REVIEWS OF MODERN PHYSICS VOLUME 34, NUMBER 4 OCTOBER 1962

The Wigner Distribution Function and Second Quantization in Phase Space*

WESLEY E. BRITTIN AND WILLARD R. CHAPPELL†
University of Colorado, Boulder, Colorado

I. INTRODUCTION

IN 1932 Wigner described a quantum mechanical phase space distribution function.[1] This function, which depends upon the coordinates and momenta of the particles comprising a given system, has the remarkable property that it can be used to calculate a class of quantum mechanical averages in the same manner as the classical phase space distribution function is used to calculate classical averages. One merely multiplies the distribution function and the classical phase space function whose average is desired, and then integrates the product over the entire phase space. Wigner has pointed out that his function is not unique, but it does have the property of being real and is in a certain sense the simplest and most natural quantum analog of the classical phase space distribution function. The Wigner distribution function has been used in a number of investigations, especially in investigations of the quantum theory of transport phenomena.[2–9]

Klimontovich[10] introduced phase space operators (actually quantum fields in phase space) which have the property that their expectation values are Wigner distribution functions.

Schönberg[11,12] has discussed the second quantization of the classical Liouville equation, but as is well known, this "quantization" has nothing to do with Planck's quantum of action. It does, however, enable one to treat classical statistical mechanics in a manner which is independent of the number of particles. Since in this review we are interested in quantum statistical mechanics, we shall not discuss this brand of second quantization further.

The purpose of this review is to introduce the phase space operators for a system of particles in a natural way, to show various relationships satisfied by them, to show their relation to the Wigner distribution function, and finally to consider distribution functions for a system of charged particles including the quantized electromagnetic field.

II. CLASSICAL THEORY

We consider a system of N identical particles interacting via two-body forces. The classical Hamiltonian is taken to be

$$H = \sum_{i=1}^{N} \mathbf{p}_i^2/2m + \sum_{i<j} V(i,j) , \qquad \text{(II.1)}$$

where $\mathbf{p}_i$ is the linear momentum of the ith particle and $V(i,j) = V(|\mathbf{r}_i - \mathbf{r}_j|)$ is the potential energy of interaction between the ith and jth particles. If $\mathbf{r}_i(t)$ and $\mathbf{p}_i(t)$ are solutions of the equations of motion corresponding to the Hamiltonian (II.1) we may define an exact microscopic one-particle density function f_1 by means of the expression

$$f_1(\mathbf{r},\mathbf{p},t) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))\delta(\mathbf{p} - \mathbf{p}_i(t)) , \qquad \text{(II.2)}$$

where δ is the three-dimensional Dirac delta function. One may think of f_1 as a Heisenberg operator for the one particle distribution function. It is a function of $\mathbf{r}$, $\mathbf{p}$, t, and the initial coordinates and momenta $\mathbf{r}_i^0$, $\mathbf{p}_i^0$. Its average value or expectation value is determined by the state of the system, which can be specified by a distribution function $f_N(\mathbf{r}_1^0,\cdots,\mathbf{r}_N^0;\mathbf{p}_1^0,\cdots\mathbf{p}_N^0)$. Thus,

$$\langle f_1(\mathbf{r},\mathbf{p},t)\rangle = \int f_1 f_N d\Omega_0 , \qquad \text{(II.3)}$$

where $d\Omega_0 = d\mathbf{r}_1^0\cdots d\mathbf{r}_N^0 d\mathbf{p}_1^0\cdots d\mathbf{p}_N^0$, and the integra-

* Research sponsored by Aeronautical Research Laboratory, Office of Aerospace Research, U. S. Air Force.
† Present Address, Harvard University, Cambridge, Massachusetts.
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[8] Yu. L. Klimontovich and S. V. Temko, Soviet Phys.—JETP **6**, 102 (1958).
[9] Yu. L. Klimontovich and V. P. Silin, Uspehki Fiz. Nauk **70**, 247 (1960).
[10] Yu. L. Klimontovich, Soviet Phys.—JETP **6**, 753 (1958).
[11] M. Schönberg, Nuovo cimento **9**, 1139 (1952).
[12] M. Schönberg, Nuovo cimento **10**, 419 (1953).

tion extends over the entire range of the indicated variables. Gross[13] has emphasized the distinction one should make between microscopic variables and macroscopic variables. We have not as yet introduced any statistical *ansatz* which would destroy the reversible nature of our equations. In fact, the time dependence of f_1 can be shifted to f_N (Schrödinger picture) with the result that (II.3) becomes the usual integral of $f_N(t)$ integrated over all but one set of phase space variables (actually it is also symmetrized and multiplied by N). This paper will be concerned mainly with the exact microscopic description, and we shall not discuss the interesting question of irreversibility. The formulation, however, lends itself very easily to such considerations.

