But this functional is easily obtained. From (6.4) and (6.15) we see that

$$w[f] = \prod_{i=1}^{n} \left[\frac{1}{nm^4} f(t, \mathbf{x}_i, \boldsymbol{\xi}_i)\right] \quad (6.22)$$

maximizes the basic entropy $S[w]$ subject to prescribed f. Hence from (2.18)

$$S_1[f] = S[w[f]] = \frac{k}{m} \int f \log f\, d\mathbf{x}\, d\boldsymbol{\xi} + kn \log (mn). \quad (6.23)$$

The additive constant is obviously superfluous in maximizing S_1. Thus, omitting the subscript 1, we set

$$S[f] = -R \int f \log f\, d\mathbf{x}\, d\boldsymbol{\xi}. \quad (6.24)$$

Here $R = k/m$ is the gas constant.

7. HYDRODYNAMIC EQUATIONS: FIVE MOMENTS

Starting with the solution f of the Boltzmann equation, we introduce a simplified description in terms of the five functions

$$\rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \boldsymbol{\xi})\, d\boldsymbol{\xi}, \quad (7.1)$$

$$\rho u_i(t, \mathbf{x}) = \int \xi_i f\, d\boldsymbol{\xi}, \quad i = 1, 2, 3, \quad (7.2)$$

$$p(t, \mathbf{x}) = \tfrac{1}{3} \int c^2 f\, d\boldsymbol{\xi}, \quad (7.3)$$

where

$$c^2 = (\boldsymbol{\xi} - \mathbf{u})^2 = \sum_{i=1}^{3} (\xi_i - u_i)^2. \quad (7.4)$$

Here we have followed the notation of Refs. 9, 16, and 17; ρ is the mass density, $\mathbf{u} = (u_1, u_2, u_3)$ is the velocity vector, and p is the scalar pressure. It is also convenient to define the kinetic temperature T by

$$p = \rho RT. \quad (7.5)$$

To apply the special principle (Sec. 3) we first maximize the entropy functional (6.24) subject to (7.1)–(7.3). By the method of Lagrange multipliers one finds easily that the maximizing f is given by the "local Maxwellian,"

$$f = f[\rho, \mathbf{u}, p] = f_0 = \frac{\rho^{\frac{5}{2}}}{(2\pi p)^{\frac{3}{2}}} \exp\left\{\frac{-\rho}{2p} (\boldsymbol{\xi} - \mathbf{u})^2\right\} = \frac{\rho}{(2\pi RT)^{\frac{3}{2}}} \exp\left\{-\frac{c^2}{2RT}\right\}. \quad (7.6)$$

According to the special principle, we see that the equations of motion for ρ, $\mathbf{u}$, p are to be obtained by applying the operator L, defined by (7.1)–(7.3), to the Boltzmann equation (6.16), and then replacing f by (7.6). A brief calculation then yields

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\nu} (\rho u_\nu) = J_0 = \int J[f_0]\, d\boldsymbol{\xi}, \quad (7.7)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_\nu} (\rho u_i u_\nu) + \frac{\partial p}{\partial x_i} = J_i = \int \xi_i J[f_0]\, d\boldsymbol{\xi}, \quad i = 1, 2, 3, \quad (7.8)$$

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_\nu} (p u_\nu) + \frac{2}{3} \left(\frac{\partial u_\nu}{\partial x_\nu}\right) p = J_4 = \int c^2 J[f_0]\, d\boldsymbol{\xi}. \quad (7.9)$$

It can be shown[9,17] that if we use (6.17) for $J[f]$, the collision terms J_ν ($\nu = 0, 1, 2, 3, 4$) are all zero. Then if we introduce the Lagrangian time derivative $d/dt = (\partial/\partial t) + u_\nu(\partial/\partial x_\nu)$, we obtain the equation of mass conservation from (7.7),

$$d\rho/dt + \rho(\partial u_\nu/\partial x_\nu) = 0, \quad (7.10)$$

the equation of momentum conservation from (7.8)

$$(du_i/dt) + (1/\rho)(\partial p/\partial x_i) = 0, \quad i = 1, 2, 3, \quad (7.11)$$

and the equation of energy conservation from (7.9),

$$(dp/dt) + \tfrac{5}{3}p(\partial u_i/\partial x_i) = 0. \quad (7.12)$$

If we introduce the internal energy per unit mass defined by

$$e = \tfrac{3}{2}RT = \tfrac{3}{2}(p/\rho), \quad (7.13)$$

then (7.12) has the alternate form

$$\rho(de/dt) + p(\partial u_i/\partial x_i) = 0. \quad (7.14)$$

These equations form a determined system, the "Euler equations," for ρ, $\mathbf{u}$, p. In these hydrodynamic equations the heat-flux vector is zero and the pressure tensor reduces to the scalar pressure p.

It is interesting to note that instead of beginning with the Boltzmann equation, we can use the Vlasov equation. To obtain the resulting hydrodynamic equations, we need only use (6.19) for J in (7.7)–(7.9). Then it is easy to show that $J_0 = J_4 = 0$, and for $\nu = 1, 2, 3$,

$$J_\nu = -\frac{1}{m}\mathcal{F}_i \int \xi_\nu \frac{\partial f_0}{\partial \xi_i}\, d\boldsymbol{\xi} = \frac{1}{m}\mathcal{F}_i \delta_{i\nu} \int f_0\, d\boldsymbol{\xi} = \frac{\rho}{m}\mathcal{F}_\nu. \quad (7.15)$$

Thus in this case, the momentum conservation equation becomes

$$\frac{du_i}{dt} + \frac{1}{\rho}\frac{\partial p}{\partial x_i} = \frac{1}{m}\mathcal{F}_i, \quad (7.16)$$

where $\mathcal{F}$ is the average interparticle force given by (6.20).

For either set of five hydrodynamic equations, we complete the description by computing the entropy functional. We just insert (7.6) in (6.24). The result is

$$S[\rho, \mathbf{u}, p] = \int \eta(\mathbf{x})\rho(\mathbf{x})\, d\mathbf{x}, \quad (7.17)$$

where η is the entropy per unit mass,

$$\eta(\mathbf{x}) = \tfrac{3}{2}R \log \frac{p}{\rho^{\frac{5}{3}}} + \text{const.} \quad (7.18)$$

8. HYDRODYNAMIC EQUATIONS: TEN MOMENTS

We begin again with the Boltzmann equation and apply the special principle to a description in terms of ten moments. The result which we describe briefly below has also been obtained by Kogan,[6] following a proposal of Koga.[18] We introduce a description in terms of

$$\rho = \int f\, d\boldsymbol{\xi}, \quad (8.1)$$

$$\rho u_i = \int \xi_i f\, d\boldsymbol{\xi}, \quad i = 1, 2, 3, \quad (8.2)$$

$$P_{ij} = \int c_i c_j f\, d\boldsymbol{\xi}, \quad i, j = 1, 2, 3; \quad (8.3)$$

where $c_i = \xi_i - u_i$. These are 10 functions in all since the pressure tensor (P_{ij}) is symmetric. We maximize the entropy (6.24) subject to (8.1)–(8.3) using the Lagrange method. If we use a coordinate system in which (P_{ij}) is diagonal, it is then easy to determine the Lagrange multipliers by using (8.1)–(8.3). In terms of the inverse (Q_{ij}) of the matrix (P_{ij}), the maximizing f is given by

$$f = f[\rho, \mathbf{u}, P] = \tilde{f} = \frac{\rho^{\frac{5}{2}}}{(2\pi)^{\frac{3}{2}}[\det(P_{ij})]^{\frac{1}{2}}} \times \exp\left\{-\frac{\rho}{2}Q_{ij}c_ic_j\right\}, \quad (8.4)$$

and if we insert (8.4) into (6.24) we obtain the entropy functional for the ten moment description,

$$S[\rho, \mathbf{u}, P] = \int \sigma(\mathbf{x})\rho(\mathbf{x})\, d\mathbf{x}, \quad (8.5)$$

where σ is the entropy per unit mass,

$$\sigma = \tfrac{3}{2}R \log\left[\frac{(\det P)^{\frac{1}{3}}}{\rho^{\frac{5}{3}}}\right] + \text{const.} \quad (8.6)$$

If we introduce the scalar pressure

$$p = \tfrac{1}{3}\operatorname{tr}(P_{ij}) = \tfrac{1}{3}\int c^2 \tilde{f}\, d\boldsymbol{\xi} \quad (8.7)$$

and set

$$p_{ij} = P_{ij} - p\delta_{ij}, \quad (8.8)$$

then (8.6) reduces to (7.18) when $p_{ij} = 0$, i.e., when the stress tensor reduces to the scalar pressure.

We now apply the special principle. This simply means that we take ten moments of the Boltzmann equation and then replace f by (8.4). A brief calculation then leads to the mass and momentum conservation equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\nu}(\rho u_\nu) = 0, \quad (8.9)$$

$$\frac{\partial u_j}{\partial t} + u_\nu \frac{\partial u_j}{\partial x_\nu} + \frac{1}{\rho}\frac{\partial}{\partial x_\nu}(P_{j\nu}) = 0, \quad j = 1, 2, 3, \quad (8.10)$$

[18] T. Koga, J. Chem. Phys. 22, 1633 (1954).

and the equations

$$\frac{\partial p_{ij}}{\partial t} + \frac{\partial}{\partial x_v}(u_v p_{ij}) + p_{iv}\frac{\partial u_j}{\partial x_v} + p_{jv}\frac{\partial u_i}{\partial x_v} - \tfrac{2}{3}\delta_{ij}\frac{\partial u_r}{\partial x_v}p_{rv} + p\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \tfrac{2}{3}\delta_{ij}\frac{\partial u_r}{\partial x_r}\right) = J_{ij}; \quad i,j = 1,2,3. \tag{8.11}$$

Here,

$$J_{ij} = \int \xi_i \xi_j J[\tilde{f}]\, d\boldsymbol{\xi} \tag{8.12}$$

and $J[f]$ is given by (6.17). The collision terms (8.12), which are originally given by eight-fold integrals can be reduced to single integrals which, in turn, can be expressed in terms of tabulated elliptic integrals. For the sake of brevity these calculations are not given here.

If we expand (8.4) for small p_{ij} [again it is convenient to use a coordinate system in which (P_{ij}) and (p_{ij}) are diagonal] we obtain, to first order,

$$\tilde{f} \approx f_0[1 + (p_{ij}c_ic_j/2pRT)]. \tag{8.13}$$

Here f_0 is given by (7.6) and T is defined by (7.5). This functional form is the basis for Grad's ten moment approximation.[19] Except for the collision term (8.12), our Eqs. (8.9)–(8.11) are identical to Grad's, and if we use the approximation (8.13) instead of (8.4) to compute (8.12), our collision term reduces exactly to his. A detailed discussion of the physical interpretation of Grad's equations is given in Ref. 16.

The application of our principle to a thirteen moment description (including the heat-flux vector) leads to difficulties, because the positive definite quadratic form in the exponent of (8.4) is replaced by a cubic and then the integrals over velocity-space diverge. As pointed out by Kogan[6] a similar difficulty occurs in Grad's treatment in that the one-particle distribution function can become negative in portions of velocity-space. An approximate treatment, in which the exponential is expanded as in (8.13), is given by Kogan, who also treats molecules with internal degrees of freedom and degenerate gases.

9. EQUILIBRIUM STATISTICAL MECHANICS

For completeness we derive the canonical distribution function of equilibrium statistical mechanics from our general principle. The derivation is essentially the same as that of Gibbs,[1] Jaynes,[2] and others. We begin with the Liouville equation and introduce the simplified description in terms of the single scalar

$$U = \int Hw\, dz, \tag{9.1}$$

where H is the Hamiltonian. It is easy to verify that if we maximize (2.18) subject to (2.22) and (9.1), the result is

$$w[U] = Z^{-1}e^{-\beta H(z)}, \tag{9.2}$$

where Z is the partition function,

$$Z = \int e^{-\beta H(z)}\, dz. \tag{9.3}$$

The Lagrange multiplier β is determined implicitly by (9.1), i.e., by

$$U = \int Hw[U]\, dz = Z^{-1}\int He^{-\beta H}\, dz. \tag{9.4}$$

[The equilibrium temperature is defined by $\theta = (k\beta)^{-1}$.] From (2.4) we see that H is invariant under the solution operator S_t. It follows that (9.2) is invariant and therefore the general principle (in either the form of Sec. 5 or Sec. 3) yields the trivial equation of motion

$$dU/dt = 0. \tag{9.5}$$

The corresponding entropy, obtained by inserting (9.2) in (2.18), is

$$S(U) = S[w[U]] = k[\log Z(U) + \beta U]. \tag{9.6}$$

In this case the equation of motion (9.5) is uninteresting but the explicit formula (9.2), the canonical distribution function, is the basis of equilibrium statistical mechanics. As is well known, the equations of macroscopic thermodynamics follow from (9.6) and (9.3).

10. IRREVERSIBLE THERMODYNAMICS

In this section we derive the equations of irreversible thermodynamics from the Liouville equation by using our general principle. A similar derivation is given by Kubo[7] in the quantum-mechanical case. We introduce a description in terms of $r + 1$ scalars

$$U_i = \int \alpha_i(z)w(z)\, dz; \quad i = 0, 1, \cdots, r. \tag{10.1}$$

Here $\alpha_0 = H$ is the Hamiltonian and the other α_i's are arbitrary time-independent symmetric phase functions corresponding to r physical observables. We maximize (2.18) subject to (2.22) and (10.1). The result is

$$w[U] = w[U_0, \cdots, U_r] = Z^{-1}\exp\left\{-\sum_{i=0}^{r}\beta_i\alpha_i(z)\right\}, \tag{10.2}$$

[19] To obtain his ten moment approximation from Grad's thirteen moment approximation, we merely take the heat flux vector to be zero. See Ref. 16, Eq. (5.18) with $S_i \equiv 0$.

where

$$Z = \int \exp\left\{-\sum_{i=0}^{r} \beta_i \alpha_i\right\} dz. \tag{10.3}$$

The β_i are functions of t determined implicitly by (10.1), i.e.,

$$U_i(t) = \int \alpha_i(z) w[U(t)]\, dz, \quad i = 0, 1, \cdots, r. \tag{10.4}$$

According to the general principle, the equation of motion for the U_i's is given by (5.5), i.e.,

$$\frac{dU_i}{dt} = \dot{U}_i(t) = \frac{1}{\tau} \int \alpha_i(z)[S_{-\tau} - 1] w[U(t)]\, dz, \quad i = 0, 1, \cdots, r. \tag{10.5}$$

We now assume that $\beta_1, \cdots, \beta_r$ are small and we expand (10.2) to first order to obtain

$$w[U] = Z_0^{-1} e^{-\beta_0 H(z)} \left[1 + \left\langle \sum_{j=1}^{r} \beta_j \alpha_j \right\rangle - \sum_{j=1}^{r} \beta_j \alpha_j(z)\right], \tag{10.6}$$

where

$$Z_0 = \int \exp\{-\beta_0 H\}\, dz \tag{10.7}$$

and, for any f,

$$\langle f \rangle = Z_0^{-1} \int e^{-\beta_0 H} f\, dz. \tag{10.8}$$

If we insert (10.6) into (10.5) we obtain

$$\dot{U}_i(t) = \frac{1}{\tau} \sum_{j=1}^{r} \beta_j(t) \langle \alpha_i(z)[\alpha_j(z) - \alpha_j(S_{-\tau} z)]\rangle, \quad i = 0, 1, \cdots, r, \tag{10.9}$$

and by inserting (10.2) in (2.18) we obtain the new entropy function

$$S(t) = S\{U(t)\} = S[w[U]] = k\left\{\log Z + \sum_{i=0}^{r} \beta_i U_i\right\}. \tag{10.10}$$

From (10.3) and (10.4),

$$\partial \log Z / \partial \beta_i = -U_i, \tag{10.11}$$

hence,

$$\frac{\partial S}{\partial U_j} = k\left\{-\sum_{i=0}^{r} U_i \frac{\partial \beta_i}{\partial U_j} + \sum_{i=0}^{r} U_i \frac{\partial \beta_i}{\partial U_j} + \beta_j\right\} = k\beta_j. \tag{10.12}$$

We define the *forces*,

$$X_j(t) = (\partial S / \partial U_j) = k\beta_j(t) \tag{10.13}$$

and the *flows*,

$$J_i = \dot{U}_i(t). \tag{10.14}$$

Then the equations of motion (10.9) reduce to the *equations of irreversible thermodynamics*,

$$J_i = \sum_{j=1}^{r} L_{ij} X_j, \quad i = 0, 1, \cdots, r, \tag{10.15}$$

where L_{ij} is the *kinetic coefficient*

$$L_{ij} = \frac{1}{k\tau} \langle \alpha_i(z)[\alpha_j(z) - \alpha_j(S_{-\tau} z)]\rangle. \tag{10.16}$$

From (10.13) and (10.14), we have the *equation of entropy production*,

$$\dot{S}(t) = \sum_{j=0}^{r} X_j J_j \tag{10.17}$$

and from the general considerations of Sec. 5 it follows that $\dot{S}(t) \geq 0$.

Under certain conditions, the matrix (L_{ij}) is symmetric. Using the definition (10.8) of $\langle\ \rangle$, we see that the change of integration variable $z \to S_\tau z$ yields

$$\langle \alpha_i(z) \alpha_j(S_{-\tau} z)\rangle = \langle \alpha_i(S_\tau z) \alpha_j(z)\rangle. \tag{10.18}$$

Now, from (2.8) we note that $S_\tau = \mathcal{R} S_{-\tau} \mathcal{R}$. If we insert this in (10.18) and replace $\mathcal{R}z$ by z, we obtain

$$\langle \alpha_i(z) \alpha_j(S_{-\tau} z)\rangle = \langle \alpha_i(\mathcal{R} S_{-\tau} z) \alpha_j(\mathcal{R} z)\rangle. \tag{10.19}$$

We now assume that the phase functions $\alpha_1, \cdots, \alpha_r$ are invariant under momentum reversal, i.e., $\alpha_i(\mathcal{R}z) = \alpha_i(z)$. [This is obviously true for $\alpha_0 = H$. See (2.6).] Then,

$$\langle \alpha_i(z) \alpha_j(S_{-\tau} z)\rangle = \langle \alpha_j(z) \alpha_i(S_{-\tau} z)\rangle, \tag{10.20}$$

and from (10.18) we obtain the *Onsager relations*,

$$L_{ij} = L_{ji}, \quad i, j = 0, 1, \cdots, r. \tag{10.21}$$

Since $\alpha_0 = H$, we see from (10.16) and (10.21) that

$$L_{i0} = L_{0i} = 0, \quad i = 0, 1, \cdots, r, \tag{10.22}$$

hence from (10.14) and (10.15) that

$$\dot{U}_0 = J_0 = 0. \tag{10.23}$$

Thus U_0 is constant. If we use only the leading term of (10.6) in (10.4), we have

$$U_0 = Z_0^{-1} \int H e^{-\beta_0 H}\, dz \tag{10.24}$$

which is the same as (9.4). Thus, to this approximation β_0 is constant and we can identify it with the equilibrium value $\beta_0 = (k\theta)^{-1}$. Similarly we may interpret $\langle\ \rangle$ as the equilibrium average in the formula (10.16) for the kinetic coefficients.

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Integral Representations of Invariant States on B^* Algebras

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Let $\mathfrak{A}$ be a B^* algebra with a group G of automorphisms and K be the set of G-invariant states on $\mathfrak{A}$. We discuss conditions under which a G-invariant state has a unique integral representation in terms of extremal points of K, i.e., extremal invariant states.

1. INTRODUCTION AND NOTATIONS

LET $\mathfrak{A}$ be a B^* algebra, G a group, and τ a (group) homomorphism of G into the * automorphisms of $\mathfrak{A}$. If $\mathfrak{A}$ has an identity, the set of G-invariant states on $\mathfrak{A}$ is compact (for the w^* topology) and one may try to obtain an integral representation of G-invariant states in terms of extremal invariant states. If G is reduced to the identity, such an integral representation is unique if and only if $\mathfrak{A}$ is Abelian. It has, however, been remarked recently that uniqueness prevails under more general circumstances (see Refs. 1 and 2, and for further information, Refs. 3 and 4). The aim of this note is to discuss the general problem of existence and uniqueness of integral representations of invariant states, using Choquet's theory of integral representations on convex compact sets. While some of our results are best possible (in particular, the characterization of G-Abelian B^* algebras, Theorem 2.3), others could certainly be improved (see Sec. 4). Questions related to the existence of a topology on G are relevant for applications to physics, but are not discussed here.

If K is a metrizable compact (phase space) and G a group of homomorphisms of K (time evolution), it is known (see Ref. 5) that a measure on K, invariant under G, can be uniquely decomposed into ergodic measures, i.e., has an integral representation in terms of extremal invariant measures. In this note we obtain an extension of this result of ergodic theory to the noncommutative case (using an algebra of operators in Hilbert space instead of the algebra of continuous functions on a compact) and we weaken the metrizability requirement. The physical problem we have in mind is that of statistical mechanics of an infinite system. An equilibrium state of such a system can be represented by a state ρ on a B^* algebra (e.g., the algebra of canonical commutation relations for a system of bosons), and we may assume invariance of ρ under some natural group G (e.g., the product of the Euclidean group and of the particle number gauge group). One can see that a decomposition of ρ into extremal G-invariant states corresponds to a decomposition into pure thermodynamic phases. Such a decomposition should thus be unique and the problem arises to study the conditions on a non-Abelian algebra and a group of automorphisms such that the invariant states have a unique integral representation in terms of extremal invariant states.

Throughout this note we use the following notations: $\mathfrak{A}$, a B^* algebra; G, a group; $\tau: g \to \tau_g$ a representation of G into the * automorphisms of $\mathfrak{A}$; $\mathfrak{A}'$, the dual of $\mathfrak{A}$ with the w^* topology; $E \subset \mathfrak{A}'$, the set of states on $\mathfrak{A}$ (if $\mathfrak{A}$ has an identity, E is compact); $\mathfrak{L}_G$, the subspace of $\mathfrak{A}$ generated by the elements $A - \tau_g A$ with $A \in \mathfrak{A}$, $g \in G$; $\mathfrak{L}_G^{\perp}$, the orthogonal complement of $\mathfrak{L}_G$ in $\mathfrak{A}'$; $E \cap \mathfrak{L}_G^{\perp}$, the set of G-invariant states.

If $\rho \in E$, we denote by $\mathfrak{H}_\rho$, the Hilbert space of the Gel'fand–Segal construction; π_ρ, the corresponding * homomorphism of $\mathfrak{A}$ into the bounded operators on $\mathfrak{H}_\rho$; $\Omega_\rho \in \mathfrak{H}_\rho$, the normalized vector, cyclic with respect to $\pi_\rho(\mathfrak{A})$ and such that $\rho(A) = (\Omega_\rho, \pi_\rho(A)\Omega_\rho)$ for all $A \in \mathfrak{A}$.

If $\rho \in E \cap \mathfrak{L}_G^{\perp}$ we denote by U_ρ, the unitary representation of G in $\mathfrak{H}_\rho$ such that $U_\rho(g)\Omega_\rho = \Omega_\rho$, $U_\rho(g)\pi_\rho(A)U_\rho(g^{-1}) = \pi_\rho(\tau_g A)$ for all $g \in G$, $A \in \mathfrak{A}$; P_ρ, the projection on the subspace of $\mathfrak{H}_\rho$ formed by the vectors invariant under $U_\rho(G)$.

2. G-ABELIAN ALGEBRAS

In Refs. 1 and 2, the group G was taken to be R^ν and it was assumed that if $A_1, A_2 \in \mathfrak{A}$ the commutator $[A_1, \tau_g A_2]$ vanishes when $g \to \infty$. A suitable generalization of this condition is the basis of our analysis; we formulate it first in a different manner.

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[2] D. Kastler and D. Robinson, Commun. Math. Phys. 3, 151 (1966).

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[4] D. Robinson and D. Ruelle, "Extremal Invariant States," Institut des Hautes Etudes Scientifiques (1966).

[5] R. Phelps, *Lectures on Choquet's Theorem* (D. Van Nostrand Company, Inc. Princeton, New Jersey, 1966).

Definition 2.1: $\mathfrak{A}$ is said to be G-Abelian if for all $\rho \in E \cap \mathfrak{L}_G^\perp$ and $A_1, A_2 \in \mathfrak{A}$,

$$[P_\rho \pi_\rho(A_1) P_\rho, P_\rho \pi_\rho(A_2) P_\rho] = 0.$$

In other words the von Neumann algebra generated by $P_\rho \pi_\rho(\mathfrak{A}) P_\rho$ is Abelian.

Theorem 2.2 (Alaoglu-Birkhoff): Let $\{U_\alpha\}_{\alpha \in I}$ be a semigroup of contractions on a Hilbert space $\mathfrak{H}$, i.e., a collection of operators such that

(1) $\|U_\alpha\| \leq 1$ for all $\alpha \in I$

(2) For any $\alpha, \beta \in I$, $U_\alpha U_\beta = U_\gamma$ for some $\gamma \in I$.

Let P be the orthogonal projection onto the set of all vectors in $\mathfrak{H}$ left invariant by all the U_α's. Then P is in the strong closure at the convex hull of $\{U_\alpha\}_{\alpha \in I}$.

This theorem is proved in Riesz–Nagy.[6] The theorem stated by Riesz and Nagy is slightly different from the one given above; what they do is to construct a net of convex linear combinations of the U_α's and show that it converges strongly. Although the fact that P is the strong limit of this net is not included in the statement of the theorem, it appears in the course of the proof.

Theorem 2.3: In order that $\mathfrak{A}$ be G-Abelian it is necessary and sufficient that, for all Hermitian A_1, $A_2 \in \mathfrak{A}$ and all $\rho \in E \cap \mathfrak{L}_G^\perp$,

$$\inf_{A_1'} |\rho([A_1', A_2])| = 0,$$

where A_1' runs over the convex hull of $\{\tau_g A_1 : g \in G\}$.

In order that $\mathfrak{A}$ be G-Abelian, it is evidently necessary and sufficient that, for any $\rho \in E \cap \mathfrak{L}_G^\perp$, $\Psi \in P_\rho \mathfrak{H}_\rho$ with $\|\Psi\| = 1$, and A_1, A_2 Hermitian elements of the unit ball of $\mathfrak{A}$, we have

$$(\Psi, \pi_\rho(A_1) P_\rho \pi_\rho(A_2) \Psi) = (\Psi, \pi_\rho(A_2) P_\rho \pi_\rho(A_1) \Psi) \quad (*).$$

We prove first the sufficiency of the criterion stated in the proposition. Let $\epsilon > 0$; then by the preceding theorem, we can find positive numbers λ_i with $\sum_i \lambda_i = 1$ and elements g_i of G such that

$$\|(\sum \lambda_i U_\rho(g_i) - P_\rho) \pi_\rho(A_1) \Psi\| \leq \tfrac{1}{2}\epsilon.$$

If we define

$$A_1' = \sum \lambda_i \tau_{g_i} A_1,$$

then both sides of (*) are unchanged if we replace A_1 by A_1', and we have

$$\begin{aligned} &\|P_\rho \pi_\rho(A_1') \Psi - U_\rho(g) \pi_\rho(A_1') \Psi\| \\ &\quad = \|P_\rho \pi_\rho(A_1) \Psi - U_\rho(g) \pi_\rho(A_1') \Psi\| \\ &\quad = \|U_\rho(g)[P_\rho \pi_\rho(A_1) \Psi - \pi_\rho(A_1') \Psi]\| \leq \tfrac{1}{2}\epsilon \end{aligned}$$

for all $g \in G$.

Using this inequality, and the fact that A_1' is Hermitian, we get for any positive numbers λ_i' with $\sum_i \lambda_i' = 1$ and any $g_i' \in G$,

$$\begin{aligned} &|(\Psi, \pi_\rho(A_1) P_\rho \pi_\rho(A_2) \Psi) - (\Psi, \pi_\rho(A_2) P_\rho \pi_\rho(A_1) \Psi)| \\ &= |(\Psi, \pi_\rho(A_1') P_\rho \pi_\rho(A_2) \Psi) - (\Psi, \pi_\rho(A_2) P_\rho \pi_\rho(A_1') \Psi)| \\ &\leq 2 \cdot \sum_i \lambda_i' \|\pi_\rho(A_2) \Psi\| \cdot \|P_\rho \pi_\rho(A_1') \Psi - U_\rho(g_i') \pi_\rho(A_1') \Psi\| \\ &\qquad + |(\Psi, \pi_\rho([\textstyle\sum \lambda_i' \tau_{g_i'} A_1', A_2]) \Psi)| \\ &\leq \epsilon + |(\Psi, \pi_\rho([\textstyle\sum \lambda_i' \tau_{g_i'} A_1', A_2]) \Psi)| . \end{aligned}$$

But by hypothesis, $|(\Psi, \pi_\rho([\sum \lambda_i' \tau_{g_i'} A_1', A_2]) \Psi)|$ can be made arbitrarily small by an appropriate choice of λ_i' and g_i', so

$$|(\Psi, \pi_\rho(A_1) P_\rho \pi_\rho(A_2) \Psi) - (\Psi, \pi_\rho(A_2) P_\rho \pi_\rho(A_1) \Psi)| \leq \epsilon.$$

Thus, (*) holds, so $\mathfrak{A}$ is G-Abelian.

Now we suppose that $\mathfrak{A}$ is G-Abelian, so (*) holds, and we let λ_i, g_i be as above. Then

$$\begin{aligned} &\left|\left(\Psi, \pi_\rho\left(\left[\sum_i \lambda_i \tau_{g_i} A_1, A_2\right]\right) \Psi\right)\right| \\ &= \left|\left(\sum_i \lambda_i U_\rho(g_i) \pi_\rho(A_1) \Psi, \pi_\rho(A_2) \Psi\right)\right. \\ &\quad \left. - \left(\pi_\rho(A_2), \sum_i \lambda_i U_\rho(g_i) \pi_\rho(A_1) \Psi\right)\right| \\ &\leq 2 \cdot \|\pi_\rho(A_2) \Psi\| \cdot \left\|\left(\sum_i \lambda_i U_\rho(g_i) - P_\rho\right) \pi_\rho(A_1) \Psi\right\| \\ &\quad + |(\Psi, \pi_\rho(A_1) P_\rho \pi_\rho(A_2) \Psi) - (\Psi, \pi_\rho(A_2) P_\rho \pi_\rho(A_1) \Psi)| \\ &\leq \epsilon, \end{aligned}$$

so

$$\inf_{A_1' \in \text{convex hull of } \{\tau_g A_1\}} |(\Psi, \pi_\rho([A_1', A_2]) \Psi)| = 0,$$

so the criterion of the proposition holds.

Corollary 2.4: Let H be a subgroup of G. Then, if $\mathfrak{A}$ is H-Abelian, it is also G-Abelian.

We need only apply the criterion of the preceding proposition, observing that $\mathfrak{L}_G^\perp$ is contained in $\mathfrak{L}_H^\perp$ and that the convex hull of $\{\tau_g A_1 : g \in G\}$ contains the convex hull of $\{\tau_h A_1 : h \in H\}$.

Corollary 2.5: $\mathfrak{A}$ is G-Abelian whenever one of the following conditions is satisfied.

[6] F. Riesz and B. Sz.-Nagy, *Functional Analysis*, translated by L. Boron (Frederick Ungar Publishing Company, New York, 1955), Sec. 146.

(i) For all $\rho \in E \cap \mathfrak{L}_G^{\perp}$ and self-adjoint $A_1, A_2 \in \mathfrak{A}$,

$$\inf_{g \in G} |\rho([A_1, \tau_g A_2])| = 0.$$

(ii) $\mathfrak{A}$ is Abelian.

(iii) $E \cap \mathfrak{L}_G^{\perp}$ is empty.

The usefulness of Definition 2.1 appears in the next two sections; we indicate here, however, the following result.

Proposition 2.6: If $\rho \in E \cap \mathfrak{L}_G^{\perp}$ and the von Neumann algebra $[P_\rho \pi_\rho(\mathfrak{A}) P_\rho]''$ generated by $P_\rho \pi_\rho(\mathfrak{A}) P_\rho$ is Abelian, then

$$P_\rho [P_\rho \pi_\rho(\mathfrak{A}) P_\rho]' = P_\rho [P_\rho \pi_\rho(\mathfrak{A}) P_\rho]''.$$

The vector Ω_ρ is cyclic for the restriction to $P_\rho \mathfrak{H}_\rho$ of $P_\rho [P_\rho \pi_\rho(\mathfrak{A}) P_\rho]''$; hence, if this von Neumann algebra is commutative, it is equal to its commutant (see Ref. 7, p. 89, Corollaire 2), namely to

$$P_\rho [P_\rho \pi_\rho(\mathfrak{A}) P_\rho]'$$

restricted to $P_\rho \mathfrak{H}_\rho$.

3. INTEGRAL REPRESENTATION OF G-INVARIANT STATES

In this and the next section, we use the theory of integral representations on convex compact sets (see Ref. 8). Let K be a convex compact set in a locally convex topological vector space. The unit mass at $\kappa \in K$ is denoted by δ_κ. We remind the reader that an order relation is defined on the positive measures of norm 1 on K by $\mu \prec u' \Leftrightarrow \mu(f) \leq \mu'(f)$ for all convex continuous f on K. A measure is called maximal if it is maximal for the order $\prec$, and K is said to be a simplex if every $\kappa \in K$ is the resultant of a *unique* maximal measure on K. In what follows we take $K = E \cap \mathfrak{L}_G^{\perp}$, where $\mathfrak{A}$ is assumed to have an identity. If $A \in \mathfrak{A}$, we denote by $\hat{A}$ the function on $E \cap \mathfrak{L}_G^{\perp}$ defined by $\hat{A}(\rho) = \rho(A)$.

Theorem 3.1: Let $\mathfrak{A}$ have an identity, $\rho \in E \cap \mathfrak{L}_G^{\perp}$, and let the von Neumann algebra generated by $P_\rho \pi_\rho(\mathfrak{A}) P_\rho$ be Abelian. Then, there exists a unique maximal measure μ_ρ on $E \cap \mathfrak{L}_G^{\perp}$ such that $\mu_\rho \succ \delta_\rho$ (i.e., μ_ρ has resultant ρ). The measure μ_ρ is determined by

$$\mu_\rho(\hat{A}_1 \cdots \hat{A}_l) = (\Omega_\rho, \pi_\rho(A_1) P_\rho \pi_\rho(A_2) P_\rho \cdots P_\rho \pi_\rho(A_l) \Omega_l). \quad (1)$$

Take $A_1, \cdots, A_l$ self-adjoint. Since the operators $P_\rho \pi_\rho(A_1) P_\rho, \cdots, P_\rho \pi_\rho(A_l) P_\rho$ commute, there exists a projection-valued measure F on R^l such that

$$P_\rho \pi_\rho(A_i) P_\rho = \int t_i \, dF(t_1, \cdots, t_l).$$

If $\mathfrak{F}$ is a complex polynomial of l variables, we have

$$\begin{aligned} &|(\Omega_\rho, \mathfrak{F}(P_\rho \pi_\rho(A_1) P_\rho, \cdots, P_\rho \pi_\rho(A_l) P_\rho) \Omega_\rho)| \\ &= \left| \left(\Omega_\rho, \int \mathfrak{F}(t_1, \cdots, t_l) \, dF(t_1, \cdots, t_l) \Omega_\rho \right) \right| \\ &\leq \sup_{\|\Phi\|=1, P_\rho \Phi = \Phi} |\mathfrak{F}((\Phi, \pi_\rho(A_1)\Phi), \cdots, (\Phi, \pi_\rho(A_l)\Phi))| \\ &\leq \sup_{\sigma \in K \cap \mathfrak{L}_G^{\perp}} |\mathfrak{F}(\sigma(A_1), \cdots, \sigma(A_l))| \\ &= \sup_{\sigma \in K \cap \mathfrak{L}_G^{\perp}} |\mathfrak{F}(\hat{A}_1(\sigma), \cdots, \hat{A}_l(\sigma))|. \end{aligned}$$

This shows that Eq. (1) defines a linear functional on the polynomials in the $\hat{A}$, which is continuous for the topology of uniform convergence on $E \cap \mathfrak{L}_G^{\perp}$. By the Stone–Weierstrass theorem, this functional extends uniquely to a measure μ_ρ on $E \cap \mathfrak{L}_G^{\perp}$, which is ≥ 0 and of norm 1.

Let $\rho_1, \cdots, \rho_m \in E \cap \mathfrak{L}_G^{\perp}$, $\lambda_1, \cdots, \lambda_m > 0$, $\sum \lambda_i = 1$ and $\rho = \sum \lambda_i \rho_i$. There exist (see Ref. 9, 2.5.1.) uniquely defined self-adjoint operators $T_i \in [\pi_\rho(\mathfrak{A})]'$ such that $0 \leq T_i \leq 1$ and for all $A \in \mathfrak{A}$.

$$\lambda_i \rho_i(A) = (T_i \Omega_\rho, \pi_\rho(A) T_i \Omega_\rho).$$

The T_i satisfy $\sum T_i^2 = 1$. If $g \in G$, we have

$$U(g) T_i U(g^{-1}) \in [\pi_\rho(\mathfrak{A})]',$$

the uniqueness of T_i and the fact that $\lambda_i \rho_i \in \mathfrak{L}_G^{\perp}$ then shows that $U(g) T_i U(g^{-1}) = T_i$, hence,

$$T_i \in [U(G)]', \quad [T_i, P_\rho] = 0.$$

By the uniqueness of the Gel'fand–Segal construction, we may identify $\mathfrak{H}_{\rho_i}$ with the closure of $\pi_\rho(\mathfrak{A}) T_i \Omega_\rho$, π_{ρ_i} with the restriction of π_ρ to $\mathfrak{H}_{\rho_i}$, and Ω_{ρ_i} with $\lambda_i^{-\frac{1}{2}} T_i \Omega_\rho$. Then U_{ρ_i} is identified with the restriction of U_ρ to $\mathfrak{H}_{\rho_i}$ and P_{ρ_i} with the restriction of P_ρ to $\mathfrak{H}_{\rho_i}$. In particular, $[P_{\rho_i} \pi_{\rho_i}(\mathfrak{A}) P_{\rho_i}]''$ is Abelian and μ_{ρ_i} is thus defined. We have

$$\begin{aligned} \mu_{\rho_i}(\hat{A}_1 \cdots \hat{A}_l) &= (\Omega_\rho, \pi_\rho(A_1) P_{\rho_i} \cdots P_{\rho_i} \pi_{\rho_i}(A_l) \Omega_{\rho_i}) \\ &= \lambda_i^{-1} (T_i \Omega_\rho, \pi_\rho(A_1) P_\rho \cdots P_\rho \pi_\rho(A_l) T_i \Omega_\rho) \\ &= \lambda_i^{-1} (\Omega_\rho, \pi_\rho(A_1) P_\rho \cdots P_\rho \pi_\rho(A_l) T_i^2 \Omega_\rho) \end{aligned}$$

so that

$$\sum \lambda_i \mu_{\rho_i}(\hat{A}_1 \cdots \hat{A}_l) = \mu_\rho(\hat{A}_1 \cdots \hat{A}_l).$$

[7] J. Dixmier, *Les algèbres d'opérateurs dans l'Espace Hilbertien*, (Gauthier-Villars, Paris, 1957).

[8] G. Choquet and P. A. Meyer, Ann. Inst. Fourier **13**, 139 (1963).

[9] J. Dixmier, *Les C*-Algèbres et leurs Représentations* (Gauthier-Villars, Paris, 1964).

Now let μ be a measure on $E \cap \mathfrak{L}_G^\perp$ such that $\mu \succ \delta_\rho$. If $\phi \in \mathfrak{C}(E \cap \mathfrak{L}_G^\perp)$ and $\epsilon > 0$, one can find a measure μ' with finite support: $\mu' = \sum \lambda_i \delta_{\rho_i}$, $\lambda_i > 0$, $\rho_i \in E \cap \mathfrak{L}_G^\perp$, such that $|\mu(\phi) - \mu'(\phi)| < \epsilon$ and $\sum \lambda_i \rho_i = \rho$ (see Ref. 10, p. 217, Prop. 3). If ϕ is convex we thus have

$$\mu(\phi) - \epsilon \leq \mu'(\phi) = \sum \lambda_i \delta_{\rho_i}(\phi) \leq \sum \lambda_i \mu_{\rho_i}(\phi) = \mu_\rho(\phi),$$

hence $\mu_\rho \succ \mu$. Since μ is an arbitrary measure on $E \cap \mathfrak{L}_G^\perp$ such that $\mu \succ \delta_\rho$, we see that μ_ρ is the unique maximal measure on $E \cap \mathfrak{L}_G^\perp$ such that $\mu_\rho \succ \delta_\rho$ which concludes the proof of the theorem.

Corollary 3.2: If $\mathfrak{A}$ has an identity and is G-Abelian, then $E \cap \mathfrak{L}_G^\perp$ is a simplex.

Remark 3.3: If $\mathfrak{A}$ is Abelian, the problem considered in this section reduces to that of decomposing an invariant measure on a compact set into ergodic measures (see Ref. 5, Sec. 10).

4. EXTREMAL G-INVARIANT STATES

Let $\mathfrak{E}(E \cap \mathfrak{L}_G^\perp)$ be the set of extremal points of $E \cap \mathfrak{L}_G^\perp$, i.e., the extremal invariant states. The following statement characterizes the elements of $\mathfrak{E}(E \cap \mathfrak{L}_G^\perp)$.

Proposition 4.1: Let $\rho \in E \cap \mathfrak{L}_G^\perp$. If $\mathfrak{A}$ is G-Abelian, the following conditions are equivalent:

(i) $\rho \in \mathfrak{E}(E \cap \mathfrak{L}_G^\perp)$.
(ii) The set $\pi_\rho(\mathfrak{A}) \cup U_\rho(G)$ is irreducible in $\mathfrak{H}_\rho$.
(iii) P_ρ is one dimensional.

The simple proof is left to the reader. We remark only that the implications (i) $\Leftrightarrow$ (ii) $\Leftarrow$ (iii) do not make use of the assumption that $\mathfrak{A}$ is G-Abelian, and that (ii) $\Rightarrow$ (iii) follows from Proposition 2.6.

The measure μ_ρ of Theorem 3.1 is in the "good cases" carried by $\mathfrak{E}(E \cap \mathfrak{L}_G^\perp)$. This is so, for instance, if $\mathfrak{A}$ is (norm-)separable, because $E \cap \mathfrak{L}_G^\perp$ is then metrizable (see Ref. 8, Corr. 14). We indicate now without proofs some more results in this direction.

[10] N. Bourbaki, *Intégration* (Hermann et Cie., Paris, 1965), 2nd ed., Chaps. 1–4.

Proposition 4.2: Let $\mathfrak{A}$ have an identity and $\mathfrak{B}$ be a self-adjoint subalgebra of $\mathfrak{A}$; define

$$\mathcal{F} = \{\sigma \in E: \text{The restriction of } \rho \text{ to } \mathfrak{B} \text{ has norm 1}\}.$$

Then,

(i) $\mathcal{F}$ is a G_δ (a countable intersection of open subsets of E).
(ii) If μ is a measure on E such that $\mu \geq 0$, $\mu(E) = 1$, and μ has resultant ρ, then
$$\rho \in \mathcal{F} \leftrightarrow \mu \text{ is carried by } \mathcal{F},$$

cf. Ref. 1, Theorem, Part 4.

Proposition 4.3: Let $(\mathfrak{A}_\alpha)$ be a countable family of sub-B^* algebras of $\mathfrak{A}$ such that $\bigcup_\alpha \mathfrak{A}_\alpha$ is dense in $\mathfrak{A}$. Let $\mathfrak{C}_\alpha$ be a separable closed two-sided ideal of $\mathfrak{A}_\alpha$ for each α, and define

$$\mathcal{F}_\alpha = \{\sigma \in E: \text{the restriction of } \sigma \text{ to } \mathfrak{C}_\alpha \text{ has norm 1}\}, \quad \mathcal{F} = \bigcap_\alpha \mathcal{F}_\alpha.$$

Then,

(i) If $\rho \in \mathcal{F}$, then $\mathfrak{H}_\rho$ is separable.
(ii) There exists a sequence (A_i) of self-adjoint elements of $\mathfrak{A}$ such that if $\rho \in \mathcal{F}$ and $\sigma \in E$, then $\rho(A_i) \neq \sigma(A_i)$ for some i.
(iii) If $\mathfrak{A}$ has an identity and is G-Abelian and if μ is a measure on $E \cap \mathfrak{L}_G^\perp$ such that $\mu \geq 0$, $\mu(E \cap \mathfrak{L}_G^\perp) = 1$ and μ has resultant $\rho \in \mathcal{F}$, then
(μ maximal on $E \cap \mathfrak{L}_G^\perp$)
$$\Leftrightarrow (\mu \text{ carried by } \mathfrak{E}(E \cap \mathfrak{L}_G^\perp)).$$

(i) and (ii) are easy, the proof of (iii) uses (ii), Corollary 3.2 and an argument in Ref. 1, Theorem, Part 5.

The usefulness of (iii) appears in statistical mechanics, where $\mathfrak{A}$ may not be norm separable but the states of interest satisfy a condition of the type $\rho \in \mathcal{F}$. One has then a unique decomposition $\rho \to \mu_\rho$ of ρ into extremal invariant states and those states are again in $\mathcal{F}$. For an explicit treatment see Ref. 11, in particular, the Appendix.

[11] D. Ruelle, "The States of Classical Statistical Mechanics," J. Math. Phys. (to be published).

Null Electromagnetic Field in the Form of Spherical Radiation

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An example is given of a differential form which leads, through Einstein's gravitational equations, to an energy tensor representing a null electromagnetic field in the form of spherical radiation.

1. INTRODUCTORY

A PREVIOUS paper[1] obtained the conditions that must be satisfied by the energy tensor of a null source-free electromagnetic field. It was also shown how the electromagnetic field can be determined when an energy tensor satisfying these conditions is given.

If $f_{\mu\nu}$ is the tensor of the electromagnetic field (we assume Heaviside–Lorentz units), then the energy tensor is

$$T_{\mu\nu} = f_{\mu\alpha}f_{\nu}^{\ \alpha} - \tfrac{1}{4}g_{\mu\nu}f_{\alpha\beta}f^{\alpha\beta}. \tag{1.1}$$

The three algebraic conditions which must be satisfied by $T_{\mu\nu}$ are

$$T_{\alpha}^{\alpha} = 0, \tag{1.2}$$

$$T_{\mu\alpha}T_{\nu}^{\alpha} = \tfrac{1}{4}g_{\mu\nu}T_{\alpha\beta}T^{\alpha\beta}, \tag{1.3}$$

which result from the form of (1.1), and

$$T_{\alpha\beta}v^{\alpha}v^{\beta} \geq 0, \tag{1.4}$$

where v^{μ} is any timelike vector. The electromagnetic field is described as null when the two invariants I_1 and I_2 vanish, where

$$I_1 = \tfrac{1}{2}f_{\alpha\beta}f^{\alpha\beta}, \quad I_2 = \tfrac{1}{2}f_{\alpha\beta}{}^{*}f^{\alpha\beta}.$$

In terms of the energy tensor, this is equivalent to

$$T_{\alpha\beta}T^{\alpha\beta} = 0, \tag{1.5}$$

and in this case (1.3) becomes

$$T_{\mu\alpha}T_{\nu}^{\alpha} = 0, \tag{1.6}$$

and we may write

$$T_{\mu\nu} = C_{\mu}C_{\nu}, \tag{1.7}$$

where C_{μ} is a null vector. Then (1.4) is automatically satisfied.

There are five differential conditions of the first order to be satisfied by C_{μ}. These are contained in the equations NEF (5.13), viz.,

$$C_{\lambda}C_{\sigma}E_{\mu\nu} + C_{\mu}C_{\nu}E_{\lambda\sigma} = C_{\lambda}C_{\mu}E_{\nu\sigma} + C_{\nu}C_{\sigma}E_{\lambda\mu}, \tag{1.8}$$

where

$$E_{\mu\nu} \equiv C_{\mu;\nu} + C_{\nu;\mu} - 2g_{\mu\nu}C_{;\alpha}^{\alpha}. \tag{1.9}$$

Finally, there are five integrablity conditions of higher order which cannot be written explicitly in terms of C_{μ}. These are given in NEF (8.10).

A special case, which the author calls the null–null case, occurs when $C_{;\alpha}^{\alpha} = 0$, and a specific example of this case was referred to, representing plane radiation. In order to find a specific example of the more general case when $C_{;\alpha}^{\alpha} \neq 0$, it is natural to consider the possibility of spherical radiation.

If we confine ourselves to the approximation of special relativity, where the space is assumed to be flat and Einstein's gravitational equations do not apply, it is not difficult to construct theoretical null electromagnetic fields consisting of spherical radiation. But if we want exact solutions, valid in general relativity, the differential form must be modified in such a way that the Ricci tensor satisfies the equation[2]

$$R_{\mu\nu} - \tfrac{1}{2}g_{\mu\nu}R = -\gamma T_{\mu\nu}. \tag{1.10}$$

By (1.2) this leads to

$$R = 0, \quad R_{\mu\nu} = -\gamma T_{\mu\nu}, \tag{1.11, 12}$$

and by (1.3) we must have

$$R_{\mu\alpha}R_{\nu}^{\alpha} = \tfrac{1}{4}g_{\mu\nu}R_{\alpha\beta}R^{\alpha\beta}. \tag{1.13}$$

For a null electromagnetic field we must have, by (1.6),

$$R_{\mu\alpha}R_{\nu}^{\alpha} = 0. \tag{1.14}$$

2. THE DIFFERENTIAL FORM

A differential form which, in special cases, can represent spherical gravitational radiation was considered by Robinson and Trautman.[3] We use this, with sign changed to give it the signature $+++-$, viz.,

$$ds^2 = \frac{\rho^2}{p^2}\left(d\xi + \frac{\partial q}{\partial \eta}\,d\sigma\right)^2 + \frac{\rho^2}{p^2}\left(d\eta + \frac{\partial q}{\partial \xi}\,d\sigma\right)^2 - 2d\rho\,d\sigma - A\,d\sigma^2, \tag{2.1}$$

[1] P. C. Bartrum, J. Math. Phys. 8, 667 (1967); This will be referred to as NEF.

[2] We omit the "cosmic" term for simplicity. Here $\gamma = 4\pi\gamma_0/c^4$, where γ_0 is the gravitational constant and $\gamma_0 = 6.664 \times 10^{-8}$ cgs units. $[\gamma] = M^{-1}L^{-1}T^2$.

[3] I. Robinson and A. Trautmann, Phys. Rev. Letters 4, 431 (1960).

where the coordinates are ξ, η, ρ, σ,

$$A = K - 2\rho H - 2m/\rho, \tag{2.2}$$

$$K = p^2\left(\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2}\right)\log p, \tag{2.3}$$

$$H = \frac{1}{p}\frac{\partial p}{\partial\sigma} + p^2\frac{\partial^2}{\partial\xi\partial\eta}\left(\frac{q}{p}\right) - pq\frac{\partial^2}{\partial\xi\partial\eta}\left(\frac{1}{p}\right); \tag{2.4}$$

p and q are functions of ξ, η, σ. m is a function of σ.

Numbering the coordinates ξ, η, ρ, σ as 1, 2, 3, 4, we find the following nonzero components of the Ricci tensor, where

$$Q = (\partial^2 q/\partial\xi^2) + (\partial^2 q/\partial\eta^2), \tag{2.5}$$

$$\begin{aligned}
R_{12} &= (\rho/p^2)Q,\\
R_{14} &= \frac{1}{2}\frac{\partial Q}{\partial\eta} + \frac{Q}{p}\left(\frac{\rho}{p}\frac{\partial q}{\partial\xi} - \frac{\partial p}{\partial\eta}\right),\\
R_{24} &= \frac{1}{2}\frac{\partial Q}{\partial\xi} + \frac{Q}{p}\left(\frac{\rho}{p}\frac{\partial q}{\partial\eta} - \frac{\partial p}{\partial\xi}\right),\\
R_{44} &= \frac{p^2}{\rho}\frac{\partial^2 Q}{\partial\xi\partial\eta} + \frac{p}{\rho}\frac{\partial Q}{\partial\xi}\left(\frac{\rho}{p}\frac{\partial q}{\partial\eta} - \frac{\partial p}{\partial\xi}\right)\\
&\quad + \frac{p}{\rho}\frac{\partial Q}{\partial\eta}\left(\frac{\rho}{p}\frac{\partial q}{\partial\eta} - \frac{\partial p}{\partial\xi}\right) + \frac{2}{\rho}Q\left(\frac{\rho}{p}\frac{\partial q}{\partial\xi} - \frac{\partial p}{\partial\eta}\right)\\
&\quad \times\left(\frac{\rho}{p}\frac{\partial q}{\partial\eta} - \frac{\partial p}{\partial\xi}\right) - \frac{2p}{\rho}Q\frac{\partial^2 p}{\partial\xi\partial\eta} + \tfrac{1}{2}Q^2\\
&\quad - \frac{1}{2}\frac{p^2}{\rho^2}\left(\frac{\partial^2 K}{\partial\xi^2} + \frac{\partial^2 K}{\partial\eta^2}\right) + \frac{2}{\rho^2}\frac{dm}{d\sigma} - \frac{6m}{\rho^2}H.
\end{aligned} \tag{2.6}$$

From these we immediately deduce

$$R = 0, \quad R_{\alpha\beta}R^{\alpha\beta} = 2Q^2/\rho^2. \tag{2.7}$$

The condition (1.11) is automatically satisfied, but (1.13) is only satisfied if $Q = 0$. In this case $R_{\alpha\beta}R^{\alpha\beta} = 0$, so that if there is an electromagnetic field it must be null. If $Q = 0$ we can deduce $q = 0$ by a coordinate transformation, and the differential form is simplified to

$$ds^2 = (\rho^2/p^2)(d\xi^2 + d\eta^2) - 2\,d\rho\,d\sigma - A\,d\sigma^2 \tag{2.8}$$

with

$$A = K - \frac{2\rho}{p}\frac{\partial p}{\partial\sigma} - \frac{2m}{\rho}, \tag{2.9}$$

$$\begin{aligned}
g^{11} = g^{22} &= p^2/\rho^2, \quad g^{33} = A,\\
g^{14} &= -1, \quad g = -(\rho/p)^4.
\end{aligned} \tag{2.10}$$

The Ricci tensor $R_{\mu\nu}$ now has only one nonzero component, R_{44}.

We write

$$\gamma E^2 \equiv \tfrac{1}{2}p^2\left(\frac{\partial^2 K}{\partial\xi^2} + \frac{\partial^2 K}{\partial\eta^2}\right) - \frac{2\,dm}{d\sigma} + \frac{6m}{p}\frac{\partial p}{\partial\sigma}. \tag{2.11}$$

Then,

$$R_{44} = -\gamma E^2/\rho^2, \tag{2.12}$$

and

$$T_{44} = E^2/\rho^2 \tag{2.13}$$

by (1.12). E is a function of ξ, η, σ.

3. THE DIFFERENTIAL CONDITIONS

$T_{\mu\nu}$ defines the null vector C_μ (except for a choice of sign which is immaterial):

$$C_\mu = (0, 0, 0, E/\rho), \quad C^\mu = (0, 0, -E/\rho, 0). \tag{3.1}$$

Proceeding as described in NEF, we get

$$C^\alpha_{;\alpha} = -E/\rho^2, \quad N = 0. \tag{3.2}$$

We find that the conditions (1.8) are satisfied without any restriction on the form of E. NEF (8.9) becomes (writing α for θ),

$$\begin{aligned}
\frac{\partial\alpha}{\partial\xi} &= -\frac{\partial}{\partial\eta}\left(\log\frac{E}{p}\right), \quad \frac{\partial\alpha}{\partial\eta} = \frac{\partial}{\partial\xi}\left(\log\frac{E}{p}\right),\\
\frac{\partial\alpha}{\partial\rho} &= 0, \quad \frac{\partial\alpha}{\partial\sigma} = \omega\frac{E}{\rho},
\end{aligned} \tag{3.3}$$

where ω is an undetermined invariant. The integrability conditions therefore reduce to

$$\left(\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2}\right)\log\frac{E}{p} = 0, \tag{3.4}$$

and the general solution is

$$\log\frac{E}{p} + i\alpha = F(\xi + i\eta, \sigma), \quad w = \frac{\rho}{E}\frac{\partial\alpha}{\partial\sigma}, \tag{3.5}$$

where F is any complex function.

We seek a symmetric solution, i.e., one which is a function of

$$\zeta = (\xi^2 + \eta^2)^{\frac{1}{2}}. \tag{3.6}$$

The most general solution of this form is when

$$F = b\log(\xi + i\eta) + \log a + i\epsilon,$$

where a, b, ϵ are real and may be functions of σ. Then,

$$E/p = a\zeta^b, \tag{3.7}$$

and

$$\alpha = b\tan^{-1}\eta/\xi + \epsilon. \tag{3.8}$$

Combining (3.7) and (2.11) we have

$$\gamma a^2\zeta^{2b} = \frac{1}{2}\left(\frac{\partial^2 K}{\partial\zeta^2} + \frac{1}{\zeta}\frac{\partial K}{\partial\zeta}\right) - \frac{2}{p^2}\frac{dm}{d\sigma} + \frac{6m}{p^3}\frac{\partial p}{\partial\sigma}, \tag{3.9}$$

where

$$K = p^2\left(\frac{\partial^2}{\partial\zeta^2} + \frac{1}{\zeta}\frac{\partial}{\partial\zeta}\right)\log p, \tag{3.10}$$

so that (3.9) is a differential equation of the fourth order for which we have to find a solution $p = p(\zeta, \sigma)$.

4. A SIMPLE SOLUTION

A simple solution is

$$p = (m/m_0)^{\frac{1}{3}}\zeta^n(1 + \tfrac{1}{4}\zeta^2), \tag{4.1}$$

where m_0 is a constant. This gives

$$K = (m/m_0)^{\frac{2}{3}}\zeta^{2n}, \tag{4.2}$$

$$E/p = n(2/\gamma)^{\frac{1}{2}}(m/m_0)^{\frac{1}{3}}\zeta^{n-1}, \tag{4.3}$$

$$R_{44} = -\frac{2n^2}{\rho^2}\left(\frac{m}{m_0}\right)^{\frac{4}{3}}\zeta^{4n-2}(1 + \tfrac{1}{4}\zeta^2)^2, \tag{4.4}$$

$$T_{44} = \frac{2}{\gamma}\frac{n^2}{\rho^2}\left(\frac{m}{m_0}\right)^{\frac{4}{3}}\zeta^{4n-2}(1 + \tfrac{1}{4}\zeta^2)^2, \tag{4.5}$$

$$A = \left(\frac{m}{m_0}\right)^{\frac{2}{3}}\zeta^{2n} - \frac{2}{3}\frac{\rho}{m}\frac{dm}{d\sigma} - \frac{2m}{\rho}. \tag{4.6}$$

The electromagnetic field is now determined with some degree of arbitrariness, as

$$\begin{aligned} f_{14} &= n(2/\gamma)^{\frac{1}{2}}(m/m_0)^{\frac{1}{3}}\zeta^{n-1}\sin\{(n-1)\tan^{-1}\eta/\xi + \epsilon\}, \\ f_{24} &= n(2/\gamma)^{\frac{1}{2}}(m/m_0)^{\frac{1}{3}}\zeta^{n-1}\cos\{(n-1)\tan^{-1}\eta/\xi + \epsilon\}, \end{aligned} \tag{4.7}$$

where m and ϵ can be any functions of σ, and m_0 is a constant. We see later that n must be a positive or negative integer.

If $n = 0$, the electromagnetic field vanishes and we are left with a gravitational field determined by m.

If $m = 0$ and $m_0 \neq 0$, then by (4.1) $p = 0$ and the differential form becomes degenerate. This must be ruled out, but if $m \to l^3 m_0 \to 0$ so that $m/m_0 \to l^3(\sigma)$, then we have a solution

$$m = 0, \quad p = l(\sigma)\zeta^n(1 + \tfrac{1}{4}\zeta^2). \tag{4.8}$$

Then

$$A = l^2\zeta^{2n} - (2\rho/l)(dl/d\sigma). \tag{4.9}$$

That is, if $m = 0$ we can substitute $l^3(\sigma)$ for m/m_0 and we have a valid solution giving a null electromagnetic field. This alternative is assumed in the equations which follow.

5. POLAR COORDINATES

Transform to the coordinates r, ϕ, θ, ct which we label in the order 1, 2, 3, 4. Here ϕ is the "colatitude" and θ the "longitude." $0 \leq \phi \leq \pi$, $0 \leq \theta \leq 2\pi$.

$$\begin{aligned} \xi &= 2\tan\phi/2\cos\theta, \quad \eta = 2\tan\phi/2\sin\theta, \\ \rho &= r, \quad \sigma = ct - r, \end{aligned} \tag{5.1}$$

so that

$$\zeta = 2\tan\phi/2, \quad 1 + \tfrac{1}{4}\zeta^2 = \sec^2\phi/2. \tag{5.2}$$

The differential form now becomes

$$\begin{aligned} ds^2 = (2 - A)\,dr^2 + Br^2(d\phi^2 + \sin^2\phi\,d\theta^2) \\ - 2(1 - A)c\,dr\,dt - Ac^2\,dt^2, \end{aligned} \tag{5.3}$$

where

$$A = \left(\frac{m}{m_0}\right)^{\frac{2}{3}}\left(2\tan\frac{\phi}{2}\right)^{2n} - \frac{2}{3}\frac{r}{m}\frac{dm}{d\sigma} - \frac{2m}{r}, \tag{5.4}$$

$$B = (m/m_0)^{-\frac{2}{3}}(2\tan\phi/2)^{-2n}. \tag{5.5}$$

Then,

$$\begin{aligned} g^{11} = A, \quad g^{22} = B^{-1}r^{-2}, \quad g^{33} = B^{-1}r^{-2}(\sin\phi)^{-2}, \\ g^{44} = -(2 - A), \quad g^{14} = -(1 - A), \\ g = -B^2r^4\sin^2\phi. \end{aligned} \tag{5.6}$$

The world lines defined by $ct - r = \text{const}$, $\phi = \text{const}$, $\theta = \text{const}$, are null geodesics.

When $n = 0$ and $m \to m_0 \to 0$, then $A = 1$, $B = 1$ and (5.3) reduces to the ordinary "flat" form. More generally it is necessary and sufficient for flatness that

$$n = 0, \quad m = 0, \quad m/m_0 \to l^3(\sigma).$$

The tensor of the electromagnetic field in these coordinates is

$$\begin{aligned} f_{13} &= f_{34} = n(2/\gamma)^{\frac{1}{2}}(m/m_0)^{\frac{1}{3}}(2\tan\phi/2)^n\cos(n\theta + \epsilon), \\ f_{12} &= f_{24} = n(2/\gamma)^{\frac{1}{2}}(m/m_0)^{\frac{1}{3}}(2\tan\phi/2)^n \\ &\quad \times \sin(n\theta + \epsilon)/\sin\phi, \end{aligned} \tag{5.7}$$

where m, ϵ may be any functions of $\sigma = ct - r$. Since θ is assumed to go from 0 to 2π there will be a discontinuity when $\theta = 2\pi$ unless n is integral positive or negative.

In these coordinates, the energy tensor has the following components:

$$\begin{aligned} T_{11} = -T_{14} = T_{44} = \frac{E^2}{r^2} \\ = \frac{2}{\gamma}\frac{n^2}{r^2}\left(\frac{m}{m_0}\right)^{\frac{4}{3}}(2\tan\phi/2)^{4n-2}\sec^4\phi/2. \end{aligned} \tag{5.8}$$

When $n = 0$, the electromagnetic field vanishes and the energy tensor vanishes. We are left with a gravitational field defined by m. Variations of m lead to gravitational waves traveling outward with the speed of light. They contribute nothing to the energy tensor and appear only as variations in the Riemann tensor. If m is constant, we can take $m = m_0$ and the differential form becomes

$$\begin{aligned} ds^2 = \left(1 + \frac{2m}{r}\right)dr^2 + r^2(d\phi^2 + \sin^2\phi\,d\theta^2) \\ - \frac{4m}{r}c\,dr\,dt - \left(1 - \frac{2m}{r}\right)c^2\,dt^2. \end{aligned} \tag{5.9}$$

This is equivalent to the Schwarzschild solution for a

point mass, and can be transformed to the better known form [e.g., Eq. (38.8) of Ref. 4] by putting

$$t = \bar{t} - (2m/c)\log[(r/2m - 1]. \tag{5.10}$$

This indicates the nature of m and suggests that when m is variable it should be confined to positive values if the results are to correspond to reality.

When $n \neq 0$, the electromagnetic field given by (5.7) represents electromagnetic radiation traveling radially outward with the speed of light in the presence of a gravitational field. This exists whether m varies or not, and the radiation need not have a wavelike structure. If m does vary we have electromagnetic and gravitational waves in phase. If we assume that m must remain positive, the sign of the electromagnetic field cannot change at a point and the electromagnetic radiation cannot have a simple harmonic wavelike form. We could, however, have, for example,

$$(m/m_0)^{\frac{1}{3}} = 1 + \kappa \sin 2\pi\nu(r/c - t),$$

where $k < 1$. In this case there would be a simple monochromatic radiation field of frequency ν, superimposed on a steady field (of zero frequency). This restriction on the form of the electromagnetic radiation in the presence of a central gravitational field is perhaps a peculiarity of our solution and not necessarily fundamental.

The situation is different when $m = 0$. As already mentioned above [following Eq. (4.9)] we may now substitute $l^3(\sigma)$ for m/m_0 so that

$$\begin{aligned} A &= l^2(2\tan\phi/2)^{2n} - (2r/l)(dl/d\sigma), \\ B &= l^{-2}(2\tan\phi/2)^{-2n}, \end{aligned} \tag{5.11}$$

$$\begin{aligned} f_{13} &= f_{34} = n(2/\gamma)^{\frac{1}{2}} l(2\tan\phi/2)^n \cos(n\theta + \epsilon), \\ f_{12} &= f_{24} = n(2/\gamma)^{\frac{1}{2}} l(2\tan\phi/2)^n \sin(n\theta + \epsilon)/\sin\phi, \end{aligned} \tag{5.12}$$

where l, ϵ may be any functions of $\sigma = ct - r$. Radiation exists whether l varies or not. If l varies it can have a simple harmonic form, i.e.,

$$l = l_0 \sin 2\pi\nu(r/c - t).$$

The differential form (5.3) becomes degenerate when $r = 0$, $m \neq 0$ and when $\phi = 0$ or π, $n \neq 0$. That is, there is a singularity at the origin when $m \neq 0$, and along a line extending "north" and "south" through the origin when $n \neq 0$. The same singularities appear in the electromagnetic and gravitational fields.

The rate of flow of electromagnetic energy outwards across an element of the surface $r = r$, $t = t$, is

$$cT^{14}(-g)^{\frac{1}{2}}\, d\phi\, d\theta = (2cn^2/\delta)(m/m_0)^{\frac{2}{3}}(2\tan\phi/2)^{2n-1} \times \sec^2\phi/2\, d\phi\, d\theta. \tag{5.13}$$

If we exclude two cones surrounding the "poles" defined by $\phi = 2\beta$, $t = t$, and $\phi = \pi - 2\beta$, $t = t$, we may integrate over the remaining surface $r = r$, $t = t$. We find that the rate of flow of electromagnetic energy across the surface is

$$(2\pi c/\gamma)(2)^{2n} n(m/m_0)^{\frac{2}{3}}\{(\tan\beta)^{-2n} - (\tan\beta)^{2n}\}. \tag{5.14}$$

This outward flow of energy occurs even when m is constant or zero. It is presumably compensated by an inflow of energy along the lines of discontinuity, i.e., from the "north" and "south." This is an adaptation of a suggestion made by P. G. Bergmann in respect of gravitational radiation (see Ref. 3, p. 431).

6. SPECIAL RELATIVITY APPROXIMATION

If we abandon Einstein's gravitational equations, we may consider the possibility in special relativity of similar electromagnetic fields existing in flat space–time. In polar coordinates we may write, corresponding to (5.12),

$$\begin{aligned} f_{13} &= f_{34} = f\tan^n\phi/2\cos(n\theta + \epsilon), \\ f_{12} &= f_{24} = f\tan^n\phi/2\sin(n\theta + \epsilon)/\sin\phi, \end{aligned} \tag{6.1}$$

where f, ϵ are any functions of $(ct - r)$. These satisfy all the necessary conditions for a null source-free electromagnetic field and represent radiation traveling radially outward with the speed of light. Note that the field does not now vanish when $n = 0$.

The ordinary vector "northward" and "eastward" components of the magnetic and electric fields are

$$\begin{aligned} H_n &= E_e = f\tan^n\phi/2\cos(n\theta + \epsilon)/r\sin\phi, \\ H_e &= -E_n = f\tan^n\phi/2\sin(n\theta + \epsilon)/r\sin\phi. \end{aligned} \tag{6.2}$$

The null electromagnetic fields considered here are such that the invariant N, defined in NEF (7.1), vanishes. This allows for the existence of the arbitrary variable ϵ in the description of the electromagnetic field, as in the case of plane radiation. It would be interesting to find, if possible, a case when $N \neq 0$.

[4] A. S. Eddinton, *The Mathematical Theory of Relativity* (Cambridge University Press, Cambridge, England, 1924), 2nd ed.

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Stress-Tensor Commutators and Schwinger Terms*

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We investigate, in local field theory, general properties of commutators involving Poincaré generators or stress-tensor components, particularly those of local commutators among the latter. The spectral representation of the vacuum stress commutator is given, and shown to require the existence of singular "Schwinger terms" at equal times, similar to those present in current commutators. These terms are analyzed and related to the metric dependence of the stress tensor in the presence of a prescribed gravitational field and some general results concerning this dependence presented. The resolution of the Schwinger paradox for the $T^{\mu\nu}$ commutators is discussed together with some of its implications, such as "nonclassical" metric dependence of $T^{\mu\nu}$. A further paradox concerning the vacuum self-stress—whether the stress tensor or its vacuum-subtracted value should enter in the commutators—is related to the covariance of the theory, and partially resolved within this framework.

I. INTRODUCTION

THE commutation relations among the generators $(P^\mu, J^{\lambda\sigma})$ of the Poincaré group, together with the existence of a unique normalizable vacuum state, require their vacuum expectation values to vanish.[1] Lorentz invariance also dictates the effect of these generators on any tensor, in particular on the symmetric stress tensor $T^{\mu\nu}$ itself, thereby placing requirements on the vacuum expectation value of the latter. While the stress tensor does not in general vanish in the vacuum, one may of course define subtracted stresses, $\bar{T}^{\mu\nu} = T^{\mu\nu} - \langle T^{\mu\nu}\rangle$. However, the commutator of any operator with $\bar{T}^{\mu\nu}$ is equal to that with $T^{\mu\nu}$. In particular, commutators such as $i[T^{00}(\mathbf{r}), T^{00}(\mathbf{r}')]$ are independent of whether T^{00} or $\bar{T}^{00}$ is used. This commutator, one of several which determine the Lorentz covariance of a theory,[2,3] has the particularly simple form $i[T^{00}(\mathbf{r}), T^{00}(\mathbf{r}')] = [T^{0k}(\mathbf{r}) + T^{0k}(\mathbf{r}')]\partial_k\delta(\mathbf{r} - \mathbf{r}')$ for fields of spin ≤ 1. The right-hand sides of such relations, on the other hand, are clearly dependent on whether $T^{\mu\nu}$ or $\bar{T}^{\mu\nu}$ is used. We may see, in going symmetrically from the Poincaré algebra, through relations of the type $[J^{\mu\nu}, T^{\lambda\sigma}]$ to $[T^{\mu\nu}, T^{\lambda\sigma}]$, that the right sides are in fact independent of whether $T^{\mu\nu}$ or $\bar{T}^{\mu\nu}$ is used, provided, as is required by Lorentz invariance, that $\langle T^{\mu\nu}\rangle = -\lambda\eta^{\mu\nu}$ (λ is constant, $\eta^{\mu\nu}$ is the Lorentz metric). Conversely, the connection of the stress tensor commutators to the Poincaré algebra will then also be verifiable in terms of either the original or the subtracted stresses. While these results are satisfactory, they are somewhat formal, for the usual evaluation of $\langle T^{\mu\nu}\rangle$ (even for free fields) yields a divergent, *noncovariant* result. (For example, the Maxwell field has $T^\mu_\mu = 0$, $\langle T^{00}\rangle > 0$.) Taking this noncovariance literally implies that a Wick ordering must be performed not only on $T^{\mu\nu}$ itself, but on all commutation relations involving $T^{\mu\nu}$ or the generators as well. This can be avoided by using extremely *ad hoc* prescriptions, which make $\langle T^{\mu\nu}\rangle$ covariant. These prescriptions are closely related to the necessity (for reasons given below) of redefining $T^{\mu\nu}$ as the limit of a spatially nonlocal operator.

Independently of the operator commutators mentioned above, the vacuum expectation values of local stress-tensor commutators $\langle[T^{\mu\nu}, T^{\lambda\sigma}]\rangle$ may be expressed in Lehmann–Källén (spectral) form solely on covariance grounds. Comparison with the operator expressions then implies, in addition to the above conditions on $\langle T^{\mu\nu}\rangle$, the necessary presence of Schwinger terms[4] [singular terms involving higher derivatives of $\delta(\mathbf{r})$] in the equal time $T^{\mu\nu}$ commutators, in close analogy to the corresponding results for current commutators. The metric dependence (of a fully quantum nature) of $T^{\mu\nu}$ in an external gravitational field implied by these terms is discussed. This dependence is in addition to the "classical" one dictated by general covariance which is also treated here. We give both general results on metric dependence of

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† John Simon Guggenheim Memorial Fellow, 1966–1967.
[1] This also follows from the absence of constant vectors or antisymmetric tensors to represent the constants $\langle P^\mu\rangle$ and $\langle J^{\mu\nu}\rangle$. We use the notation $\langle A\rangle$ to denote the vacuum expectation value, where the vacuum is assumed to be unique, normalizable, and invariant under the inhomogeneous Lorentz group.
[2] J. Schwinger, Phys. Rev. 127, 324 (1962); 130, 406, 800 (1963).
[3] P. A. M. Dirac, Rev. Mod. Phys. 34, 1 (1962).
[4] J. Schwinger, Phys. Rev. Letters 3, 259 (1959).

$T^{\mu\nu}$ and also, in the canonical formulation of specific local fields, the explicit (classical) dependence on the components $g_{0\mu}$ needed to evaluate the commutator expressions.

II. COMMUTATORS INVOLVING GENERATORS

Lorentz invariance is established in a field theory when the existence of Poincaré generators can be demonstrated. What is often actually exhibited, in a manifestly covariant theory, is not the Poincaré algebra of the $(P^\mu, J^{\lambda\sigma})$ but rather their effects as generators of field transformations:

$$i[\psi(x), P^\mu] = \partial^\mu\psi(x), \tag{1a}$$

$$i[\psi(x), J^{\mu\nu}] = (x^\mu\partial^\nu - x^\nu\partial^\mu)\psi(x) + iS^{\mu\nu}\psi(x), \tag{1b}$$

the matrices $S^{\mu\nu}$ realizing a finite dimensional representation of the Lorentz group. If Eqs. (1) hold for a complete set of fields ψ, they define the generators uniquely to within an additive c number. We now invoke the group structure implicit in Eqs. (1) and observe that, by the Jacobi identity, the operators $(\bar{P}^\mu, \bar{J}^{\mu\nu})$ defined by the right-hand sides of

$$i[P^\mu, P^\nu] = 0, \tag{2a}$$

$$i[P^\mu, J^{\lambda\sigma}] = \eta^{\mu\lambda}\bar{P}^\sigma - \eta^{\mu\sigma}\bar{P}^\lambda, \tag{2b}$$

$$i[J^{\mu\nu}, J^{\lambda\sigma}] = \eta^{\mu\lambda}\bar{J}^{\sigma\nu} - \eta^{\mu\sigma}\bar{J}^{\lambda\nu} + \eta^{\nu\lambda}\bar{J}^{\mu\sigma} - \eta^{\nu\sigma}\bar{J}^{\mu\lambda}, \tag{2c}$$

generate the same Lorentz transformations [Eqs. (1)] as do $(P^\mu, J^{\lambda\sigma})$. The $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$ then differ at most by a c number from $(P^\mu, J^{\lambda\sigma})$; further, Eqs. (2), together with the existence of a unique (invariant) normalizable vacuum, require that $\langle\bar{P}^\mu\rangle = 0 = \langle\bar{J}^{\lambda\sigma}\rangle$, but *not*, of course, that $\langle P^\mu\rangle = 0 = \langle J^{\lambda\sigma}\rangle$. The $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$ are completely fixed by this requirement, for any other set would differ by a c number and hence not vanish in the vacuum. We may then, if we like, rewrite Eqs. (2) as the usual algebra of generators with vanishing vacuum values simply by putting bars over the $(P^\mu, J^{\lambda\sigma})$ on the left sides:

$$i[\bar{P}^\mu, \bar{P}^\lambda] = 0, \tag{3a}$$

$$i[\bar{P}^\mu, \bar{J}^{\lambda\sigma}] = \eta^{\mu\lambda}\bar{P}^\sigma - \eta^{\mu\sigma}\bar{P}^\lambda, \tag{3b}$$

$$i[\bar{J}^{\mu\nu}, \bar{J}^{\lambda\sigma}] = \eta^{\mu\lambda}\bar{J}^{\sigma\nu} - \eta^{\mu\sigma}\bar{J}^{\lambda\nu} + \eta^{\nu\lambda}\bar{J}^{\nu\sigma} - \eta^{\nu\sigma}\bar{J}^{\mu\lambda}. \tag{3c}$$

We emphasize that Lorentz invariance requires not only the vanishing in the vacuum of the right sides of Eqs. (2) [or the members of the algebra of Eqs. (3)], but that the commutators on the left must automatically produce the correct $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$ generators.

Consider now the effect of the generators on an arbitrary symmetric second-rank tensor $T^{\mu\nu}(x)$; the commutators must take the form

$$i[T^{\mu\nu}(x), P^\lambda] = \partial^\lambda T^{\mu\nu}(x), \tag{4a}$$

$$i[T^{\mu\nu}(x), J^{\lambda\sigma}] = (x^\lambda\partial^\sigma - x^\sigma\partial^\lambda)T^{\mu\nu}(x) + \eta^{\mu\lambda}T^{\sigma\nu}(x) - \eta^{\mu\sigma}T^{\lambda\nu}(x) + \eta^{\nu\lambda}T^{\mu\sigma}(x) - \eta^{\nu\sigma}T^{\mu\lambda}(x). \tag{4b}$$

As before, the left sides of Eqs. (4) must vanish in the vacuum. For consistency then, Eq. (4a) requires that $\langle T^{\mu\nu}\rangle$ be constant,

$$\partial^\lambda\langle T^{\mu\nu}(x)\rangle = 0 \tag{5a}$$

while Eq. (4b) requires in addition that the constant be invariant, namely that

$$\langle T^{\mu\nu}(x)\rangle = -\lambda\eta^{\mu\nu}. \tag{5b}$$

Equations (5) just express the well-known translation and rotation invariance requirements on the vacuum expectation of any local symmetric second-rank tensor. If, in particular, $T^{\mu\nu}(x)$ is chosen to be the stress tensor of a local field theory,[5] we see that Lorentz invariance [as expressed by Eqs. (4)] does not require that $\langle T^{\mu\nu}(x)\rangle$ vanish, but only that it satisfy Eqs. (5). However, precisely the conditions expressed by Eqs. (5) are sufficient for the right sides of Eqs. (4) to have the same form in terms of $\bar{T}^{\mu\nu}(x) = T^{\mu\nu}(x) - \langle T^{\mu\nu}\rangle$, as is easily verified. We may then write

$$i[T^{\mu\nu}(x), P^\lambda] = \partial^\lambda\bar{T}^{\mu\nu}(x), \tag{6a}$$

$$i[T^{\mu\nu}(x), J^{\lambda\sigma}] = (x^\lambda\partial^\sigma - x^\sigma\partial^\lambda)\bar{T}^{\mu\nu}(x) + \eta^{\mu\lambda}\bar{T}^{\sigma\nu}(x) - \eta^{\mu\sigma}\bar{T}^{\lambda\nu}(x) + \eta^{\nu\lambda}\bar{T}^{\mu\sigma}(x) - \eta^{\nu\sigma}\bar{T}^{\mu\lambda}(x). \tag{6b}$$

From Eqs. (6), one may now conclude that if the $T^{\mu\nu}$ on the left are integrated[6] to yield P^λ or $J^{\lambda\sigma}$ [or if one puts $\bar{T}^{\mu\nu}$ on the left and integrates them to $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$] the corresponding integrals on the right are represented by the correct $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$ as required by Eqs. (2) or (3). [Some care must be taken in establishing this; if one starts from Eqs. (4) in terms of the original $T^{\mu\nu}$ on the right, the required integrations by parts yield nonvanishing surface terms here since $T^{\mu\nu}$, unlike $\bar{T}^{\mu\nu}$, does not vanish at infinity.[7]]

[5] $T^{\mu\nu}$ is not necessarily a local function of the canonical variables even if the Lagrangian is local (e.g., the Maxwell field with sources or the gravitational field). Even where $T^{\mu\nu}$ is a local function, as for the free spin-two massless field, the commutator $[T^{00}(\mathbf{r}), T^{00}(\mathbf{r}')]$, for example, is not necessarily local. See S. Deser, J. Trubatch, and S. Trubatch, Nuovo Cimento **39**, 1159 (1965).

[6] The generators P^μ and $J^{\lambda\sigma}$ can, of course, be written in terms of the stress tensor $T^{\mu\nu}$ through the relations $P^\mu = \int d^3r T^{0\mu}(x)$, $J^{\lambda\sigma} = \int d^3r[x^\lambda T^{0\sigma}(x) - x^\sigma T^{0\lambda}(x)]$. The same relations then obviously hold.

[7] We here assume that any physical system is sufficiently well localized that $(x^l)^4\bar{T}^{0\nu}(x) \to 0$ as $r \to \infty$. This will insure that the generators $(\bar{P}^\mu, \bar{J}^{\lambda\sigma})$ have finite matrix elements between physical states.

III. STRESS-TENSOR COMMUTATORS

We now consider a general set of local equal-time commutation relations[8] among the $T^{\mu\nu}(x)$ which, upon integration,[6] yield the Poincaré algebra, Eqs. (2) and (3), as well as Eqs. (4):

$$i[T^{00}(\mathbf{r}), T^{00}(\mathbf{r}')] = (T^{0k}(\mathbf{r}) + T^{0k}(\mathbf{r}'))\partial_k\delta(\mathbf{r}-\mathbf{r}') - \bar{\tau}^{00,00}(\mathbf{r},\mathbf{r}'), \quad (7a)$$

$$i[T^{00}(\mathbf{r}), T^{0m}(\mathbf{r}')] = (T^{mn}(\mathbf{r}) + T^{00}(\mathbf{r}')\delta^{mn})\partial_n\delta(\mathbf{r}-\mathbf{r}') - \bar{\tau}^{00,0m}(\mathbf{r},\mathbf{r}'), \quad (7b)$$

$$i[T^{00}(\mathbf{r}), T^{mn}(\mathbf{r}')] = (-\partial^0 T^{mn}(\mathbf{r}) + T^{0m}(\mathbf{r}')\partial^n + T^{0n}(\mathbf{r}')\partial^m)\delta(\mathbf{r}-\mathbf{r}') - \bar{\tau}^{00,mn}(\mathbf{r},\mathbf{r}'), \quad (7c)$$

$$i[T^{0k}(\mathbf{r}), T^{0m}(\mathbf{r}')] = (T^{0m}(\mathbf{r})\partial^k + T^{0k}(\mathbf{r}')\partial^m)\delta(\mathbf{r}-\mathbf{r}') - \bar{\tau}^{0k,0m}(\mathbf{r},\mathbf{r}'), \quad (7d)$$

$$i[T^{0k}(\mathbf{r}), T^{mn}(\mathbf{r}')] = (T^{mn}(\mathbf{r})\delta^{kl} - T^{ml}(\mathbf{r}')\delta^{nk} - T^{nl}(\mathbf{r}')\delta^{mk})\partial_l\delta(\mathbf{r}-\mathbf{r}') - \bar{\tau}^{0k,mn}(\mathbf{r},\mathbf{r}'). \quad (7e)$$

The operators $\bar{\tau}^{\mu\nu,\lambda\sigma}(\mathbf{r},\mathbf{r}')$ in Eqs. (7) are, in general, model dependent; they are, however, constrained to have certain integrals and moments vanishing. These constraints arise as the explicit $T^{\mu\nu}$ dependence on the right sides of Eqs. (7) is precisely such as to yield Eqs. (4) when integrating (or taking first moments) over $\mathbf{r}$ or $\mathbf{r}'$ [and, of course, yields Eqs. (2, 3) when integrated over both variables]. Thus, for

$$\bar{\tau}^{00,00}(\mathbf{r},\mathbf{r}') = -\bar{\tau}^{00,00}(\mathbf{r}',\mathbf{r}),$$

we must have in general that

$$\int d^3r\bar{\tau}^{00,00}(\mathbf{r},\mathbf{r}') = 0 = \int d^3r x^k\bar{\tau}^{00,00}(\mathbf{r},\mathbf{r}').$$

Relations (7) do not form an algebra, partly because of the $\bar{\tau}$, partly because no condition from the Poincaré relations is available to specify $[T^{kl}, T^{mn}]$ in a model independent way. We are, of course, assured by the earlier discussion that, upon integration of Eqs. (7), the right sides will be expressible in terms of the $\bar{T}^{\mu\nu}$. We may now ask if this is also the case for Eqs. (7) themselves? The condition $\langle T^{\mu\nu}\rangle = -\lambda\eta^{\mu\nu}$ clearly ensures that Eqs. (7a)–(7d) hold also in terms of $\bar{T}^{\mu\nu}$. However, Eq. (7e) changes form, by a term

$$\sim\lambda(\delta^{mn}\delta^{kl} - \delta^{mk}\delta^{nl} - \delta^{ml}\delta^{nk})\partial_l\delta(\mathbf{r}-\mathbf{r}')$$

when $T^{\mu\nu}$ is replaced by $\bar{T}^{\mu\nu} + \lambda\eta^{\mu\nu}$. This difference has a vanishing integral over $\mathbf{r}$ and a vanishing antisymmetric first moment; hence it can be absorbed into the $\bar{\tau}^{0k,mn}(\mathbf{r},\mathbf{r}')$ term, leaving a formally identical expression for the model-independent stress-tensor parts in terms of the $\bar{T}^{\mu\nu}$ together with an appropriately redefined $\bar{\tau}^{0k,mn}(\mathbf{r},\mathbf{r}')$. We will see, in fact, in terms of the spectral form for $\langle[T^{\mu\nu}(x), T^{\lambda\sigma}(x')]\rangle$, that a sum rule relates certain integrals of spectral functions for $\langle T^{mn}\rangle$ and $\langle\bar{\tau}^{0k,mn}\rangle$ or, equivalently, these integrals to $\langle\bar{T}^{mn}\rangle$ and the redefined $\langle\bar{\tau}^{0k,mn}\rangle$.

[8] Some of these relations are given in Refs. 2 and 3.

IV. SPECTRAL FORM OF VACUUM COMMUTATORS

If the $T^{\mu\nu}(x)$ are local operators and transform as tensors under proper Lorentz transformations, the vacuum expectation of the stress tensor commutators can be given a Lehmann–Källén representation.[9] For an arbitrary conserved symmetric second-rank tensor, there are two independent weight functions specifying the vacuum commutator;

$$\langle 0|\,[T^{\mu\nu}(x), T^{\lambda\sigma}(x')]\,|0\rangle = \int_0^\infty ds\{\rho_2(s)[\theta^{\mu\lambda}\theta^{\nu\sigma} + \theta^{\mu\sigma}\theta^{\nu\lambda} - \tfrac{2}{3}\theta^{\mu\nu}\theta^{\lambda\sigma}] + \rho_0\theta^{\mu\nu}\theta^{\lambda\sigma}\}\Delta(x-x',s), \quad (8)$$

where $\theta^{\mu\nu} \equiv \eta^{\mu\nu} - s^{-1}\partial^\mu\partial^\nu$ is conserved [i.e., $\partial_\nu\theta^{\mu\nu} \times \Delta(x,s) = 0$] and $\Delta(x-x',s)$ is the causal propagator with the property that $\Delta(x-x',s) = 0$ and

$$\partial^0\Delta(x-x',s) = i\delta(\mathbf{r}-\mathbf{r}')$$

for $x^0 = x'^0$. The functions $\rho_2(s)$ and $\rho_0(s)$, representing the contributions of intermediate states of mass $s^{\frac{1}{2}}$ and spin 2 and 0 respectively are nonnegative if the Hilbert space metric is positive definite.[10]

The only nonvanishing equal-time commutators are those with an odd number of temporal indices [since $\Delta(x,s)$ is odd in x^0]:

$$\langle 0|\,[T^{00}(\mathbf{r}), T^{0k}(\mathbf{r}')]\,|0\rangle = -i\int_0^\infty ds\, s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)](-\nabla^2)\partial^k\delta(\mathbf{r}-\mathbf{r}') \quad (9a)$$

$$\langle 0|\,[T^{0k}(\mathbf{r}), T^{mn}(\mathbf{r}')]\,|0\rangle = -i\int_0^\infty ds\{s^{-1}\rho_2(s)(\delta^{mk}\delta^{nl} + \delta^{nk}\delta^{ml} - \tfrac{2}{3}\delta^{kl}\delta^{mn}) \times \partial_l\delta(\mathbf{r}-\mathbf{r}') + s^{-1}\rho_0(s)\delta^{kl}\delta^{mn}\partial_l\delta(\mathbf{r}-\mathbf{r}') + s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)](-\partial^k\partial^m\partial^n)\delta(\mathbf{r}-\mathbf{r}')\}. \quad (9b)$$

[9] There are systems which violate these assumptions. For zero mass fields with spin $\geq\frac{3}{2}$; the Lorentz transformations induce additional gauge transformations on $\bar{T}^{\mu\nu}$ [see Ref. 5, and C. M. Bender and B. M. McCoy, Phys. Rev. **148**, 1375 (1966)], and so the latter do not transform as Lorentz tensors. There are, however, no restrictions on the singularity of the $\langle T^{\mu\nu}(x)T^{\lambda\sigma}(x')\rangle$ function. If the Wightman function exists, then the spectral form does also; see K. Bardacki and B. Schroer, J. Math. Phys. **7**, 10 (1966).

[10] This condition includes the radiation gauge formulation of electrodynamics which possesses a positive definite metric and a gauge invariant stress tensor.

Comparing the equal-time forms with Eqs. (7) and using $\langle T^{\mu\nu}\rangle = -\lambda\eta^{\mu\nu}$, we find first, from the vanishing components, that

$$\langle\bar{\tau}^{00,00}\rangle = 0 = \langle\bar{\tau}^{00,mn}\rangle = 0 = \langle\bar{\tau}^{0m,0n}\rangle, \quad (10a)$$

while Eq. (9a) yields

$$\langle\bar{\tau}^{0k,00}(\mathbf{r},\mathbf{r}')\rangle = -\int_0^\infty ds\, s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)] \times (-\nabla^2)\partial^k\delta(\mathbf{r}-\mathbf{r}'). \quad (10b)$$

The right side of Eq. (9b) has both a $\partial^k\delta(\mathbf{r}-\mathbf{r}')$ and a $\partial^k\partial^m\partial^n\delta(\mathbf{r}-\mathbf{r}')$ part, and so must $\langle\bar{\tau}^{0k,mn}(\mathbf{r},\mathbf{r}')\rangle$. Equating first derivatives yields a sum rule between $\int_0^\infty ds\, s^{-1}\rho_2(s)$, $\int_0^\infty ds\, s^{-1}\rho_0(s)$, λ, and the $\partial^k\delta(\mathbf{r}-\mathbf{r}')$ part of $\langle\bar{\tau}^{0k,mn}\rangle$, or, alternatively, between these integrals and the redefined $\langle\bar{\tau}^{0k,mn}\rangle$. The part of $\langle\bar{\tau}^{0k,mn}\rangle$ which is proportional to $\partial^k\partial^m\partial^n\delta(\mathbf{r}-\mathbf{r}')$ satisfies

$$\langle\bar{\tau}^{0k,mn}(\mathbf{r},\mathbf{r}')\rangle = \int_0^\infty ds\, s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)] \times \partial^k\partial^l\partial^m\delta(\mathbf{r}-\mathbf{r}'). \quad (10c)$$

Note that the $(\partial)^3\delta(\mathbf{r}-\mathbf{r}')$ terms in both $\langle\bar{\tau}^{00,0m}\rangle$ and $\langle\bar{\tau}^{0k,mn}\rangle$ involve the same nonnegative integral

$$\int_0^\infty ds\, s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)].$$

Equations (10) are, for our purposes, the most important consequences of the spectral relations (9). They imply that singular Schwinger terms[4] proportional to $(\partial)^3\delta(\mathbf{r}-\mathbf{r}')$ must be present in the operator relations, Eqs. (7b) and (7e), if the operator $T^{\mu\nu}$ itself is not to vanish. For, since ρ_2 and ρ_0 are separately nonnegative, they would each have to vanish if the $(\partial)^3\delta(\mathbf{r}-\mathbf{r}')$ terms in Eqs. (10) were absent. However, we could then conclude from the Wightman product corresponding to Eq. (8), that $\langle T^{\mu\nu}(x)T^{\lambda\sigma}(x')\rangle = 0$, and hence (since $T^{\mu\nu}$ is Hermitian) that $T^{\lambda\sigma}(x)\,|0\rangle = 0$. This follows from the fact that the Wightman product differs from Eq. (8) only by the replacement of $\Delta(x-x',s)$ by $\Delta^{(+)}(x-x',s)$, but has the same spectral functions. But, by the Federbush–Johnson theorem,[11] $T^{\mu\nu}$ itself must vanish (as an operator) if $T^{\mu\nu}(x)\,|0\rangle$ vanishes.[12] Thus, positive Hilbert space metric, positive energy spectrum, proper Lorentz covariance and locality by themselves require the presence of singular terms in $\bar{\tau}^{00,0m}$ and $\bar{\tau}^{0k,mn}$, i.e., in the commutators of Eqs. (7b) and (7e). As in the case of currents, naive application of canonical commutation or anticommutation relations, even for free spin 0, $\frac{1}{2}$, or 1 fields yield, paradoxically, no Schwinger terms. Hence, the singular operator $T^{\mu\nu}$ must be redefined, in analogy with the procedure for currents, as the limit of a nonlocal $T^{\mu\nu}$ in which the constituent field operators are separated by a space like distance and the commutators evaluated before taking the limit. This prescription does yield nonvanishing $(\partial)^3\delta(\mathbf{r}-\mathbf{r}')$ contributions, at least for free systems whose $T^{\mu\nu}$ are bilinear in the fields. For interacting fields, $T^{\mu\nu}$ contains, of course, higher powers of field operators. This case has not been investigated, but it seems likely that the essence of the problem resides in the kinematical free field parts.

V. METRIC DEPENDENCE AND STRESS-TENSOR COMMUTATORS

We discuss here the general dependence of the stress tensor on a weak external metric $g_{\mu\nu}$; our treatment is essentially a generalization of the analysis of the second paper of Ref. 2, which treated the case of a weak external g_{00} (this being sufficient for the $[T^{00}, T^{00}]$ commutator). These considerations bring out some properties of the functions $\bar{\tau}$ of Eqs. (7), constituting, in fact, a derivation of the latter equations. We also remark on a more specific problem: the dependence on an arbitrary metric of the stress tensor for local dynamical fields. The dependence on the four components $g_{0\nu}$, needed to evaluate the right sides of Eqs. (7), is explicitly exhibited for fields of spin $\lesssim 1$, and seen to be in accord with the requirements for a Hamiltonian formulation of the coupled matter and gravitational fields.

We begin with the definition of the stress tensor of a dynamical system as the coefficient of the variation of an external metric in the generally covariant form of its action[13] according to

$$\delta W_M = \int dx\tfrac{1}{2}\delta g_{\mu\nu}(x)\mathfrak{T}^{\mu\nu}(x),$$

where $\mathfrak{T}^{\mu\nu}(x)$ is the metric dependent symmetric tensor density. Thus a general matrix element in a prescribed classical external $g_{\mu\nu}$ obeys

$$-2i[\delta\langle a \mid b\rangle/\delta g_{\mu\nu}(x)] = \langle a|\,\mathfrak{T}^{\mu\nu}(x)\,|b\rangle \quad (11a)$$

and a second variation then yields the stress-tensor correlation function

$$2[\delta\langle a|\,\mathfrak{T}^{\mu\nu}(x)\,|b\rangle/\delta g_{\lambda\sigma}(x')] = i\,\langle a|\,[\mathfrak{T}^{\mu\nu}(x)\mathfrak{T}^{\lambda\sigma}(x')]_+\,|b\rangle + 2\,\langle a|\,\delta\mathfrak{T}^{\mu\nu}(x)/\delta g_{\lambda\sigma}(x')\,|b\rangle. \quad (11b)$$

[11] P. Federbush and K. Johnson, Phys. Rev. **120**, 1926 (1960). The essential point is that any local operator which annihilates the vacuum must vanish identically. See also R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics and All That* (W. A. Benjamin, Inc., New York, 1964), Chap. 4.

[12] This derivation is quite similar to that used elsewhere for vector currents: D. G. Boulware and S. Deser, Phys. Letters **22**, 99 (1966); Phys. Rev. **151**, 1278 (1966).

[13] A complementary problem is the use of prescribed external $T^{\mu\nu}$ in probing the properties of a dynamical metric field, which has been discussed by the authors, Nuovo Cimento **30**, 1009 (1963).

The last term takes into account the explicit $g_{\lambda\sigma}$ dependence of $\mathcal{C}^{\mu\nu}$ (in analogy with terms $\delta j^\mu/\delta A_\lambda$ in electrodynamics[2]). Note the reciprocity

$$\delta\mathcal{C}^{\mu\nu}(x)/\delta g_{\lambda\sigma}(x') = \delta\mathcal{C}^{\lambda\sigma}(x')/\delta g_{\mu\nu}(x).$$

The conservation law for $\mathcal{C}^{\mu\nu}$ is now the covariant one,

$$\mathcal{C}^{\mu\nu};\,\nu \equiv \mathcal{C}^{\mu\nu},\,\nu + \mathcal{C}^{\alpha\beta}\Gamma^\mu_{\alpha\beta} = 0. \tag{12}$$

If we vary a matrix element of this equation, we obtain from

$$\delta/\delta g_{\lambda\sigma}\,\langle a|\,\mathcal{C}^{\mu\nu};\,\nu\,|b\rangle \equiv 0$$

and from Eqs. (11) and (12), the relation

$$\partial_\nu\,\langle a|\,i[\mathcal{C}^{\mu\nu}(x)\mathcal{C}^{\lambda\sigma}(x')]_+\,|b\rangle + \partial_\nu\,\langle a|\,2\frac{\delta\mathcal{C}^{\mu\nu}(x)}{\delta g_{\lambda\sigma}(x')}\,|b\rangle + 2\frac{\delta\Gamma^\mu_{\alpha\beta}(x)}{\delta g_{\lambda\sigma}(x')}\,\langle a|\,\mathcal{C}^{\alpha\beta}(x)\,|b\rangle + \Gamma^\mu_{\alpha\beta}2\frac{\delta\,\langle a|\,\mathcal{C}^{\alpha\beta}(x)\,|b\rangle}{\delta g_{\lambda\sigma}(x')} = 0. \tag{13}$$

While relation (13) holds in the presence of an arbitrary metric, we are primarily interested here in the flat space limit $g_{\mu\nu} \to \eta_{\mu\nu}$. Then Γ is zero and the variation of Γ,

$$\delta\Gamma^\mu_{\alpha\beta} = -g^{\mu\lambda}\delta g_{\lambda\sigma}\Gamma^\sigma_{\alpha\beta} + \tfrac{1}{2}g^{\mu\rho}(\partial_\alpha\delta g_{\rho\beta} + \partial_\beta\delta g_{\rho\alpha} - \partial_\rho\delta g_{\alpha\beta}), \tag{14}$$

reduces to the three $\partial\delta g$ terms. We may then conclude from Eqs. (13) and (14) that, in the flat space limit,

$$\partial_\nu\left\{i[T^{\mu\nu}(x)T^{\lambda\sigma}(x')]_+ + 2\frac{\delta\mathcal{C}^{\mu\nu}(x)}{\delta g_{\lambda\sigma}(x')}\right\} + [\eta^{\mu\lambda}T^{\sigma\nu}(x) + \eta^{\mu\sigma}T^{\lambda\nu}(x) - \eta^{\mu\nu}T^{\lambda\sigma}(x)] \times \partial_\nu\delta(x - x') = 0. \tag{15}$$

In Eq. (15) we have returned to the flat space tensor $T^{\mu\nu}$ (which is, of course, identical to the tensor density $\mathcal{C}^{\mu\nu}$ in the limit), except in $\delta\mathcal{C}/\delta g$ where the distinction must be kept. On the other hand, the discontinuity of the time-ordered product at $x^0 = x'^0$ now yields

$$i[T^{0\mu}(x),\,T^{\lambda\sigma}(x')]\delta(x^0 - x'^0) = [\eta^{\mu\nu}T^{\lambda\sigma}(x) - \eta^{\mu\lambda}T^{\nu\sigma}(x) - \eta^{\mu\sigma}T^{\nu\lambda}(x)] \times \partial_\nu\delta(x - x') - 2\partial_\nu[\delta\mathcal{C}^{\mu\nu}(x)/\delta g_{\lambda\sigma}(x')]. \tag{16}$$

The absence of a $[T^{kl}, T^{mn}]$ relation here reflects the fact that T^{kl} does not obey a (partial) conservation law. The commutator terms arise exclusively from the discontinuities of the time-ordered products, which yield commutators when differentiated with respect to time in the course of applying Eq. (15).

Equation (16) is nearly of the form of Eqs. (7) with $2\partial_\nu(\delta\mathcal{C}^{\mu\nu}/\delta g_{\lambda\sigma})$ playing the role of the (model-dependent) $\bar{\tau}^{0\mu,\lambda\sigma}$; however, the right side of Eq. (16) contains explicit time derivatives of the delta function which are inconsistent with the equal time nature of the commutator. There must therefore be terms in $\delta\mathcal{C}^{0\mu}/\delta g_{\lambda\sigma}$ which cancel these time derivatives (there are also other, time local, parts of $\delta\mathcal{C}/\delta g$). The analysis of the various terms can most easily be presented by defining functions $t^{\mu\nu,\lambda\sigma}$:

$$t^{0\nu,00}(x, x') = 2[\delta\mathcal{C}^{0\nu}(x)/\delta g_{00}(x')] + T^{00}(x)\eta^{0\nu}\delta(x - x'), \tag{17a}$$

$$t^{0\nu,0m}(x, x') = 2[\delta\mathcal{C}^{0\nu}(x)/\delta g_{0m}(x')] + T^{00}(x)\eta^{\nu m}\delta(x - x'), \tag{17b}$$

$$t^{0\nu,mn}(x, x') = 2[\delta\mathcal{C}^{0\nu}(x)/\delta g_{mn}(x')] + [T^{0m}(x)\eta^{\nu n} + T^{0n}(x)\eta^{\nu m} - T^{0m}(x)\eta^{0\nu}] \times \delta(x - x'), \tag{17c}$$

$$t^{k\nu,0m}(x, x') = 2[\delta\mathcal{C}^{k\nu}(x)/\delta g_{0m}(x')] + [T^{0k}(x)\eta^{\nu m} + T^{0\nu}(x)\eta^{km}] \times \delta(x - x'), \tag{17d}$$

$$t^{k\nu,mn}(x, x') = 2[\delta\mathcal{C}^{k\nu}(x)/\delta g_{mn}(x')]. \tag{17e}$$

The $t^{\mu\nu,\lambda\sigma}(x, x')$ are symmetric,

$$t^{\mu\nu,\lambda\sigma}(x, x') = t^{\lambda\sigma,\mu\nu}(x', x)$$

and, comparing with Eqs. (7), we have the relation

$$\partial_\nu t^{\mu\nu;\lambda\sigma}(x, x') = \bar{\tau}^{0\mu,\lambda\sigma}(x, x') \tag{18}$$

As an example of how these equations are derived, we consider Eq. (17a). Equation (16) states that

$$i[T^{00}(x),\,T^{00}(x')]\delta(x^0 - x'^0) = 2T^{0k}(x)\partial_k\delta(x - x') + T^{00}(x)\partial_0\delta(x - x') - 2\partial_0[\delta\mathcal{C}^{00}(x)/\delta g_{00}(x')] - 2\partial_k[\delta\mathcal{C}^{0k}(x)/\delta g_{00}(x')].$$

Then, the definition

$$2[\delta\mathcal{C}^{00}(x)/\delta g_{00}(x')] = T^{00}(x)\delta(x - x') + t^{00,00}(x, x')$$

explicitly cancels the undesirable $T^{00}(x)\partial_0\delta(x - x')$ term. To see whether a similar redefinition is needed for the $\delta\mathcal{C}^{0k}(x)/\delta g_{00}(x')$ term, consider

$$i[T^{0k}(x),\,T^{00}(x')]\delta(x^0 - x'^0) = T^{00}(x)\partial^k\delta(x - x') - 2\partial_\nu[\delta\mathcal{C}^{k\nu}(x)/\delta g_{00}(x')].$$

Clearly, none is required, since there are no explicit $\partial_0\delta$ terms on the right. Thus, we arrive at Eq. (17a),

$$t^{0\nu,00}(x, x') = 2[\delta\mathcal{C}^{0\nu,00}(x)/\delta g_{00}(x')] + T^{00}(x)\eta^{0\nu}\delta(x - x')$$

and obtain the expression

$$i[T^{00}(x),\,T^{00}(x')]\delta(x^0 - x'^0) = [T^{0k}(x) + T^{0k}(x')]\partial_k\delta(x - x') - \partial_\nu t^{0\nu,00}(x, x') \tag{19}$$

A similar analysis yields the remainder of Eqs. (17) together with the analogs of Eq. (19).

The $\bar{\tau}$ of Eqs. (7) are antisymmetric, $\bar{\tau}^{\mu\nu,\lambda\sigma}(x, x') = -\bar{\tau}^{\lambda\sigma,\mu\nu}(x', x)$, hence, using Eq. (18), the symmetry of the t, the antisymmetry of the $\bar{\tau}$, and the integral conditions which enforce the vanishing of the moments of $\bar{\tau}$, the following expressions are obtained.

$$t^{00,00}(x, x') = \partial_k\partial_l\partial'_m\partial'_n\sigma^{kl,mn}(x, x'), \tag{20a}$$

$$t^{0k,00}(x, x') = \partial_l\partial'_m\partial'_n[\tau_1^{kl,mn}(x, x') - \partial_0\sigma^{kl,mn}(x, x')], \tag{20b}$$

$$t^{0k,0m}(x, x') = \partial_l\partial'_n[\tau_2^{kl,mn}(x, x') + \tfrac{1}{2}(\partial_0 - \partial'_0) \times \tau_1^{kl,mn}(x, x') + \partial_0\partial'_0\sigma^{kl,mn}(x, x')], \tag{20c}$$

$$t^{00,mn}(x, x') = -\partial_k\partial_l[\tau_2^{kl,mn}(x, x') - \tfrac{1}{2}(\partial_0 + 3\partial'_0) \times \tau_1^{kl,mn}(x, x') - \partial_0'^2\sigma^{kl,mn}(x, x')], \tag{20d}$$

$$t^{0k,mn}(x, x') = -\partial_l[\tau_3^{kl,mn}(x, x') + \partial'_0(\tau_2^{kl,mn}(x, x') + \tfrac{1}{2}(\partial_0 - \partial'_0)\tau_1^{kl,mn}(x, x') + \partial_0\partial'_0\sigma^{kl,mn}(x, x'))], \tag{20e}$$

$$t^{kl,mn}(x, x') = \tau_4^{kl,mn}(x, x') + \tfrac{1}{2}(\partial_0 - \partial'_0)\tau_3^{kl,mn}(x, x') + \partial_0\partial'_0[\tau_2^{kl,mn}(x, x') + \tfrac{1}{2}(\partial_0 - \partial'_0) \times \tau_1^{kl,mn}(x, x')] + \partial_0^2\partial_0'^2\sigma^{kl,mn}(x, x'), \tag{20f}$$

where $\sigma^{kl,mn}(x, x')$, $\tau_2^{kl,mn}(x, x')$, and $\tau_4^{kl,mn}(x, x')$ are symmetric under $\tau^{kl,mn}(x, x') \to \tau^{mn,kl}(x', x)$ and τ_3 and τ_1 are antisymmetric. Furthermore,

$$\tau_i^{kl,mn}(x, x') = \tau_i^{lk,mn}(x, x').$$

We have inferred from the integral statements [$\int d^3r\bar{\tau}^{0k,mn}(x, x')$, for example] that $\bar{\tau}^{0k,mn}(x, x') = \partial_l\bar{\tau}^{lk,mn}(x, x')$. This conclusion holds if $\bar{\tau}(x, x')$ is local, as we assume here. For then, the matrix element,

$$\langle p|\,\bar{\tau}(x, x')\,|0\rangle = \exp(-i)p\tfrac{1}{2}(x + x')\sum_n f^{(n)}(p)\delta^{(n)}(x - x'),$$

where $\langle p|$ is an arbitrary state (by the Federbush–Johnson theorem, we do not need to consider more general matrix elements[11]), is a finite sum of derivatives of $\delta(x - x')$. Then the Fourier transform with respect to x at $x' = 0$ is $\sum_n[i(k + \frac{1}{2}p)]^n f^{(n)}_{(p)}$, a finite polynomial in k. If $\int d^3r\bar{\tau}(x, x') = 0$, then the leading term must be k, and we can re-express $\bar{\tau}^{0\cdots}$ as $\partial_l\bar{\tau}^{l\cdots}$. For $\bar{\tau}^{00,00}$ we can similarly conclude that $\bar{\tau}^{00,00} = \partial'_m\partial'_n\partial_k\partial_l\bar{\tau}^{kl,mn}$. If the $\bar{\tau}$'s are nonlocal,[9] the argument breaks down and one can no longer assume the derivative form in all cases.

Equations (16)–(18) and Eq. (20) may then be used to determine the equal-time commutators

$$i[T^{00}(x), T^{00}(x')]\delta(x^0 - x'^0) = [T^{0k}(x) + T^{0k}(x')]\partial_k\delta(x - x') - \partial_k\partial_l\partial'_m\partial'_n\tau_1^{kl,mn}(x, x'), \tag{21a}$$

$$i[T^{00}(x), T^{0m}(x')]\delta(x^0 - x'^0) = [T^{ml}(x) + T^{00}(x')\delta^{ml}]\partial_l\delta(x - x') - \partial_k\partial_l\partial'_n[\tau_2^{kl,mn}(x, x') - \tfrac{1}{2}(\partial_0 + \partial'_0)\tau_1^{kl,mn}(x, x')], \tag{21b}$$

$$i[T^{00}(x), T^{mn}(x')]\delta(x^0 - x'^0) = [-\partial^0 T^{mn}(x) + T^{0m}(x')\partial^n + T^{0n}(x')\partial^m]\delta(x - x') + \partial_k\partial_l[\tau_3^{kl,mn}(x, x') + (\partial_0 + \partial'_0)\tau_2^{kl,mn}(x, x') - \tfrac{1}{2}(\partial_0 + \partial'_0)^2\tau_1^{kl,mn}(x, x')], \tag{21c}$$

$$i[T^{0k}(x), T^{0m}(x')]\delta(x^0 - x'^0) = [T^{0m}(x)\partial^k + T^{0k}(x')\partial^m]\delta(x - x') - \partial_l\partial'_n\tau_3^{kl,mn}(x, x'), \tag{21d}$$

$$i[T^{0k}(x), T^{mn}(x')]\delta(x^0 - x'^0) = [T^{mn}(x)\delta^{kl} - T^{ln}\delta^{mk} - T^{lm}\delta^{nk}]\partial_l\delta(x - x') - \partial_l[\tau_4^{kl,mn}(x, x') - \tfrac{1}{2}(\partial_0 + \partial'_0)\tau_3^{kl,mn}(x, x')]. \tag{21e}$$

This is the most general form of the stress-tensor commutation relations consistent with the Poincaré algebra and locality. The form of the relations has been obtained here from the metric dependence of $\mathcal{C}^{\mu\nu}$, the τ_i functions representing model-dependent parts. The structures are consistent with the time locality of the commutators since time derivatives only occur in the combination $\partial_0 + \partial'_0$ which cannot generate any derivatives of a delta function $\delta(x^0 - x'^0)$, but only the time derivative (or commutator with P^0) of the operator coefficient of the delta function. Hence, we conclude that the functions τ_i must be local in time. There is no such direct requirement on σ since it does not appear in any of the commutators. These statements do not imply that $\mathcal{C}^{\mu\nu}$ is independent of time derivatives of $g_{\lambda\sigma}$, but only restrict the form of the dependence to that implicit in Eqs. (17) and (20). The spectral functions ensure that τ_2 and τ_4 cannot be zero. Their vacuum expectation values must be

$$\partial_k\partial_l\partial'_n\langle\tau_2^{kl,mn}(x, x')\rangle = \int_0^\infty ds s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)]\nabla^2\partial^m\delta(x - x'), \tag{22a}$$

$$\partial_l\langle\tau_4^{kl,mn}(x, x')\rangle = -\int_0^\infty ds\{s^{-1}\rho_2(s)[\delta^{mk}\delta^{nl} + \delta^{ml}\delta^{nk} - \tfrac{2}{3}\delta^{mn}\delta^{lk}] + s^{-1}\rho_0(s)\delta^{kl}\delta^{mn}\}\partial_l\delta(x - x') + \int_0^\infty ds s^{-2}[\tfrac{4}{3}\rho_2(s) + \rho_0(s)]\partial^k\partial^m\partial^n\delta(x - x'). \tag{22b}$$

The time derivative terms cannot contribute in the vacuum, since they are commutators with P^0, hence only the above terms survive if we express the relations in terms of $\bar{T}$. The single derivative term is highly model dependent and occurs "classically" in the spin $\frac{1}{2}$ case, for example.

The general results embodied in Eq. (16) and the subsequent form Eq. (21) determine the equal-time commutators once the metric dependence (both classical and quantum) of the stress tensor of a particular system is known. It is interesting that for an important class of systems, namely local dynamical fields of low spin (≤ 1), this dependence (more precisely, its classical part) can be inferred explicitly in a uniform way. One takes the field's flat space action in terms of canonical variables[14] (π_A, ϕ_A) and expresses it in a generally covariant form. It is then possible to redefine the canonical variables in the presence of $g_{\mu\nu}$ such that the flat space canonical form

$$W_M = \int dx[\sum \pi_A \partial_0 \phi_A - \mathcal{H}(\pi_A, \phi_A; \eta)] \quad (23)$$

only changes by $\mathcal{H}(\pi, \phi; \eta) \to \mathcal{H}(\pi, \phi, g)$. This may be accomplished[14] essentially by defining π_A so as to absorb the $(-g_4)^{\frac{1}{2}}$ of the volume element.

The energy density $\mathcal{H}$ now takes the form

$$\mathcal{H}(\pi_A, \phi_A; g) = -N\Theta_0^0(\pi_A, \phi_A, g_{ij}) - N^i\Theta_i^0(\pi_A, \phi_A, g_{ij})$$

in terms of the convenient notation $N_i \equiv g_{0i}$, $N^i \equiv {}^3g^{ij}N_j$, $N \equiv (-g^{00})^{-\frac{1}{2}} = (N_iN^i - g_{00})^{\frac{1}{2}}$, where the contravariant metric ${}^3g^{ij}$ is the inverse of the spatial part of $g_{\mu\nu}$: ${}^3g^{ij}g_{jk} = \delta_k^i$. The fundamental point is that the Θ_μ^0 are functions only of the spatial components and *not* of the $g_{0\mu}$, the full dependence on the latter being through the linear coefficients N, N^i. In the flat space limit, the Θ_μ^0 are just the energy momentum density components. Thus, for the Maxwell field, $-\Theta_\eta^0 = \frac{1}{2}g^{-\frac{1}{2}}[g_{ij}(\epsilon^i\epsilon^j + \mathcal{B}^i\mathcal{B}^j)]$, $\Theta_i^0 = \epsilon_{ijk}\epsilon^j\mathcal{B}^k$, and $\epsilon^i = (-g_4)^{\frac{1}{2}}F^{0i}$, $\mathcal{B}^i = \epsilon^{ijk}\partial_j A_k$. The correct variables here are the contravariant densities ϵ^i and $\mathcal{B}^i$ while g is the three-dimensional determinant and $-g_4$ represents the four-dimensional one.

Now, if one varies the combined Einstein-matter action,

$$W = W_E + W_M, \; W_E = K^{-1}\int dx(-g_4)^{\frac{1}{2}}R$$

the quantities Θ_μ^0 are precisely the sources of the G_μ^0 components of the Einstein tensor, referred to a time constant surface. For W_E itself may be written in the form[14]

$$W_E = \int dx[\pi^{ij}\partial_0 g_{ij} - NR_0(\pi^{ij}, g_{ij}) - N^iR_i(\pi^{ij}, g_{ij})],$$

the R_μ being linear combinations of the G_μ^0 and depending only on g_{ij} and its conjugate variable π^{ij} but not on N or N_i. The four equations $R_\mu = -K\Theta_0^\mu$ are in fact the four constraint equations corresponding to $\nabla \cdot E = j^0$ in electrodynamics and Θ_μ^0 are then clearly linear combinations of the correct energy momentum density source of the Einstein field.

The energy momentum density Θ_μ^0 depends only, as it must for a correct formulation of the initial value problem (Cauchy data), on quantities which transform as tensors under coordinate transformations within the t = const surface and are invariant under coordinate transformations off the surface, namely on π_A, ϕ_A, and g_{ij}. The gauge quantities N, N^i (or, equivalently, the $g_{0\mu}$), on the other hand, are altered by coordinate changes off the surface (they correspond to the gauge variable A^0 in electrodynamics) which is why they are not desirable in a correct Θ_μ^0.[14]

The Θ_μ^0 may now be used to evaluate the stress-density $\mathcal{T}^{\mu\nu}$ defined according to $W_M = \frac{1}{2}\int dx\delta g_{\mu\nu}\mathcal{T}^{\mu\nu}$, which enters in the general commutation relations. The Θ_μ^0 and $\mathcal{T}^{0\mu}$ are not identical since they are the coefficients of (N, N^i) and (g_{00}, g_{0i}), respectively, in the action. Thus we find from $-\frac{1}{2}\mathcal{T}^{\mu\nu} = \delta\mathcal{H}/\delta g_{\mu\nu}$ that

$$\mathcal{T}^{00} = -N^{-1}\Theta_0^0, \quad \mathcal{T}^{0i} = {}^3g^{ij}[\Theta_j^0 + N_iN^{-1}\Theta_0^0], \quad (24)$$

which gives the explicit dependence of the $\mathcal{T}^{0\mu}$, for example, on $g_{0\mu}$ and thus also defines the ("classical" part of) $\delta\mathcal{T}^{0\mu}/\delta g_{\lambda\sigma}$. Note that in the limit $g_{\mu\nu} = \eta_{\mu\nu}$ the $\mathcal{T}^{0\nu}$ and $\Theta^{0\mu}$ coincide. However, in computing the $\delta\mathcal{T}/\delta g$ terms, the relations (24) must be used. For fields of spin ≤ 1, including electrodynamics, these results (which hold for arbitrary g) may be used to calculate the $[T^{0\mu}, T^{\lambda\sigma}]$ relations. They agree with direct calculations using canonical commutation

[14] These results arise from the canonical analysis of coupled gravitational and matter fields: R. Arnowitt, S. Deser, and C. W. Misner, J. Math. Phys. **1**, 434 (1960), and Phys. Rev. **120**, 313 (1960) for derivations and explicit examples (including the Maxwell field). For the canonical form of the spinor field (which is somewhat more complicated, involving essentially derivative coupling to the metric) see T. W. B. Kibble, J. Math. Phys. **4**, 1433 (1963). Higher spin cases, where the constraints among matter field components complicate matters are dealt with in their g_{00} dependence, which is relevant to the $[T^{00}, T^{00}]$ relation in Ref. 2. Here, the process of eliminating constraints to reach canonical form in terms of the independent modes may bring in more metric dependence than that given in the text for low spins. In particular, the Θ_μ^0 may acquire N, N^i dependence when expressed in terms of the reduced variables. In view of the subsequent discussion, this may be regarded as a strong argument against the physical significance of elementary higher spin systems; for the latter would then not have the desired property of a system in time development from a given set of Caudy data, the energy momentum density being dependent at any instant on the physically meaningless choice of coordinates N, N^i, as well as on the dynamical variables. This would also raise analogous difficulties in the Einstein constraint equations $R_\mu = -K\Theta_\mu^0$.

relations and keeping $g_{\mu\nu} = \eta_{\mu\nu}$.[15] One may also recover the results of Ref. 2 for a weak external g_{00}. In particular these forms imply that there are no additional $\bar{\tau}^{00,00}$ terms in the $[T^{00}, T^{00}]$ relations for low spins.

We emphasize that the general metric dependence obtained here is the classical one and does not include the purely quantum dependence on the metric which is required to yield the Schwinger terms. Indeed, there is here a curious contrast to the situation for currents. There,[12] "classical" dependence of the current on the corresponding external field (e.g., the Maxwell field) may or may not be present, depending on whether or not the system has spin $\frac{1}{2}$. If there is classical (A^2) dependence, it automatically gives rise to Schwinger type terms. Here, on the other hand, there is always classical metric dependence on $\mathcal{T}^{\mu\nu}$, irrespective of spin, but this dependence turns out never to be sufficient to yield Schwinger terms (at least for spin ≤ 1). Thus, for all fields, one must redefine $\mathcal{T}^{\mu\nu}$ as the limit of a spatially nonlocal operator to obtain the terms.

In our framework, involving an external (or dynamical) metric, one must simultaneously insert an appropriate quantum metric dependence in this redefined $\mathcal{T}^{\mu\nu}$. The necessity for this prescription may also be inferred either from general covariance (for a "split" $\mathcal{T}^{\mu\nu}$ without extra dependence no longer transforms as a coordinate tensor) or, in terms of a dynamical gravitational field, along lines similar to those of Ref. 12 for currents coupled to a Bose field. The Schwinger terms will then correspond to the nonclassical part of $\delta\mathcal{T}/\delta g$. The elaboration of these remarks regarding the nonclassical metric dependence and nonlocal $\mathcal{T}^{\mu\nu}$ constitutes a separate program, which we do not pursue here.

Some general conclusions may be drawn, however, from the $\partial^3\delta$ nature of the Schwinger terms, together with the fact that they must arise from $\partial_j\delta\mathcal{T}^{ij}/\delta g_{00}$ or $\partial_i(\delta\mathcal{T}^{0i}/\delta g_{0j})$ and $\partial_j(\delta\mathcal{T}^{ij}/\delta g_{kl})$ in $[T^{00}, T^{0j}]$ and $[T^{0i}, T^{kl}]$, respectively. There must be at least the following nonclassical dependence: $\mathcal{T}^{0i}[\partial^2_{kl}g_{0i}]$, $\mathcal{T}^{00}[\partial^2_{kl}g_{mn}]$, and $\mathcal{T}^{ij}[\partial^2_{kl}g_{mn}]$, and $\mathcal{T}^{ij}[\partial^2_{kl}g_{00}, \partial^2_{kl}g_{mn}]$.

An alternate argument leading to these dependences in the $\mathcal{T}^{\mu\nu}$ is as follows. In electrodynamics, $[j^0, j^i] \neq 0$ and Gauss's equation $\nabla \cdot E = j^0$ implies that $[\mathbf{E}^L, j^i] \neq 0$, where $\mathbf{E}^L$ is the longitudinal electric filed. Lorentz invariance then requires that the transverse part $\mathbf{E}^T$ also fail to commute, i.e., that $[\mathbf{E}^T, j] \neq 0$, and hence that $\mathbf{j} = \mathbf{j}(A^T)$. Similarly the constraint equations $G^0_\mu = -\kappa T^0_\mu$ require that $[G^0_0, T^{0i}]$, $[G^0_i, T^{00}]$ and $[G^0_i, T^{kl}]$ not vanish. In the linearized approximation, where $G^0_0 \approx \nabla^2 g_{ij}$ and $G^0_i \sim \pi^{ij},_j$ Lorentz invariance then requires that $\mathcal{T}^{0i}$ depend on the variables π^{ij} conjugate to g_{ij} which means in particular that it involves $\partial^2_{kl}g_{0j}$ (since π^{ij} is by its definition proportional to $g_{0i,j}$). Likewise $\mathcal{T}^{00}$ and $\mathcal{T}^{kl}$ must depend on $\partial^2_{kl}g_{ij}$. It is hoped to return to these questions elsewhere.

[15] Explicit calculations on these questions have been carried out by J. Trubatch (unpublished).

VI. SUMMARY

We have examined a number of consistency conditions on the commutation relation among the Poincaré generators and the stress-tensor components in local field theory. In particular, the apparent difficulty that, while the right sides of such relations should vanish in vacuum, they actually involve the unsubtracted (nonvanishing in vacuum) stresses or their integrals, was resolved by the Lorentz covariance requirement that $\langle T^{\mu\nu}\rangle = -\lambda\eta^{\mu\nu}$. The latter ensured that the right side could simultaneously satisfy both these apparently contradictory conditions.

The general form of the equal-time stress-tensor commutation relations compatible with the Poincaré algebra was exhibited, and compared with the Lehmann–Källén representation[16] for

$$\langle 0|\,[T^{\mu\nu}(x), T^{\lambda\sigma}(x')]\,|0\rangle.$$

The latter depends only on the locality and Lorentz transformation properties of $T^{\mu\nu}$, and involves two nonnegative weight functions for conserved $T^{\mu\nu}$ when the Hilbert space metric is positive. The main result of the spectral representation (and hence a consequence of only locality, proper Lorentz covariance, positive energy spectrum, and positive Hilbert space metric) was the necessary existence of Schwinger terms, of the form $\partial^3\delta(\mathbf{r} - \mathbf{r}')$ in the equal-time commutators $[T^{00}(\mathbf{r}), T^{0m}(\mathbf{r}')]$, and $[T^{0k}(\mathbf{r}), T^{mn}(\mathbf{r}')]$.

Paradoxically, straightforward calculations from canonical commutation relations (even for free fields) yields neither Schwinger terms nor the covariant form $\lambda\eta^{\mu\nu}$ for $\langle T^{\mu\nu}\rangle$. If the stress tensor is defined as the limit of a spatially nonlocal operator, the Schwinger terms required by the spectral forms appear. However, this prescription does not simultaneously reinstate the covariance of $\langle T^{\mu\nu}\rangle$. We have been able to achieve the latter only by extremely artificial means, such as regularization with indefinite weight functions which would probably introduce negative energy states or a limiting process in which the spacelike separation was not along a $t = \text{const}$ surface. Thus, while it is likely

[16] The Lehmann–Källén representation is, of course, valid only in the flat space limit $g \to \eta$. We have used the more general metric as a device for studying the flat space limit, but many of our results will be reflected in the full nonlinear theory.

that the singularity of the strictly local product is responsible both for loss of Lorentz covariance and the Schwinger paradox, a unified prescription for removing both problems has not been found. Incidentally, the above difficulties are most apparent in the vacuum expectation values, since the operator products are most singular when associated with creation and annihilation of excitations at the same point. For a free field, however, it is possible to calculate $\langle 0|\, T^{\mu\nu}(x)T^{\lambda\sigma}(x')\,|0\rangle$ for unequal times. This form is manifestly covariant (with the exception of the $\langle 0|\, T^{\mu\nu}\,|0\rangle\langle 0|\, T^{\lambda\sigma}\,|0\rangle$ terms) and satisfies the Lehmann–Källén representation. If this is used to calculate the commutators $\langle [T^{\mu\nu}, T^{\lambda\sigma}]\rangle$, we find that the right sides have all the requisite properties in the vacuum. It is, of course, impossible to calculate $\langle \bar{T}^{\mu\nu}\rangle = -\lambda\eta^{\mu\nu}$ by this method, but it does establish the form for $\langle \bar{T}^{\mu\nu}\rangle$. It is clear from the discussion in Sec. II that $\bar{T}^{\mu\nu}$ rather than $T^{\mu\nu}$ is the tensor, otherwise J would have to be expressed in terms of T rather than $\bar{T}$. The source of the difficulty can be understood somewhat better by considering the case of a free spin 0 field. The term from which the trouble stems is $\phi^{\mu}(x)\phi^{\nu}(x)$, which must be written

$$\phi^{\mu}(x + \tfrac{1}{2}\xi)\phi^{\nu}(x - \tfrac{1}{2}\xi) \equiv \mathbf{T}^{\mu\nu}(x, \xi).$$

Then

$$\begin{aligned} i[\mathbf{T}^{\mu\nu}(x, \xi), J^{\lambda\sigma}] &= (x^{\lambda}\partial_x^{\sigma} - x^{\sigma}\partial_x^{\lambda})\mathbf{T}^{\mu\nu}(x, \xi) + g^{\mu\lambda}\mathbf{T}^{\sigma\nu}(x, \xi) \\ &\quad - g^{\mu\sigma}\mathbf{T}^{\lambda\nu}(x, \xi) + g^{\nu\lambda}\mathbf{T}^{\mu\sigma}(x, \xi) - g^{\nu\sigma}\mathbf{T}^{\mu\lambda}(x, \xi) \\ &\quad + (\xi^{\lambda}\partial_{\xi}^{\sigma} - \xi^{\sigma}\partial_{\xi}^{\lambda})\mathbf{T}^{\mu\nu}(x, \xi). \end{aligned}$$

In the limit $\xi \to 0$, the last term never appears; however, in the vacuum expectation value, that term is essential for the proper covariance, *even in the limit* $\xi \to 0$. Thus, the noncovariance of

$$T^{\mu\nu}(x) = \lim_{\xi \to 0} T^{\mu\nu}(x, \xi),$$

is due to extra terms which are not transformed properly as $\xi \to 0$. Once these terms are subtracted, the remainder $\bar{T}^{\mu\nu}$ does transform correctly.

We have further exhibited the dependence of the stress tensor on $g_{\mu\nu}$ which is forced by the structure constants of the Poincaré algebra and compatible with the most general additional "nonalgebra" terms. These considerations are consistent with the (classical) explicit metric dependence of $\mathcal{T}^{\mu\nu}$ which was obtained in the generally covariant canonical formulation of matter fields of spin ≤ 1.

The nonlocal prescription for $\mathcal{T}^{\mu\nu}$ requires, in order to maintain general covariance, that explicit dependence on the metric be inserted into the "spread" $\mathcal{T}^{\mu\nu}$, which would otherwise no longer transform as a tensor under general coordinate transformations. Now, by direct calculation[15] in terms of canonical commutation relations with $g_{\mu\nu} = \eta_{\mu\nu}$, spreading the points in $\mathcal{T}^{\mu\nu}$ is actually sufficient to produce terms proportional to $(\partial)^3\delta(\mathbf{r} - \mathbf{r}')$ in the $[T^{00}, T^{0m}]$ and $[T^{0k}, T^{mn}]$ commutators. In the presence of an external metric (or in terms of the general $\delta\mathcal{T}/\delta g$), the additional metric dependence must of course be used. The specific form of this dependence {which corresponds to the definition

$$j^{\mu}(x) = e\bar{\psi}(x + \epsilon)\gamma^{\mu} \exp\left[ie\int_x^{x+\epsilon} dy_{\mu}A^{\mu}(y)\psi(x)\right]$$

in electrodynamics} and the (presumed) consistency of the general covariance and Schwinger term requirements are separate questions which we have not studied in detail here. We have only given necessary conditions of the dependence of $\mathcal{T}^{\mu\nu}$ on second derivatives of $g_{\mu\nu}$.

However, from purely geometrical considerations, it may be shown that the necessary nonclassical dependence on the metric appears in restoring the coordinate tensor nature of the "split" $T^{\mu\nu}$, say $\phi_{\mu}(x + \epsilon)\phi_{\nu}(x)$, by use of parallel transfer to make it a tensor at one point. An operator ${}^{\mu}D(x, x')_{\nu}$ such that ${}^{\mu}D(x, x')_{\nu}\phi^{\nu}(x')$ is a vector at x may be defined and is essentially a path integral over the affinity

$${}^{\mu}D(x, x')_{\nu} = {}^{\mu}\left\{\exp\left[\int_{x'}^{x} dy^{\alpha}\Gamma_{\alpha}(y)\right]\right\}_{+\nu}.$$

It is hoped to return to this elsewhere.

Some speculations on the role of these terms when the gravitational field itself is dynamical and quantized may be of interest, however. In electrodynamics, the additional A_{μ} dependence ensures the preservation of gauge invariance in at least two situations.[17] The first is in the maintenance of zero photon self-mass in the closed loop diagram, the second the elimination of finite, but gauge dependent, terms in the "box" diagram (scattering of light by light). Similarly, it may be that some of the difficulties encountered in renormalizing the interaction of a scalar field with the quantized Einstein field can be avoided if the correct form for $\mathcal{T}^{\mu\nu}[g]$ is employed. In electrodynamics, where the current correlation function $\delta\langle j\rangle/\delta A$ differs from the time-ordered product $i\langle (jj)_+\rangle$ by the explicit dependence $\langle \delta j/\delta A\rangle$,[18] the additional term is needed both for covariance and for charge conservation.

[17] D. G. Boulware, Phys. Rev. **151**, 1024 (1966).

[18] See Ref. 2, K. A. Johnson, Nucl. Phys. **31**, 464 (1962); L. S. Brown, Phys. Rev. **150**, 1338 (1966). The additional dependence discussed here may or may not be reflected in the Feynman rules of the resultant theory; this question can only be decided by a detailed analysis of the role of the extra terms.

The latter property ensures a vanishing photon self mass. It seems likely that there is a closed analogy in our case, where (covariant) conservation requires the explicit $\delta\mathfrak{G}/\delta g$ term of Eq. (11b); a nonconserved correlation function would correspond to a graviton mass (in the language of the linearized theory at least). There are probably also terms in the graviton–graviton scattering through virtual matter pairs with difficulties similar to those of the box diagram in quantum electrodynamics. Certainly, unless the metric dependence is inserted, no interaction is possible with the gravitational field at all, just as the exp $(ie \int dy_\mu A^\mu)$ term is essential for a nonvanishing current in electrodynamics. Another interesting problem has to do with the resulting lack of commutation, at equal times, between the matter $\mathfrak{G}^{\mu\nu}$ and the gravitational field variables. For, just as in electrodynamics, where [**E**, **j**] fails to vanish as a consequence of the A dependence of j, the corresponding commutators between $\mathfrak{G}^{\mu\nu}$ and the canonical Einstein variables will be nonzero. Since the Einstein equations are nonlinear, the computation of this noncommutativity is not so direct as for vector currents coupled to, say, a spin one field[12]; also it is presumably necessary to split the points in the nonlinear terms of the Einstein equations (which correspond to the $\mathfrak{G}^{\mu\nu}$ of the gravitational field) in order to avoid similar paradoxes for the Einstein field itself.

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Note on the Kerr Metric and Rotating Masses

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(Received 17 November 1966)

Kerr's metric is often said to describe the geometry exterior to a body whose mass and rotation are measured by Kerr's parameters m and a, respectively, even though no interior solution is known. In this paper we give an interior solution valid in the limit when the rotation parameter a is sufficiently small so that terms of higher power than the first are negligible, but the mass parameter m is allowed to be large. This is accomplished by bringing Kerr's exterior metric into the form of the metric for a slowly rotating mass shell. Also, the connection is found between Kerr's parameters and the physical parameters characterizing the rotating body.

I. INTRODUCTION

IN 1963, Kerr[1] gave the exact stationary but not static exterior solution to Einstein's equations:

$$ds^2 = \Sigma(d\theta^2 + \sin^2\theta\, d\bar{\phi}^2) + 2(dU + a\sin^2\theta\, d\bar{\phi})(dr + a\sin^2\theta\, d\bar{\phi}) - (1 - 2mr\Sigma^{-1})(dU + a\sin^2\theta\, d\bar{\phi})^2, \quad (1)$$

where

$$\Sigma = R^2 + a^2\cos^2\theta, \quad (2)$$

$$U = t + R, \quad (3)$$

and m and a are constants. Kerr claims that this metric (1) is the metric exterior to a rotating body. The parameter a is related to the rate of rotation, and m is the mass parameter. Since the appearance of Kerr's paper there has been a search for an interior solution. If any interior solution exists, there must in particular be interior solutions in the case when a is sufficiently small that terms of higher power than the first in a can be neglected. The purpose of this paper is to provide such an interior solution which matches the Kerr solution at a radius r_0 to first order in a, *but for any* m whose gravitational radius does not exceed r_0.

This is accomplished in Sec. III via coordinate transformations which bring the Kerr exterior metric into the form of the metric for a thin slowly rotating mass shell.[2] For completeness, the exterior and interior metrics associated with a thin slowly rotating mass shell are given in Sec. II.

* Atomic Energy Commission, Postdoctoral Fellow.

[1] R. Kerr, Phys. Rev. Letters **11**, 237 (1963).

[2] D R. Brill and J. M. Cohen, Phys. Rev. **143**, 1011 (1966).

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This is accomplished in Sec. III via coordinate transformations which bring the Kerr exterior metric into the form of the metric for a thin slowly rotating mass shell.[2] For completeness, the exterior and interior metrics associated with a thin slowly rotating mass shell are given in Sec. II.

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II. INTERIOR SOLUTION

It has recently been shown[2] that the metric associated with a thin slowly rotating mass shell of radius r_0 is

$$ds^2 = \psi^4[dr^2 + r^2\,d\theta^2 + r^2\sin^2\theta(d\phi - \Omega\,dt)^2] - V^2\,dt^2, \quad (4)$$

where

$$\begin{aligned} V &= (r_0 - \alpha)/(r_0 + \alpha), \\ \psi &= \psi_0 = 1 + \alpha r_0^{-1}, \\ \Omega &= \Omega_0, \quad \text{for} \quad r < r_0, \end{aligned} \quad (5)$$

while

$$\begin{aligned} V &= (r - \alpha)/(r + \alpha), \\ \psi &= 1 + \alpha r^{-1}, \\ \Omega &= (r_0\psi_0^2/r\psi^2)^3\Omega_0, \quad \text{for} \quad r > r_0. \end{aligned} \quad (6)$$

Here the constants have the values

$$\Omega_0 = \omega_s/(1 + [3(r_0 - \alpha)/8\alpha(1 + \beta_0)]); \quad (7)$$

$$\beta_0 = \alpha/2(r_0 - \alpha); \quad (8)$$

2α is the mass of the shell as seen by an observer at infinity, and ω_s is the angular velocity of the mass shell; the elastic stress in the shell is proportional to β_0.

III. COORDINATE TRANSFORMATION

The coordinate transformation

$$\begin{aligned} \bar{\phi} &= \phi + ak\coth^{-1}k(R - m), \\ U &= t + R + m\ln\Delta - 2m^2k\coth^{-1}k(R - m) \end{aligned} \quad (9)$$

with

$$k = (m^2 - a^2)^{-\frac{1}{2}}, \quad (10)$$

$$\Delta = R^2 - 2mR + a^2, \quad (11)$$

eliminates U from the Kerr metric (1) and brings it into the form[3]

$$ds^2 = \Sigma(dR^2\Delta^{-1} + d\theta^2) + (R^2 + a^2)\sin^2\theta\,d\phi^2 - dt^2 + 2mR\,\Sigma^{-1}(dt + a\sin^2\theta\,d\phi)^2. \quad (12)$$

To first order in a, the metric (12) becomes

$$ds^2 = (1 - 2mR^{-1})^{-1}dR^2 + R^2\,d\theta^2 + R^2\sin^2\theta\,d\phi^2 + 4maR^{-1}\sin^2\theta\,d\phi\,dt - (1 - 2mR^{-1})\,dt^2. \quad (13)$$

The spacelike part of the metric (13) can be transformed to isotropic form via the coordinate transformation:

$$R = r\psi^2, \quad (14)$$

where

$$\psi = 1 + \alpha r^{-1}, \quad (15)$$

$$\alpha = \tfrac{1}{2}m. \quad (16)$$

In these coordinates the four-dimensional metric becomes

$$ds^2 = \psi^4(dr^2 + r^2\,d\theta^2 + r^2\sin^2\theta\,d\phi^2) - V^2\,dt^2 + (4ma/r\psi^2)\sin^2\theta\,d\phi\,dt, \quad (17)$$

where

$$V = (r - \alpha)/(r + \alpha). \quad (18)$$

This metric (17) is the same as the exterior part of the metric (4), i.e., when $r > r_0$, if we set

$$2ma = -(r_0\psi_0^2)^3\Omega_0. \quad (19)$$

Equations (19) and (7) give the connection between Kerr's rotation parameter a and the *physical* parameters m, r_0 and ω_s of the rotating body.

Thus, *when a is* sufficiently *small* so that terms of higher power than the first are negligible but *m is allowed to be large, Kerr's exterior solution can be matched to an interior solution.*[4]

By integration of the conservation laws over all space–time and application of Stokes theorem to this integral, it can be shown that the following quantity is conserved:

$$J = \tfrac{2}{3}m(1 + \beta_0)r_0^2\psi_0^5(\omega_s - \Omega_0)/V_0. \quad (20)$$

For $r_0 \gg \alpha$, this expression (20) reduces to the Newtonian expression for the angular momentum of a rotating mass shell. Thus it seems reasonable to define J as the relativistic generalization of the angular momentum of the shell. Note that the elastic stress in the shell and the gravitational potential contribute to the angular momentum J.

When the relation (7) between Ω_0, ω_s, and r_0 is substituted into the above expression (2) for the angular momentum J, there results

$$2J = (r_0\psi_0^2)^3\Omega_0. \quad (21)$$

Comparison with Eq. (19) gives

$$J = -ma. \quad (22)$$

Thus it can be concluded that, when a is sufficiently small so that terms of higher power than the first are negligible, $|ma|$ is the angular momentum of the shell and the rotation is retrograde[5] for $a > 0$.

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[3] This form of the Kerr metric was first shown to me by Robert H. Boyer (private communication). It appears, e.g., in a paper by R. H. Boyer and R. W. Lindquist, J. Math. Phys. **8**, 265 (1967).

[4] The thin spherical rotating mass shell is by no means the only possible source for the Kerr solution to first order in a. For example, using the method described in this paper, it can be shown that a slowly rotating solid sphere of perfect fluid can also be the source for Kerr's exterior metric with small a.

[5] For the case of both m and a small, Boyer and Price [Proc. Cambridge Phil. Soc. **61**, 531 (1965)] noticed that the motion was retrograde in their investigation of a slowly rotating sphere of perfect fluid.

Particlelike Solutions of a Class of Nonlinear Field Equations*

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A procedure for generating integral relations satisfied by particlelike solutions of the class of nonlinear field equations $\Delta\phi = F^{I}(\phi)$ is proposed and used to develop the first few such relations. The relations are used to reduce the expression for the "energy" associated with the system; as an example, the case $F^{I}(\phi) = \phi - \phi^3$ is treated. It is shown generally that the variational bound to any of the possible energy values will approach the exact value from above if the trial functions are chosen to satisfy one of the integral relations, which is satisfied identically by the exact solutions.

1. INTRODUCTION

THROUGH the years various authors have proposed and investigated nonlinear field equations in attempts to find models for extended elementary particles.[1–6] In many cases these equations reduce, in the simplest static case and in suitable units, to the form[5,6]

$$\Delta\phi = F^{I}(\phi) \quad (\equiv dF/d\phi), \tag{1}$$

where $F(\phi)$ is some simple, differentiable function of ϕ.[7] Various properties of the solutions of the class of elliptic partial differential equations (1) have been investigated to date, such as the existence and uniqueness of the solutions,[8] their stability,[9–11] etc. In Sec. 2 of this paper we establish a scheme by means of which integral relations satisfied by particlelike[12] solutions of (1) may be generated. One application of these integral relations, in obtaining alternate expressions for the energy

$$E = \frac{1}{2\pi}\int [\tfrac{1}{2}(\nabla\phi)^2 + F(\phi)]\, d^3x \tag{2}$$

associated with the system described by (1), is illustrated for the most commonly considered nonlinear field equation, for which $F^{I}(\phi) = \phi - \phi^3$.

Generally speaking, it is not possible to obtain solutions of (1) explicitly and various approximation techniques are used. In the case of one dimension, approximate solutions are readily obtained by numerical integration, while in two or three dimensions, the variational method is often useful.[13] In Sec. 3 we make use of the integral relations developed in Sec. 2 to establish criteria under which variational approximations yield upper bounds to the energy (2) associated with the particlelike solutions.

2. INTEGRAL RELATIONS

Some integral relations satisfied by particlelike solutions of equations of type (1) have been obtained previously[5,10] with the aid of the energy (2), which is extremized by these solutions. It is apparent, however, that these (and other) properties of the solutions should be obtainable from (1) without recourse to the energy.

The procedure for obtaining integral relations consists, in essence, of partially integrating the identity[14]

$$\int \phi\xi_i^n \frac{\partial^n}{\partial\xi_i^n}(\Delta_\xi\phi)\, d^3\xi = \int \phi\xi_i^n \frac{\partial^n}{\partial\xi_i^n} F^{I}(\phi)\, d^3\xi, \tag{3}$$

for $i = 1, 2, 3$ and $n = 1, 2, \cdots$. In (3) (ξ_1, ξ_2, ξ_3) is a set of coordinates spanning the region of space under consideration and Δ_ξ is the Laplacian operator expressed in these coordinates. In this paper we derive some of the integral relations obtainable when ξ_i are taken to be rectangular Cartesian and the radial polar coordinates, and the integrations are taken over all space. First we note that all integral

* This work is part of a thesis submitted by the first author to the University of Alberta in partial fulfilment of the requirements for the Ph.D. degree.

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[1] G. Mie, Ann. Physik **37**, 511 (1912); **39**, 1 (1912); **40**, 1 (1913).

[2] M. Born, Proc. Roy. Soc. (London) **A143**, 410 (1934); M. Born and L. Infeld, *ibid.* **144**, 425 (1934); **147**, 522 (1934); **150**, 41 (1935).

[3] W. Heisenberg, Rev. Mod. Phys. **29**, 269 (1947).

[4] L. I. Schiff, Phys. Rev. **84**, 1 (1951).

[5] H. Schiff, Proc. Roy. Soc. (London) **A269**, 277 (1962).

[6] V. Enz, Phys. Rev. **131**, 1392 (1963).

[7] Such equations arise also in other branches of science and engineering; see, for example, H. T. Davis, *Introduction to Nonlinear Differential and Integral Equations* (Dover Publications, Inc., New York, 1962).

[8] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1962), Vol. II, p. 369.

[9] R. H. Hobart, Proc. Roy. Soc. (London) **82**, 201 (1963).

[10] G. H. Derrick, J. Math. Phys. **5**, 1252 (1964).

[11] G. Rosen, J. Math. Phys. **6**, 1269 (1965).

[12] In this paper, a particlelike solution ϕ is one for which ϕ, its derivatives, and all physical quantities derivable from them are well behaved (exist, continuous, and single valued).

[13] D. D. Betts, H. Schiff, and W. B. Strickfadden, J. Math. Phys. **4**, 334 (1963).

[14] The use of this identity, which follows from (1), is suggested by the work of D. J. Morgan and P. T. Landsberg, Proc. Phys. Soc. (London) **86**, 261 (1965).

relations obtainable from (3) with $n = 0, 1, 2, \cdots, k$ are also obtainable from (3) with $n = k + 1$, since the "order" n of the identity may be reduced by one, by partially integrating both sides of (3) once and making use of (1). It is simpler, however, to start with $n = 0$. In this case (3) implies, simply,

$$\int \phi \Delta\phi \, d^3x = \int \phi F^{\mathrm{I}}(\phi) \, d^3x,$$

or

$$\int [\nabla \cdot (\phi \nabla\phi) - (\nabla\phi)^2] \, d^3x = \int \phi F^{\mathrm{I}}(\phi) \, d^3x.$$

Using the divergence theorem,[15] we obtain

$$\int [(\nabla\phi)^2 + \phi F^{\mathrm{I}}(\phi)] \, d^3x = 0. \tag{4}$$

Taking ξ_i to be x, one of the rectangular Cartesian coordinates, (3) becomes, with $n = 1$

$$\int \phi x \frac{\partial}{\partial x}(\Delta\phi) \, d^3x = \int \phi x \frac{\partial}{\partial x} F^{\mathrm{I}}(\phi) \, d^3x$$

or

$$\int x\phi \Delta\left(\frac{\partial\phi}{\partial x}\right) d^3x = -\int x \frac{\partial}{\partial x} [F(\phi) - \phi F^{\mathrm{I}}(\phi)] \, d^3x.$$

Using Green's theorem on the left and integrating partially on the right, we get

$$\int \frac{\partial\phi}{\partial x} \Delta(x\phi) \, d^3x = \int [F(\phi) - \phi F^{\mathrm{I}}(\phi)] \, d^3x. \tag{5}$$

But

$$\begin{aligned}
&\int \frac{\partial\phi}{\partial x} \Delta(x\phi) \, d^3x \\
&\quad = \int \frac{\partial\phi}{\partial x}\left(x\Delta\phi + 2\frac{\partial\phi}{\partial x}\right) d^3x \\
&\quad = \int \left[x \frac{\partial}{\partial x} F(\phi) + 2\left(\frac{\partial\phi}{\partial x}\right)^2\right] d^3x \text{ using (1),} \\
&\quad = \int \left[2\left(\frac{\partial\phi}{\partial x}\right)^2 - F(\phi)\right] d^3x \text{ after partial integration.}
\end{aligned}$$

Thus (5) becomes

$$2\int \left(\frac{\partial\phi}{\partial x}\right)^2 d^3x = \int [2F(\phi) - \phi F^{\mathrm{I}}(\phi)] \, d^3x.$$

Similar expressions hold for the other two Cartesian coordinates, so that

$$\begin{aligned}
\int \left(\frac{\partial\phi}{\partial x}\right)^2 d^3x &= \int \left(\frac{\partial\phi}{\partial y}\right)^2 d^3x = \int \left(\frac{\partial\phi}{\partial z}\right)^2 d^3x \\
&= \tfrac{1}{3}\int (\nabla\phi)^2 \, d^3x \\
&= \int [F(\phi) - \tfrac{1}{2}\phi F^{\mathrm{I}}(\phi)] \, d^3x.
\end{aligned} \tag{6}$$

[15] For the sake of simplicity we consider here only "localized" particlelike solutions, for which ϕ and its derivatives vanish at infinity. The somewhat more general case is treated in G. Darewych, Ph.D. thesis, University of Alberta (1966).

When $\xi_i = x$ and $n = 2$, a relation identical to (6) is obtained. With $n = 3$, (3) becomes

$$\begin{aligned}
\int \phi x^3 \Delta\left(\frac{\partial^3\phi}{\partial x^3}\right) d^3x = \int x^3\phi \Big[&\left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{IV}} \\
&+ 3\left(\frac{\partial\phi}{\partial x}\right)\left(\frac{\partial^2\phi}{\partial x^2}\right) F^{\mathrm{III}} + F^{\mathrm{II}} \frac{\partial^3\phi}{\partial x^3}\Big] d^3x
\end{aligned}$$

Using Green's theorem on the left, and (1) we get

$$\begin{aligned}
&6\int x^2 \frac{\partial^3\phi}{\partial x^3}\frac{\partial\phi}{\partial x} \, d^3x + 6\int x \frac{\partial^3\phi}{\partial x^3} \phi \, d^3x \\
&\quad = \int x^3 \Big[\phi\left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{IV}} + 3\phi \frac{\partial\phi}{\partial x}\frac{\partial^2\phi}{\partial x^2} F^{\mathrm{III}} \\
&\qquad + (\phi F^{\mathrm{II}} - F^{\mathrm{I}}) \frac{\partial^3\phi}{\partial x^3}\Big] d^3x.
\end{aligned}$$

Integrating partially on the left,

$$\begin{aligned}
&-6\int \frac{\partial^2\phi}{\partial x^2}\left(x^2 \frac{\partial^2\phi}{\partial x^2} + 2x\frac{\partial\phi}{\partial x}\right) d^3x \\
&\qquad - 6\int \frac{\partial^2\phi}{\partial x^2}\left(\phi + x\frac{\partial\phi}{\partial x}\right) d^3x \\
&\qquad = \int x^3 \left[\frac{\partial^3}{\partial x^3}(\phi F^{\mathrm{I}} - 2F) - \left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{III}}\right] d^3x,
\end{aligned}$$

or

$$\begin{aligned}
&6\int x^2 \left(\frac{\partial^2\phi}{\partial x^2}\right)^2 d^3x + 9\int x \frac{\partial}{\partial x}\left[\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2\right] d^3x \\
&\qquad + 6\int \phi \frac{\partial^2\phi}{\partial x^2} \, d^3x \\
&\qquad = 6\int (\phi F^{\mathrm{I}} - 2F) \, d^3x + \int x^3 \left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{III}} \, d^3x.
\end{aligned}$$

Further partial integration of the integrals on the left implies that

$$\begin{aligned}
&6\int x^2 \left(\frac{\partial^2\phi}{\partial x^2}\right)^2 d^3x - 15\int \left(\frac{\partial\phi}{\partial x}\right)^2 d^3x \\
&\qquad = 6\int (\phi F^{\mathrm{I}} - 2F) \, d^3x + \int x^3 \left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{III}} \, d^3x.
\end{aligned}$$

Finally, using (6) we obtain the relation

$$\int \left(\frac{\partial\phi}{\partial x}\right)^2 d^3x = 2\int \left[x^2 \left(\frac{\partial^2\phi}{\partial x^2}\right)^2 - \tfrac{1}{6}x^3 \left(\frac{\partial\phi}{\partial x}\right)^3 F^{\mathrm{III}}\right] d^3x, \tag{7}$$

and similar expressions for y and z. When ξ_i is taken to be r, the radial spherical polar coordinate then, for $n = 0$, 1, 2 no new relations are obtained. When $n = 3$ we obtain, as shown in the Appendix, the relation

$$\begin{aligned}
\tfrac{1}{3}\int (\nabla\phi)^2 \, d^3x = \tfrac{1}{20}\int \Big[&\tfrac{1}{6} r^3 \left(\frac{\partial\phi}{\partial r}\right)^3 F^{\mathrm{III}} \\
&- \left(r^2 \frac{\partial^2\phi}{\partial r^2} - 3r\frac{\partial\phi}{\partial r} + 4\phi\right) F^{\mathrm{I}}\Big] d^3x.
\end{aligned} \tag{8}$$

Still other integral relations may be obtained from (3) by using higher values of n and other coordinates ξ_i.

These relations may be used, for example, to obtain alternate expression for the energy (2). A frequently encountered nonlinear field equation of type (1) corresponds to $F^{\mathrm{I}}(\phi) = \phi - \phi^3$. The integral relations (4), (6), (7), and (8) in this case imply that the energy of this system

$$E = \frac{1}{4\pi}\int [\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}\phi^2 - \tfrac{1}{4}\phi^4]\, d^3x,$$

may be expressed equivalently as

$$E = \frac{1}{4\pi}\int \phi^2\, d^3x = \frac{1}{16\pi}\int \phi^4\, d^3x = \frac{1}{12\pi}\int (\nabla\phi)^2\, d^3x, \tag{9}$$

$$E_x = \frac{1}{4\pi}\int \left(\frac{\partial\phi}{\partial x}\right)^2 d^3x \tag{10}$$

and similar expressions for y and z,

$$E_r = \frac{1}{4\pi}\frac{2}{5}\int \left[\phi\left(\frac{\partial\phi}{\partial r}\right)^3 r^3 + r^2(3\phi^2 - 1)\left(\frac{\partial\phi}{\partial r}\right)^2\right] d^3x \tag{11}$$

or

$$E_{xx} = \frac{2}{4\pi}\int \left[x^2\left(\frac{\partial^2\phi}{\partial x^2}\right)^2 + x^3\phi\left(\frac{\partial\phi}{\partial x}\right)^3\right] d^3x, \tag{12}$$

and similar expressions for y and z.

3. VARIATIONAL UPPER BOUNDS

The fact that the solutions of (1) extremize the energy (2) suggests that a variational principle based on (2) may be used to obtain approximations to the solutions of (1).[16] If ϕ is a solution of (1) and $\psi = \phi + u$ some suitable variational trial function (u being an arbitrary but small perturbation) consider the nature of the bound $E(\psi)$ to $E(\phi)$:

$$E(\psi) = E(\phi) + \frac{1}{4\pi}\int [\nabla\phi\cdot\nabla u + uF^{\mathrm{I}}(\phi)]\, d^3x + \frac{1}{4\pi}\int [\tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{2}u^2F^{\mathrm{II}}(\phi)]\, d^3x + \frac{1}{4\pi}\sum_{l=3}^{\infty}\int \frac{u^l}{l!}F^{(l)}(\phi)\, d^3x. \tag{13}$$

Using the identity $\nabla\cdot(u\nabla\phi) = \nabla u\cdot\nabla\phi + u\Delta\phi$, Gauss' theorem and (1), it is clear that the term which is of first order in u vanishes in (13) and, for $|u|$ sufficiently small, the nature of the variational bound is determined by the second-order term

$$\delta^2E = \frac{1}{4\pi}\int [\tfrac{1}{2}(\nabla u)^2 + \tfrac{1}{2}u^2F^{\mathrm{II}}(\phi)]\, d^3x. \tag{14}$$

[16] Such a procedure has been used[13] to obtain approximations to eigensolutions of $\Delta\phi = \phi - \phi^3$.

Since, in general, $F^{\mathrm{II}}(\phi)$ is indefinite, so presumably is the variational bound $E(\psi)$ to $E(\phi)$. Suppose, however, that the variational trial functions ψ are restricted to those which satisfy the integral relation[17]

$$\int [(\nabla\psi)^2 + 6F(\psi)]\, d^3x = 0, \tag{15}$$

which relation, as is clear from (4) and (6), is satisfied identically by the solutions of (1). Replacing ψ by $\phi + u$ in (15) we get, to second order in u

$$\int \tfrac{1}{2}u^2F^{\mathrm{II}}(\phi)\, d^3x = -\int [\tfrac{1}{3}\nabla\phi\cdot\nabla u + \tfrac{1}{6}(\nabla u)^2 + uF^{\mathrm{I}}(\phi)]\, d^3x.$$

Thus, to second order in u, (13) becomes

$$E(\psi) = E(\phi) + \frac{1}{4\pi}\int \tfrac{2}{3}\nabla\phi\cdot\nabla u\, d^3x + \frac{1}{4\pi}\int \tfrac{1}{3}(\nabla u)^2\, d^3x. \tag{16}$$

Since ϕ is a solution of (1), it extremizes E, hence the first-order term in (16) vanishes while the second-order term is now positive definite. We conclude then, that if the variational trial function ψ is chosen to satisfy (15), then $E(\psi)$ provides an upper bound to $E(\phi)$, provided $|\psi - \phi|$ is sufficiently small. It should be noted that this applies quite generally to all particlelike solutions of (1) not only the "ground state" solution [for which $E(\phi)$ is smallest].

4. CONCLUSIONS

We have proposed a scheme by means of which integral relations, satisfied by particlelike solutions of a wide class of nonlinear field equations (1), may be generated. We have used this scheme to obtain the first few such integral relations. One use of these integral relations, in providing alternate expressions for the energy associated with a system described by (1), was demonstrated for the particular case $\Delta\phi = \phi - \phi^3$. The variational bound to the energy associated with a particlelike solution of (1) was considered, and it was shown that if the variational trial functions are chosen to satisfy one of the integral relations, then the variational energy will approach the exact result from above.

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[17] As is evident from the work of Schiff[5] and Derrick,[10] this is equivalent to requiring that the variational trial function be an extremum with respect to a radial scale parameter ν, ψ being otherwise arbitrary: $(\partial/\partial\nu)E[\psi(\nu r, \cdots)] = 0$.

APPENDIX. AN INTEGRAL RELATION

Consider the identity

$$\int \phi r^3 \frac{\partial^3}{\partial r^3}(\Delta\phi)\, d^3x = \int \phi r^3 \frac{\partial^3}{\partial r^3} F^{\mathrm{I}}(\phi)\, d^3x, \quad \text{(A1)}$$

and

$$\frac{\partial^3}{\partial r^3}(\Delta\phi) = \Delta\left(\frac{\partial^3\phi}{\partial r^3}\right) - \frac{6}{r}\Delta\left(\frac{\partial^2\phi}{\partial r^2}\right) + \frac{18}{r^2}\Delta\left(\frac{\partial\phi}{\partial r}\right) - \frac{24}{r^3}\Delta\phi + \frac{6}{r}\frac{\partial^4\phi}{\partial r^4} - \frac{12}{r^2}\frac{\partial^3\phi}{\partial r^3} + \frac{36}{r^4}\frac{\partial\phi}{\partial r}.$$

Making use of Green's theorem, and noting that for the localized, particlelike solutions considered here, the surface terms vanish; we find that

$$\int \phi r^3 \Delta\left(\frac{\partial^3\phi}{\partial r^3}\right) d^3x = \int \frac{\partial^3\phi}{\partial r^3}\left(r^3\Delta\phi + 6r^2\frac{\partial\phi}{\partial r} + 12r\phi\right) d^3x,$$

$$\int \phi r^2 \Delta\left(\frac{\partial^2\phi}{\partial r^2}\right) d^3x = \int \frac{\partial^2\phi}{\partial r^2}\left(r^2\Delta\phi + 4r\frac{\partial\phi}{\partial r} + 6\phi\right) d^3x,$$

and

$$\int \phi r \Delta\left(\frac{\partial\phi}{\partial r}\right) d^3x = \int \frac{\partial\phi}{\partial r}\left(r\Delta\phi + 2\frac{\partial\phi}{\partial r} + \frac{2}{r}\phi\right) d^3x.$$

Thus, (A1) becomes

$$\int\left[6r^2\frac{\partial^3\phi}{\partial r^3}\frac{\partial\phi}{\partial r} - 24r\frac{\partial^2\phi}{\partial r^2}\frac{\partial\phi}{\partial r} - 36\phi\frac{\partial^2\phi}{\partial r^2} + 36\left(\frac{\partial\phi}{\partial r}\right)^2 + \frac{72}{r}\phi\frac{\partial\phi}{\partial r} + 6r^2\phi\frac{\partial^4\phi}{\partial r^4} + \left\{r^3\frac{\partial^3\phi}{\partial r^3} - 6r^2\frac{\partial^2\phi}{\partial r^2} + 18r\frac{\partial\phi}{\partial r} - 24\phi\right\}\Delta\phi\right] d^3x$$

$$= \int r^3\phi\left[\left(\frac{\partial\phi}{\partial r}\right)^3 F^{\mathrm{IV}} + 3\frac{\partial\phi}{\partial r}\frac{\partial^2\phi}{\partial r^2}F^{\mathrm{III}} + \frac{\partial^3\phi}{\partial r^3}F^{\mathrm{II}}\right] d^3x,$$

$$\int\left[6r^2\frac{\partial^3\phi}{\partial r^3}\frac{\partial\phi}{\partial r} - 24r\frac{\partial^2\phi}{\partial r^2}\frac{\partial\phi}{\partial r} - 36\phi\frac{\partial^2\phi}{\partial r^2} + 36\left(\frac{\partial\phi}{\partial r}\right)^2 + \frac{72}{r}\phi\frac{\partial\phi}{\partial r} + 6r^2\phi\frac{\partial^4\phi}{\partial r^4} - 6\left(r^2\frac{\partial^2\phi}{\partial r^2} - 3r\frac{\partial\phi}{\partial r} + 4\phi\right)\Delta\phi\right] d^3x$$

$$= \int r^3\left[\phi\left(\frac{\partial\phi}{\partial r}\right)^3 F^{\mathrm{IV}} + 3\phi\frac{\partial\phi}{\partial r}\frac{\partial^2\phi}{\partial r^2}F^{\mathrm{III}} + (\phi F^{\mathrm{II}} - F^{\mathrm{I}})\frac{\partial^3\phi}{\partial r^3}\right] d^3x. \quad \text{(A2)}$$

Integrating by parts,

$$\int r^2\left(\frac{\partial^3\phi}{\partial r^3}\frac{\partial\phi}{\partial r} + \phi\frac{\partial^4\phi}{\partial r^4}\right) d^3x = \int r^2\frac{\partial}{\partial r}\left(\phi\frac{\partial^3\phi}{\partial r^3}\right) d^3x = -4\int r\phi\frac{\partial^3\phi}{\partial r^3}\, d^3x,$$

$$\int r\left(\frac{\partial^2\phi}{\partial r^2}\frac{\partial\phi}{\partial r} + \phi\frac{\partial^3\phi}{\partial r^3}\right) d^3x = \int r\frac{\partial}{\partial r}\left(\phi\frac{\partial^2\phi}{\partial r^2}\right) d^3x = -3\int\phi\frac{\partial^2\phi}{\partial r^2}\, d^3x,$$

and

$$\int \frac{1}{r}\phi\frac{\partial\phi}{\partial r}\, d^3x = \frac{1}{2}\int\phi\frac{\partial\phi}{\partial r}\, d(r^2)\, d\Omega = -\frac{1}{2}\int\left[\left(\frac{\partial\phi}{\partial r}\right)^2 + \phi\frac{\partial^2\phi}{\partial r^2}\right] d^3x$$

where $r^2\, dr\, d\Omega \equiv d^3x$. Thus (A2) becomes

$$-6\int\left[r^2\frac{\partial^2\phi}{\partial r^2} - 3r\frac{\partial\phi}{\partial r} + 4\phi\right]\Delta\phi\, d^3x = \int r^3\left[\frac{\partial^3}{\partial r^3}(\phi F^{\mathrm{I}} - 2F) - r^3\left(\frac{\partial\phi}{\partial r}\right)^3 F^{\mathrm{III}}\right] d^3x.$$

Using (1) and integrating partially on the right,

$$\int\left[r^2\frac{\partial^2\phi}{\partial r^2} - 3r\frac{\partial\phi}{\partial r} + 4\phi\right]F^{\mathrm{I}}(\phi)\, d^3x = \int\left[10(\phi F^{\mathrm{I}} - 2F) + \tfrac{1}{6}r^3\left(\frac{\partial\phi}{\partial r}\right)^3 F^{\mathrm{III}}\right] d^3x.$$

Finally, using (6), we obtain the relation (8).

Quantum Correlation Function for the Noninteracting Particle System

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A method for determining the quantum correlation functions of the noninteracting particle system in thermal equilibrium is developed. It is designed to reduce the labor involved in treating the large number of permutation operators of the symmetric group that occurs. An alternate form of the n-particle correlation function is obtained in order to simplify computation. The London–Placzek formula is derived as a check. The error in Kirkwood's superposition approximation for this system is investigated, and the exact relationship between the two- and three-particle correlation functions is found. Finally, a method determining the pair correlation function in the Hartree–Fock approximation of a pair-interacting particle system at a finite temperature is presented.

I. INTRODUCTION

In recent years, many important studies of the many-body problem of quantum statistics have been done successfully by using the concept of the grand canonical ensemble on the basis of the method of second quantization in quantum field theory. In their study of the pair correlation function, Fujita, Isihara, and Montroll[1] have, by using the idea of "torons" introduced firstly by Montroll and Ward,[2] shown that the pair correlation function in the grand canonical ensemble[3] can be expressed in terms of the two-body Green's function corresponding to the scattering in reciprocal temperature–position space. Subsequently, Fujita has, in a simple and straightforward way, proved again the validity of this theorem by using the familiar and easier procedure of second quantization in the Schrödinger picture.[4] According to him, the form of the pair correlation function $g(\mathbf{r}_1\mathbf{r}_2)$ [Eq. (2.8) of the first of Ref. 4] is, in terms of the annihilation and creation operators $\Psi(\mathbf{r}_1)$ and $\Psi^+(\mathbf{r}_2)$ in the configuration representation, given by

$$g(\mathbf{r}_1\mathbf{r}_2) = (V/\bar{N})^2 \operatorname{Tr}\left[\Psi(\mathbf{r}_2)\Psi(\mathbf{r}_1)e^{-\beta\mathfrak{L}}\Psi^+(\mathbf{r}_1)\Psi^+(\mathbf{r}_2)\right] \div \operatorname{Tr}(e^{-\beta\mathfrak{L}}). \quad (1)$$

Here the trace is taken in Fock space, and $\mathfrak{L} \equiv H - \mu N$ with the Hamiltonian operator H of the system having the total particle-number operator N. $\bar{N}$ is the average of the total particle number, i.e.,

$$\bar{N} \equiv \operatorname{Tr}(e^{-\beta\mathfrak{L}}N) \div \operatorname{Tr}(e^{-\beta\mathfrak{L}}),$$

and V, the volume of the system. The constant β is the reciprocal temperature parameter of the system defined by $\beta \equiv (KT)^{-1}$ with the Boltzmann constant K and the temperature T. The c number μ is the chemical potential.

Equation (1) is also consistent with the definition of the pair correlation function given by Lee, Huang, and Yang,[5] and can be easily extended to give the n particle correlation function taking the form

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = (V/\bar{N})^n \operatorname{Tr}\left[\Psi(\mathbf{r}_n)\cdots\Psi(\mathbf{r}_2)\Psi(\mathbf{r}_1) \times e^{-\beta\mathfrak{L}}\Psi^+(\mathbf{r}_1)\Psi^+(\mathbf{r}_2)\cdots\Psi^+(\mathbf{r}_n)\right] \div \operatorname{Tr}(e^{-\beta\mathfrak{L}}) \quad (n \ll \bar{N}). \quad (2)$$

In this paper, we show that Eq. (2) leads to

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = n!\left(\frac{V}{\bar{N}}\right)^n \langle \mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n | S_n \prod_{\lambda=1}^{n} \{e^{\beta(h_\lambda-\mu)} - \eta\}^{-1} \times |\mathbf{r}_n, \cdots, \mathbf{r}_2, \mathbf{r}_1\rangle \quad (3)$$

in the noninteracting particle system, where S_n is the symmetrizer for bosons, or the antisymmetrizer for fermions,[6] and h_λ ($\lambda = 1, 2, \cdots, n$), the n single-particle Hamiltonians corresponding to the n particles. The numerical constant η takes $+1$ for bosons and -1 for fermions. Next we very simply determine the explicit form of the n particle correlation function for the noninteracting spinless particle system from Eq. (3) with the application of the symmetric group of order $n!$. Finally, the order of the accuracy of Kirkwood's superposition approximation is investigated for the noninteracting particle system. Our theory will also be applied for finding the pair correlation function in the Hartree–Fock approximation in the

[1] S. Fujita, A. Isihara, and E. W. Montroll, Bull. Cl. Sci. Acad. Roy. Belg. **44**, 1018 (1958).
[2] E. W. Montroll and J. C. Ward, Phys. Fluids **1**, 55 (1958).
[3] There is no distinction between the pair correlation functions of canonical and grand canonical ensembles in the calculation of the thermodynamical property of the system in thermal equilibrium. See T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), p. 236 *et seq.*
[4] S. Fujita and R. Hirota, Phys. Rev. **118**, 6 (1960); S. Fujita, *ibid.* **115**, 1335 (1959).
[5] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1136, Eq. (42) (1957).
[6] See S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson and Company, Evanston, Illinois, 1961), Eq. (70) of p. 133 and Eq. (99b) of p. 140.

temperature region $\beta < \infty$ in the interacting-particle system with non-hard core potential such as the screened Coulomb potential of electron gas.

II. A PRELIMINARY THEOREM

Let $|j_\lambda\rangle$ be the normalized energy-eigenket vector of the λth single particle corresponding to the energy eigenvalue ϵ_{j_λ}. As is well known, the Hermitian scalar product between $|j_\lambda\rangle$'s and the position eigenket vector $|r_\lambda\rangle$ is then given by

$$\langle j_\lambda \mid j_\nu\rangle = \delta_{j_\lambda j_\nu}, \quad \langle \mathbf{r}_\lambda \mid j_\lambda\rangle = e^{i\mathbf{r}_\lambda\cdot\mathbf{k}_\lambda}/V^{\frac{1}{2}} \tag{4}$$

with

$$\mathbf{k}_\lambda \equiv 2\pi \mathbf{l}_{j_\lambda} V^{-\frac{1}{3}}.$$

Here $\mathbf{l}_{j_\lambda}$ is the lattice vector of the quantum number for the momentum of single particle, and the relationship between two quantum numbers j_λ and $\mathbf{l}_{j_\lambda}$ depends upon the shape of the box V.

The Hermitian scalar product between two direct products given by

$$|\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n\rangle \equiv \prod_{\lambda=1}^{n} |\mathbf{r}_\lambda\rangle,$$

$$|j_1, j_2, \cdots, j_n\rangle \equiv \prod_{\lambda=1}^{n} |j_\lambda\rangle,$$

is defined by

$$\langle \mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n \mid j_n, \cdots, j_2, j_1\rangle \equiv \prod_{\lambda=1}^{n} \langle \mathbf{r}_\lambda \mid j_\lambda\rangle,$$

which is normalized to unity. Now we introduce the symmetrized (or antisymmetrized) position-eigenket vector $|\mathbf{r}\rangle$ and energy eigenket vector $|\mathbf{J}\rangle$ of n particles by the following definitions:

$$|\mathbf{r}\rangle \equiv |\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n\rangle \equiv S_n |\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n\rangle,$$
$$|\mathbf{J}\rangle \equiv |j_1 j_2 \cdots j_n\rangle \equiv S_n |j_1, j_2, \cdots, j_n\rangle.$$

We can construct the Hermitian scalar product between them by noting $S_n^2 = S_n$, to have

$$\langle \mathbf{r} \mid \mathbf{J}\rangle \equiv \langle \mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n \mid j_n\cdots j_2 j_1\rangle = \frac{1}{n!} \times \begin{cases} \det(\langle \mathbf{r}_\lambda \mid j_\nu\rangle) \\ \mathrm{pet}(\langle \mathbf{r}_\lambda \mid j_\nu\rangle) \end{cases} \tag{5}$$

with the normalization condition given by

$$\langle \mathbf{J} \mid \mathbf{J}\rangle \equiv \langle j_1 j_2 \cdots j_n \mid j_n \cdots j_2 j_1\rangle = \begin{cases} (n!)^{-1} \prod_{\lambda<\nu}^{n} (1 - \delta_{j_\lambda j_\nu}) \\ (n!)^{-1} \prod_{\lambda=1}^{n} \sum_{\nu=1}^{\lambda} \delta_{j_\lambda j_\nu}, \end{cases} \tag{6}$$

respectively. "det" represents "determinant," and "pet," "permanent" of the elements $\langle \mathbf{r}_\lambda \mid j_\nu\rangle$ ($\lambda, \nu = 1, 2, 3, \cdots, n$), valid for fermions and bosons, respectively. Equation (5) is the symmetrized (or antisymmetrized) wavefunction of n identical, indistinguishable particle systems with nonnormalization to unity. Therefore, its completeness condition is given by

$$\sum_{\mathbf{J}} \frac{|\mathbf{J}\rangle\langle\mathbf{J}|}{\langle \mathbf{J} \mid \mathbf{J}\rangle} = I \text{ (identity)}, \tag{7}$$

and the operator $f(h_1, h_2, \cdots, h_n)$ given by

$$\langle \mathbf{J}| f(h_1, h_2, \cdots, h_n) |\mathbf{J}\rangle = F(\mathbf{J}) \text{ (known)} \tag{8}$$

has the following expansion form in terms of the projection operators $|\mathbf{J}\rangle\langle\mathbf{J}|$'s:

$$f(h_1, h_2, \cdots, h_n) = \sum_{\mathbf{J}} |\mathbf{J}\rangle \frac{F(\mathbf{J})}{(\langle \mathbf{J} \mid \mathbf{J}\rangle)^2} \langle \mathbf{J}|. \tag{9}$$

Theorem: Let $(a_{j_\lambda}^+, a_{j_\lambda})$ be the pair of the creation and annihilation operators in the momentum representation. For both fermion and boson, we have then,

$$n!\langle \mathbf{J} \mid \mathbf{J}\rangle \prod_{\lambda=1}^{n} \{e^{\beta(\epsilon_{j_\lambda}-\mu)} - \eta\}^{-1} = \mathrm{Tr}\,(e^{-\beta\mathfrak{L}} A_{\mathbf{J}}^+ A_{\mathbf{J}}) \div \mathrm{Tr}\,(e^{-\beta\mathfrak{L}}), \tag{10}$$

where the trace is taken in Fock space, and $\langle \mathbf{J} \mid \mathbf{J}\rangle$ is defined by Eq. (6), and $A_{\mathbf{J}}^+ \equiv \prod_{\lambda=1}^{n} a_{j_\lambda}^+$ so that $A_{\mathbf{J}} \equiv (\prod_{\lambda=1}^{n} a_{j_\lambda}^+)^+$.

Proof Case 1: $j_1 \neq j_2 \neq \cdots \neq j_n$. Let us express the numerator in the right-hand side of Eq. (10) by $\Omega(n)$. We have then,

$$\Omega(n) = \eta\,\mathrm{Tr}\,(e^{-\beta\mathfrak{L}} a_{j_1}^+ a_{j_2}^+ \cdots a_{j_{n-1}}^+ \times (a_{j_n} a_{j_n}^+ - 1) a_{j_{n-1}} \cdots a_{j_2} a_{j_1})$$

by using the commutation, or anticommutation rule given by $a_{j_n}^+ a_{j_n} = \eta(a_{j_n} a_{j_n}^+ - 1)$. Using the commutation rule[7] given by

$$e^{-\beta\mathfrak{L}} a_{j_n} = e^{\beta(\epsilon_{j_n}-\mu)} a_{j_n} e^{-\beta\mathfrak{L}}, \tag{11}$$

and $a_{j_\lambda}^+ a_{j_n} = \eta a_{j_n} a_{j_\lambda}^+$, $a_{j_\lambda} a_{j_n} = \eta a_{j_n} a_{j_\lambda}$ ($\lambda = 1, 2, \cdots, n-1$), and the trace theorem; we can easily lead this equation to the following recurrence formula:

$$\Omega(n) = \{e^{\beta(\epsilon_{j_n}-\mu)} - \eta\}^{-1} \Omega(n-1),$$

and, therefore,

$$\Omega(n) = \mathrm{Tr}\,(e^{-\beta\mathfrak{L}}) \prod_{\lambda=1}^{n} \{e^{\beta(\epsilon_{j_\lambda}-\mu)} - \eta\}^{-1}. \tag{12}$$

From Eqs. (12) and (6), we see that both sides of Eq. (10) are equal to each other, showing that Eq. (10) is valid for both fermion and boson when

$$j_1 \neq j_2 \neq \cdots \neq j_n.$$

[7] C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc., New York, 1963), p. 408.

Proof Case 2: The several j's among $(j_1 j_2 \cdots j_n)$ are equal to each other.

(*a*) *Fermion case:* For example, let $j_n = j_{n-1} = \cdots$, we then have

$$\text{THE LEFT-HAND SIDE OF EQ. (10)} = 0$$

in accordance with Eq. (6), while

$$\text{THE RIGHT-HAND SIDE OF EQ. (10)} = \text{Tr}\,[e^{-\beta\mathfrak{L}} a_{j_1}^{+} \cdots a_{j_{n-2}}^{+} (n_{j_n}^2 - n_{j_n}) a_{j_{n-2}} \cdots a_{j_1}]$$

by using the definition of the occupation number operator $n_{j_n} \equiv a_{j_n}^{+} a_{j_n}$ and the commutation rule of $n_{j_n} a_{j_n} = a_{j_n}(n_{j_n} - 1)$ valid for both fermion and boson. Thus, noting that $n_{j_n}^2 = n_{j_n}$ for fermion, we see that Eq. (10) is always valid for fermion irrespective of the values $(j_1 j_2 \cdots j_n)$.

(*b*) *Boson case:* Let $(j_1 j_2 \cdots j_n)$ be composed of the same j's of $m_1, m_2, \cdots, m_\lambda, \cdots$ in number, respectively, i.e.,

$$\sum_{\lambda=1}^{n} m_\lambda = n, \tag{13}$$

where some m_λ are zero, and, also, may be 1. We collect together the a^{+}'s and a's with the same j's, referring to the commutation rule of boson. We have, then,

$$\Omega(n) \equiv \text{Tr}\left[e^{-\beta\mathfrak{L}} \prod_{\lambda=1}^{n} \left\{ \prod_{s=0}^{m_\lambda - 1} (n_{j_\lambda} - s) \right\}\right], \tag{14}$$

where we have defined

$$\prod_{s=0}^{-1} (n_{j_\lambda} - s) = I \,(\text{identity}).$$

Splitting the last factor $(n_{j_1} - m_1 + 1)$ of the operator $\prod_{s=0}^{m_1 - 1}(n_{j_1} - s)$ into two parts and using the definition of the occupation number operator $n_{j_1} \equiv a_{j_1}^{+} a_{j_1}$, Eq. (14) is changed into the following form:

$$\Omega(n) = \text{Tr}\left[e^{-\beta\mathfrak{L}} n_{j_1}(n_{j_1} - 1) \cdots (n_{j_1} - m_1 + 2) a_{j_1}^{+} a_{j_1} \times \prod_{\lambda=2}^{n} \left\{ \prod_{s=0}^{m_\lambda - 1} (n_{j_\lambda} - s) \right\}\right]$$

$$- (m_1 - 1)\,\text{Tr}\left[e^{-\beta\mathfrak{L}} n_{j_1}(n_{j_1} - 1) \cdots (n_{j_1} - m_1 + 2) \times \prod_{\lambda=2}^{n} \left\{ \prod_{s=0}^{m_\lambda - 1} (n_{j_\lambda} - s) \right\}\right].$$

Now, we make the following procedure: (1) We replace $a_{j_1}^{+} a_{j_1} = a_{j_1} a_{j_1}^{+} - 1$ in the first term to combine the part of the coefficient (-1) with the second term. (2) In the first term, we bring the destruction operator a_{j_1} at the position right after the operator $e^{-\beta\mathfrak{L}}$ by using the commutation rule of $n_{j_1} a_{j_1} = a_{j_1}(n_{j_1} - 1)$. (3) We use Eq. (11). (4) We bring the destruction operator a_{j_1} to the last position by using the trace theorem. (5) We bring it to its original position to combine again with the creation operator $a_{j_1}^{+}$ to form the occupation number operator n_{j_1} by using the commutability of a_{j_1} and $\prod_{\lambda=2}^{n}\{\prod_{s=0}^{m_\lambda - 1}(n_{j_\lambda} - s)\}$.

After this procedure, we obtain the following recurrence formula:

$$\Omega(n) = m_1 \{e^{\beta(\epsilon_{j_1} - \mu)} - 1\}^{-1} \Omega(n - 1).$$

The same procedure continues $(m_1 - 1)$ times for the remaining a_{j_1} of $(m_1 - 1)$ in number, to give

$$\Omega(n) = m_1! \{e^{\beta(\epsilon_{j_1} - \mu)} - 1\}^{-m_1} \Omega(n - m_1).$$

Next, we carry out the same procedure, also, for a_{j_2}, a_{j_3}, and so on. Then we finally arrive at

$$\Omega(n) = \text{Tr}\,(e^{-\beta\mathfrak{L}}) \prod_{\lambda=1}^{n} \frac{m_\lambda!}{\{e^{\beta(\epsilon_{j_\lambda} - \mu)} - 1\}^{m_\lambda}}, \tag{15}$$

where the m_λ's satisfy Eq. (13).

From Eqs. (15) and (6), we see that both sides of Eq. (10) are equal to each other, showing the validity of Eq. (10) even for this case of bosons. Thus, we have proved that Eq. (10) is always valid for both fermion and boson.

The above procedure of proof is useful, also, for finding the grand-canonical ensemble average of an observable expressed in terms of the destruction and creation operators. For example, the grand-canonical ensemble average of the quantity n^m, i.e., the m powers of an occupation number operator n, is found by a recurrence formula given by

$$\text{Tr}\,(e^{-\beta\mathfrak{L}} n^m) = \frac{(m-1)q + 1}{q - 1} \text{Tr}\,(e^{-\beta\mathfrak{L}} n^{m-1}) - \frac{q}{q-1} \sum_{s=2}^{m-1} (-1)^s \frac{(m-1)!}{s!(m-s-1)!} \text{Tr}\,(e^{-\beta\mathfrak{L}} n^{m-s}) \qquad (q \equiv e^{\beta(\epsilon - \mu)}) \tag{16}$$

and, in the case of boson,

$$\text{Tr}\,(e^{-\beta\mathfrak{L}} n) = \frac{1}{q-1} \text{Tr}\,(e^{-\beta\mathfrak{L}}),$$

$$\text{Tr}\,(e^{-\beta\mathfrak{L}} n^2) = \frac{q+1}{(q-1)^2} \text{Tr}\,(e^{-\beta\mathfrak{L}}), \tag{17}$$

$$\text{Tr}\,(e^{-\beta\mathfrak{L}} n^3) = \frac{q^2 + 4q + 1}{(q-1)^3} \text{Tr}\,(e^{-\beta\mathfrak{L}}), \quad \text{etc.}$$

In the case of fermion, we have simply

$$\text{Tr}\,(e^{-\beta\mathfrak{L}} n^m) = [1/(q+1)]\,\text{Tr}\,(e^{-\beta\mathfrak{L}}) \tag{18}$$

for all $m \geq 1$, in accordance with the special character of the occupation number operator given by $n^m = n$. All results obtained above are in agreement

with those obtained at an earlier time by Schrödinger through his c-number theory.[8]

Using Eq. (9), we can write Eq. (10) in the following alternative form:

$$n!\prod_{\lambda=1}^{n}\{e^{\beta(h_\lambda-\mu)}-\eta\}^{-1} = (\mathrm{Tr}\,(e^{-\beta\mathfrak{L}}))^{-1}\sum_{\mathbf{J}}|\mathbf{J}\rangle\frac{\mathrm{Tr}\,(e^{-\beta\mathfrak{L}}A_{\mathbf{J}}^{\dagger}A_{\mathbf{J}})}{(\langle\mathbf{J}\,|\,\mathbf{J}\rangle)^2}\langle\mathbf{J}|. \quad (19)$$

III. DERIVATION OF EQ. (3)

The well-known Jordan–Wigner rule is given by[6]

$$(n!)^{\frac{1}{2}}\langle\mathbf{r}| = \langle 0|\prod_{\lambda=1}^{n}\Psi(\mathbf{r}_\lambda), \quad (20)$$

where $\langle 0|$ is the bra vector of the vacuum state. We expand the operator $\prod_{\lambda=1}^{n}\Psi(\mathbf{r}_\lambda)$ in the form given by

$$\prod_{\lambda=1}^{n}\Psi(\mathbf{r}_\lambda) = \sum_{\mathbf{J}}A_{\mathbf{J}}\langle\mathbf{r}\,|\,\mathbf{J}\rangle C(\mathbf{J}), \quad (21)$$

and determine the c-number coefficient $C(J)$ by using Eq. (20). From Eqs. (21) and (20), we have

$$(n!)^{\frac{1}{2}}\langle\mathbf{r}| = \langle\mathbf{r}|\sum_{\mathbf{J}}|\mathbf{J}\rangle\, C(\mathbf{J})\,\langle 0|\,A_{\mathbf{J}}. \quad (22)$$

It is easy to see, from the property of the destruction operator a_{j_λ} and Eq. (6), that

$$\langle 0|\,A_{\mathbf{J}} = \langle\mathbf{J}|\,(n!)^{\frac{1}{2}}. \quad (23)$$

The combination of Eq. (22) with Eq. (23) requires

$$\sum_{\mathbf{J}}|\mathbf{J}\rangle\, C(\mathbf{J})\,\langle\mathbf{J}| = I\ (\text{identity}). \quad (24)$$

We compare Eq. (24) with Eq. (7) to have $C(\mathbf{J}) = 1/\langle\mathbf{J}\,|\,\mathbf{J}\rangle$, and therefore, Eq. (21) is written as

$$\prod_{\lambda=1}^{n}\Psi(\mathbf{r}_\lambda) = \sum_{\mathbf{J}}A_{\mathbf{J}}\langle\mathbf{r}\,|\,\mathbf{J}\rangle \div \langle\mathbf{J}\,|\,\mathbf{J}\rangle. \quad (25)$$

The Hermitian conjugate to Eq. (25) is

$$\prod_{\lambda=1}^{n}\Psi^{+}(\mathbf{r}_{n+1-\lambda}) = \sum_{\mathbf{J}}\langle\mathbf{J}\,|\,\mathbf{r}\rangle\, A_{\mathbf{J}}^{\dagger} \div \langle\mathbf{J}\,|\,\mathbf{J}\rangle. \quad (26)$$

We substitute Eqs. (26) and (25) into Eq. (2), to have

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = (V/\bar{N})^n(\mathrm{Tr}\,(e^{-\beta\mathfrak{L}}))^{-1}\sum_{\mathbf{J},\mathbf{J}'}\mathrm{Tr}\,[e^{-\beta\mathfrak{L}}A_{\mathbf{J}}^{\dagger}A_{\mathbf{J}'}\langle\mathbf{r}\,|\,\mathbf{J}'\rangle\langle\mathbf{J}\,|\,\mathbf{r}\rangle \div \{\langle\mathbf{J}\,|\,\mathbf{J}\rangle\langle\mathbf{J}'\,|\,\mathbf{J}'\rangle\}].$$

We note here, that all parts behind the operator $a_{j'}$ is a c number to be taken out from the trace parenthesis, and

$$\mathrm{Tr}\,(e^{-\beta\mathfrak{L}}A_{\mathbf{J}}^{\dagger}A_{\mathbf{J}'}) = \mathrm{Tr}\,(e^{-\beta\mathfrak{L}}A_{\mathbf{J}}^{\dagger}A_{\mathbf{J}})\delta_{\mathbf{J},\mathbf{J}'}.$$

[8] E. Schrödinger, Physik. Z. 27, 95 (1926), Eq. (25) *et seq.*

Thus, it reduces to

$$= \left(\frac{V}{\bar{N}}\right)^n\langle\mathbf{r}|\,\{\mathrm{Tr}\,(e^{-\beta\mathfrak{L}})\}^{-1}\sum_{\mathbf{J}}|\mathbf{J}\rangle\frac{\mathrm{Tr}\,(e^{-\beta\mathfrak{L}}A_{\mathbf{J}}^{\dagger}A_{\mathbf{J}})}{(\langle\mathbf{J}\,|\,\mathbf{J}\rangle)^2}\langle\mathbf{J}\,|\,\mathbf{r}\rangle.$$

We compare this equation with Eq. (19). We then have

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = n!\left(\frac{V}{\bar{N}}\right)^n\langle\mathbf{r}|\prod_{\lambda=1}^{n}\{e^{\beta(h_\lambda-\mu)}-\eta\}^{-1}|\mathbf{r}\rangle = n!\left(\frac{V}{\bar{N}}\right)^n\langle\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_n|\,S_n\prod_{\lambda=1}^{n}\{e^{\beta(h_\lambda-\mu)}-\eta\}^{-1} \times|\mathbf{r}_n,\cdots,\mathbf{r}_2,\mathbf{r}_1\rangle. \quad (27)$$

This proves that Eq. (3) is correct. Since the quantity $g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n)V^{-n}$ represents the statistical probability of finding simultaneously n particles (among $\bar{N}$ particles) per unit volumes at the n points $(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_n)$ in the volume V irrespective of what the remaining other $(\bar{N}-n)$ particles are doing; the operator $P(123\cdots n)$ given by

$$P(123\cdots n) \equiv \frac{n!}{\bar{N}^n}\prod_{\lambda=1}^{n}\{e^{\beta(h_\lambda-\mu)}-\eta\}^{-1} \quad (28)$$

can be interpreted as the statistical probability density operator correlating n particles with each other. Thus, the n particle correlation function is simply regarded as V^n times the expectation value of the statistical probability density operator $P(123\cdots n)$ of Eq. (28) at the state $|\mathbf{r}\rangle$, or the diagonal element of the representatives of the operator $P(123\cdots n)$ in the symmetrized configuration representation of n particles. Therefore, the statistical probability density $f(\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_n)$ of n particles in the momentum space (or representation) must be given by

$$f(\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_n) \equiv \langle\mathbf{k}|\,P(123\cdots n)\,|\mathbf{k}\rangle = n!\bar{N}^{-n}\langle\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_n|\,S_n\prod_{\lambda=1}^{n}\{e^{\beta(h_\lambda-\mu)}-\eta\}^{-1} \times|\mathbf{k}_n,\cdots,\mathbf{k}_2,\mathbf{k}_1\rangle = n!(\bar{N})^{-n}\langle\mathbf{J}\,|\,\mathbf{J}\rangle\prod_{\lambda=1}^{n}\{e^{\beta(\epsilon_{j_\lambda}-\mu)}-\eta\}^{-1}, \quad (29)$$

with the definition of Eq. (6). Equation (29) can be regarded, also, as the function proportional to the n particle correlation function in the momentum space. In this way, we can determine the correlation function in arbitrary representation by finding the corresponding expectation value of the operator $P(123\cdots n)$.

The reasonableness of Eq. (28) can be understood also by the following elementary discussion: As is well known in the elementary c-number theory of quantum

statistics, the statistical probability p_j of finding a particle in its energy eigenstate $|j\rangle$ is given by

$$p_j = \bar{N}^{-1}\{e^{\beta(\epsilon_j-\mu)} - \eta\}^{-1}, \quad \bar{N} = \sum_j \{e^{\beta(\epsilon_j-\mu)} - \eta\}^{-1}. \tag{30}$$

Since p_j can be regarded as the expectation value of an operator $P(1)$ at the state $|j\rangle$, we must have

$$\langle j|\, P(1)\,|j\rangle \equiv p_j = \langle j|\, \bar{N}^{-1}\{e^{\beta(h_1-\mu)} - \eta\}^{-1}\,|j\rangle.$$

This equation leads to

$$P(1) = \bar{N}^{-1}\{e^{\beta(h_1-\mu)} - \eta\}^{-1}, \tag{31}$$

since it is valid for an arbitrary element $|j\rangle$ of the orthonormalized complete set of the energy eigenket vectors $|j\rangle$. Therefore, the statistical probability density operator $P(123\cdots n)$ of finding simultaneously n identical, indistinguishable particles is given by $n!$ times the product of n individual statistical probability operators $P(\lambda)$ $(\lambda = 1, 2, \cdots, n)$, i.e.,

$$P(123\cdots n) = n!\prod_{\lambda=1}^{n} P(\lambda),$$

by assuming the validity of the theorem of probability operator product,[9] where the factorial $n!$ comes from the identical and indistinguishable character of n particles. The combination of Eq. (31) with this equation gives Eq. (28).

IV. EXPLICIT FORM OF THE CORRELATION FUNCTION

We show explicitly the correctness of the above formalism by determining the correlation functions and comparing them with the results obtained by other methods. In our subsequent discussion, an element of the symmetric group of order $n!$ denoted by

$$\begin{pmatrix} 1 & 2 & \cdots & n \\ j_1 & j_2 & \cdots & j_n \end{pmatrix}$$

represents an exchange operation which replaces 1 by j_1, 2 by j_2, and so on. We also use the identity operator I taking the following form:

$$I \equiv \sum_{\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_n} |\mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_n\rangle\langle\mathbf{k}_n, \cdots, \mathbf{k}_2, \mathbf{k}_1| \tag{32}$$

in the propagation-vector (or momentum) representation $|\mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_n\rangle$ of n particles. Note that

$$\langle \mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n| \begin{pmatrix} 1 & 2 & \cdots & n \\ j_1 & j_2 & \cdots & j_n \end{pmatrix} |\mathbf{k}_n, \cdots, \mathbf{k}_2, \mathbf{k}_1\rangle \equiv \prod_{\lambda=1}^{n} \langle \mathbf{r}_\lambda \,|\, \mathbf{k}_{j_\lambda}\rangle \tag{33}$$

with $\langle \mathbf{r}_\lambda \,|\, \mathbf{k}_{j_\lambda}\rangle \equiv \langle \mathbf{r}_\lambda \,|\, j_\lambda\rangle$ defined in Eq. (4).

(a) One-particle correlation function: The one-particle correlation function for any kind of system is unity. Our foregoing formalism leads correctly to this universal result. According to Eq. (27), the one-particle correlation function $g(\mathbf{r}_1)$ for an ideal particle system is given by

$$g(\mathbf{r}_1) = \lim_{\substack{\bar{N}\to\infty \\ V\to\infty}} \frac{V}{\bar{N}} \langle \mathbf{r}_1|\, \{e^{\beta(h_1-\mu)} - \eta\}^{-1}\,|\mathbf{r}_1\rangle,$$

since we have $S_1 = I$ (identity) for one particle. Now, we insert the identity operator of Eq. (32) with $n = 1$ between the ket vector $|\mathbf{r}_1\rangle$ and the statistical probability density operator $\{e^{\beta(h_1-\mu)} - \eta\}^{-1}$, and note that

$$h_1\,|\mathbf{k}_1\rangle = \alpha\mathbf{k}_1^2\,|\mathbf{k}_1\rangle,$$

where α is the reciprocal of Schrödinger's constant defined by $\alpha \equiv \hbar^2/2m$ for the single particle having mass m. Then, using Eqs. (4) and (30), we have

$$g(\mathbf{r}_1) = 1 \tag{34}$$

in agreement with the above statement.

(b) Two-particle correlation function: Likewise, from Eq. (27) the pair correlation function $g(\mathbf{r}_1\mathbf{r}_2)$ is given by

$$g(\mathbf{r}_1\mathbf{r}_2) = 2!\lim_{\substack{\bar{N}\to\infty \\ V\to\infty}} \left(\frac{V}{\bar{N}}\right)^2 \langle \mathbf{r}_1, \mathbf{r}_2|\, \prod_{\lambda=1}^{2} \{e^{\beta(h_\lambda-\mu)} - \eta\}^{-1} S_2\,|\mathbf{r}_2, \mathbf{r}_1\rangle.$$

If we insert the identity operator of Eq. (32) with $n = 2$ between two operators $\{e^{\beta(h_\lambda-u)} - \eta\}^{-1}$ and S_2 using the explicit form of S_2:

$$S_2 = \frac{1}{2!}\left\{\begin{pmatrix} 1 & 2 \\ 1 & 2 \end{pmatrix} \pm \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix}\right\}.$$

Then, we have

$$\begin{aligned} g(\mathbf{r}_1\mathbf{r}_2) = \lim_{\substack{\bar{N}\to\infty \\ V\to\infty}} \left(\frac{V}{\bar{N}}\right)^2 &\times \sum_{(\mathbf{k}_1,\mathbf{k}_2)} \prod_{\lambda=1}^{2} \{e^{\beta(\alpha\mathbf{k}_\lambda^2-\mu)} - \eta\}^{-1} \\ &\times \left\{\frac{1}{V^2} \pm \langle \mathbf{r}_1, \mathbf{r}_2 \,|\, \mathbf{k}_2, \mathbf{k}_1\rangle \right. \\ &\times \left. \langle \mathbf{k}_1, \mathbf{k}_2|\, \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} |\mathbf{r}_2, \mathbf{r}_1\rangle\right\} \\ = 1 + \eta\{L_\eta(\mathbf{r}_2 - \mathbf{r}_1)\}^2, \end{aligned} \tag{35}$$

where $L_\eta(\mathbf{x})$ is the London–Placzek function defined by

$$L_\eta(\mathbf{x}) \equiv \bar{N}^{-1}\sum_{\mathbf{k}} \{e^{\beta(\alpha\mathbf{k}^2-\mu)} - \eta\}^{-1} e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{36}$$

It is obvious that $2 \geq g(\mathbf{r}_1\mathbf{r}_2) > 1$ for the boson system, and $0 \leq g(\mathbf{r}_1\mathbf{r}_2) < 1$ for the fermion system from Eq. (35). We note, here, that the London–Placzek function defined by Eq. (36) is a real function of the variable $\mathbf{x}$, since we have always the pair terms corresponding to the pair of $(\mathbf{k}, -\mathbf{k})$ in the summation, and as $(\bar{N}, V) \to (\infty, \infty)$ it approaches to the function given by[10]

$$L_\eta(|\mathbf{x}|) \equiv \frac{1}{2\pi^2\rho x}\int_0^\infty dk\, \frac{k\sin(kx)}{e^{\beta(\alpha k^2-\mu)} - \eta}, \quad (\rho \equiv \bar{N}/V). \tag{37}$$

[9] Actually, Eq. (10) guarantees this statement.

[10] Note, in this derivation, that the number of states per the volume element $d^3\mathbf{k}$ in $\mathbf{k}$ space is given by $(2\pi)^{-3}Vd^3\mathbf{k}$.

TABLE I. The structures of classes of the symmetric group of order 4!.

	1st class	2nd class	3rd class	4th class	5th class	
Cyclic structure	$(1^4, 2^0, 3^0, 4^0)$	$(1^2, 2^1, 3^0, 4^0)$	$(1^0, 2^2, 3^0, 4^0)$	$(1^1, 2^0, 3^1, 4^0)$	$(1^0, 2^0, 3^0, 4^1)$	
p	+	−	+	+	−	Total
ν	1	6	3	8	6	24

Equation (35) is the well-known London–Placzek formula obtained previously by other methods.[11–13]

(c) *Three-particle correlation function:* The three-particle correlation function $g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ is similarly given by

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = 3! \lim_{\substack{N\to\infty \\ V\to\infty}} \left(\frac{V}{N}\right)^3 \langle \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3| \times \prod_{\lambda=1}^{3} \{e^{\beta(\alpha h_\lambda - \mu)} - \eta\}^{-1} S_3 |\mathbf{r}_3, \mathbf{r}_2, \mathbf{r}_1\rangle$$

with the explicit form of the symmetrizer S_3 given by

$$S_3 \equiv \frac{1}{3!}\left\{\begin{pmatrix}1&2&3\\1&2&3\end{pmatrix} + \eta\begin{pmatrix}1&2&3\\1&3&2\end{pmatrix} + \eta\begin{pmatrix}1&2&3\\3&2&1\end{pmatrix} + \eta\begin{pmatrix}1&2&3\\2&1&3\end{pmatrix} + \begin{pmatrix}1&2&3\\2&3&1\end{pmatrix} + \begin{pmatrix}1&2&3\\3&1&2\end{pmatrix}\right\}.$$

We obtain the following form of $g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ by using the similar procedure used in (a) and (b):

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = 1 + \eta L_\eta(\mathbf{r}_1 - \mathbf{r}_2)^2 + \eta L_\eta(\mathbf{r}_2 - \mathbf{r}_3)^2 + \eta L_\eta(\mathbf{r}_3 - \mathbf{r}_1)^2 + 2L_\eta(\mathbf{r}_1 - \mathbf{r}_2)L_\eta(\mathbf{r}_2 - \mathbf{r}_3)L_\eta(\mathbf{r}_3 - \mathbf{r}_1), \quad (38)$$

which is also in agreement with the result obtained by another method.[14] We observe, in the right-hand side of Eq. (38), that the first term corresponds to the element of the class with the structure of three unary cycles. The next three terms correspond to the three elements of the class with the structure of one unary and one binary cycle. The last term corresponds to the two elements of the class with the ternary cyclic structure of the symmetric group of order 3!.

(d) *Four-particle correlation function:* In order to find the four-particle correlation function $g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4)$, we first analyze the structure of the symmetric group of order $4! = 24$. The number $C(4)$ of distinct classes of this group is equal to the number of positive integer solutions to the algebraic equation $x_1 + 2x_2 + 3x_3 + 4x_4 = 4$. This equation has five kinds of positive-integer solutions. Therefore, $C(4) = 5$. We use the conventional notation $(1^{x_1}, 2^{x_2}, 3^{x_3}, 4^{x_4})$ with the parity $(-1)^{x_2+x_4}$ in representing the cyclic structure of each class. As is well known, the number ν of distinct elements contained in each class is given by

$$\nu = 4! \Big/ \prod_{j=1}^{4} j^{x_j} x_j!. \quad (39)$$

The cyclic structure, parity p, and number ν of distinct elements of each of five classes are as given in Table I.

Let us introduce a notation defined by

$$L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix} \equiv L_\eta(\mathbf{r}_1 - \mathbf{r}_{j_1})L_\eta(\mathbf{r}_2 - \mathbf{r}_{j_2})L_\eta(\mathbf{r}_3 - \mathbf{r}_{j_3})L_\eta(\mathbf{r}_4 - \mathbf{r}_{j_4}).$$

The function $g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4)$ is then given by

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4) = \sum(\eta^0, \text{ or } \eta)L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix}, \quad (40)$$

i.e., the summation over all 24 elements where $\eta^0 \equiv 1$ stands for even parity and η, for odd parity of the permutation $(j_1j_2j_3j_4)$. Referring to Table I, we divide Eq. (40) into five subsummations taking the form

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4) = 1 + \eta\sum_{2}^{6} L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix} + \sum_{3}^{3} L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix}, + \sum_{4}^{8} L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix} + \eta\sum_{5}^{6} L_\eta\begin{pmatrix}1&2&3&4\\j_1&j_2&j_3&j_4\end{pmatrix}, \quad (41)$$

where $\sum_\lambda^\nu$ denotes the subsummation over all ν distinct elements of the λth class. From the cyclic structure of each class from $\lambda = 2$ to $\lambda = 5$, each of the subsummations is easily found. The result is

$$\begin{aligned} g(\mathbf{r}_1\,\mathbf{r}_2\,\mathbf{r}_3\,\mathbf{r}_4) &= 1 + \eta\{L_\eta(\mathbf{r}_1 - \mathbf{r}_2)^2 + L_\eta(\mathbf{r}_1 - \mathbf{r}_3)^2 + L_\eta(\mathbf{r}_1 - \mathbf{r}_4)^2 \\ &\quad + L_\eta(\mathbf{r}_2 - \mathbf{r}_3)^2 + L_\eta(\mathbf{r}_2 - \mathbf{r}_4)^2 + L_\eta(\mathbf{r}_3 - \mathbf{r}_4)^2\} \\ &\quad + \{L_\eta(\mathbf{r}_1 - \mathbf{r}_2)^2 L_\eta(\mathbf{r}_3 - \mathbf{r}_4)^2 + L_\eta(\mathbf{r}_1 - \mathbf{r}_3)^2 \\ &\quad \times L_\eta(\mathbf{r}_2 - \mathbf{r}_4)^2 + L_\eta(\mathbf{r}_1 - \mathbf{r}_4)^2 L_\eta(\mathbf{r}_2 - \mathbf{r}_3)^2\} \\ &\quad + 2\{L_\eta(\mathbf{r}_2 - \mathbf{r}_3)L_\eta(\mathbf{r}_3 - \mathbf{r}_4)L_\eta(\mathbf{r}_4 - \mathbf{r}_2) \\ &\quad + L_\eta(\mathbf{r}_3 - \mathbf{r}_4)L_\eta(\mathbf{r}_4 - \mathbf{r}_1)L_\eta(\mathbf{r}_1 - \mathbf{r}_3) \\ &\quad + L_\eta(\mathbf{r}_4 - \mathbf{r}_1)L_\eta(\mathbf{r}_1 - \mathbf{r}_2)L_\eta(\mathbf{r}_2 - \mathbf{r}_4) + L_\eta(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad \times L_\eta(\mathbf{r}_2 - \mathbf{r}_3)L_\eta(\mathbf{r}_3 - \mathbf{r}_1)\} + 2\eta\{L_\eta(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad \times L_\eta(\mathbf{r}_2 - \mathbf{r}_3)L_\eta(\mathbf{r}_3 - \mathbf{r}_4)L_\eta(\mathbf{r}_4 - \mathbf{r}_1) \\ &\quad + L_\eta(\mathbf{r}_1 - \mathbf{r}_2)L_\eta(\mathbf{r}_2 - \mathbf{r}_4)L_\eta(\mathbf{r}_3 - \mathbf{r}_1)L_\eta(\mathbf{r}_4 - \mathbf{r}_3) \\ &\quad + L_\eta(\mathbf{r}_1 - \mathbf{r}_4)L_\eta(\mathbf{r}_2 - \mathbf{r}_3)L_\eta(\mathbf{r}_3 - \mathbf{r}_1)L_\eta(\mathbf{r}_4 - \mathbf{r}_2)\}. \end{aligned} \quad (42)$$

[11] F. London, J. Chem. Phys. 11, 203 (1943).
[12] G. Placzek, *Proceeding of the Second Berkeley Symposium on Mathematical Statistics and Probability* (University of California Press, Berkeley, California, 1951), p. 581.
[13] See Appendix III of the second paper of Ref. 4.
[14] F. Lado and T. Dunn (private communications).

(e) *The n particle correlation function:* The n particle correlation function defined by Eq. (27) reduces to

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = \lim_{\substack{\bar{N}\to\infty \\ V\to\infty}} \left(\frac{V}{\bar{N}}\right)^n \sum_{(\mathbf{k}_1,\mathbf{k}_2,\cdots,\mathbf{k}_n)} \prod_{\lambda=1}^{n} \{e^{\beta(\alpha\mathbf{k}\lambda^2-\mu)} - \eta\}^{-1} \times V^{-n/2} \exp\left(i\sum_{\lambda=1}^{n} \mathbf{k}_\lambda\cdot\mathbf{r}_\lambda\right) \cdot \langle \mathbf{k}_1, \mathbf{k}_2, \cdots, \mathbf{k}_n| \times \sum_p (\pm 1)^p p\, |\mathbf{r}_n, \cdots, \mathbf{r}_2, \mathbf{r}_1\rangle \quad (43)$$

by the use of the identity given by Eq. (32). Furthermore, taking out the operator $\sum_p (\pm 1)^p$ before the coefficient $(V/\bar{N})^n$ in Eq. (43) and referring to Eq. (36), we have then,

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = 1 + \sum_p (\pm)^p \prod_{\lambda=1}^{n} L_\eta(\mathbf{r}_\lambda - p\mathbf{r}_\lambda) = 1 + \sum(\eta^0, \text{or } \eta) L_\eta\begin{pmatrix} 1 & 2 & 3 & \cdots & 4 \\ j_1 & j_2 & j_3 & \cdots & j_n \end{pmatrix}. \quad (44)$$

We follow the same idea as that for the derivation of Eq. (41). We have then,

$$g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n) = 1 + \sum_{s=2}^{c(n)} \eta^{p_s} \sum_{s}^{\nu_s} L_\eta\begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ j_1 & j_2 & j_3 & \cdots & j_n \end{pmatrix}, \quad (45)$$

where $c(n)$ is the total number of classes in the symmetric group of order $n!$, and $\sum_s^{\nu_s}$, the subsummation over all ν_s distinct elements contained in the sth class with its parity p_s. The number ν_s is given by

$$\nu_s = n! \Big/ \prod_{j=1}^{n} j^{x_j^{(s)}} \cdot x_j^{(s)}!; \quad \sum_{j=1}^{n} j x_j^{(s)} = n, \quad (46)$$

in the sth class with the cyclic structure of

$$(1^{x_1^{(s)}}, 2^{x_2^{(s)}}, \cdots, n^{x_n^{(s)}}),$$

and the parity p_s is given by

$$p_s = x_2^{(s)} + x_4^{(s)} + x_6^{(s)} + \cdots.$$

The total number $c(n)$ of classes is equal to the total number of the positive integer solutions $(x_1^{(s)}, x_2^{(s)}, x_3^{(s)}, \cdots, x_n^{(s)})$ to the algebraic equation given by the second of Eq. (46). Therefore, if we find all positive-integer solutions of this algebraic equation, the n particle correlation function $g(\mathbf{r}_1\mathbf{r}_2\cdots\mathbf{r}_n)$ of Eq. (45) is completely determined in its explicit form in terms of the London–Placzek function by analyzing the cyclic structures of all classes of the symmetric group of order $n!$. The systematic table of the cyclic structures can be found in many references by which we can find the correlation functions for $n = 5, 6$, and so on.

V. KIRKWOOD'S SUPERPOSITION APPROXIMATION

It would be instructive to see how much Kirkwood's superposition approximation agrees in the case of the ideal particle system. Kirkwood's superposition approximation states that[15]

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) \approx g(\mathbf{r}_1\mathbf{r}_2)g(\mathbf{r}_2\mathbf{r}_3)g(\mathbf{r}_3\mathbf{r}_1). \quad (47)$$

Let us express the right-hand side of Eq. (47) in terms of the function $L_\eta(\mathbf{x})$ defined by Eq. (36) by using the London–Placzek formula of Eq. (35). It is

$$\begin{aligned} &g(\mathbf{r}_1\mathbf{r}_2)g(\mathbf{r}_2\mathbf{r}_3)g(\mathbf{r}_3\mathbf{r}_1) \\ &= 1 + \eta L_\eta(\mathbf{r}_1-\mathbf{r}_2)^2 + \eta L_\eta(\mathbf{r}_2-\mathbf{r}_3)^2 \\ &\quad + \eta L_\eta(\mathbf{r}_3-\mathbf{r}_1)^2 + L_\eta(\mathbf{r}_1-\mathbf{r}_2)^2 L_\eta(\mathbf{r}_2-\mathbf{r}_3)^2 \\ &\quad + L_\eta(\mathbf{r}_2-\mathbf{r}_3)^2 L_\eta(\mathbf{r}_3-\mathbf{r}_1)^2 + L_\eta(\mathbf{r}_3-\mathbf{r}_1)^2 \\ &\quad \times L_\eta(\mathbf{r}_1-\mathbf{r}_2)^2 + \eta L_\eta(\mathbf{r}_1-\mathbf{r}_2)^2 L_\eta(\mathbf{r}_2-\mathbf{r}_3)^2 \\ &\quad \times L_\eta(\mathbf{r}_3-\mathbf{r}_1)^2. \end{aligned} \quad (48)$$

Thus, the comparison of Eq. (48) with Eq. (38) shows that the last term of Eq. (38) is approximated by the last four terms of Eq. (48) in Kirkwood's superposition approximation.

We can find the exact relationship between the pair correlation function and the three-particle correlation function by eliminating the London–Placzek function L_η in Eqs. (38) and (35). From Eq. (35) we have

$$L_\eta(\mathbf{r}_\lambda - \mathbf{r}_\nu)^2 = \eta\{g(\mathbf{r}_\lambda, \mathbf{r}_\nu) - 1\} \quad (\lambda, \nu = 1, 2, 3; \lambda \neq \nu). \quad (49)$$

When this is substituted into Eq. (38), we obtain

$$g(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3) = g_{12} + g_{23} + g_{31} + 2 \times [\{\eta(g_{12}-1)(g_{23}-1)(g_{31}-1)\}^{\frac{1}{2}} - 1], \quad (50)$$

where $g_{\lambda\nu} \equiv g(\mathbf{r}_\lambda, \mathbf{r}_\nu)$. This equation is exact for the noninteracting particle system.

The exact error of Kirkwood's superposition approximation is, thus, given by the following function $E_\eta(g_1, g_2, g_3)$:

$$E_\eta \equiv g_1 + g_2 + g_3 + 2[\{\eta(g_1-1)(g_2-1)(g_3-1)\}^{\frac{1}{2}} - 1] - g_1g_2g_3 \quad (51)$$

with the further definition of $g_1 \equiv g_{23}$, $g_2 \equiv g_{31}$, and $g_3 \equiv g_{12}$. This error function E_η varies with the changes of the values g_j $(j = 1, 2, 3)$, or $r_1 \equiv |\mathbf{r}_3 - \mathbf{r}_2|$, $r_2 \equiv |\mathbf{r}_1 - \mathbf{r}_3|$, and $r_3 \equiv |\mathbf{r}_2 - \mathbf{r}_1|$. The pair correlation function g_j varies in the open–closed range $(1, 2]$ for bosons, and in the closed–open range $[0, 1)$ for fermions, with the change of the pair distance r_j in its closed-open interval $[0, \infty)$ as stated already in Sec. IV(b). For example, at $r_j = 0$ $(j = 1, 2, 3)$, we have

[15] J. G. Kirkwood, J. Chem. Phys. 3, 300 (1935).

$g_j = 2$ and $E_+ = -2$ for bosons, and $g_j = 0$, $E_- = 0$ for fermions, respectively. Therefore, Eq. (47) is, for fermions, correct at the generic configuration where three particles come simultaneously together at a point, while incorrect with the large error -2 for bosons. At the generic configuration where $g_1 = g_2 = g_3$ equal to 1.5 for bosons, and 0.5 for fermions, we have $E_+ = -0.167\cdots$ and $E_- = 0.082\cdots$, respectively, showing that the error for bosons is much larger than that for fermions as in the previous case of $r_j = 0$. However, at a large distance of $r_j \approx \infty$, i.e., $g_j \approx 1$ $(j = 1, 2, 3)$, we have $E_\eta \approx 0$, to show that the Kirkwood's superposition approximation is effective in the large distance region for both bosons and fermions. It seems, from the above discussion, that Kirkwood's superposition approximation is, as a whole, more effective for fermions than bosons.

Next, we are interested in finding the generic configuration where the error function of Eq. (51) attains its maximum or minimum. This is simply an elementary extremum problem. The values (g_1, g_2, g_3) for this extremum are found by the roots of the simplified algebraic equation $g_1^3 + g_1^2 - g_1 - (1 + \eta) = 0$, and $g_1 = g_2 = g_3$. After a check of the condition for the maximum, or minimum, we obtain the following result: The error E_η attains at its maximum $E_+ = 0.0412\cdots$ at $g_1 = g_2 = g_3 = 1.205\cdots$ for bosons, while at its minimum $E_- = 0.0901\cdots$ at $g_1 = g_2 = g_3 = 0.618\cdots$ for fermions, respectively. Therefore, the ranges of the errors are given by $-2 \leq E_+ \leq 0.0412\cdots$ for bosons, and $0 \leq E_- \leq 0.0901\cdots$ for fermions, respectively.

This incorrectness is not a surprising result, because this approximation has, without any statistical-mechanical points of view, been introduced originally by Kirkwood[15] only for the purpose of simplifying the mathematical manipulation concerned with the hierarchy of the exact coupled integral equations for the determination of the classical pair correlation function, as pointed out by Fisher.[16] Therefore, it is desirable, on the basis of Eq. (50), to suggest the following approximation:

$$g'_{123} \approx g'_{12} + g'_{23} + g'_{31} + 2[\{\eta(g'_{12} - 1)(g'_{23} - 1)(g'_{31} - 1)\}^{\frac{1}{2}} - 1] \quad (52)$$

in the weak-interacting particle system, where $g'_{123} \equiv g'(\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3)$ is the exact three-particle correlation function, and g'_{ij} $(i, j = 1, 2, 3; i \neq j)$, the corresponding exact pair correlation functions of the system. This new approximation would give a better answer than that of Kirkwood's superposition approximation. The proof is as follows:

Let us suppose that a weak interaction is coupled pairwise between all particles of the system under consideration. Then, the form of the pair correlation function g'_j $(\equiv g'_{23}, g'_{31}, g'_{12})$ is changed by a small amount from its original form g_j into $g'_j \equiv g_j + \delta g_j$ with $\delta g_j \to 0$ as the interaction goes to zero. We can safely assume that the function g'_{123} is split into two parts of the form

$$g'_{123} = \Theta(g'_1, g'_2, g'_3) + \delta\Theta' \quad (53)$$

with a certain function Θ going to the form Θ_0 given by the right-hand side of Eq. (50), and $\delta\Theta' \to 0$, as the interaction goes to zero, where $\delta\Theta'$ is very small compared with Θ, or Θ_0, and also may generally contain the higher-order (than g'_{123}) correlation functions coupled with g'_j $(j = 1, 2, 3)$, just as in the classical case. Then, the right-hand side of Eq. (52) is expressed notationally by $\Theta_0(g'_1, g'_2, g'_3)$, and the error function E_1 for the new approximation of Eq. (52) is given by

$$E_1 \equiv \Theta(g_j + \delta g_j) + \delta\Theta' - \Theta_0(g_j + \delta g_j).$$

Let us make the Taylor expansion of this function E_1 with respect to the variation δg_j. We then have

$$E_1 = \delta\Theta(g_j) + \delta\Theta' + [\partial\delta\Theta(g_j)/\partial g_j]\delta g_j + (\text{the higher-order terms than the first order } \delta g_j).$$

Since all the terms below the third terms in this expansion are, in general, higher orders than the first two terms, we have, in first-order approximation,

$$E_1 \approx \delta\Theta(g_j) + \delta\Theta'. \quad (54)$$

On the other hand, the error function E_2 for the Kirkwood's superposition approximation is given by

$$E_2 = \Theta(g_j + \delta g_j) + \delta\Theta' - \prod_{j=1}^{3}(g_j + \delta g_j).$$

We add

$$0 \equiv -\Theta_0(g_j + \delta g_j) + \Theta_0(g_j + \delta g_j)$$

to the right-hand side of this equation, and then, make its Taylor expansion with respect to δg_j. We obtain, then,

$$E_2 = E_\eta + \delta\Theta(g_j) + \delta\Theta' + (\partial E_\eta/\partial g_j)\delta g_j + (\text{higher-order terms}),$$

where E_η is defined by Eq. (51). In first-order approximation, we have, therefore,

$$E_2 \approx E_\eta + \delta\Theta(g_j) + \delta\Theta' + (\partial E_\eta/\partial g_j)\delta g_j, \quad (55)$$

[16] I. Z. Fisher, *Statistical Theory of Liquids* (The University of Chicago Press, Chicago, 1964), p. 131 *et seq.*

to show that the error E_2 accompanies always a definite value E_η (the same order of g_j as seen previously) in addition to the small value represented by all the terms below the second term of Eq. (55). The comparison of Eq. (55) with Eq. (54) shows that the previous statement can be recognized.

In closing this section, it should be pointed out that an arbitrary n-particle correlation function in a noninteracting particle system can, in general, be expressed in terms of the corresponding pair correlation functions of $\frac{1}{2}n(n-1)$ in number. This statement is guaranteed by the last discussion of Sec. IV.

VI. THE PAIR CORRELATION FUNCTION IN THE HARTREE–FOCK APPROXIMATION

If the Hamiltonian operator of the single particle is the function $\epsilon(\mathbf{p})$ of only the single-particle momentum operator $\mathbf{p}$, i.e., the energy eigenvalue of the single particle is given by a function $\epsilon(\mathbf{k})$ in the noninteracting particle system, the London–Placzek function of Eq. (35) takes, then, an extended form given by

$$L_\eta(\mathbf{r}) \equiv 2\pi^{-3}\rho^{-1}\int_\infty d^3\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}[e^{\beta\{\epsilon(\mathbf{k})-\mu\}}-\eta]^{-1}. \quad (56)$$

As is well known in the Green's function theory of equilibrium statistical mechanics by Martin and Schwinger,[17] the function $\epsilon(\mathbf{k})$ is the Hartree–Fock approximation of a pair-interacting system is found by the solution to the following integral equation:

$$\epsilon(\mathbf{k}) = \alpha\mathbf{k}^2 + \rho\phi(0) + \eta(2\pi)^{-3}\int_\infty d^3\mathbf{k}'\phi(\mathbf{k}-\mathbf{k}') \times [e^{\beta\{\epsilon(\mathbf{k}')-\mu\}}-\eta]^{-1}, \quad (57)$$

where $\phi(\mathbf{k})$ is the Fourier transform of the pair potential $\phi(\mathbf{r})$, i.e.,

$$\phi(\mathbf{k}) = \int_\infty d^3\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}}\phi(\mathbf{r}),$$

and $\phi(0) \equiv \phi\ (\mathbf{k}=0)$. For example, in the electron gas with the screened Coulomb pair-potential given by

$$\phi(r) \equiv e^2\exp(-\sigma r)/r$$

($e \equiv$ electron charge, $\sigma \equiv$ a parameter),

Eq. (57) takes the following explicit form:

$$\epsilon(k) = \alpha k^2 + 4\pi\rho e^2/\sigma^2 - e^2(2\pi k)^{-1}\int_0^\infty x[e^{\beta\{\epsilon(x)-\mu\}}+1]^{-1}\ln[\{\sigma^2+(k+x)^2\} \div \{\sigma^2+(k-x)^2\}]\,dx. \quad (58)$$

In this sense, the Hartree–Fock approximation can be regarded as an operation making the single-particle Hamiltonian of an interacting particle system be a function of the single-particle momentum only.

An iteration method would be applicable for finding the solution $\epsilon(\mathbf{k})$ to Eq. (57) by assuming that the iteration series and the value $\phi(0)$ are convergent.[18] This is easily done numerically also by the Fortran program of a computing machine, even if the Fourier transform $\phi(\mathbf{k})$ is a complicated function. The substitution of $\epsilon(\mathbf{k})$ (known in this way) into Eq. (35) through Eq. (56) enables us to determine the pair correlation function $g(\mathbf{r}_1\mathbf{r}_2)$ in the Hartree–Fock approximation of a pair-interacting particle system.

The method presented in this section is useful for the determination of the Hartree–Fock energy in finding the correlation energy at a finite temperature in an interacting system with a non-hard-core pair potential.

Finally, it should be mentioned that Eq. (27) can, also, be applied for the noninteracting particle system placed in a stationary external potential field. For example, in the case of pair correlation function, it is done simply as follows: We insert the identity operator I constructed from the simultaneous energy-eigenket vectors $|\mathbf{j},\mathbf{j}'\rangle$ of the two commutable Hamiltonian operators h_1 and h_2 corresponding to their energy eigenvalues $\epsilon(\mathbf{j})$ and $\epsilon(\mathbf{j}')$, i.e.,

$$I \equiv \sum_{\mathbf{j},\mathbf{j}'} |\mathbf{j},\mathbf{j}'\rangle\langle\mathbf{j}',\mathbf{j}|,$$

between two operators $[e^{\beta(h_\lambda-\mu)}-\eta]^{-1}$, $(\lambda=1,2)$, in Eq. (27), and then, step the same procedure as done in Sec. IV(b), by noting the direct product $|\mathbf{j},\mathbf{j}'\rangle$ and the orthonormalized character $\langle\mathbf{j}\,|\,\mathbf{j}'\rangle = \delta(\mathbf{j},\mathbf{j}')$ of the single-particle energy-eigenket vectors $|\mathbf{j}\rangle$'s. We find, then,

$$g(\mathbf{r}_1\mathbf{r}_2) = 1 + \eta\bar{N}^{-1}\left|\sum_{\mathbf{j}}\{e^{\beta(\epsilon(\mathbf{j})-\mu)}-\eta\}^{-1} \times U_{\mathbf{j}}^*(\mathbf{r}_1)U_{\mathbf{j}}(\mathbf{r}_2)\right|^2, \quad (59)$$

where $U_{\mathbf{j}}(\mathbf{r}) \equiv \langle\mathbf{r}\,|\,\mathbf{j}\rangle$. The function forms of $\epsilon(\mathbf{j})$ and $U_{\mathbf{j}}(\mathbf{r})$ depend upon the external potential field. The second term of Eq. (59) is an extended London–Placzek function, which does, in general, not have a pair character as in the noninteracting particle system.

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[17] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959), Eq. (5.44); or L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962), p. 26, Eq. (3-29).

[18] $\phi(0)$ is not convergent for hard-core pair potential such as Lennard–Jones' potential.

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Characteristic Hypersurfaces in General Relativity. I*

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Lightlike (null) hypersurfaces are treated by means of an intrinsic Ricci rotation coefficient technique. This provides an effective way of dealing with the various types of geometry on a null hypersurface. The formalism is used to examine inner affinities, differential invariants, local features such as asymptotic and shear directions and geodesic lines, and to give a short description of null hypersurfaces in flat space–time. Applications to gravitational radiation theory and cosmology are briefly mentioned.

1. INTRODUCTION

THERE are several reasons, apart from its intrinsic interest, for an investigation of isotropic hypersurfaces in a pseudo-Riemannian manifold. One is connected with gravitational waves. A suitable description of a general outgoing gravitational wave can be given in terms of a one-parameter set of propagation fronts $\mathfrak{U}$ which are null hypersurfaces, and a set of "conjugate null hypersurfaces" $\mathfrak{V}$ intersecting the set of propagation fronts $\mathfrak{U}$ in two-dimensional spacelike surfaces. Intrinsic structures on each hypersurface $V \in \mathfrak{V}$ measure the intensity of the outgoing gravitational wave.[1] Note that the set $\mathfrak{V}$ could be interpreted as a system of incoming wavefronts, with the intrinsic structure of the hypersurfaces $\mathfrak{U}$ measuring the intensity of the incoming waves.[2]

Another reason for considering isotropic hypersurfaces comes from cosmology. As Heckmann and Schucking pointed out in 1958,[3] the cosmological problem should be formulated as a characteristic initial value problem on the past null cone of the observer. Most relations between observable quantities can be written in a form involving only those geometrical quantities which are related to the inner geometry of the past cone. Moreover, because of the uniqueness of the characteristic initial value problem inside the past cone, the cone geometry together with quantities describing the matter distribution on the cone can be used to characterize a world model. Evidently, an appropriate technique for treating the geometry of light cones is needed.

The study of the differential geometry of general null hypersurfaces is still in its initial stages.[4] In this paper a kind of spin coefficient technique is presented, which provides an effective way of dealing with the various types of geometry on a null hypersurface. This formalism is used to examine inner affinities (Sec. 2), differential invariants (Sec. 4), local features such as asymptotic and shear directions (Sec. 5), and geodesic lines (Sec. 6), and to give a short description of the special lightlike hypersurfaces appearing in flat space–time (Sec. 7).

A null hypersurface is defined intrinsically as a three-dimensional manifold of class $n \geq 2$ in the sense of Veblen and Whitehead[5] on which is given a degenerate metric tensor field $\gamma_{ik}(x^i)$ $(i, k = 1, 2, 3)$. The tensor γ_{ik} has, in general, rank 2, class C^2 at least and signature (0, 1, 1). Since the appearance of focal points can violate the rank condition, it is useful to define a regular point P with coordinates x^i as a point satisfying the condition $rk\gamma_{ik}(x^i) = 2$. Local properties of null hypersurfaces are considered for domains containing only regular points.

At a regular point, γ_{ik} determines one and only one eigendirection ϵ^k with eigenvalue 0:

$$\gamma_{ik}\epsilon^k = 0. \tag{1}$$

A contravariant vector is called spacelike, if $\gamma_{ik}a^ia^k > 0$, and null, if $\gamma_{ik}a^ia^k = 0$. a^i being null implies $a^i = a\epsilon^i$; every (real) direction in a null hypersurface is either null or spacelike. The curves to which the directions ϵ^i are tangents are the solutions of the differential equations

$$\epsilon^k(x^k) = dx^k/dv, \tag{2}$$

* The main results of this paper were presented at the London conference on general relativity, London (1965).

[1] G. Daŭtcourt, to be published.

[2] The reciprocity between wavefronts and intensity measuring fronts with regard to incoming and outgoing radiation follows essentially from the geometrical nature of gravitational waves. Naturally the splitting into incoming and outgoing radiation is not in general a unique one.

[3] O. Heckmann and E. Schucking, *La structure et l'evolution de l'univers* (Reinhold Europe, Brussels, 1959).

[4] R. Penrose, *Null Hypersurface Initial Data for Classical Fields of Arbitrary Spin and for General Relativity*, preprint (1961); I. Ozsváth, E. Schucking, *Recent Developments in General Relativity* (Warschau, 1962), p. 339; R. Sachs, J. Math. Phys. 3, 908 (1962); G. Lemmer, Nuovo Cimento 37, 1959 (1965); M. Crampin and J. Foster, Proc. Cambridge Phil. Soc. 62, 269 (1966).

[5] O. Veblen and J. H. C. Whitehead, *Foundations of Differential Geometry* (Cambridge, 1932).

these curves are called *generators* of the null hypersurface. They are lightlike geodesics when the hypersurface is embedded in four-dimensional space. In what sense they may be considered as geodesics of the inner geometry also is made clear shortly. The general solution of (2) is of the form

$$x^i = x^i(w^A, v), \tag{3}$$

where the two parameters w^A [arbitrary up to $w^{A'} = w^{A'}(w^A)$] fix a generator, and v, which is determined up to $v' = v'(v, w^A)$, $\partial v'/\partial v \neq 0$, ∞ is a parameter along each fixed ray. Note that v need not be an affine parameter.

From the assumptions made above, it follows that there are two vectors (spacelike directions) π^i and $\tilde{\pi}^i$, satisfying both

$$\begin{aligned} \pi^i\gamma_{ik} &\equiv \pi_k \neq 0, \\ \tilde{\pi}^i\gamma_{ik} &\equiv \tilde{\pi}_k \neq 0, \end{aligned} \tag{4}$$

and the further condition, that ϵ^i, π^i, $\tilde{\pi}^i$ form a linearly independent triad. Defining a third covariant vector by

$$\gamma_i = \epsilon_{ikl}\pi^k\tilde{\pi}^l/\epsilon_{rst}\epsilon^r\pi^s\tilde{\pi}^t \tag{5}$$

(where ϵ_{ikl} is the three-dimensional Levi-Civita symbol), one obtains a linearly independent covariant triad π_k, $\tilde{\pi}_k$, γ_k. However, even if the additional conditions

$$\begin{aligned} &\pi^i\pi_i = \tilde{\pi}^i\tilde{\pi}_i = 1, \\ &\pi^i\tilde{\pi}_i = \tilde{\pi}^i\pi_i = \pi^i\gamma_i = \tilde{\pi}^i\gamma_i = 0, \\ &\epsilon^i\pi_i = \epsilon^i\tilde{\pi}_i = 0, \quad \epsilon^i\gamma_i = 1 \end{aligned} \tag{6}$$

are imposed, the triad is not uniquely determined. It is easy to show that the remaining freedom at each point is that of null rotations, that is, the subgroup of the Lorentz transformations, which leaves one null direction (the generator direction) unchanged:

$$\begin{aligned} t'_i &= e^{i\mu}t_i, \\ t^{i'} &= e^{i\mu}(t^i - \bar{\kappa}\lambda\epsilon^i), \\ \epsilon^{i'} &= \lambda\epsilon^i, \\ \gamma'_i &= (1/\lambda)\gamma_i + \kappa t_i + \bar{\kappa}\bar{t}_i, \end{aligned} \tag{7}$$

where

$$t_i = (1/\sqrt{2})(\pi_i + i\tilde{\pi}_i)$$

(κ complex, λ, μ real). The 4-parameter group (7) splits into three commutative subgroups characterized by (a) $\kappa = \lambda - 1 = 0$, (b) $\mu = \kappa = 0$, (c) $\mu = \lambda - 1 = 0$. (a) corresponds to an ordinary rotation of the complex null vectors, (b) to a change in the parameter v (scale transformation), and (c) to a null rotation, that is, a reassignment of the spacelike plane element spanned by t^i. Obviously, the inner metric, expressed in terms of the triad by

$$\gamma_{ik} = \pi_i\pi_k + \tilde{\pi}_i\tilde{\pi}_k = \bar{t}_it_k + t_i\bar{t}_k \tag{8}$$

is invariant with respect to (7). Because of the degeneracy of γ_{ik} there is no contravariant metric tensor γ^{ik} satisfying $\gamma^{ik}\gamma_{il} = \delta^k_l$. However, there are solutions ϵ^{ik} of the equations

$$\gamma_{ri}\gamma_{sk}\epsilon^{ik} = \gamma_{rs}, \tag{9}$$

valid even if γ_{ik} is degenerate. In particular to every triad there corresponds a solution

$$\epsilon^{ik} = t^i\bar{t}^k + \bar{t}^it^k \tag{10}$$

of (9). This quantity is introduced as a substitute contravariant metric. Under (7) ϵ^{ik} transforms according to

$$\begin{aligned} \epsilon^{ik'} &= \epsilon^{ik} + a^i\epsilon^k + a^k\epsilon^i, \\ a' &= \lambda(\kappa\bar{\kappa}\epsilon^i - \kappa t^i - \bar{\kappa}\bar{t}^i). \end{aligned} \tag{11}$$

Furthermore, ϵ^{ik} satisfies

$$\begin{aligned} \epsilon^{ik}\gamma_k &= 0, \\ \epsilon^{kl}\gamma_{li} &= \delta^k_i - \epsilon^k\gamma_i. \end{aligned} \tag{12}$$

The relation between the co- and contravariant triads is

$$\begin{aligned} &\gamma_i = (i/\Delta)\epsilon_{ikl}t^k\bar{t}^l, \quad \epsilon^i = i\Delta\epsilon^{ikl}t_k\bar{t}_l, \\ &t_i = (i/\Delta)\epsilon_{ikl}\epsilon^k t^l, \quad t^i = i\Delta\epsilon^{ikl}\gamma_k\bar{t}_l, \\ &\Delta = i\epsilon_{ikl}\epsilon^i t^k\bar{t}^l = 1/i\epsilon^{ikl}\gamma_i t_k\bar{t}_l. \end{aligned} \tag{13}$$

2. AFFINITY

It is easy to show, by using the transformation law for γ_{ik}, that because of the degeneracy of γ_{ik} there is no uniquely determined affinity Γ^l_{ik} depending only on the inner metric γ_{ik} and its first derivatives. One way out of this uncomfortable situation would be to use affinities of higher order (depending on higher derivatives of γ_{ik}). In fact affinities of this type do exist. Alternatively, one may introduce a *class* of affinities and demand all relevant equations to be invariant with respect to a change of the affinity within this class. This can be done in the following way:

Any affinity ${}'\Gamma^l_{ik} = {}'\Gamma^l_{ki}$ must satisfy an equation

$${}'\nabla_l\gamma_{ik} \equiv \gamma_{ik,l} - {}'\Gamma^m_{kl}\gamma_{im} - {}'\Gamma^m_{il}\gamma_{km} = K_{ikl}. \tag{14}$$

Cyclic interchange of ikl and addition and subtraction gives

$$\begin{aligned} {}'\Gamma^m_{ik}\gamma_{ml} &= \Gamma_{ikl} + \Lambda_{ikl}, \\ \Lambda_{ikl} &= \tfrac{1}{2}(K_{ikl} - K_{lki} - K_{lik}). \end{aligned} \tag{15}$$

Transvecting with ϵ^l gives the condition

$$\Gamma_{ikl}\epsilon^l + \Lambda_{ikl}\epsilon^l = 0 \tag{16}$$

and $K_{ikl} = 0$ requires

$$h_{ik} \equiv \Gamma_{ikl}\epsilon^l = 0. \tag{17}$$

Despite its definition (17), h_{ik} behaves as a tensor with regard to arbitrary coordinate transformations $x^i \to x^{i'} = x^{i'}(x^k)$ and is multiplied by λ under a

triad transformation (7). Note the transversal character of h_{ik}: $h_{ik}\epsilon^k = 0$. In fact, h_{ik} is, apart from a factor 2, the Lie derivative of γ_{ik} with respect to the generator congruence $\epsilon^i(x^k)$.[6] Equation (17) implies a strong restriction on the type of null hypersurface considered; one may not assume $K_{ikl} = 0$ in the general case. The general solution of (15) turns out to be

$$'\Gamma^m_{ik} = \epsilon^m\lambda_{ik} + \epsilon^{mr}(\Gamma_{ikr} + \Lambda_{ikr}). \tag{18}$$

In order that $'\Gamma^m_{ik}$ transform as an affinity, the transformation law of λ_{ik} has to be

$$\bar{\lambda}_{ik} = \frac{\partial x^l}{\partial \bar{x}^i}\frac{\partial x^m}{\partial \bar{x}^k}\gamma_{lm} + \gamma_l\frac{\partial^2 x^l}{\partial \bar{x}^i \partial \bar{x}^k}. \tag{19}$$

The most general quantity λ_{ik} satisfying this transformation law is

$$\lambda_{ik} = \tfrac{1}{2}(\gamma_{i,k} + \gamma_{k,i}) + \mu_{ik}, \tag{20}$$

μ_{ik} being an arbitrary tensor field. The affinity is therefore

$$'\Gamma^m_{ik} = \epsilon^{mr}\Gamma_{ikr} + \tfrac{1}{2}\epsilon^m(\gamma_{i,k} + \gamma_{k,i}) + \epsilon^m\mu_{ik} + \gamma^{mr}\Lambda_{ikr}.$$

This is the sum of two tensorial terms, $\epsilon^m\mu_{ik}$ and $\gamma^{mr}\Lambda_{ikr}$, and a quantity transforming as an affinity. Obviously, the quantity

$$\Gamma^l_{ik} = \epsilon^{lm}\Gamma_{ikm} + \tfrac{1}{2}\epsilon^l(\gamma_{i,k} + \gamma_{k,i}) \tag{21}$$

may be used as an affinity on the null surface. To every given triad ϵ^i, t^i (or γ_i, t_i) there corresponds one affinity (21), satisfying

$$\nabla_l\gamma_{ik} = h_{il}\gamma_k + h_{kl}\gamma_i. \tag{22}$$

Clearly,

$$\epsilon^k\nabla_k\epsilon^i = 0 \tag{23}$$

is an identity for every affinity (21): the generators are geodesics with respect to the inner affinity Γ^l_{ik}. In contrast to the usual geodesic equation, a change of the parameter v in $\epsilon^i = dx^i/dv$ does not change (23), because Γ^l_{ik} transforms in a complementary way [see Eq. (28) below].

Further consequences of (22) are

$$\epsilon^l\nabla_l\gamma_{ik} = 0 \tag{24}$$

and

$$\nabla_l\epsilon^{ik} = -\epsilon^{ir}\epsilon^k\nabla_l\gamma_r - \epsilon^{kr}\epsilon^i\nabla_l\gamma_r.$$

From (24) it follows that $\nabla_l\epsilon^{ik} = 0$ is equivalent to γ_i being a gradient. For $\nabla_l\epsilon^{ik} = 0 \Leftrightarrow \nabla_k\gamma_i = 0$ and from (21),

$$\nabla_k\gamma_i = \tfrac{1}{2}(\gamma_{i,k} - \gamma_{k,i}). \tag{25}$$

If we perform a transformation (7), Γ^l_{ik} will in general transform according to

$$\Gamma^{l'}_{ik} = \Gamma^l_{ik} - \kappa\lambda h_{ik}t^l - \bar{\kappa}\lambda h_{ik}\bar{t}^l + m_{ik}\epsilon^l \tag{26}$$

with

$$\frac{2}{\lambda}m_{ik} = 4\kappa\bar{\kappa}\lambda h_{ik} + \kappa_{,i}t_k + \kappa_{,k}t_i + \bar{\kappa}_{,i}\bar{t}_k + \bar{\kappa}_{,k}\bar{t}_i - \lambda_{,i}\gamma_k/\lambda^2 - \lambda_{,k}\gamma_i/\lambda^2 + \kappa(\nabla_k t_i + \nabla_i t_k) + \bar{\kappa}(\nabla_k\bar{t}_i + \nabla_i\bar{t}_k). \tag{27}$$

A change in scale transforms Γ^l_{ik} according to

$$\Gamma^{l'}_{ik} = \Gamma^l_{ik} - \tfrac{1}{2}\epsilon^l(\gamma_k\lambda_{,i}/\lambda^2 + \gamma_i\lambda_{,k}/\lambda^2). \tag{28}$$

However, Γ^l_{ik} is invariant with respect to spacelike rotations.

It is clear from these considerations that an affinity is fixed in a unique manner, if a covariant tensor field is specified on the null hypersurface. Using the gradient of a differential invariant of γ_{ik} for γ_i, we could obtain uniquely defined affinities of higher degree. Nevertheless it seems natural to use (21). Later it is shown in detail that (21) is obtained by projecting the Christoffel affinity of the embedding space into the null hypersurface.

3. ROTATION COEFFICIENTS

Using the affinity introduced in Sec. 2 and expressing the covariant derivatives of the triad ϵ^i, t^i and γ_i, t_i in terms of the triad itself, one obtains

$$\nabla_k\epsilon^i = -(\rho\bar{t}_k + \sigma t_k)t^i - (\rho t_k + \bar{\sigma}\bar{t}_k)\bar{t}^i + \chi t_k\epsilon^i + \bar{\chi}\bar{t}_k\epsilon^i, \tag{29}$$

$$\nabla_k t^i = (\tau t_k - \bar{\tau}\bar{t}_k + iv\gamma_k)t^i + (i\varphi t_k - \chi\gamma_k)\epsilon^i, \tag{30}$$

$$\nabla_k\gamma_i = i\varphi(t_i\bar{t}_k - \bar{t}_i t_k) + \chi(t_i\gamma_k - \gamma_i t_k) + \bar{\chi}(\bar{t}_i\gamma_k - \gamma_i\bar{t}_k), \tag{31}$$

$$\nabla_k t_i = \tau t_i t_k - \bar{\tau}t_i\bar{t}_k + iv\gamma_k t_i + \rho\gamma_i t_k + \bar{\sigma}\gamma_i\bar{t}_k. \tag{32}$$

On the right-hand sides there appear the nine independent Ricci rotation coefficients ρ, v, φ (real), σ, τ, χ (complex). The equations

$$\rho + iv = \epsilon^i t^k(\nabla_k\bar{t}_i - \nabla_i\bar{t}_k) = \epsilon^i t^k(\bar{t}_{i,k} - \bar{t}_{k,i}), \tag{33}$$

$$\sigma = \epsilon^i\bar{t}^k\nabla_k\bar{t}_i = \epsilon^i\bar{t}^k(\bar{t}_{i,k} - \bar{t}_{k,i}), \tag{34}$$

$$\tau = \bar{t}^i\bar{t}^k\nabla_k t_i = \bar{t}^i t^k(\bar{t}_{i,k} - \bar{t}_{k,i}), \tag{35}$$

$$\chi = \bar{t}^i\epsilon^k\nabla_k\gamma_i = \tfrac{1}{2}\bar{t}^i\epsilon^k(\gamma_{i,k} - \gamma_{k,i}), \tag{36}$$

$$i\varphi = \bar{t}^i t^k\nabla_k\gamma_i = \tfrac{1}{2}\bar{t}^i t^k(\gamma_{i,k} - \gamma_{k,i}), \tag{37}$$

are equivalent to (29)–(32). Under a transformation (7) they become

$$\rho' = \lambda\rho, \tag{38}$$

$$\sigma' = \lambda e^{-2i\mu}\sigma, \tag{39}$$

$$\tau' = e^{-i\mu}(\tau + i\bar{\delta}\mu - i\kappa\lambda D\mu - iv\kappa\lambda + \bar{\kappa}\lambda\sigma - \kappa\lambda\rho), \tag{40}$$

$$v' = \lambda v + \lambda D\mu, \tag{41}$$

[6] A detailed treatment of Lie displacements with regard to a null congruence is given by F. A. E. Pirani and A. Schild, Hlavaty-Festschrift (to be published).

$$\chi' = e^{-i\mu}[\chi + (\bar{\delta}\lambda/2\lambda) - \tfrac{1}{2}\kappa\rho\lambda + \tfrac{1}{2}\upsilon\kappa\lambda - \tfrac{1}{2}\sigma\bar{\kappa}\lambda + \tfrac{1}{2}\lambda D\kappa], \quad (42)$$

$$i\varphi' = i\varphi/\lambda + \tfrac{1}{2}(-\kappa\bar{\tau} + \bar{\kappa}\tau + \delta\kappa - \bar{\delta}\bar{\kappa}) + \tfrac{1}{2}\kappa(2\bar{\chi} + \delta\lambda/\lambda - i\kappa\lambda\upsilon - \kappa\lambda\bar{\sigma} + \lambda D\bar{\kappa}) - \tfrac{1}{2}\kappa(2\chi + \bar{\delta}\lambda/\lambda + i\kappa\lambda\upsilon - \bar{\kappa}\lambda\sigma + \lambda D\kappa). \quad (43)$$

The intrinsic derivatives are written

$$D = \epsilon^i\partial_i, \quad \delta = t^i\partial_i, \quad \bar{\delta} = \bar{t}^i\partial_i. \quad (44)$$

Applied to scalar quantities, they satisfy the commutation relations

$$D\delta - \delta D = (\rho + i\upsilon)\delta + \bar{\sigma}\bar{\delta} - 2\bar{\chi}D, \quad (45)$$

$$\delta\bar{\delta} - \bar{\delta}\delta = \bar{\tau}\bar{\delta} - \tau\delta - 2i\varphi D. \quad (46)$$

Here ρ and σ represent the rotation and shear of the generator congruence (see Sec. 5 for the well-known geometrical interpretation of ρ and σ). They also satisfy

$$h_{ik} = \rho\gamma_{ik} + \sigma t_i t_k + \bar{\sigma}\bar{t}_i\bar{t}_k; \quad (47)$$

χ and φ turn out to have no intrinsic geometrical meaning. The vector γ_i is hypersurface orthogonal if and only if φ vanishes; if, furthermore, γ_i is a gradient, then χ is also zero. If triads with γ_i a gradient vector are used (as is in fact very convenient), the transformations preserving this condition must satisfy the further restrictions

$$\delta\lambda = -\lambda^2(D\bar{\kappa} - i\bar{\kappa}\upsilon - \bar{\kappa}\rho - \kappa\bar{\sigma}), \quad \bar{\delta}\bar{\kappa} - \delta\kappa = \bar{\kappa}\tau - \kappa\bar{\tau}. \quad (48)$$

The quantity τ is connected with the inner geometry of a set of spacelike wave surfaces spanning the null hypersurface. If γ_i is the gradient of the function v, constant on each surface of this set,

$$K = 2\tau\bar{\tau} - \bar{\delta}\bar{\tau} - \delta\tau \quad (49)$$

is the Gaussian curvature of the wave surfaces. The last coefficient, $\upsilon = (1/i)\nabla_k t_i\epsilon^k\bar{t}^i$ describes the deviation of the transport of t^i in the ray direction from parallel transport with respect to the affinity Γ^l_{ik}, $\upsilon = 0$ being equivalent to parallel transport. This condition is preserved under transformation (7) if we restrict (7) through $D\mu = 0$.

The Riemann tensor constructed from the affinity Γ^l_{ik}, namely

$$R_{ikl}{}^{m} = \Gamma^m_{kl,i} - \Gamma^m_{il,k} + \Gamma^m_{ir}\Gamma^r_{kl} - \Gamma^m_{kr}\Gamma^r_{il}, \quad (50)$$

satisfies the usual identities

$$R_{(ik)l}{}^{m} = 0, \quad R_{\{ikl\}}{}^{m} = 0, \quad \nabla_{\{i}R_{kl\}m}{}^{r} = 0, \quad (51)$$

but has in general an antisymmetric contraction

$$V_{ik} = R_{ikl}{}^{l} = -2R_{[ik]} = \Gamma_{k,i} - \Gamma_{i,k}. \quad (52)$$

Here $R_{ik} = R_{lik}{}^{l}$ is the Ricci tensor and $\Gamma_i = \Gamma^l_{il}$. V_{ik} is given in terms of the rotation coefficient by

$$V_{ik} = \frac{i}{2}(t_i\bar{t}_k - \bar{t}_i t_k)(D\varphi + \rho\varphi) + \tfrac{1}{2}(t_i\gamma_k - \gamma_i t_k)(D\chi + i\upsilon\chi + \tfrac{1}{2}\rho\chi + \tfrac{1}{2}\sigma\bar{\chi}) + \tfrac{1}{2}(\bar{t}_i\gamma_k - \gamma_i\bar{t}_k)(D\bar{\chi} - i\upsilon\bar{\chi} + \tfrac{1}{2}\rho\bar{\chi} + \tfrac{1}{2}\bar{\sigma}\chi). \quad (53)$$

The expression V_{ik} vanishes if γ_i is a gradient, then additionally $\gamma_m R_{kli}{}^{m} = 0$. The remaining nonvanishing components can be written

$$\begin{aligned}
t^k\epsilon^l\epsilon^i R_{kli}{}^{m}\bar{t}_m &\equiv \omega = D\rho - \rho^2 - \sigma\bar{\sigma},\\
\bar{t}^k\epsilon^l\epsilon^i R_{kli}{}^{m}\bar{t}_m &\equiv \psi = D\sigma - 2\sigma(\rho - i\upsilon),\\
t^k\bar{t}^l\epsilon^i R_{kli}{}^{m}\bar{t}_m &= \bar{\delta}\rho - \delta\sigma + 2\sigma\bar{\tau} + \sigma\bar{\chi} - \rho\chi,\\
\epsilon^k t^l t^i R_{kli}{}^{m}\bar{t}_m &= -D\bar{t} - i\delta\upsilon + \bar{\tau}\rho - \tau\bar{\sigma} + i\upsilon\bar{\tau} + i\bar{\chi}\upsilon - \rho\bar{\chi},\\
\epsilon^k\bar{t}^l t^i R_{kli}{}^{m}\bar{t}_m &= D\tau - i\bar{\delta}\upsilon - \tau\rho + \bar{\tau}\sigma + i\upsilon\tau + 2i\upsilon\chi - \sigma\bar{\chi},\\
\bar{t}^k t^l t^i R_{kli}{}^{m}\bar{t}_m &= 2\tau\bar{\tau} - \bar{\delta}\bar{\tau} - \delta\tau + \varphi(2\upsilon + i\rho),\\
\epsilon^k t^l\bar{t}^i R_{kli}{}^{m}\bar{t}_m &= -\rho\chi,\\
\epsilon^k\bar{t}^l\bar{t}^i R_{kli}{}^{m}\bar{t}_m &= -\sigma\chi,\\
t^k\bar{t}^l\bar{t}^i R_{kli}{}^{m}\bar{t}_m &= -i\varphi\sigma.
\end{aligned} \quad (54)$$

The equations $R_{(kli)}{}^{m} = 0$ lead to the important identities

$$D\tau = \bar{\delta}(\rho + i\upsilon) - \delta\sigma + \tau(\rho - i\upsilon) + \bar{\tau}\sigma - 2\chi(\rho + i\upsilon) + 2\bar{\chi}\sigma, \quad (55)$$

$$iD\varphi = \delta\chi - \bar{\delta}\bar{\chi} + 2i\varphi\rho + \bar{\chi}\tau - \chi\bar{\tau}. \quad (56)$$

4. DIFFERENT GEOMETRIES

So far we have been concerned only with the inner geometry of a null hypersurface, that is, with those propositions which depend only on the inner metric, or alternatively which depend on the triad but are invariant with respect to the 4-parameter group (7). In this sense the group (7) can be considered as the inner geometry group. This type of characterization of a geometry by means of a group of triad transformations can be used to generalize the notion of inner geometry.[7]

First we consider the hierarchy of conformal geometries. The strong conformal geometry on the null surface is fixed if γ_{ik} is given up to a conformal factor ν ($\nu_{,i} \neq 0$), or by demanding all propositions to be invariant with regard to the group

$$t^{i'} = (1/\nu)(e^{i\mu}t^i - \bar{\kappa}\lambda e^{i\mu}\epsilon^i), \quad \epsilon^{i'} = \lambda\epsilon^i, \quad (57)$$

[7] See also R. Penrose, Ref. 4, for different types of geometries on a null hypersurface.

or

$$t_i' = \nu e^{i\mu} t_i,$$
$$\gamma_i' = (1/\lambda)\gamma_i + \kappa t_i + \bar{\kappa} \bar{t}_i. \tag{58}$$

This geometry is the geometry induced on the null hypersurfaces of a conformal 4-space. Restricting ν by $D\nu = 0$ or $\nu = \text{const}$ we obtain further geometries ("restricted conformal geometry" or "weak conformal geometry"); $\nu = 1$ gives the inner geometry.

Restrictions on the transformations of the scale parameter v lead to another hierarchy. If v is required to be an affine parameter on the generators, the resulting geometry is called the affine geometry. The group (7) must be restricted by $D\lambda = 0$ in order to preserve this property of v. The relation between the inner and affine geometry is of primary importance in understanding the embedding of null hypersurfaces, for example into an Einstein space. For special null surfaces there are further specializations of the geometry. The focal points of a null surface (points of intersection of neighboring generators) may be used as zero points for the affine parameter, so that only transformations of the type $v' = \alpha v$ are allowed. An observer at the vertex of a cone determines an affine parameter in a unique way, inducing therefore a further type of geometry. Still another geometry will be determined if a set of two-dimensional spacelike wave surfaces is fixed in the surface (for some physical or symmetry reason). It may be noted that both types of hierarchy just mentioned may be mixed together: affine conformal geometry for example arises when an affine parameter is introduced into the strong conformal geometry. The different geometries become clearer, when the differential invariants belonging to each geometry have been constructed.

5. DIFFERENTIAL INVARIANTS

A differential invariant of the first or second order of the inner geometry is a function of γ_{ik}, its first and eventually second derivatives with the property

$$I\left(\gamma_{ik}, \frac{\partial \gamma_{ik}}{\partial x^l}, \frac{\partial^2 \gamma_{ik}}{\partial x^l \partial x^m}\right) = I\left(\gamma'_{ik}, \frac{\partial \gamma'_{ik}}{\partial x^{l'}}, \frac{\partial^2 \gamma'_{ik}}{\partial x^{l'} \partial x^{m'}}\right). \tag{59}$$

In terms of the rotation coefficients and their intrinsic derivatives, the inner invariants may be described as functions of these quantities which are invariant with respect to the inner group (7). In the same way differential invariants of other geometries may be defined in terms of the appropriate group of triad transformations.

One of the peculiarities of null surfaces is the existence of a first-order invariant. The invariant of the first-order depends on the nine rotation coefficients $\rho, \sigma, \tau, v, \chi, \varphi$; invariants of the second order on the $3 \cdot 9 = 27$ intrinsic derivatives of these coefficients. In order to simplify the calculation, it is assumed—as is permitted—$v = \chi = \varphi = 0$. To preserve this condition the transformation functions κ, λ, μ, ν must be restricted by

$$\delta\lambda = -\lambda^2(D\bar{\kappa} - \bar{\kappa}\rho - \kappa\bar{\sigma}),$$
$$\bar{\delta}\bar{\kappa} - \delta\kappa = \bar{\kappa}\tau - \kappa\bar{\tau}, \tag{60}$$

$$D\mu = 0. \tag{61}$$

For different geometries, additional restrictions must be made. Invariants of the transformations (60), (57) with (61) are the strong conformal invariants, written in the special class of triads with $v = \chi = \varphi = 0$. In a similar way the invariants of the restricted conformal geometries are obtained by imposing the conditions $D\nu = 0$, $\nu = \text{const}$. The affine-conformal invariants are obtained from (57) and (61) by imposing the condition $D(\lambda\nu) = 0$. Invariants of the inner geometry are obtained by demanding invariance with respect to (7) together with (60). For the affine geometry, the additional condition is $D\lambda = 0$. Every invariant of a geometry is an invariant of the weaker geometries in the appropriate hierarchy. The results are: there is no first-order strong conformal or affine conformal invariant. The inner, affine and restricted conformal geometries possess exactly one first-order invariant,

$$j = \rho/|\sigma| \tag{62}$$

(or any function of j). The second-order invariants are considered only for the strong conformal, inner, and affine geometry. If the shear does not vanish in the domain considered, there is one strong conformal invariant, linear in the second derivatives:

$$I_1 = \frac{i}{2|\sigma|}\left(\frac{D\bar{\sigma}}{\bar{\sigma}} - \frac{D\sigma}{\sigma}\right) + \frac{2v}{|\sigma|} = (Ds + 2v)/|\sigma| \tag{63}$$

with

$$\sigma = |\sigma| e^{is}$$

(written with respect to a general triad). If $|\sigma| = 0$ in this domain, there is no conformal invariant. Turning to the inner geometry, in a domain with $|\sigma| \neq 0$, $\rho \neq 0$ and $I_2^2 + (I_1^2 - 4[1 - j^2])^2 \neq 0$ [I_2 defined by (64)], that is in the general case, four invariants exist, two linear in the second derivatives:

$$I = I_1 + iI_2 = i(D\rho/\rho - D\sigma/\sigma)/|\sigma| + 2v/|\sigma| \tag{64}$$

and two nonlinear:

$$J = e^{is}[(\beta\bar{\beta} - 4)(\delta\sigma/\sigma - \delta\rho/\rho) + (\alpha\bar{\beta} - 4) \times (\delta\bar{\sigma}/\bar{\sigma} - \delta\rho/\rho) + 2\bar{\beta}(\alpha - \beta)\tau] + 2e^{-is}(\alpha - \beta)(2\tau + \bar{\delta}\sigma/\sigma - \bar{\delta}\rho/\rho), \tag{65}$$

$$\alpha = 2j - iI,$$
$$\beta = 2j - iI.$$

If $I_2 = 0$ and $I_1^2 = 4(1 - j^2)$, J drops out and besides I there are three further inner invariants:

$$L = e^{is/2}(\delta\sigma/\sigma - \delta\rho/\rho - 2\bar{\tau}) + \tfrac{1}{2}\bar{\alpha}e^{-is/2}(\bar{\delta}\bar{\sigma}/\bar{\sigma} - \bar{\delta}\rho/\rho - 2\tau), \quad (66)$$

$$M = e^{is/2}(\delta\sigma/\sigma - \delta\bar{\sigma}/\bar{\sigma} - 2\delta\rho/\rho) \equiv -2e^{is}\delta j/j$$

(with $2L = \bar{L}$). If the shear vanishes in the domain considered, but the divergence is still different from zero, no inner invariant exists. In the opposite case of vanishing divergence, but nonvanishing shear,[8] two cases are to be considered: If $|I_1| \neq 2$, only the conformal invariant I_1 exists. However if $|I_1| = 2$, there is the inner invariant

$$N = e^{is/2}(\delta\sigma/\sigma - \delta\bar{\sigma}/\bar{\sigma}) + \tfrac{1}{2}iI_1e^{-is/2}(\bar{\delta}\sigma/\sigma - \bar{\delta}\bar{\sigma}/\bar{\sigma}) + 2iI_1e^{-is/2}\tau - 4e^{is/2}\bar{\tau} \quad (67)$$

$$(\bar{N} = 2iN/I_1).$$

If both divergence and shear vanish (as for the Schwarzschild surface), only one inner invariant exists, namely

$$K = 2\tau\bar{\tau} - \delta\tau - \bar{\delta}\bar{\tau} + 2\varphi v. \quad (68)$$

As remarked, for a hypersurface-orthogonal γ_i ($\varphi = 0$), K represents the Gaussian curvature of the spacelike two-dimensional surfaces spanning the three-dimensional null hypersurface. (For the Schwarzschild surface $K = 1/4m^2$, where m is the mass constant.)

The invariants for the affine geometry turn out to be the same as for the inner geometry with the exception that for $\rho \neq 0$ $D\rho/\rho^2$ represents an additional invariant. For $\rho = 0$, $|\sigma| \neq 0$ there is besides I_1 one further invariant

$$(D\sigma/\sigma\,|\sigma|) + (2iv/|\sigma|). \quad (69)$$

6. ASYMPTOTIC AND SHEAR DIRECTIONS

Let us consider a point P on a generator w^A with coordinates x^i or intrinsic coordinates v, w^A. The direction dx^i to the point Q on a neighboring generator $w^A + dw^A$ is given by

$$dx^i = (\partial x^i/\partial w^A)\,dw^A + (\partial x^i/\partial v)\,dv, \quad (70)$$

the distance by

$$dl^2 = \gamma_{ik}\,dx^i\,dx^k = (\partial x^i/\partial w^A)(\partial x^k/\partial w^B)\gamma_{ik}\,dw^A\,dw^B. \quad (71)$$

Here dl does not depend on the location of Q on the neighboring generator (provided Q is in an infinitesimal distance from P). A short calculation gives, for the change in dl if P moves along its generator

$$D(dl^2) = -2h_{ik}\,dx^i\,dx^k. \quad (72)$$

[8] Note that hypersurfaces of this type cannot appear in Einstein spaces whereas all others can.

The shear directions dx^i are defined as directions with extremal change of distance. Asymptotic directions are defined as directions with vanishing change of distance, if any exist.

Setting

$$l^i = lt^i + \bar{l}\bar{t}^i + L\epsilon^i \quad (73)$$

for a shear direction one finds from the extremum condition the eigenvalue equation

$$(h_{ik} - \Lambda\gamma_{ik})l^k = 0, \quad (74)$$

which leads to

$$l(\rho - \Lambda) + \bar{l}\sigma = 0 \quad (75)$$

with

$$\Lambda_{1,2} = \rho \pm |\sigma| \quad (76)$$

and

$$l_1^i = e^{is/2}t^i/\sqrt{2} + e^{-is/2}\bar{t}^i/\sqrt{2} + L_1\epsilon^i, \quad (77)$$

$$l_2^i = -ie^{is/2}t^i/\sqrt{2} + ie^{-is/2}\bar{t}^i/\sqrt{2} + L_2\epsilon^i \quad (78)$$

as the general expression for both spacelike shear directions, normed to 1. l_1^i and l_2^i are orthogonal to each other. Equations (77) and (78) do not each determine one spacelike direction but rather a lightlike plane element, spanned by the generator direction and any of the spacelike directions contained in (77) or (78). The shear plane element could be described likewise by its covariant tangent vector $\overset{(1)}{l}_i = \epsilon_{ikl}l_1^k\epsilon^l/\Delta$.

If asymptotic directions are represented by

$$a^i = at^i + \bar{a}\bar{t}^i + A\epsilon^i, \quad (79)$$

then from $h_{ik}\,dx^i\,dx^k = 0$ it follows that

$$2\rho a\bar{a} + a^2\bar{\sigma} + \bar{a}^2\sigma = 0. \quad (80)$$

For a solution of (80) to exist the inequality $\rho^2 - \sigma\bar{\sigma} \leq 0$ must be satisfied. This is equivalent to h_{ik} not being positive definite. According to the existence of asymptotic directions (or equivalently the value of the first-order invariant j) the points on a null surface divide into four classes as shown in Table I.

The asymptotic directions (normed to 1) are given by

$$a_1^i = t^ie^{i(s+\vartheta)/2}/\sqrt{2} + \bar{t}^ie^{-(s+\vartheta)/2}/\sqrt{2} + A_1\epsilon^i, \quad (81)$$

$$a_2^i = t^ie^{i(s-\vartheta)/2}/\sqrt{2} + \bar{t}^ie^{-(s-\vartheta)/2}/\sqrt{2} + A_2\epsilon^i. \quad (82)$$

TABLE I. Classification of null hypersurface points in terms of asymptotic directions.

rkh_{ik}			No. of asymptotical plane elements
2	$\rho^2 - \sigma\bar{\sigma} > 0$	elliptic point	0
2	$\rho^2 - \sigma\bar{\sigma} < 0$	hyperbolic point	2
1	$\rho^2 = \sigma\bar{\sigma}$, $\rho \neq 0$	parabolic point	1
0	$\rho = \lvert\sigma\rvert = 0$	planar point	∞

The angle ϑ, defined by

$$\cos\vartheta = -j, \quad \sin\vartheta = (1-j^2)^{\frac{1}{2}} \tag{83}$$

is the angle between both asymptotic directions. The corresponding plane elements become identical in parabolic points ($j = \pm 1$). If there are asymptotic directions ($|j| \leq 1$), the shear direction l_1^i bisects the angle ϑ. The geometrical meaning of the classification[9] given in the table is obvious: if $\rho = |\sigma| = 0$ (planar points), the distance to the neighboring generators remains constant along the given generator. In elliptic points the distance to all directions will change in the same sense. Hyperbolic (respectively parabolic) points show 2 (respectively 1) directions with no change of distance. In hyperbolic points, there are four disconnected sets of directions, separated by asymptotic directions, with the same sense of change of distance in opposite directions; expansion and contraction occur in alternate regions. A polar diagram similar to Dupin's indicatrix can be used to picture the different situations. If the normed spacelike direction is represented by

$$dx^i/dl = e^{i\beta}t^i/\sqrt{2} + e^{-i\beta}\bar{t}^i/\sqrt{2} + B\epsilon^i,$$

then $D(dl)/dl = -|\sigma|\cos(2\beta - s) - \rho$ gives the change of distance in this direction; β varies from 0 to 2π.

The meaning of I_2 can be seen from $Dj = \rho I_2$: I_2 represents some invariant measure of the change of j. The equation

$$D\vartheta = -I_2\rho/(1-j^2)^{\frac{1}{2}} \tag{84}$$

expresses the change of angle ϑ between the asymptotic directions in terms of I_2. I_1 has a different interpretation. In the general null surface, there will be a rotation of the shear directions with regard to the ray congruence along the given generator. The normed spacelike direction from the generator w^A to the generator $w^A + dw^A$ is given by

$$m^i = (e^{im}t^i + e^{-im}\bar{t}^i)/\sqrt{2} + M\epsilon^i \tag{85}$$

with

$$e^{2im} = \frac{\partial x^i}{\partial w^A}\bar{t}_i\,dw^A \Big/ \frac{\partial x^k}{\partial w^B}t_k\,dw^B. \tag{86}$$

From (86) follows

$$Dm = -v + (\bar{\sigma}/2i)e^{2im} - (\sigma/2i)e^{-2im}. \tag{87}$$

Let

$$n^i = (e^{in}t^i + e^{-in}\bar{t}^i)/\sqrt{2} + N\epsilon^i \tag{88}$$

be any other spacelike direction. The angle between (85) and (88) is determined by $\beta = n - m$ (since $\cos\beta = n^i m^k \gamma_{ik}$) and the change of β along the ray is given by

$$d\beta/dv = Dn + v + \sigma e^{-2in}/2i - \bar{\sigma}e^{2in}/2i. \tag{89}$$

If n^i represents either of the two shear directions then

$$d\beta/dv = \tfrac{1}{2}|\sigma|\,I_1. \tag{90}$$

I_1 therefore turns out to be a measure of the velocity of rotation of the shear directions. For hyperbolic points the rotation velocity of the asymptotic directions is given by

$$\tfrac{1}{2}|\sigma|\{I_1 \pm [I_2 j/(1-j^2)^{\frac{1}{2}} - 2(1-j^2)^{\frac{1}{2}}]\}.$$

In general the shear surface elements and asymptotic surface elements cannot be extended to form finite two-dimensional lightlike surfaces. The condition for surface forming is the same as for nonrotation of the corresponding shear and asymptotic directions, as may easily be seen either from a geometrical consideration or from the following calculation. If the surface element is spanned by n^i in (88) and ϵ^i, its tangential vector can be written

$$p_i = \epsilon_{ikl}n^k\epsilon^l/\Delta. \tag{91}$$

The condition for p_i to generate finite surfaces is

$$\epsilon^{ikl}p_{i,k}p_l = 0; \tag{92}$$

explicitly

$$nD\bar{n} - \bar{n}Dn - 2ivn\bar{n} + \bar{\sigma}n^2 - \sigma\bar{n}^2 = 0. \tag{93}$$

For shear directions this turns out to be $|\sigma|\,I_i = 0$[10] and for asymptotic directions $I_1 \pm (I_2 j/(1-j^2)^{\frac{1}{2}} - 2(1-j^2)^{\frac{1}{2}}] = 0$. Nontrivial shear surfaces ($I_1 = 0$, $|\sigma| \neq 0$; if $|\sigma| = 0$, all lightlike two-surfaces on the null hypersurface are shear surfaces) will appear for instance on null hypersurfaces in conformally flat space times. This follows from the conformal invariance of I_1 and the fact (compare Sec. 7) that I_1 vanishes for null hypersurfaces in flat space. Null surfaces with vanishing I_1 have simple properties with regard to focal points, for a given generator intersects the neighboring generators only on the shear surfaces.

7. GEODESIC LINES

A geodesic is a solution of the differential equation

$$a^k\nabla_k a^i = la^i, \quad a^i = dx^i/dl. \tag{94}$$

It can easily be shown that (94) expresses a condition invariant with respect to the inner geometry if and

[9] For a general conformal transformation of the triad $\sigma' = \lambda e^{-2i\mu}\sigma$, $\rho' = \lambda\rho - \lambda D\ln\nu$. It follows that the above distinction is invariant for all geometries considered in Sec. 3, with exception of the strong conformal and affine-conformal geometry. Here the notion of asymptotic directions becomes meaningless, but shear directions still exist.

[10] Note $|\sigma| \neq 0$ at hyperbolic points.

only if $a^k \sim \epsilon^k$ [when the right-hand side of (94) must also vanish]. In this case the a^i curves have zero metrical lengths and so are the shortest curves on the hypersurface. For spacelike curves this second definition of geodesic line must be used. The condition for the arc length integral

$$l = \int_P^Q \left(\frac{dx^i}{dl}\frac{dx^k}{dl}\gamma_{ik}\right)^{\frac{1}{2}} dl \tag{95}$$

to have an extremum with fixed end points P and Q is

$$\gamma_{ik}\frac{d^2x^k}{dl^2} + \Gamma_{kli}\frac{dx^k}{dl}\frac{dx^l}{dl} = \tfrac{1}{2}\gamma_{ik}\frac{dx^k}{dl}\frac{d\ln f}{dl} \tag{96}$$

with $f = (dx^i/dl)(dx^k/dl)\gamma_{ik}$. In contrast to (94), this equation is invariant also for spacelike curves. Using the arc length as parameter ($f = 1$) in (96) gives

$$h_{ik}(dx^i/dl)(dx^k/dl) = 0, \tag{97}$$

which says that spacelike extremal curves on null hypersurfaces must be asymptotic lines: They appear only in nonelliptical domains. Write $dx^i/dl = a^i$ with a^i equal to (81) or (82). The further two relations contained in (96) for the asymptotic lines to be geodesic are, in a hyperbolic domain

$$\begin{aligned} A_\pm|\sigma|\,[I_1 \pm 2(1-j^2)^{\frac{1}{2}} \pm I_2 j/(1-j^2)^{\frac{1}{2}}] \\ = i\sqrt{2}(\tau e^{-i(s\pm\vartheta)/2} - \bar{\tau}e^{i(s\pm\vartheta)/2}) \\ - e^{i(s\pm\vartheta)/2}(\delta s \pm \delta\vartheta)/\sqrt{2} \\ - e^{-i(s\pm\vartheta)/2}(\bar{\delta}s \pm \bar{\delta}\vartheta)/\sqrt{2}, \end{aligned} \tag{98}$$

here + and − refer to the two asymptotic directions at every point. There are various different cases to be considered. If both invariants $I_1 \pm 2(1-j^2)^{\frac{1}{2}} \pm I_2 j/(1-j^2)^{\frac{1}{2}}$ are different from zero, A_+ and A_- can be calculated from (98) and a geodesic asymptotic line is fixed. In this (general) case the hyperbolic domain on the null hypersurface contains two spacelike congruences of geodesic asymptotic lines. If one or both of the invariants vanishes,[10] there are in general no geodesic asymptotic lines. However, if the right-hand side of (98) vanishes (say for one sign), every asymptotic line (of the corresponding sign) becomes geodesic. The expression on the right-hand side of (98) is a real invariant of second order. If $I_2 \neq 0$ the right-hand side of (98) is

$$k_{(\pm)}J + \bar{k}_{(\pm)}\bar{J} \tag{99}$$

with

$$k_{(-)} = e^{i\vartheta/2}(1-j^2)^{\frac{1}{2}}/4I_2^2, \quad k_{(+)} = -\bar{k}_{(-)}. \tag{100}$$

If $I_2 = 0$, then $I_1^2 = 4(1-j^2)$. The complex invariant J does not exist in this case (*vide* the Appendix). Using here the invariants L, M, $\bar{M}$, the right-hand side of (98) now becomes

$$\begin{aligned} ie^{\pm i\vartheta/2}(\tfrac{1}{2}M) \mp e^{\pm 3i\vartheta/2}M/4(1-j^2)^{\frac{1}{2}} \\ \mp e^{\mp 3i\vartheta/2}\bar{M}/4(1-j^2)^{\frac{1}{2}}. \end{aligned} \tag{101}$$

Equation (96) holds only in a hyperbolic domain. At a parabolic point[11] there is only one asymptotic direction. The condition corresponding to (98) is ($j = 1$):

$$\begin{aligned} |\sigma|\,I_1 A = -i\sqrt{2}e^{is/2}\bar{\tau} + i\sqrt{2}e^{-is/2}\tau \\ - (\delta s e^{is/2} + \bar{\delta}s e^{-is/2})/\sqrt{2}. \end{aligned} \tag{102}$$

If $I_1 \neq 0$, there is a preferred congruence of geodesic asymptotic lines. If I_1 vanishes, either there is no geodesic line or, if

$$\begin{aligned} -ie^{is/2}\bar{\tau} + ie^{-is/2}\tau - (d s e^{is/2} + \bar{\delta}s e^{-is/2})/2 \\ \equiv \tfrac{1}{2}i(\tfrac{1}{2}\bar{M} - \tfrac{1}{2}M + L) = 0 \end{aligned} \tag{103}$$

is satisfied,[12] every asymptotic line is geodesic. The situation is different for planar null surfaces. Here (97) is satisfied automatically and (94) gives one condition, and there are ∞^1 geodesic lines through every point.

8. NULL SURFACES IN FLAT SPACE

Some remarks may be made about embedding restrictions. As will be shown in a forthcoming paper, an embedding of a given lightlike hypersurface into an Einstein space does not restrict the inner geometry locally, so long as only finite domains are considered for which $\rho \neq 0$. Every null hypersurface in an Einstein space will ultimately develop caustics, if there is no intrinsic lightlike group of motions on the hypersurface. A null hypersurface with an inner geometry given globally without both focal points and a lightlike group of motions cannot be embedded globally into an Einstein space—there must occur singularities or regions with $T_{\mu\nu} \neq 0$. Also there are local restrictions of the affine geometry (one affine invariant has to vanish).

For an embedding into flat space even the inner geometry is locally restricted. If $j \neq 0$, the conditions

$$I_1 = 0, \tag{104}$$

$$I_2 = (1/j) - j \tag{105}$$

are necessary and sufficient for local embedding. If $j = 0$, in addition to ρ the shear $|\sigma|$ and the invariant K must vanish; the last condition expresses the fact that the only planar null surfaces are null planes

[11] It is assumed that the parabolic domain is three dimensional; in general, however, there are only parabolic two-surfaces on a null surface, dividing domains of elliptic and hyperbolic points.

[12] Because of $j = -1$ here again the particular case $I_2 = 0$, $I_1^2 = 4(1-j^2)$ applies.

[with the metric $ds^2 = (dx^2)^2 + (dx^3)^2$ in special coordinates].

The restrictions for the affine geometry turn out to be[13] $\psi = 0$, $\omega = 0$ in general. Their integration gives the explicit dependence of ρ and σ on the affine parameter v:

$$\rho = (\rho^0 + v[\bar{\sigma}^0\sigma^0 - \rho^{02}])/([1 - v\rho^0]^2 - v^2\sigma^0\bar{\sigma}^0) \quad (106)$$

$$\sigma = \sigma^0/([1 - v\rho^0]^2 - v^2\sigma^0\bar{\sigma}^0). \quad (107)$$

Furthermore,

$$j = j_0 + v\rho^0(1/j_0 - j_0). \quad (108)$$

Except in the cases $\sigma = 0$, $\rho \neq 0$ (cone), $\sigma = \rho = 0$ (null plane), $\rho^2 = \sigma\bar{\sigma}$ or $j^2 = 1$ (parabolic null surface), every null hypersurface possesses two distinct caustics for $v = (\pm 1 - j_0)/\rho^0(1/j_0 - j_0)$, consisting of the focal points of the corresponding set of shear surfaces. From (108) it is seen that $j = \pm 1$ at a focal point and I and J vanish there. A general null hypersurface in flat space exhibits the following behavior as one moves along a given ray: at infinity the surface consists of elliptic points; after passing the first (parabolic) focal point the ray enters the hyperbolic domain until the second focal point is reached. Then elliptical points follow until infinity is reached again. Introducing the invariant areal distance r by

$$r = r_0 \exp\left\{-\int_{v_0}^{v} \rho\, dv\right\} \quad (109)$$

(the integral is an integral invariant of the inner geometry), (106)–(108) may be written

$$\begin{aligned} \rho &= \pm(r_0\rho^0/r)(1 - 1/j_0^2 + r_0^2/j_0^2r^2)^{\frac{1}{2}}, \\ \sigma &= \sigma^0 r_0^2/r^2, \\ r &= r_0[(1 - j^2)/(1 - j_0^2)]^{\frac{1}{2}}, \end{aligned} \quad (110)$$

r becomes null in focal points. With respect to r the null hypersurface can be divided into four regions extending from $\rho = 0$ to $\rho \to \pm\infty$, respectively. In every region, both r and the affine parameter v are related in a one-to-one manner.

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[13] ψ and ω do not behave as affine invariants in the strict sense, but acquire factors $\lambda^2 e^{-2i\mu}$, λ^2 under transformation. However, their vanishing is an invariant statement in the affine geometry. The invariants constructed from ψ and ω are $\psi/\rho\sigma$, ω/ρ^2, respectively; if these invariants are used, the cases $\rho = 0$ and $|\sigma| = 0$ must be considered separately.

APPENDIX

Using infinitesimal transformations

$$\begin{aligned} \lambda &= 1 + \check{\lambda}, \\ e^{i\mu} &= 1 + i\check{\mu}, \\ \kappa &= \check{\kappa}, \end{aligned} \quad (A1)$$

[note κ, λ, μ are restricted by (60), (61)] we obtain for inner invariants of the first order from $I(\rho', \sigma', \tau') = I(\rho, \sigma, \tau)$ the system:

$$\begin{aligned} &\check{\lambda}[\rho(\partial I/\partial\rho) + \sigma(\partial I/\partial\sigma) + \bar{\sigma}(\partial I/\partial\bar{\sigma})] \\ &\quad + i\check{\omega}[-2\sigma(\partial I/\partial\sigma) + 2\bar{\sigma}(\partial I/\partial\bar{\sigma}) \\ &\quad - \tau(\partial I/\partial\tau) + \bar{\tau}(\partial I/\partial\bar{\tau})] \\ &\quad + \check{\kappa}[-\rho(\partial I/\partial\tau) + \bar{\sigma}(\partial I/\partial\bar{\tau})] \\ &\quad + \check{\bar{\kappa}}[-\rho(\partial I/\partial\bar{\tau}) + \sigma(\partial I/\partial\tau)] \\ &\quad + i\delta\check{\omega}(\partial I/\partial\tau) - i\bar{\delta}\check{\omega}(\partial I/\partial\bar{\tau}) = 0. \end{aligned} \quad (A2)$$

Choosing $\check{\lambda} = \check{\omega} = \check{\kappa} = 0$, it follows

$$\partial I/\partial\tau = 0, \quad \partial I/\partial\bar{\tau} = 0.$$

Using this in (A2):

$$\rho\partial I/\partial\rho + \sigma\partial I/\partial\sigma + \bar{\sigma}\partial I/\partial\bar{\sigma} = 0,$$

$$\sigma\partial I/\partial\sigma - \bar{\sigma}\partial I/\partial\bar{\sigma} = 0$$

is obtained. The general solution is given by

$$I = I(\rho/|\sigma|) = I(j). \quad (A3)$$

It is convenient to choose $I = j$. j is not an invariant of the conformal geometry: No conformal invariant of the first order does exist. j however is the one and only first-order invariant of the restricted conformal geometries (with exception of the affine conformal geometry). j is also the only invariant of the affine geometry.

The invariants of second order depend on the 18 quantities

$$\begin{aligned} &x^1 = D\rho, \quad x^2 = D\sigma, \quad x^3 = D\bar{\sigma}, \\ &x^4 = \delta\rho, \quad x^5 = \bar{\delta}\rho, \quad x^6 = \delta\sigma, \\ &x^7 = \bar{\delta}\sigma, \quad x^8 = \delta\bar{\sigma}, \quad x^9 = \bar{\delta}\bar{\sigma}, \\ &x^{10} = \delta\tau, \quad x^{11} = \bar{\delta}\tau, \quad x^{12} = \delta\bar{\tau}, \\ &x^{13} = \bar{\delta}\bar{\tau}, \quad x^{14} = \rho, \quad x^{15} = \sigma, \\ &x^{16} = \bar{\sigma}, \quad x^{17} = \tau, \quad x^{18} = \bar{\tau}. \end{aligned} \quad (A4)$$

Because of (55) and (56), they do not depend on $D\tau$ and $D\bar{\tau}$. The condition $I(x^i) = I(x^{i'})$ leads for infinitesimal transformations (A1) and $\nu = 1 + \check{\nu} \neq 1$

(strong conformal geometry) to the basic system

$$
\begin{aligned}
0 = {} & \check{\lambda}(2D\rho I^1 + 2D\sigma I^2 + 2D\bar{\sigma} I^3 + \delta\rho I^4 + \bar{\delta}\rho I^5 + \delta\sigma I^6 \\
& + \bar{\delta}\sigma I^7 + \delta\bar{\sigma} I^8 + \bar{\delta}\bar{\sigma} I^9 + \rho I^{14} + \sigma I^{15} + \bar{\sigma} I^{16}) \\
& + D\check{\lambda}(\rho I^1 + \sigma I^2 + \bar{\sigma} I^3) \\
& + i\check{\mu}(-2D\sigma I^2 + 2D\bar{\sigma} I^3 + \delta\rho I^4 - \bar{\delta}\rho I^5 - \delta\sigma I^6 \\
& - 3\bar{\delta}\sigma I^7 + 3\delta\bar{\sigma} I^8 + \bar{\delta}\bar{\sigma} I^9 + 2\delta\bar{\tau} I^{11} - 2\bar{\delta}\bar{\tau} I^{12} \\
& - 2\sigma I^{15} + 2\bar{\sigma} I^{16} - \tau I^{17} + \bar{\tau} I^{18}) \\
& + i\delta\check{\mu}(-2\tau I^{10} + \tau I^{11} - I^{18} - 2\sigma I^6 + 2\bar{\sigma} I^8) \\
& + i\bar{\delta}\check{\mu}(-\tau I^{12} + \bar{\tau} I^{13} + I^{17} - 2\sigma I^7 + 2\bar{\sigma} I^9 + \bar{\tau} I^{10}) \\
& + \delta\check{\lambda}(\rho I^4 + \sigma I^6 + \bar{\sigma} I^8) + \bar{\delta}\check{\lambda}(\rho I^5 + \sigma I^7 + \bar{\sigma} I^9) \\
& + \check{\nu}(-I^4\delta\rho - I^5\bar{\delta}\rho - \delta\sigma I^6 - \bar{\delta}\sigma I^7 - \delta\bar{\sigma} I^8 \\
& - \bar{\delta}\bar{\sigma} I^9 - 2\delta\tau I^{10} - 2\delta\bar{\tau} I^{11} - 2\bar{\delta}\tau I^{12} - 2\bar{\delta}\bar{\tau} I^{13} \\
& - \tau I^{17} - \bar{\tau} I^{18}) \\
& + D\check{\nu}(-I^{14}) + \delta\check{\nu}(-\bar{\tau} I^{11} - I^{18}) + \bar{\delta}\check{\nu}(-\bar{\tau} I^{10} - \tau I^{12} \\
& - \bar{\tau} I^{13} - I^{17}) \\
& + \check{\kappa}(-D\rho I^4 - D\sigma I^6 - D\bar{\sigma} I^8 + \delta\sigma I^{10} - D\tau I^{10} \\
& - \delta\rho I^{11} - D\bar{\tau} I^{11} + \bar{\delta}\sigma I^{12} - \bar{\delta}\rho I^{13} + \sigma I^{17} \\
& - \rho I^{18}) \\
& + \check{\varkappa}(-D\rho I^5 - D\sigma I^7 - D\bar{\sigma} I^9 - \delta\rho I^{10} + \delta\bar{\sigma} I^{11} \\
& - \bar{\delta}\rho I^{12} - D\tau I^{12} + \bar{\delta}\bar{\sigma} I^{13} - D\bar{\tau} I^{13} - \rho I^{17} + \bar{\sigma} I^{18}) \\
& + \delta\check{\kappa}(\sigma I^{10} - \rho I^{11}) + \delta\check{\varkappa}(\sigma I^{11} - \rho I^{10}) \\
& + \bar{\delta}\check{\varkappa}(-\rho I^{12} + \bar{\sigma} I^{13}) \\
& + \bar{\delta}\check{\kappa}(\sigma I^{12} - \rho I^{13}) \\
& - I^1 D^2\check{\nu} - \delta D\check{\nu} I^4 - \bar{\delta} D\check{\nu} I^5 \\
& - \delta\delta\check{\nu} I^{11} - i\delta\delta\check{\mu} I^{11} - \bar{\delta}\bar{\delta}\check{\nu} I^{12} + i\bar{\delta}\bar{\delta}\check{\mu} I^{12} \\
& - \bar{\delta}\delta\check{\nu}(I^{10} + I^{13}) + i\bar{\delta}\delta\check{\mu}(I^{10} - I^{13}).
\end{aligned}
$$

Here, $\partial I/\partial x^i \equiv I^i$. From the arbitrariness of the second derivatives, it follows immediately that

$$I^1 = I^4 = I^5 = I^{10} = I^{11} = I^{12} = I^{13} = 0.$$

Assuming $|\sigma| \neq 0$ (if $|\sigma| = 0$, no conformal invariant exists), from the rest of the system (A5) follows

$$
\begin{aligned}
I^6 = I^7 = I^8 = I^9 = I^{14} = I^{17} = I^{18} &= 0, \\
D\sigma I^2 + D\bar{\sigma} I^3 &= -\tfrac{1}{2}\sigma I^{15} - \tfrac{1}{2}\bar{\sigma} I^{16}, \\
D\sigma I^2 - D\bar{\sigma} I^3 &= \bar{\sigma} I^{16} - \sigma I^{15}, \\
\sigma I^2 + \bar{\sigma} I^3 &= 0.
\end{aligned}
$$

The general solution of this involutive system of differential equations is given by[14]

$$I_1 \overset{*}{=} i(\sigma D\bar{\sigma} - \bar{\sigma} D\sigma)/2\,|\sigma|^3 \tag{A7}$$

[14] An asterisk denotes an equation valid only for the class of triads with $v = \chi = \varphi = 0$.

or an arbitrary function of I_1. For a general triad

$$
\begin{aligned}
I_1 &= i(\sigma D\bar{\sigma} - \bar{\sigma} D\sigma)/2\,|\sigma|^3 + 2v/|\sigma| \\
&= (Ds - 2v)/|\sigma|.
\end{aligned} \tag{A8}
$$

I_1 represents the only strong conformal invariant of second order.

For the first restricted conformal geometry ($Dv = 0$), if $\rho \neq 0$, $|\sigma| \neq 0$, $\bar{\sigma} D\sigma + \sigma D\bar{\sigma} - 2D\rho\,|\sigma|^2/\rho \neq 0$, a similar system follows from (A5). The general solution here is given by

$$I = i(D\rho/\rho - D\sigma/\sigma)/|\sigma| + 2v/|\sigma| = I_1 + iI_2. \tag{A9}$$

In the particular case $|\sigma| = 0$, no invariant of this geometry exists. If $\rho = 0$, $|\sigma| \neq 0$, one obtains I_1. The other case is $\rho \neq 0$, $|\sigma| \neq 0$, but $I_2 = 0$. Besides I_1 there is

$$e^{is}\frac{2\rho - je^{is}\delta\bar{\sigma} - je^{-is}\delta\sigma}{2\bar{\delta}\rho - j\bar{\delta}\sigma e^{-is} - j\bar{\delta}\bar{\sigma} e^{is}} \tag{A10}$$

an unimodular invariant, if the denominator in (A10) is different from zero; if it is zero, besides I_1 there is no additional invariant.

For the inner geometry $^{\nu} = 0$ in (A5). The second transversal derivatives here give

$$I^{11} = I^{12} = 0, \quad I^{10} = I^{13},$$

the following system is obtained with the use of (59):

$$
\begin{aligned}
2D\rho I^1 + 2D\sigma I^2 + 2D\bar{\sigma} I^3 + \delta\rho I^4 + \bar{\delta}\rho I^5 + \delta\sigma I^6 \\
+ \bar{\delta}\sigma I^7 + \delta\bar{\sigma} I^8 + \bar{\delta}\bar{\sigma} I^9 + \rho I^{12} + \sigma I^{13} + \bar{\sigma} I^{14} = 0, \\
\rho I^1 + \sigma I^2 + \bar{\sigma} I^3 = 0, \\
-2D\sigma I^2 + 2D\bar{\sigma} I^3 + \delta\rho I^4 - \bar{\delta}\rho I^5 - \delta\sigma I^6 - 3\bar{\delta}\sigma I^7 \\
+ 3\delta\bar{\sigma} I^8 + \bar{\delta}\bar{\sigma} I^9 - 2\sigma I^{13} + 2\bar{\sigma} I^{14} - \tau I^{15} + \bar{\tau} I^{16} = 0. \\
I^{15} = 2\sigma I^7 - 2\bar{\sigma} I^9, \\
I^{16} = 2\bar{\sigma} I^8 - 2\sigma I^6, \\
\rho I^4 + \sigma I^6 + \bar{\sigma} I^8 = 0, \\
\rho I^5 + \sigma I^7 + \bar{\sigma} I^9 = 0, \\
D\rho I^4 + D\sigma I^6 + D\bar{\sigma} I^8 - \sigma I^{15} + \rho I^{16} = 0, \\
D\rho I^5 + D\sigma I^7 + D\bar{\sigma} I^9 + \rho I^{15} - \bar{\sigma} I^{16} = 0.
\end{aligned} \tag{A11}
$$

The involutive system (A11) consists of 9 equations with 14 independent variables. When $\rho \neq 0$, $|\sigma| \neq 0$, $I_2^2 + (I_1^2 - 4[1 - j^2])^2 \neq 0$, the rank of the coefficient matrix is 9. In this general case an integral basis consists of 5 integrals. One verifies that apart from I in (A9) and j, (65) also satisfies (A11). In the particular case $I_2 = 0$, $I_1^2 = 4(1 - j^2)$ the equations (A11) are not independent. Here, the four independent variables j and (66) do exist (the rank of the corresponding system of differential equations is 8, there are 12 independent variables). Other particular cases can be treated in the same way. For the affine invariants, because of the restriction $D\check{\lambda} = 0$, the condition $\rho I^1 + \sigma I^2 + \bar{\sigma} I^3 = 0$ drops out, and the number of invariants increases in general by one.

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Decomposition of Tensors of the Classical Groups

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A tensor symmetrization procedure obtained in a recent publication [Phys. Rev. Letters **16**, 1058 (1966)] is shown to support rather than disprove Weyl's tensor symmetrization theorem. This "extended" symmetrization procedure differs from Weyl's approach in that to construct a subspace irreducible under $GL(n, c)$ one starts with a set of formal states (symmetrized tensors with formal index values) spanning an irreducible representation of the permutation group rather than starting with a single formal state. Extended symmetrization is often more useful than Weyl's approach because the states obtained are highly organized and because it also yields an efficient independent state selection method for the symmetrization procedures using modified Young symmetrizers and Wigner projection operators. The state organization obtained makes it possible to show that the nonorthogonality which is present for bases obtained with Young symmetrizers can be easily removed. The state organization also makes it possible to simplify the task of recoupling symmetrized tensor representations to gain a simply-coupled form. This form enlarges the class of Clebsch–Gordan and recoupling coefficients which can be evaluated by tensor methods. Group matrices and Lie group generator matrix elements are also obtained by tensor methods. Extended symmetrization using unitary representation Wigner projection operators based on unitary representations is shown to result in orthogonal states although usually not the orthogonal states desired. The usual Young symmetrizers are shown to often be more useful than modified Young symmetrizers or Wigner projection operators.

1. INTRODUCTION

A RECENT publication[1] examined Weyl's tensor symmetrization theorem using the fact that a symmetrized tensor subspace irreducibly invariant under $GL(n, c)$ must be a direct sum of subspaces irreducibly invariant under the permutation group. The mathematical results of Ref. 1 are also contained in the next section [Eqs. (2.8)]. At first sight the formal results obtained appeared to disprove Weyl's theorem when actually they support it.[2] In fact, the independent states among those provided are the same as the independent states among those provided by Weyl's theorem. To see how all this is so, we first note that the permutation group operations act on the indices as a function of their initial position rather than as a function of their position after some permutation operation. Now consider the following pair of bases[1] belonging to Young pattern (2, 1):

$$A_1^{(2,1)} \equiv (PQ)_{i_1 i_2, i_3} T_{i_1 i_2 i_3},$$
$$A_2^{(2,1)} \equiv (PQ)_{i_1 i_3, i_2} L_{(i_2 i_3)} T_{i_1 i_2 i_3},$$
$$B_1^{(2,1)} \equiv (PQ)_{i_1 i_2, i_3} L_{(i_2 i_3)} T_{i_1 i_2 i_3},$$
$$B_2^{(2,1)} \equiv (PQ)_{i_1 i_3, i_2} T_{i_1 i_2 i_3},$$

where commas separate tableau rows and $L_{(ij)}$ denotes an element of the permutation group. Clearly $(PQ)_{i_1 i_3, i_2} L_{(i_2 i_3)} T_{i_1 i_2 i_3} = (PQ)_{i_1 i_3, i_2} T_{i_1 i_3 i_2}$, so this really represents the same operation as that for state $A_1^{(2,1)}$, although the state obtained differs from $A_1^{(2,1)}$ in that the values of the second and third indices of the tensor have been transposed. Similarly, the state $B_1^{(2,1)}$ is found to be derived from the same Young symmetrizer operation as state $B_2^{(2,1)}$ after the values of the second and third indices of the tensor have been transposed. This is consistent with Weyl's theorem which applies a single Young symmetrizer to a tensor form and then enters all arrangements of each set of index values to get n^r tensors (r and n denote rank and dimension) spanning a subspace irreducibly invariant under $GL(n, c)$. Referring to the first column of Eqs. (2.8) in the text, which is the same as Eqs. (6) in Ref. 1, we see that: in the first basis, the operation S_{j1} brings the indices of $T_{i_1 \cdots i_r}$ into the same correspondence with $(PQ)_j^\mu$ as that found for $(PQ)_1^\mu T_{i_1 \cdots i_r}$; in the second basis, the operation S_{j2} brings the indices of $T_{i_1 \cdots i_r}$ into the same correspondence with $(PQ)_j^\mu$ as that found for $(PQ)_2^\mu T_{i_1 \cdots i_r}, \cdots$; and in the mth basis, the operation S_{jm} brings the

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[1] D. R. Tompkins, Phys. Rev. Letters **16**, 1058 (1966); **17**, 739E (1966).

[2] H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1946), p. 129. Weyl's theorem, in describing symmetrized tensors from a traditional viewpoint [one formal state for each subspace irreducibly invariant under $GL(n, c)$], evidently left some confusion about the explicit role of permutation group symmetry in symmetrized tensor bases of $GL(n, c)$. This confusion may be the reason why some authors fail to properly use Young symmetrizers to construct bases for the permutation group [see footnote 7 in Ref. 1. However, contrary to this reference, M. Hamermesh was seeking to construct basis functions for the permutation group rather than for $GL(n, c)$.] Because the pair of states given by R. E. Behrends, J. Dreitlein, C. Fronsdal, and W. Lee (see Ref. 4) conform to Weyl's theorem, they do not need to be extended (contrary to footnote 5 in Ref. 1) before entering index values to complete bases for two equivalent (but not orthogonal) representations of $SU(m)$.

indices of $T_{i_1 \cdots i_r}$ into the same correspondence with $(PQ)^{\mu}_{j}$ as that found for $(PQ)^{\mu}_{m} T_{i_1 \cdots i_r}$. This plus the above discussion show the new symmetrization procedure to be entirely consistent with Weyl's theorem and to yield the same independent *explicit* states (symmetrized tensors with explicit index values). The new symmetrization procedure differs from Weyl's approach in that to construct a subspace irreducibly invariant under $GL(n, c)$, one starts with an "extended" set of N^{μ} *formal* states (symmetrized tensors with formal index values) which span an irreducible representation (μ) of the permutation group rather than starting with a single formal state of representation (μ). Weyl's single initial state is always one member of the corresponding "extended" set of initial states. Because of this, it could be appropriate to call the new procedure an extended symmetrization procedure.

With an extended symmetrization procedure, it is only necessary to consider a single arrangement of each set of tensor index values in order to obtain a set of independent states which spans a subspace irreducibly invariant under $GL(n, c)$. Weyl's theorem admits all arrangements of each set of index values thereby obtaining a large number of dependent states. Weyl's theorem plus the rule of admitting only index values which, when entered into the standard tableaux of index positions, result in standard tableaux of independent states spanning a subspace irreducibly invariant under $GL(n, c)$. Thus the large number of dependent states provided by Weyl's theorem presents no problem. This independent state selection rule is proven by the extended symmetrization procedure.[3]

The state organization provided by the extended symmetrization concept makes it possible to develop a simple independent state selection method which applies not only when using Young symmetrizers but also when using modified Young symmetrizers or Wigner projection operators. It is well known that bases obtained with Young symmetrizers are nonorthogonal.[4] The state organization makes it possible to show that this nonorthogonality has a simple structure and can be easily removed. We are concerned not only with the orthogonality of the states within each representation but also with the orthogonality between representations because, in order to reasonably invert the similarity transformation which decomposes a tensor, it is necessary that *all* states of the decomposed tensor be orthogonal (the initial tensor is, of course, assumed orthogonal). Finally, the state organization makes it possible to prove that symmetrized tensor bases can always be brought to a simply-coupled form by using recoupling coefficients which do not depend on the individual states within the representations. Bases with simple coupling form are orthogonal when simply-coupled constituents are orthogonal.

Orthogonal symmetrized tensors make it possible to obtain many detailed properties of classical group representations by tensor methods. A particular example is Clebsch–Gordan coefficients coupling orthogonal symmetrized tensor bases. Orthogonal symmetrized tensors in Kronecker product form also allowed one to use tensor methods to evaluate the usual Clebsch–Gordan coefficients for the decomposition of Kronecker products. Such results are also obtained for classical groups not possessing inner products. The term inner product is here used inclusively for the Hermitian product or for any scalar product, while the term scalar product is reserved to express use of a metric tensor.

Symmetrization of a tensor always decomposes it as a representation of any matrix group on the underlying space, but this may not yield irreducible tensors. For the classical groups, the additional tensor operations needed to get irreducible tensors are well known and that is why here we principally address ourselves to these groups. The reduction of symmetrized tensors of semisimple Lie groups can be completed by using "shift" operations of the Lie algebra. Starting with an appropriate initial state, such "shift" operations can be used to complete a basis of an irreducible representation of the Lie algebra. Baird and Biedenharn[5] obtain bases for the groups $U(n)$ and $SU(n)$ by using Weyl's theorem to construct highest-weight states of $U(n-1) \subset U(n)$ and then complete these $U(n-1)$ multiplets with shift operations. This

[3] An invariant (tensor) subspace is always completed by entering all distinct arrangements of all sets of index values into the formal expression of any single state in the subspace. If the subspace is in decomposed form, then one such formal state from each invariant subspace is needed. This is why a tensor can be described by a single formal state (or a single formal state from each invariant subspace of a decomposed form). For Cartesian tensors this traditional state selection method is completely efficient, but for symmetrized tensors it results in some dependent states. Cartesian tensors can also be described by being formally extended before state selection. For a tensor of rank r this approach consists of using the $r!$ group operations of S_r to construct the formal states of the $r!$ dimensional (reducible) representation of S_r and then completing the tensor by entering (in all $r!$ states) a single arrangement of each set of index values. Here a Cartesian tensor is described by $r!$ formal states. It is clear that both descriptions are equally general. Except for Cartesian tensors, the extended approach always yields fewer dependent states.

[4] R. E. Behrends, J. Dreitlein, C. Fronsdal, and W. Lee, Rev. Mod. Phys. **34**, 1 (1962).

[5] G. E. Baird and L. C. Biedenharn, J. Math. Phys. **4**, 1449 (1963). The Gel'fand–Zetlin method described by these authors is more elegant than what the above text explains. In particular, it yields general expressions (rather than algorithms) for generator matrix elements.

has the advantage of yielding a basis with precisely the desired orthogonality. Moshinsky[6] has shown that certain "special Gel'fand" states in a Gel'fand basis of $U(n)$ constitute an irreducible basis of a permutation group S_n which is defined on the index *values* of the self-representation of $U(n)$ rather than on index positions.

As pointed out by Baird and Biedenharn (p. 1458),[5] the integral approach (tensors with permutational symmetry) has been used most at the level of implicit states. For these and other features of current tensor methods, the literature may be consulted.[7] The methods to be pursued here are oriented entirely toward explicit states.

2. EXTENDED SYMMETRIZATION PROCEDURES AND STATE SELECTION

For any given Young tableau $\mathcal{C}_i^\mu$, a Young symmetrizer is defined by $(PQ)_i^\mu \equiv \sum_{pq} pq\delta_q$, where δ_q is $+(-)$ as q is even (odd). The two-sided ideals obtained from the Young symmetrizers of all Young patterns of the permutation group $\mathcal{S}_r$ are linearly independent and span the whole group ring. The identity element (e) is resolved into generating units $[\sum_i (PQ)_i^\mu]$ of such ideals by

$$e = \sum_\mu (N^\mu/r!)^2 \left[\sum_i (PQ)_i^\mu\right], \tag{2.1}$$

where N^μ is the dimension of representation type (μ) and the sums include all tableaux of all patterns of $\mathcal{S}_r$.

Young actually worked with certain modified Young symmetrizers which he termed natural units. The resulting representations of the permutation group have been called the natural representations. With $Q_i p_{ia} = p_{ia} Q_a$, where p_{ia} is an element of the (p) group of standard tableaux $\mathcal{C}_a^\mu$, Young's modified symmetrizers PQ' are defined by[8]

$$(PQ')_i^\mu \equiv (PQ)_i^\mu - (P)_i^\mu p_{ia}(Q')_a - (P)_i^\mu p_{ib}(Q')_b - \cdots, \tag{2.2a}$$

$$Q'_j(P)_k^\mu = \delta_{jk}(QP)_j^\mu. \tag{2.2b}$$

The minimal left ideals obtained from modified Young symmetrizers of standard tableaux are linearly independent and span the group ring. Because these (essentially idempotent) generating units also annul one another, then the identity element can be (Peirce) resolved into generating units $(PQ')_i^\mu$ of minimal left ideals by

$$e = \sum_{i,\mu} \left[\frac{N^\mu}{r!}\right](PQ')_i^\mu, \tag{2.3}$$

where the sums include all standard tableaux of all patterns of $\mathcal{S}_r$.

The unmodified Young symmetrizers of the standard tableaux also furnish generating units for independent minimal left ideals which span the group ring. Because these (essentially idempotent) generating units do not in general all annul one another, their sum does not in general form a resolution of the identity element. A basis of the left ideal generated by $(PQ)_k^\mu$ is given by $\{S_{jk}(PQ)_k^\mu\}$, where j ranges over all standard tableaux and S_{jk} is the permutation relating standard tableaux $\mathcal{C}_j^\mu$ and $\mathcal{C}_k^\mu$ as

$$\mathcal{C}_j^\mu = S_{jk}\mathcal{C}_k^\mu, \tag{2.4}$$

so that

$$(PQ)_j^\mu = S_{jk}(PQ)_k^\mu S_{kj}. \tag{2.5}$$

We only use S_{jk} to relate standard tableaux although Eqs. (2.4) and (2.5) apply to all tableaux. From Eq. (2.1) it is clear that an arbitrary tensor can be expanded as

$$T_{i_1 \cdots i_r} = \sum_{i,\mu} \left(\frac{N^\mu}{r!}\right)^2 (PQ)_i^\mu T_{i_1 \cdots i_r}. \tag{2.6}$$

To obtain a basis of representation (μ), we start with any arrangement of the initial tensor indices $i_1 \cdots i_r$ and any standard tableau $\mathcal{C}_k^\mu$ and select the components

$$\{S_{jk}(PQ)_k^\mu T_{i_1 \cdots i_r}\}$$

(j ranges over all standard tableaux). These components all appear in Eq. (2.6) because $S_{jk}T_{i_1 \cdots i_r}$ certainly appears as an index arrangement and we can use Eq. (2.5) in the form

$$S_{jk}(PQ)_k^\mu T_{i_1 \cdots i_r} = (PQ)_j^\mu S_{jk} T_{i_1 \cdots i_r}. \tag{2.7}$$

From Eqs. (2.2) and (2.3) it is clear that these components would also appear in a Peirce-resolved tensor, so the above argument can instead be based on such an expansion.

Because the minimal left ideals of distinct standard tableaux are independent, a second independent basis is obtained with the components

$$\{S_{ji}(PQ)_i^\mu T_{i_1 \cdots i_r}\},$$

where $i \neq k$, index j ranges over all standard tableaux, and the indices $i_1 \cdots i_r$ have the same arrangement as before. Proceeding in this way, all standard tableaux are exhausted to obtain a complete set of independent bases of representation type (μ). The set is complete because all basic states appear among the components of the resolved tensor and the number of independent

[6] M. Moshinsky, J. Math. Phys. 7, 691 (1966).

[7] H. Jahn and H. van Wieringen, Proc. Roy. Soc. (London) **A209**, 502 (1951); J. P. Elliott, J. Hope, and H. A. Jahn, Phil. Trans. Roy. Soc. London **A246**, 241 (1953); J. P. Elliott, Proc. Roy. Soc. (London) **A245**, 128 (1958); A. R. Edmonds, Proc. Roy. Soc. (London) **A268**, 567 (1962); A. Pais, Rev. Mod. Phys. **38**, 215 (1966).

[8] H. Boerner, *Representations of Groups* (North-Holland Publishing Company, Amsterdam, 1963).

bases obtained is equal to the number of standard tableaux. Independent bases of type (μ) are now given in two useful forms:

First basis

$$A_1^\mu \equiv (PQ)_1^\mu T_{i_1 \cdots i_r} = (PQ)_1^\mu T_{i_1 \cdots i_r},$$
$$A_2^\mu \equiv (PQ)_2^\mu S_{21} T_{i_1 \cdots i_r} = S_{21}(PQ)_1^\mu T_{i_1 \cdots i_r},$$
$$\cdots$$
$$A_m^\mu \equiv (PQ)_m^\mu S_{m1} T_{i_1 \cdots i_r} = S_{m1}(PQ)_1^\mu T_{i_1 \cdots i_r}.$$

Second basis

$$B_1^\mu \equiv (PQ)_1^\mu S_{12} T_{i_1 \cdots i_r} = (PQ)_1^\mu S_{12} T_{i_1 \cdots i_r},$$
$$B_2^\mu \equiv (PQ)_2^\mu T_{i_1 \cdots i_r} = S_{21}(PQ)_1^\mu S_{12} T_{i_1 \cdots i_r},$$
$$\cdots \qquad (2.8)$$
$$B_m^\mu \equiv (PQ)_m^\mu S_{m2} T_{i_1 \cdots i_r} = S_{m1}(PQ)_1^\mu S_{12} T_{i_1 \cdots i_r}.$$
$$\cdots$$

mth basis ($m = N^\mu$)

$$D_1^\mu \equiv (PQ)_1^\mu S_{1m} T_{i_1 \cdots i_r} = (PQ)_1^\mu S_{1m} T_{i_1 \cdots i_r},$$
$$D_2^\mu \equiv (PQ)_2^\mu S_{2m} T_{i_1 \cdots i_r} = S_{21}(PQ)_1^\mu S_{1m} T_{i_1 \cdots i_r},$$
$$\cdots$$
$$D_m^\mu \equiv (PQ)_m^\mu T_{i \cdots i_r} = S_{m1}(PQ)_1^\mu S_{1m} T_{i_1 \cdots i_r}.$$

Note that the initial tensor $T_{i_1 \cdots i_r}$ is not required to be Cartesian. Similar tensor bases can be obtained from the minimal right ideals (see the Appendix).

The right column of the above equations shows that the kth basis state $S_{i1}(PQ)_1^\mu S_{1k} T_{i_1 \cdots i_r}$ is obtained from the first basis state $S_{i1}(PQ)_1^\mu T_{i_1 \cdots i_r}$ by permuting the indices of the Cartesian constituents of the initial tensor in the first basis state as a function of their symmetrized tensor position.

For definiteness and because symmetrization alone yields irreducible representations of the full linear group $GL(n, c)$, we refer to this group in the present discussion. Each subspace of a rank r tensor which is irreducibly invariant under $GL(n, c)$ is a direct sum of subspaces which are irreducibly invariant under S_r. These distinct subspaces belonging to a single irreducible representation of $GL(n, c)$ have distinct sets of index values and all arise from a *single* irreducible representation of S_r on a rank r tensor having arbitrary indices. In this way each independent irreducible representation of S_r on a tensor with arbitrary indices yields at most one independent representation of $GL(n, c)$. If repeated index values occur, then in general the dimension of the representation of S_r is reduced by some states either becoming identical or vanishing. We now show how to select independent states of $GL(n, c)$ by considering the initial states of S_r given by Eqs. (2.8).[9] Using commas to separate tableau rows, we illustrate the following discussion with the states

TABLE I. Decomposition of a third-rank tensor on a three-dimensional space. The states of $\{A\}$ and $\{B\}$ are described by Eqs. (2.9) and (2.10).

Tensor components	States: First basis	Second basis	Symmetric	Anti-symmetric
123, 132, 213	$A_1(123)$	$B_1(123)$	$Y(123)$	$Z(123)$
231, 312, 321	$A_2(123)$	$B_2(123)$		
112, 121, 211	$A_1(112)$	$B_1(112)$	$Y(112)$	
113, 131, 311	$A_1(113)$	$B_1(113)$	$Y(113)$	
221, 121, 122	$A_1(221)$	$B_1(221)$	$Y(221)$	
223, 232, 322	$A_1(223)$	$B_1(223)$	$Y(223)$	
331, 313, 133	$A_1(331)$	$B_1(331)$	$Y(331)$	
332, 323, 233	$A_1(332)$	$B_1(332)$	$Y(332)$	
111			$Y(111)$	
222			$Y(222)$	
333			$Y(333)$	
Number of states	8	8	10	1

$$A_1(i_1 i_2 i_3) = (PQ)_{i_1 i_2, i_3} T_{i_1 i_2 i_3},$$
$$A_2(i_1 i_2 i_3) = (PQ)_{i_1 i_3, i_2} T_{i_1 i_3 i_2} \qquad (2.9a)$$

and

$$B_1(i_1 i_2 i_3) = (PQ)_{i_1 i_2, i_3} T_{i_1 i_3 i_2},$$
$$B_2(i_1 i_2 i_3) = (PQ)_{i_1 i_3, i_2} T_{i_1 i_2 i_3}. \qquad (2.9b)$$

To bring some order into the numerous index arrangements, we admit only the index complexions $i_1 < i_2 < i_3$, $i_1 = i_2 < i_3$, $i_1 < i_2 = i_3$, and $i_1 = i_2 = i_3$. This allows a single arrangement of each set of index values and that is what we want. For $i_1 < i_2 < i_3$ the states of Eqs. (2.9a) and (2.9b) are all independent. Considering the other cases for the states of Eqs. (2.9a) we have

$i_1 = i_2 < i_3$,

$$-\tfrac{1}{2} A_1(i_1 i_1 i_3) = A_2(i_1 i_1 i_3) = (T_{i_3 i_1 i_1} - T_{i_1 i_1 i_3}), \qquad (2.10a)$$

$i_1 < i_2 = i_3$,

$$A_1(i_1 i_2 i_2) = A_2(i_1 i_2 i_2) = (T_{i_1 i_2 i_2} - T_{i_2 i_2 i_1}), \qquad (2.10b)$$

$i_1 = i_2 = i_3$,

$$A_1(i_1 i_1 i_1) = A_2(i_1 i_1 i_1) = 0. \qquad (2.10c)$$

Equations (2.9a), (2.10a), and (2.10b) yield independent states which are used in the decomposition of a third rank tensor on a three-dimensional space as shown in Table I. The second column of Eqs. (2.8) shows that,

[9] Using either modified Young symmetrizers or permutation group Wigner projection operators to construct a single formal symmetrized tensor state, it is possible to complete a basis for $GL(n, c)$ [or a $GL(n, c)$ subgroup] by admitting all arrangements of all sets of index values. However, the selection of independent states is usually difficult and the states obtained usually do not coincide with those obtained with the corresponding extended symmetrization procedures.

except for a uniform initial permutation of indices, corresponding states of equivalent representations are obtained with identical operations, so that for the equivalent representation $\{B\}$ the same results hold. The bases $\{A\}$ and $\{B\}$ obtained are independent. This approach is general. When the dimension of the underlying space is less than the rank of the tensor, some states of the expanded tensor [Eq. (2.6)] will vanish. If a state in the tensor expansion vanishes, but not all of its partners [as displayed in Eqs. (2.8)] vanish, then the representation formally associated with this state still appears.

A basis of the minimal left ideal generated by the modified idempotent $(PQ')^{\mu}_{j}$ is given by $\{S_{ij}(PQ')^{\mu}_{j}\}$. Modified idempotents of distinct standard tableaux generate independent bases. Independent tensor bases of the equivalent representations belonging to the standard tableaux of Young pattern (μ) are then:

First basis

$$\{S_{j1}(PQ')^{\mu}_{1}T_{i_1\cdots i_r}\}_{j=1,2,\cdots m}.$$

Second basis

$$\{S_{j2}(PQ')^{\mu}_{2}T_{i_1\cdots i_r}\}_{j=j,2,\cdots m}.$$

$$\cdot \qquad (2.11)$$

$$\cdot$$

$$\cdot$$

mth basis $(m = N^{\mu})$

$$\{S_{jm}(PQ')^{\mu}_{m}T_{i_1\cdots i_r}\}_{j=1,2,\cdots m},$$

where the initial tensor is not required to be Cartesian. Using page-ordered standard tableaux, Eqs. (2.2) show that $(PQ')^{\mu}_{m} = (PQ)^{\mu}_{m}$, so the mth basis of Eqs. (2.11) is identical to the mth basis of Eqs. (2.8); in general such pairs of bases are not identical. These natural representation bases can be used to form subspaces irreducibly invariant under $GL(n, c)$ in the same way as was done for the bases derived from the usual Young symmetrizers. These bases are not as highly organized as those of Eqs. (2.8) because in general it does not seem possible to write them in a form analogous to that shown by the right column of Eqs. (2.8).

Wigner[10] showed that one could construct a basis of a group representation by using projection operators formed with the representation matrices themselves. Thus using group representation matrices the minimal left ideal of row q of representation $[\mathfrak{D}^{\mu}]$ of $\mathcal{S}_r$ has basic elements $\{\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{qi}L_{\gamma}\}_{(\text{all } i)}$. Using the permutation group matrices of the states of Eqs. (2.8) to construct Wigner projection operators $\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{qq}L_{\gamma}$, one finds that in general these projection operators do not coincide with $(PQ)^{\mu}_{q}$. This is seen from the fact that Young symmetrizers do not in general all annul one another while the Wigner projection operators do, i.e.,

$$\left(\frac{N^{\mu}}{r!}\right)^2 \sum_{\alpha}[\mathfrak{D}^{\mu}_{\alpha^{-1}}]_{qq}L_{\alpha}\sum_{\beta}[\mathfrak{D}^{\mu}_{\beta^{-1}}]_{ll}L_{\beta} = \frac{\delta_{ql}N^{\mu}}{r!}\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{qq}L_{\gamma}.$$

Thus symmetrized tensor bases obtained with Young symmetrizers are generally quite distinct from those obtained with Wigner projection operators. This does not contradict $\sum_{\alpha i}[\mathfrak{D}^{\mu}_{\alpha^{-1}}]_{ij}L_{\alpha}\Psi^{s\mu}_{i} = \Psi^{s\mu}_{j}$ because to obtain symmetrized tensor bases the Wigner projection operators are applied to a general tensor. Using Wigner projection operators, a Peirce resolved tensor appears as

$$T_{i_1\cdots i_r} = \sum_{l\mu}(N^{\mu}/r!)\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{ll}L_{\gamma}T_{i_1\cdots i_r},$$

where the sums include all group elements, all representations, and all rows. Here the basic states generally do not all appear explicitly in the Peirce resolved tensor. Using Wigner projection operators, the tensor bases of $\mathcal{S}_r$ have the form:

First basis

$$\left\{\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{1j}L_{\gamma}T_{i_1\cdots i_r}\right\}_{j=1,2,\cdots m},$$

Second basis

$$\left\{\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{2j}L_{\gamma}T_{i_1\cdots i_r}\right\}_{j=1,2,\cdots m}, \qquad (2.12)$$

$$\cdot$$

$$\cdot$$

$$\cdot$$

mth basis $(m = N^{\mu})$

$$\left\{\sum_{\gamma}[\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{mj}L_{\gamma}T_{i_1\cdots i_r}\right\}_{j=1,2,\cdots m},$$

where the initial tensor is not required to be Cartesian.

A direct sum consisting of one such basis belonging to one arrangement of each set of index values forms a subspace irreducibly invariant under $GL(n, c)$. Dependent states resulting from repeated index values can be eliminated in the same way as was done for the states of Eqs. (2.8). Due to the work of Yamanouchi[11] the matrices of the unitary representations of the permutation group are readily available, and, when

[10] E. P. Wigner, *Group Theory* (Academic Press, New York, 1959). Actually Wigner followed a projection operation ("row" operation) with a "partner" operation. More recent authors combine these into a single operation. A set of such operations result in which only one is idempotent and hence only one is a true projection operation.

[11] T. Yamanouchi, Proc. Phys. Soc. Japan **19**, 436 (1937).

using such matrices, we shall write

$$U^{\mu}_{lq} \equiv (N^{\mu}/r!) \sum_{\gamma} [\mathfrak{D}^{\mu}_{\gamma^{-1}}]_{ql} L_{\gamma}.$$

In addition to the self-representation where $\mathcal{A}$ represents an element α of some complex classical group, we also have the complex conjugate self-representation where α is represented by $\mathcal{A}^*$ rather than $\mathcal{A}$. Denoting repeated Kronecker products by exponentiation, we find the representations $(\mathcal{A})^u \times (\mathcal{A}^*)^k$ are carried by tensors $T_{i_1 \cdots i_u j_1 \cdots j_k}$ with indices $i_1 \cdots i_u$ transforming as $(\mathcal{A})^u$ and indices $j_1 \cdots j_k$ transforming as $(\mathcal{A}^*)^k$. For the groups $GL(n, c)$ and $SL(n, c)$ irreducible tensors are obtained by separately symmetrizing the indices $i_1 \cdots i_u$ and $j_1 \cdots j_k$. We can also have indices of opposite variance. Thus a tensor $T^{i_1 \cdots i_v j_1 \cdots j_l}_{i_1 \cdots i_u j_1 \cdots j_k}$ of $GL(nc)$ or $SL(nc)$, with indices $i_1 \cdots i_u$ and $i_1 \cdots i_v$ having opposite variances of $\mathcal{A}$ and indices $j_1 \cdots j_k$ and $j_1 \cdots j_l$ having opposite variances of $\mathcal{A}^*$, is irreducibly decomposed by separately symmetrizing each set of the four kinds of indices and then using the "trace" condition[12] of contracting opposing variance indices belonging to the same complex conjugation.[13] The metric tensors of $O(n, c)$ and $Sp(n, c)$ make opposite variance indices of the same kind one-to-one equivalent for these groups. For the unitary groups complex conjugation plus transposition coincide with a change of variance and thus such tensors carry only two kinds of indices, which are of opposing variance. Another kind of nontrivial "mixed" tensor is one carrying indices of both a group and its cover group. An important case of this is tensors of $SO(3)$–$SU(2)$ on space-spin coordinates. The usual approach[14] of obtaining symmetric "traceless" projections uses the fact that all irreducible representations of $SO(3)$ can be described by "traceless" symmetric tensors.[15] However, to decompose the whole tensor, we must also consider the representations with other symmetry. Thus, to decompose a tensor $T_{m_1 \cdots m_j \alpha_1 \cdots \alpha_k}$ with vector indices $m_1 \cdots m_j$ and spinor indices $\alpha_1 \cdots \alpha_k$, we use Eqs. (2.8) or (2.11) or (2.12) to symmetrize separately the vector and spinor indices; apply to all vector indices conditions of the form

$$\sum_{uv} G^{uv} T_{m_1 \cdots u \cdots v \cdots m_j \alpha_1 \cdots \alpha_k} = 0;$$

and finally apply to all vector and spinor indices the conditions

$$\sum_{\beta w p} G^{wp} T_{m_1 \cdots w \cdots m_j \alpha_1 \cdots \beta \cdots \alpha_k} (\sigma_p)^{\beta}_{\gamma} = 0,$$

where σ is the Pauli vector operator represented in the same coordinate system as the initial and metric tensors.

3. ORTHOGONALITY AND RECOUPLING

The unitary groups leave the Hermitian product invariant. The orthogonal groups have a scalar product using a symmetric metric tensor and the real orthogonal groups are unitary. For the symplectic groups we can use symplectic coordinates[15] which are based on a scalar product using a skew metric, and for the unitary symplectic groups we can also use the Hermitian product.

For a Hermitian product

$$L_{\alpha} T_j = \sum_i T_i [\mathfrak{D}_{\alpha}]_{ij} \Leftrightarrow L^{\dagger}_{\alpha} \tilde{T}^*_j = \sum_i \tilde{T}^*_i [\tilde{\mathfrak{D}}_{\alpha}]^*_{ij}.$$

If the representation matrices are unitary, then this implies $L^{\dagger}_{\alpha} = L_{\alpha^{-1}}$ so that

$$([\mathfrak{D}^{\mu}_{\alpha^{-1}}]_{vu} L_{\alpha})^{\dagger} = [\mathfrak{D}^{\mu}_{\alpha^{-1}}]^*_{vu} L_{\alpha^{-1}},$$

and by linearity we obtain the unitary representation adjoint Wigner projection operator.

$$U^{\dagger}_{uv} \equiv \frac{N^{\mu}}{r!} \sum_{\alpha} [\mathfrak{D}^{\mu}_{\alpha^{-1}}]^*_{vu} L_{\alpha^{-1}}.$$

Writing $\alpha^{-1}\beta = \gamma$ so that

$$[\mathfrak{D}^{\mu}_{\alpha^{-1}}]^*_{vu} = \sum_i [\mathfrak{D}^{\mu}_{\gamma}]^*_{vi} [\mathfrak{D}^{\mu}_{\beta^{-1}}]^*_{iu}$$

and using real unitary matrices, we find

$$\langle T_{i_1 \cdots i_r} \mid (U^{\mu}_{uv})^{\dagger} U^{\nu}_{fg} T_{j_1 \cdots j_r} \rangle = \delta_{\mu\nu} \delta_{uf} \langle T_{i_1 \cdots i_r} \mid (U^{\mu}_{gv})^{\dagger} T_{j_1 \cdots j_r} \rangle. \quad (3.1)$$

These equations establish orthogonality between the states within a representation as well as showing that states of equivalent representations ($g \neq v$) are orthogonal if $u \neq f$. For components with distinct index values and which are derived from an orthogonal initial tensor, the only nonvanishing contribution to the right side of Eq. (3.1) is from $[\mathfrak{D}_e]^*_{gv} L_e$ and this contribution vanishes unless $g = v$. These results still leave the possibility of nonorthogonality between corresponding states (with repeated index values) of equivalent representations. The proof of Eqs. (3.4) requires identical representations, and Wigner projection operators provide this. This shows that if some corresponding states of equivalent representations are orthogonal then all are orthogonal, so that with an

[12] The term "trace condition" will be applied to a general class of tensor subsidiary conditions.

[13] M. A. Rashid, Nuovo Cimento **26**, 118 (1962); N. Mukunda and T. F. Jordan, J. Math. Phys. **7**, 849 (1966).

[14] Charles Zemach, Phys. Rev. **140**, B97 (1964); B. Barsella and E. Fabri, Nuovo Cimento Suppl. **11**, 293 (1964).

[15] M. Hamermesh, *Group Theory* (Addison-Wesley Publishing Company, Inc., Reading, Mass., 1962).

orthogonal initial tensor

$$\langle T_{i_1\cdots i_r} \mid (U^{\mu}_{uv})^{\dagger} U^{\nu}_{fg} T_{j_1\cdots j_r}\rangle = \delta_{\mu\nu}\delta_{uf}\delta_{vg}\langle T_{i_1\cdots i_r} \mid T_{j_1\cdots j_r}\rangle. \quad (3.2)$$

To show that the above results also apply to the scalar product of $O(n, c)$, we first note that the (diagonal form) metric tensor of $O(n, c)$ effects a transposition by changing row (column) states into column (row) states. By using *real* unitary matrices of S_r the above adjoint is also an adjoint projection operator for this scalar product.

Returning to the representations given by Eqs. (2.8), we note that the orthogonality of bases of such inequivalent representations follows from Eqs. (3.2) and the similarity of a "Young pattern subspace" derived from Young symmetrizers, and the corresponding "Young pattern subspace" derived from unitary representation Wigner projection operators. A "Young pattern subspace" is the space spanned by all equivalent representations belonging to a Young pattern. We have already seen that the second column of Eqs. (2.8) shows that the independent equivalent bases differ only in the way they are entered on the tensor indices. Thus these equivalent representations are identical and their bases have identical inner product structures, i.e.,

$$\langle A^{\mu}_t(i_1, \cdots, i_r) \mid A^{\mu}_f(j_1, \cdots, j_r)\rangle = \langle B^{\mu}_t(i_1, \cdots, i_1) \mid B^{\mu}_f(j_1, \cdots, j_r)\rangle = \cdots = \langle D^{\mu}_t(i_1, \cdots, i_r) \mid D^{\mu}_f(j_1, \cdots, j_r)\rangle. \quad (3.3)$$

As a corollary to the recoupling theorem, it is shown that the inner products between the bases of equivalent representations have essentially this same structure, i.e.,

$$\begin{aligned}
&\langle A^{\mu}_t(i_1, \cdots, i_r) \mid A^{\mu}_f(j_1, \cdots, j_r)\rangle \\
&\quad = \lambda(A, B)\langle A^{\mu}_t(i_1, \cdots, i_r) \mid B^{\mu}_f(j_1, \cdots, j_r)\rangle = \cdots \\
&\quad = \lambda(A, D)\langle A^{\mu}_t(i_1, \cdots, i_r) \mid D^{\mu}_f(j_1, \cdots, j_r)\rangle \\
&\lambda(B, A)\langle B^{\mu}_t(i_1, \cdots, i_r) \mid A^{\mu}_f(j_1, \cdots, j_r)\rangle \\
&\quad = \langle B^{\mu}_t(i_1, \cdots, i_r) \mid B^{\mu}_f(j_1, \cdots, j_r)\rangle = \cdots \\
&\quad = \lambda(B, D)\langle B^{\mu}_t(i_1, \cdots, i_r) \mid D^{\mu}_f(j_1, \cdots, j_r)\rangle \\
&\quad \vdots \\
&\lambda(D, A)\langle D^{\mu}_t(i_1, \cdots, i_r) \mid A^{\mu}_f(j_1, \cdots, j_r)\rangle \\
&\quad = \lambda(D, B)\langle D^{\mu}_t(i_1, \cdots, i_r) \mid B^{\mu}_f(j_1, \cdots, j_r)\rangle = \cdots \\
&\quad = \langle D^{\mu}_t(i_1, \cdots, i_r) \mid D^{\mu}_f(j_1, \cdots, j_r)\rangle, \qquad (3.4)
\end{aligned}$$

where λ never depends on labels t or f or on indices $i_1, \cdots, i_r$ or $j_1, \cdots, j_r$, and can be zero. The above argument for Eqs. (3.3) and the argument for Eqs. (3.4) given later are based on the initial tensor being Cartesian; however, in an added note, generalized results for non-Cartesian tensors are obtained.

Equations (3.4) show that orthogonalizing all equivalent representation bases in the same way, which by Eqs. (3.3) is always possible, also diagonalizes the inner products between equivalent representation bases. This remaining nonorthogonality can then be easily removed by recoupling whole bases rather than by separately recoupling individual states. Such recoupling does not affect the orthogonality obtained within the equivalent representation bases.

The nonorthogonality of the states of Eqs. (2.11) remains a severe problem since it does not seem possible to put them into a form analogous to that shown by the right column of Eqs. (2.8).

The orthogonality provided by the unitary representations of S_r usually does not coincide with that needed for reduction relative to a particular embedding of some particular matrix subgroup, and so such states having a common weight (Lie group) usually need to be rearranged to also gain the desired orthogonality. Thus the additional rearrangement which states obtained from Eqs. (2.8) require is that of making equivalent representations mutually orthogonal and that has been shown to be easily achieved. On the other hand, using unitary representations of S_r to symmetrize a rank r tensor becomes very tedious as r increases because it is necessary to obtain and use the representation matrices of all $r!$ group elements. This is a feature of any symmetrization procedure using Wigner projection operators.

While the subsidiary conditions for tensors of $O(n, c)$ are based on a scalar product, the resulting states can in the case of the real orthogonal groups $O(n)$, also be used with a Hermitian product. Using the metric tensor inner product, the operation of "trace" extraction orthogonally partitions a tensor (Reference 15, p. 392). For the symplectic groups $Sp(n, c)$ "trace" operations are based on the symplectic scalar product but for the unitary symplectic groups $Sp(n)$ the resulting states can also be used with a Hermitian product. For the unitary symplectic groups one would almost certainly want to use the Hermitian product. "Trace" extraction with a symplectic metric also partitions a tensor orthogonally relative to the Hermitian product. If instead we stay with the scalar product of $Sp(n, c)$ and if initial and final tensors have respective metrics G and $\bar{G}$, where $G^2 = \bar{G}^2 = 1$ and $\bar{G} = W^{-1}GW^{-1}$, then

$$\tilde{W}^{-1} = -GW\bar{G}, \quad (3.5)$$

where $\tilde{W}$ denotes the transpose of W.

We find that we are already able to use tensor

methods to obtain many detailed properties of group representations and certain recoupling results allow us to get further properties. If E_a denotes a generator of the self-representation (classical group), then, with exponents symbolizing repeated Kronecker products, the generators for a tensor of rank r are

$$\mathbf{E}_a = \sum_{k=1}^{r} (I)^{k-1} \times E_a \times (I)^{r-k}, \tag{3.6}$$

where exponentiation of power zero signifies 1 (not I). The generator matrix elements are obtained by applying these operators to the Cartesian tensor components of the states. This only uses properties of an individual representation and not properties requiring a fully decomposed tensor. Explicit states are not even required in order to evaluate the matrix elements of the commuting generators $H_1, \cdots, H_h$ as is now shown. This has also been shown by Weyl[16] for antisymmetric states and by Baird and Biedenharn[5] in a boson operator context. The eigenvalues of the maximal set of diagonal generators are the weight vector components and we assume the first rank tensors to be eigenstates of these commuting generators. If $A_q(w_1, \cdots w_n)$ is a state obtained from the reduction of a tensor on an n-dimensional space and if the entries of the state consist of w_1 entries of 1, w_2 entries of 2, $\cdots$, and w_n entries of n, then

$$\mathbf{H}_f A_q(w_1 \cdots w_n) = [w_1(\mathbf{H}_f)_1 + w_2(\mathbf{H}_f)_2 + \cdots + w_n(\mathbf{H}_f)_n] A_q(w_1 \cdots w_n), \tag{3.7}$$

so that the weight vector components of $A_q(w_1 \cdots w_n)$ are

$$\begin{aligned} &w_1(\mathbf{H}_1)_1 + w_2(\mathbf{H}_1)_2 + \cdots + w_n(\mathbf{H}_1)_n, \\ &w_1(\mathbf{H}_2)_1 + w_2(\mathbf{H}_2)_2 + \cdots + w_n(\mathbf{H}_2)_n, \\ &\cdot \\ &\cdot \\ &\cdot \\ &w_1(\mathbf{H}_h)_1 + w_2(\mathbf{H}_h)_2 + \cdots + w_n(\mathbf{H}_h)_n. \end{aligned} \tag{3.8}$$

The multiplicity of each weight vector is simply the multiplicity of each index value assignment. Tensor states having distinct weight vectors are linearly independent. This does not require the group to be semisimple but when such is the case further useful weight vector properties are ensured.

If $\mathcal{A}$ and $\mathcal{A}'$ are contravariant (covariant) self-representation transformations of $SO(3)$ and $SU(2)$, respectively, then the group transformations of a decomposed $SO(3)$–$SU(2)$ tensor having a single $SU(2)$ index are $W^{-1}[(\mathcal{A})^{q-1} \times \mathcal{A}' \times (\mathcal{A})^{r-q}]W$, where the qth tensor index is $SU(2)$. It is clear that here properties of the whole decomposed tensor are being used. We can obtain the generator matrix elements from these expressions by differentiation or else by using the matrix equation

$$\mathbf{I} + \delta_a \mathbf{E}_a = W^{-1}[(I + \delta_a E_a)^{q-1} \times (I + \delta_a E'_a) \times (I + \delta_a E_a)^{r-q}]W,$$

where δ_a is infinitesimal. The operator of Eq. (3.6) was not symmetrized (hence absence of W) because it was used according to an operational rather than matrix definition.

Denoting Kronecker products by exponentation and with $\theta, \varphi, \cdots$ denoting the parameters of a Lie group, we see that $W\mathcal{A}^k(\theta, \varphi, \cdots)W^{-1}$ yields irreducible representation matrices. These matrix element functions, which the Peter–Weyl and Wigner–Stone theorems are concerned with[17] (compact group), may also be individually useful, e.g., those of $SO(3)$ are symmetric top eigenfunctions.[18]

We now take up the evaluation of Clebsch–Gordan and recoupling coefficients by tensor methods. Our approach will differ from some usual methods[19] in that Clebsch–Gordan coefficients are directly evaluated without first being factorized. The Clebsch–Gordan and recoupling coefficients which we evaluate couple symmetrized tensor representations. Later we show how to recouple tensor representations in order to get states which are composed of simple couplings. With this we are able to use tensor methods to also evaluate the usual Clebsch–Gordan and recoupling coefficients. Due to the use of tensor methods, we can proceed without introducing operators to label representations and states. By $\bigoplus_{\lambda} T^{\lambda}_{i_1 \cdots i_r}$ we denote an irreducibly decomposed tensor of rank r and by $\hat{T}_{i_1 \cdots i_r}$ we mean a Cartesian tensor. We are interested in evaluating the coefficients of

$$\left(\bigoplus_{\lambda} T^{\lambda}_{i_1 \cdots i_r}\right)\left(\bigoplus_{\mu} T^{\mu}_{i_1 \cdots i_s}\right) C(r, s) = \bigoplus_{\zeta} T^{\zeta}_{i_1 \cdots i_{r+s}}. \tag{3.9}$$

The matrix $C(r, s)$ contains the Clebsch–Gordan coefficients of any irreducible representation appearing in a rank $r + s$ tensor which is obtained by the coupling of the irreducible representations appearing in a rank r tensor with the irreducible representations appearing in a rank s tensor. For mixed tensors one often wants to retain a certain index configuration. Considering $SO(3)$-$SU(2)$ tensors, one might want to have at most only one spinor index. Although

[16] H. Weyl, "The Structure and Representations of Continuous Groups," The Institute of Advanced Study, 1935 (unpublished).

[17] L. C. Biedenharn, in *Lectures in Theoretical Physics 5*, W. E. Britten and J. Downs, Eds. (John Wiley and Sons, New York, 1963).

[18] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).

[19] J. J. DeSwart, Rev. Mod. Phys. 35, 916 (1963); D. Lurie and A. J. Macfarlane, J. Math. Phys. 5, 565 (1964).

Eq. (3.9) does not immediately maintain such a configuration, the states of irreducible representations with two spinor indices can be mapped one-to-one onto the states of irreducible representations with no spinor indices, thereby recovering the desired index configuration. Returning to a general consideration of Clebsch–Gordan coefficients, we have

$$\bigoplus_{\zeta} T^{\zeta}_{i_1\cdots i_{r+s}} = \hat{T}_{i_1\cdots i_{r+s}} W(r+s) \tag{3.10}$$

and

$$\left(\bigoplus_{\lambda} T^{\lambda}_{i_1\cdots i_r}\right)\left(\bigoplus_{\mu} T^{\mu}_{i_1\cdots i_s}\right) = \hat{T}_{i_1\cdots i_{r+s}}[W(r)\times W(s)], \tag{3.11}$$

where the Cartesian components were assumed to be organized so that

$$(\hat{T}_{i_1\cdots i_r}W(r))(\hat{T}_{i_1\cdots i_s}W(s)) = \hat{T}_{i_1\cdots i_{r+s}}[W(r)\times W(s)].$$

Combining Eqs. (3.9) and (3.11) gives

$$\left(\bigoplus_{\zeta} T^{\zeta}_{i_1\cdots i_{r+s}}\right)C^{-1}(r,s) = \hat{T}_{i_1\cdots i_{r+s}}[W(r)\times W(s)]. \tag{3.12}$$

Using Eq. (3.10) and rearranging yields

$$[W(r)\times W(s)]^{-1}W(r+s) = C(r,s). \tag{3.13}$$

To evaluate (recoupling) coefficients which reorder successive couplings suppose we have the coupling

$$\left(\bigoplus_{\lambda} T^{\lambda}_{i_1\cdots i_r}\right)\left(\bigoplus_{\mu} T^{\mu}_{i_1\cdots i_s}\right)\left(\bigoplus_{\eta} T^{\eta}_{i_1\cdots i_v}\right)C(r,s)C(u,v) = \hat{T}_{i_1\cdots i_{u+v}}W(u+v), \tag{3.14}$$

where

$$\left(\bigoplus_{\lambda} T^{\lambda}_{i_1\cdots i_r}\right)\left(\bigoplus_{\mu} T^{\mu}_{i_1\cdots i_s}\right)C(r,s) = \bigoplus_{\xi} T^{\xi}_{i_1\cdots i_u}$$

and the coupling

$$\left(\bigoplus_{\alpha} T^{\alpha}_{i_1\cdots i_j}\right)\left(\bigoplus_{\beta} T^{\beta}_{i_1\cdots i_k}\right)\left(\bigoplus_{\gamma} T^{\gamma}_{i_1\cdots i_g}\right)C(j,k)C(f,g) = \hat{T}_{i_1\cdots i_{f+g}}W(f+g), \tag{3.15}$$

where $u+v=f+g$ and

$$\left(\bigoplus_{\alpha} T^{\alpha}_{i_1\cdots i_j}\right)\left(\bigoplus_{\beta} T^{\beta}_{i_1\cdots i_k}\right)C(j,k) = \bigoplus_{\pi} T^{\pi}_{i_1\cdots i_f}.$$

Then using

$$\left(\bigoplus_{\lambda} T^{\lambda}_{i_1\cdots i_r}\right)\left(\bigoplus_{\mu} T^{\mu}_{i_1\cdots i_s}\right)\left(\bigoplus_{\eta} T^{\eta}_{i_1\cdots i_v}\right) = \hat{T}_{i_1\cdots i_{r+s+v}}[W(r)\times W(s)\times W(v)]$$

and

$$\left(\bigoplus_{\alpha} T^{\alpha}_{i\cdots i_j}\right)\left(\bigoplus_{\beta} T^{\beta}_{i\cdots i_k}\right)\left(\bigoplus_{\gamma} T^{\gamma}_{i\cdots i_g}\right) = \hat{T}_{i_1\cdots i_{j+k+g}}[W(j)\times W(k)\times W(g)],$$

where $r+s+v=j+k+g$, we find

$$[W(j)\times W(k)\times W(g)]^{-1}[W(r)\times W(s)\times W(v)] \times C(r,s)C(u,v)W^{-1}(u+v)W(f+g) = C(j,k)C(f,g) \tag{3.16}$$

and

$$\bigoplus_{\rho} T^{\rho}_{i_1\cdots i_{u+v}} = \left(\bigoplus_{\sigma} T^{\sigma}_{i_1\cdots i_{f+g}}\right)C^{-1}(f,g)C^{-1}(j,k) \times [W(j)\times W(k)\times W(g)]^{-1} \times [W(r)\times W(s)\times W(v)] \times C(r,s)C(u,v). \tag{3.17}$$

The task of constructing W^{-1} is reasonable only when W is unitary. It has been shown that one can orthogonalize symmetrized tensors of $U(n)$ quite easily and thus obtain unitary similarity transformations W. Since the tensors of the nonunitary classical groups $GL(n,c)$, $GL(n,R)$, $SL(n,c)$, and $SL(n,R)$ are irreducibly decomposed by symmetrization plus mixed variance trace operations in the same way as tensors of $U(n)$, then the unitary similarity transformations for tensors of $U(n)$ can also be used for tensors of these nonunitary classical groups. It was for this reason that the coupling coefficient results were given in terms of similarity transformations W rather than in terms of inner products. It might also be worth while to note the reason for using postmultiplicative similarity transformations. Group representations are usually defined postmultiplicatively as

$$L_\alpha\psi_i = \sum_j \psi_j[\mathfrak{D}_\alpha]_{ji}$$

(so that for an orthogonal basis $[\mathfrak{D}_\alpha]_{ji} = \langle\psi_j \mid L_\alpha\psi_i\rangle$) and in such a case $T' = TW$ is associated with

$$\mathfrak{D}' = W^{-1}\mathfrak{D}W.$$

Some developments are now illustrated using $SU(3)$. The weights of the states of the self-representation of $SU(3)$ are the eigenvalues in the following equations:

$$H_1T_1 = (1/2\sqrt{3})T_1, \quad H_1T_2 = -(1/2\sqrt{3})T_2, \quad H_1T_3 = OT_3, \tag{3.18a}$$

$$H_2T_1 = \tfrac{1}{6}T_1, \quad H_2T_2 = \tfrac{1}{6}T_2, \quad H_2T_3 = -\tfrac{1}{3}T_3. \tag{3.18b}$$

The nonvanishing shift operations are

$$E_{i,j}T_j = (1/6^{\frac{1}{2}})T_i,$$

where

$$(i,j) = \{(1,2),(2,1),(1,3),(3,1),(2,3),(3,2)\}. \tag{3.19}$$

Because of Eqs. (3.5) and (3.6), we can make the octets mutually orthogonal by using the following normalized states, where the states $A_2(123) \pm B_2(123)$ have been additionally modified to obtain orthogonal isospin multiplets of the $SU(2)$ embedding generated

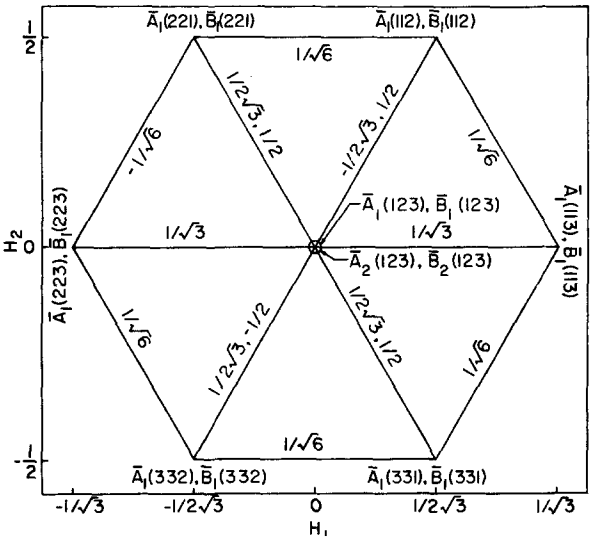

FIG. 1. Octet weight diagram. Tensor states and nonvanishing generator matrix elements are shown for two superimposed octets $\{\bar{A}\}$ and $\{\bar{B}\}$.

by $E_{1,2}$, $E_{2,1}$ and $(1/\sqrt{3})H_1$. Due to the absence of numerical factors, $\cong$ is used. Here the tensors T_{ijk} are Cartesian.

$$\bar{A}_1(iij) = (1/6^{\frac{1}{2}})[T_{iij} + T_{iji} - 2T_{jii}] \cong A_1(iij) + B_1(iij), \quad i < j,$$

$$\bar{A}_1(ijj) = (1/6^{\frac{1}{2}})[-T_{jji} - T_{jij} + 2T_{iij}] \cong A_1(ijj) + B_1(ijj), \quad i < j,$$

$$\bar{A}_1(123) = (1/12^{\frac{1}{2}})[T_{123} + T_{213} + T_{132} + T_{231} - 2T_{312} - 2T_{321}] \cong A_1(123) + B_1(123),$$

$$\bar{A}_2(123) = \tfrac{1}{2}\sqrt{3}\,[T_{123} + T_{132} - T_{213} - T_{231}] \cong 2[A_2(123) + B_2(123)] + [A_1(123) + B_1(123)], \quad (3.20a)$$

$$\bar{B}_1(iij) = (1/\sqrt{2})[T_{iij} - T_{iji}] \cong A_1(iij) - B_1(iij), \quad i < j,$$

$$\bar{B}_1(ijj) = (1/\sqrt{2})[T_{jij} - T_{jji}] \cong A_1(ijj) - B_1(ijj), \quad i < j,$$

$$\bar{B}_1(123) = \tfrac{1}{2}[T_{123} + T_{213} - T_{132} - T_{231}] \cong A_1(123) - B_1(123),$$

$$\bar{B}_2(123) = (1/(12)^{\frac{1}{2}})[-T_{123} + T_{132} + T_{213} - T_{231} + 2T_{312} - 2T_{321}] \cong 2[A_2(123) - B_2(123)] + [A_1(123) - B_1(123)]. \quad (3.20b)$$

The signs have been chosen to agree with the phase convention proposed by Baird and Biedenharn.[20] Normalized states of the decouplet and singlet are indicated in Table I. Using Eqs. (3.6) and (3.8) with these octet states, we obtain the weight diagrams and generator matrix elements shown in Fig. 1. These states also allow us to do the same for the embedded subgroups.

The states of Eqs. (3.20a) and (3.20b) plus the third rank symmetric and antisymmetric states yield a fully orthogonal tensor so that $W^{-1} = \tilde{W}$. The singlet, decouplet, and octet group matrices can then be easily evaluated in the form of homogeneous polynomials.

The octet states of Eqs. (3.20a) and (3.20b) have the interesting property of having a simply-coupled form as shown in Table II. That is, all terms in all states of octet $\{\bar{A}\}$ appear as a Kronecker product of the first rank triplet with the second rank sextet and all terms in all states of $\{\bar{B}\}$ appear as a Kronecker product of first and second rank triplets. Here as well as elsewhere, we adopt the convention that $T_{ijk}\cdots$ of $Z(ijk\cdots)$ is positive. The states of the octets obtained from Eqs. (2.9) and (2.10) are composed of nonsimple couplings which mix irreducible lower rank representations. The same is true of states obtained with unitary representation Wigner projection operators. We now wish to investigate the recoupling of states in order to get simple coupling. In Sec. 2 we found each symmetrized tensor representation of the matrix group on the underlying space to be derived from a *single* representation of $\mathcal{S}_r$ so at first we only work with representations of $\mathcal{S}_r$ belonging to a single arbitrary set of index values. Let ψ and φ be decomposed representations of $\mathcal{S}_r$ (e.g., $\{A(ijk)\} \oplus \{B(ijk)\}$ and $\{A(ijk) + B(ijk)\} \oplus \{A(ijk) - B(ijk)\}$, respectively). We assume ψ and φ each provide a direct sum of identical representations of $\mathcal{S}_r$ [this is true if both are derived from bases lying entirely in a set of equivalent representations of $\mathcal{S}_r$ given by either Eqs. (2.8) or (2.12)] and we assume φ to have bases with simple couplings. Certainly if there exists a set of bases with simple couplings, then their direct sum can be brought to a form yielding a (decomposed) representation identical to that of any equivalent initial basis.

TABLE II. The couplings among first and second rank constituents of the octets. Normalization factors are omitted and $Y(ij) \equiv T_{ij} + T_{ji}$, $Z(ij) = T_{ij} - T_{ji}$

State	Coupling
$\bar{A}_1(iij)$	$T_iY(ij) - T_jY(ii)$
$\bar{A}_2(ijj)$	$-T_jY(ij) + T_iY(jj)$
$\bar{A}_1(123)$	$T_1Y(23) + T_2Y(13) - 2T_3Y(12)$
$\bar{A}_2(123)$	$T_1Y(23) - T_2Y(13)$
$\bar{B}_1(iij)$	$T_iZ(ij)$
$\bar{B}_1(ijj)$	$T_jZ(ij)$
$\bar{B}_1(123)$	$T_1Z(23) + T_2Z(13)$
$\bar{B}_2(123)$	$T_1Z(32) + T_2Z(13) + 2T_3Z(12)$

[20] G. E. Baird and L. C. Biedenharn, J. Math. Phys. 5, 1723 (1964).

TABLE III. The Hermitian products among the states shown. Here the unnormalized states of Eqs. (2.9a) and (2.9b) and $Y(ij) = T_{ij} - T_{ji}$ and $Z(ij) = T_{ij} - T_{ji}$ are used. The selection $i = 1, j = 2, k = 3$ emphasizes that distinct index values are used here.

States	$T_1Y(23)$	$T_2Y(13)$	$T_3Y(12)$	$T_1Z(23)$	$T_2Z(13)$	$T_3Z(12)$
$aA_1(123) + bB_1(123)$	$a+b$	$a+b$	$-2(a+b)$	$a-b$	$a-b$	0
$aA_2(123) + bB_2(123)$	$a+b$	$-2(a+b)$	$a+b$	$b-a$	0	$a-b$

Thus there exists a similarity transformation $\varphi = Q\psi$ such that $\{\psi\}$ and $\{\varphi\}$ provide identical representations of $\mathcal{S}_r$, so $L_\alpha Q = QL_\alpha$ for all L_α of $\mathcal{S}_r$ and using $L_\alpha\psi_v = \sum_w \psi_w[\mathfrak{D}_\alpha]_{wv}$ we have

$$L_\alpha Q\psi_u = \sum_{v,w} \Psi_v Q_{vw}[\mathfrak{D}_\alpha]_{wu},$$
$$QL_\alpha\psi_u = \sum_{v,w} \Psi_v[\mathfrak{D}_\alpha]_{vw}Q_{wu},$$

yielding

$$\sum_w (Q_{vw}[\mathfrak{D}_\alpha]_{wu} - [\mathfrak{D}_\alpha]_{vw}Q_{wu}) = 0. \qquad (3.21)$$

Now we assume the bases ψ and φ to be decomposed into identical equivalent irreducible representations $\mathfrak{D}^\mu_\alpha$ of $\mathcal{S}_r$. Then Eq. (3.21) reads

$$\begin{bmatrix} \mathfrak{D}^\mu_\alpha & 0 & \cdots & 0 \\ 0 & \mathfrak{D}^\mu_\alpha & \cdots & \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 0 & & \cdots & \mathfrak{D}^\mu_\alpha \end{bmatrix} \begin{bmatrix} Q'_{11} & Q'_{12} & \cdots & Q'_{1g} \\ Q'_{21} & Q'_{22} & \cdots & \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ Q'_{g1} & \cdots & & Q'_{gg} \end{bmatrix}$$
$$- \begin{bmatrix} Q'_{11} & Q'_{12} & \cdots & Q'_{1g} \\ Q'_{21} & Q'_{22} & \cdots & \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ Q'_{g1} & \cdots & & Q'_{gg} \end{bmatrix} \begin{bmatrix} \mathfrak{D}^\mu_\alpha & 0 & \cdots & 0 \\ 0 & \mathfrak{D}^\mu_\alpha & \cdots & \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 0 & \cdots & & \mathfrak{D}^\mu_\alpha \end{bmatrix} = 0,$$

where Q'_{fh} are submatrices conforming to the irreducible representation matrices $\mathfrak{D}^\mu_\alpha$. This yields

$$\{\mathfrak{D}^\mu_\alpha Q'_{1j} - Q'_{1j}\mathfrak{D}^\mu_\alpha = 0\}_{j=1,2,\cdots m},$$
$$\{\mathfrak{D}^\mu_\alpha Q'_{2j} - Q'_{2j}\mathfrak{D}^\mu_\alpha = 0\}_{j=1,2,\cdots m},$$
$$\cdot$$
$$\cdot$$
$$\cdot$$
$$\{\mathfrak{D}^\mu_\alpha Q'_{gj} - Q'_{gj}\mathfrak{D}^\mu_\alpha = 0\}_{j=1,2,\cdots m},$$

so by Schur's lemma

$$Q = \begin{bmatrix} \mu_{11}I & \mu_{12}I & \cdots & \mu_{1g}I \\ \mu_{21}I & \mu_{22}I & \cdots & \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ \mu_{g1}I & \cdots & & \mu_{gg}I \end{bmatrix} \qquad (3.22)$$

Since the permutation group constituents of a symmetrized tensor basis do not intersect, then we only couple states belonging to identical sets of index values. Thus Eq. (3.22) is valid for the permutation group constituents of each set of index values. In general μ_{fh} may depend on index value. These results mean we can obtain simple couplings by recoupling in the same way all pairs of corresponding states of a pair of symmetrized tensor bases providing identical representations of $\mathcal{S}_r$. These conclusions are also valid for symmetrized tensor bases of the underlying matrix group because of the way such bases have been shown to be composed. The representations with a simply-coupled form need not be orthogonal; but they are if the states of the constituent representations are orthogonal. One would certainly seek such orthogonality.

The problem of recoupling bases to obtain a simply-coupled form has been simplified and we now see how it reduces to solving linear equations. Table III gives the Hermitian products of the states shown. Only states with distinct indices were entered because the simply-coupled form of such states implies a simply-coupled form for the states with repeated indices. For the resulting linear equations we seek two solutions $(a, b)_1$ and $(a, b)_2$, one which makes all entries of the first three columns vanish and one which makes all entries of the last three columns vanish. Discarding the trivial solution which makes all entries of all columns vanish, the solutions sought are $a, b = 1, -1$ and $a, b = 1, 1$. In matrix form this recoupling appears as

$$[A_1(ijk), A_2(ijk), B_1(ijk), B_2(ijk)] \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$$
$$= [A_1(ijk) + B_1(ijk), A_2(ijk) + B_2(ijk),$$
$$A_1(ijk) - B_1(ijk), A_2(ijk) - B_2(ijk)].$$

This recoupling matrix is seen to have the form given by Eq. (3.22). After entering appropriate index values, these states still do not quite agree with those of Eqs. (3.20a) and (3.20b) because the states of Eqs.

(3.20a) and (3.20b) have been further modified to make isospin multiplets orthogonal. Making such a modification before recoupling does not affect the validity of the recoupling theorem [Eq. (3.22)] because both equivalent representations are modified in the same way. The availability of such orthogonal states in a simply-coupled form allows us to use tensor methods to obtain Clebsch–Gordan coefficients for the reduction of any Kronecker product of symmetrized tensor representations. Recoupling matrix solutions obtained using Hermitian products also apply to those nonunitary classical groups whose tensors decompose in the same way as those of $U(n)$.

Since the $SU(n)$ generators can be mapped one-to-one onto the states of the $SU(n)$ adjoint representation,[21] then reducing a Kronecker product of adjoint representations results in certain tensor operators being obtained as generator polynomials. This can be carried out by tensor methods because all representations of $SU(n)$ appear as tensor representations.

We now return to the proof of Eqs. (3.4). First we note that the proof of the recoupling theorem required only that all initial (final) bases provided identical representations of S_r [and $GL(n, c)$] and that the initial and final representations were identical. Thus starting with a set of bases which provide identical representations [Eqs. (2.8)] and have identical inner product structures [Eqs. (3.3) provide this; actually only inner product structures which are identical up to a factor are needed], we can recouple such bases to obtain the condition where bases of distinct (identical) representations are orthogonal to each other (without necessarily having a simply-coupled form) and within each basis the inner product structure is the same. The existence of orthogonal bases providing identical representations is assured by the fact that, due to the complete reducibility of all representations of S_r, a transformation making equivalent representations mutually orthogonal is independent of that making equivalent representations identical. Now invert this process by starting with the final set of bases and recouple them to recover the initial bases given by Eqs. (2.8). Because the final bases are orthogonal to each other and have a common inner product structure, then it is clear that they recouple back to yield bases which satisfy both Eqs. (3.3) and (3.4).

CONCLUSIONS

The tensor symmetrization procedure derived in Ref. 1 is shown to support rather than disprove Weyl's tensor symmetrization theorem. This extended symmetrization procedure is shown to be more useful than Weyl's approach because it organizes the states and can be usefully generalized. The generalizations described are extended symmetrization procedures using modified Young symmetrizers and Wigner projection operators.

The bases obtained from modified Young symmetrizers do not in general seem sufficiently organized to be useful, but the fact that a tensor can always be Peirce-resolved with these symmetrizers will, in a subsequent publication, be shown to have an important application. The orthogonal states obtained with unitary representation Wigner projection operators are shown to be not usually those desired and also one is then required to obtain and use all $r!$ group matrices in order to form the Wigner projection operators.

The state organization provided by Eqs. (2.8) makes it possible to show that such symmetrized tensors can easily be made orthogonal. The state organization [Eqs. (2.8) or (2.12)] shows that bases having Kronecker product form can be obtained with recoupling coefficients which do not depend on individual states within the representations.

Group matrices and Lie group generators are obtained by tensor methods. In particular, tensor methods based on Young symmetrizers are shown to be useful because, using Eqs. (3.3) and (3.4), such tensors can easily be made orthogonal.

In addition to the usual orthogonality relations provided by the unitary Wigner projection operator algebra,[22] an additional orthogonality relation [Eq. (3.2)] is obtained for bases "projected" out of an orthogonal tensor.

Note added in proof:

Lemma: On Cartesian tensors $T'_{i_1 \cdots i_r}$, $T''_{i_1 \cdots i_r}, \cdots$ we construct bases $\{A'\}$, $\{A''\}, \cdots$ of equivalent irreducible representations of S_r. Some of these bases may coincide, but otherwise they do not intersect.

Proof. The bases $\{A'\}$, $\{A''\}, \cdots$ cannot intersect the basis of an inequivalent irreducible representation of S_r and so must span $\{A'\} + \{A''\} + \cdots$, where the sums are direct except for those members which coincide.

Theorem 1: For bases $\{A\}$, $\{B\}, \cdots, \{D\}$ (of equivalent representations) constructed on a non-Cartesian tensor according to Eqs. (2.8) we find

$$\langle A_t \mid A_f \rangle = \zeta(A, B)\langle B_t \mid B_f \rangle = \cdots = \zeta(A, D)\langle D_t \mid D_f \rangle;$$

[21] G. E. Baird and L. C. Biedenharn, J. Math. Phys. 5, 1731 (1964).

[22] R. D. Poshusta and F. A. Matsen, J. Math. Phys. 7, 711 (1966).

ζ is always independent of state labels t and f and also independent of index values.

Proof. Writing $T_{i_1\cdots i_r} = T'_{j_1\cdots j_r} + T''_{k_1\cdots k_r} + \cdots$ to expand a non-Cartesian tensor in terms of Cartesian tensors and symmetrizing according to Eqs. (2.8), we obtain the bases (of equivalent representations):

$$\{A\} = \{A'\} + \{A''\} + \cdots,$$
$$\{B\} = \{B'\} + \{B''\} + \cdots,$$
$$\cdot$$
$$\cdot$$
$$\cdot$$
$$\{D\} = \{D'\} + \{D''\} + \cdots,$$

so that

$$\langle A_t \mid A_f\rangle = \langle A'_t \mid A'_f\rangle + \langle A''_t \mid A''_f\rangle + \cdots + \langle A'_t \mid A''_f\rangle + \cdots,$$
$$\langle B_t \mid B_f\rangle = \langle B'_t \mid B'_f\rangle + \langle B''_t \mid B''_f\rangle + \cdots + \langle B'_t \mid B''_f\rangle + \cdots,$$
$$\cdot$$
$$\cdot$$
$$\cdot$$
$$\langle D_t \mid D_f\rangle = \langle D'_t \mid D'_f\rangle + \langle D''_t \mid D''_f\rangle + \cdots + \langle D'_t \mid D''_f\rangle + \cdots.$$

By Eqs. (3.3) we have

$$\langle A'_t \mid A'_f\rangle = \langle B'_t \mid B'_f\rangle = \cdots = \langle D'_t \mid D'_f\rangle,$$
$$\langle A''_t \mid A''_f\rangle = \langle B''_t \mid B''_f\rangle = \cdots = \langle D''_t \mid D''_f\rangle,$$

etc. By the preceding lemma either $\{A'\}$ coincides with $\{A''\}$ [hence $\langle A'_t \mid A''_f\rangle = \langle A'_t \mid A'_f\rangle$] or else $\{A'\}$ and $\{A''\}$ do not intersect and [by Eqs. (3.3)] we have $\langle A'_t \mid A''_f\rangle\lambda(A', A'') = \langle A'_t \mid A'_f\rangle$. This argument can be applied to all cross terms to prove the theorem.

Theorem 2: Equations (3.4) also apply to a set of bases (of equivalent representations) obtained by symmetrizing non-Cartesian tensors according to Eqs. (2.8). The numbers $\lambda(A, B)$, etc., which appear in Eqs. (3.4) will depend on the initial tensor.

Proof. The proof follows by essentially the same method as that used for Theorem 1.

APPENDIX

The usual Young symmetrizers of the standard tableaux are also generating units for linearly independent minimal right ideals which span the permutation group ring. The right ideal bases $\{(PQ)^\mu_i S_{ij}\}$ yield the linearly independent tensor bases:

First basis

$$\{(PQ)^\mu_1 S_{1j} T_{i_1\cdots i_r}\}_{j=1,2,\cdots m};$$

Second basis

$$\{(PQ)^\mu_2 S_{2j} T_{i_1\cdots i_r}\}_{j=1,2,\cdots m};$$

$$\cdot$$
$$\cdot$$
$$\cdot$$

mth basis ($m = N^\mu$)

$$\{(PQ)^\mu_m S_{mj} T_{i_1\cdots i_r}\}_{j=1,2,\cdots m}.$$

Using Eq. (2.5), the kth and gth bases are related as

$$S_{gk}(PQ)^\mu_k S_{kj} T_{i_1\cdots i_r} = (PQ)^\mu_g S_{gj} T_{i_1\cdots i_r},$$

so here the operator S_{gk} permutes indices as a function of their position in the initial Cartesian tensor. Because these states are formed with right instead of left ideals, the operation L_α of $\mathfrak{S}_r$ on state $(PQ)^\mu_i S_{ij} T_{i_1\cdots i_r}$ appears as $(PQ)^\mu_i S_{ij} L_\alpha T_{i_1\cdots i}$. These operators L_α thus have the effect of permuting the indices of the Cartesian constituents of the initial tensor as a function of their symmetrized tensor position.

The right ideal version of Weyl's theorem is to apply a single Young symmetrizer to the n^r tensors obtained by entering all arrangements of each set of index values into an initial tensor form.

All results in this appendix as well as the corresponding results in Sec. 2 can be given equivalently in terms of QP Young symmetrizers.