If Eq. (II.2) is integrated over momentum space, there results

$$n_1(\mathbf{r},t) = \int f_1(\mathbf{r},\mathbf{p},t)d\mathbf{p} = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) \,, \quad \text{(II.4)}$$

which is the density operator in ordinary space. If n_1 is integrated over $\mathbf{r}$, there results the normalization condition

$$N = \int n_1(\mathbf{r},t)d\mathbf{r} \,. \qquad \text{(II.5)}$$

In a similar manner one can introduce higher order distribution functions. For example, f_2 is defined by

$$f_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}',t) = \sum_{i\neq j} \delta(\mathbf{r} - \mathbf{r}_i)\delta(\mathbf{r}' - \mathbf{r}_j) \times \delta(\mathbf{p} - \mathbf{p}_i)\delta(\mathbf{p}' - \mathbf{p}_j) \,, \quad \text{(II.6)}$$

and has the following properties:

$$\int f_2 d\mathbf{r}'d\mathbf{p}' = (N-1)f_1(\mathbf{r},\mathbf{p},t) \,, \qquad \text{(II.7)}$$

and

$$f_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}',t) = f_1(\mathbf{r},\mathbf{p},t)f_1(\mathbf{r}',\mathbf{p}',t) - \delta(\mathbf{r} - \mathbf{r}')\delta(\mathbf{p} - \mathbf{p}')f_1(\mathbf{r},\mathbf{p},t) \,. \quad \text{(II.8)}$$

The equation of motion for f_1 can be obtained from those of $\mathbf{r}_i$ and $\mathbf{p}_i$, and if one uses the properties of δ functions one finds directly that

$$\frac{\partial f_1}{\partial t} + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{r}} f_1 = \int \frac{\partial}{\partial \mathbf{r}} V(\mathbf{r} - \mathbf{r}') \times \frac{\partial}{\partial \mathbf{p}} f_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}',t)d\mathbf{r}'d\mathbf{p}' \,. \quad \text{(II.9)}$$

Equation (II.9), which was obtained by Klimontovich[10] and by Gross,[13] has precisely the form of the first member of the BBKGY hierarchy. Since Eq. (II.9) is linear in the distribution functions, the first member of the hierarchy can be obtained by forming its expectation value:

$$\frac{\partial}{\partial t}\langle f_1\rangle + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{r}}\langle f_1\rangle = \int \frac{\partial}{\partial \mathbf{r}} V(\mathbf{r} - \mathbf{r}') \times \frac{\partial}{\partial \mathbf{p}} \langle f_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}',t)\rangle d\mathbf{r}'d\mathbf{p}' \,. \quad \text{(II.10)}$$

However, if f_2 from (II.8) is substituted into (II.9), there results the following expression which involves f_1 alone:

$$\frac{\partial f_1}{\partial t} + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial \mathbf{r}} f_1 = \int \frac{\partial}{\partial \mathbf{r}} V(\mathbf{r} - \mathbf{r}') \times \frac{\partial}{\partial \mathbf{p}} f_1(\mathbf{r},\mathbf{p},t)f_1(\mathbf{r}',\mathbf{p}',t)d\mathbf{r}'d\mathbf{p}' \,. \quad \text{(II.11)}$$

Equation (II.11) has the form of the collisionless Boltzmann equation. However, as was pointed out by Gross,[13] it has an extremely rich variety of solutions. In fact, among its solutions are those corresponding to the exact N-body dynamical problem for arbitrary N.

If one includes the electromagnetic field, one finds in a similar manner that the one-particle exact distribution function is coupled to the electromagnetic field through the Vlasov equations.[14] Further, these coupled equations have among their solutions those corresponding to the exact N-particle electrodynamic problem for arbitrary N.

We shall show in parts III and IV that the classical results considered here have analogous counterparts in quantum theory.

III. QUANTUM THEORY: PARTICLES

If one wishes to find the quantum mechanical operator corresponding to $f_1(\mathbf{r},\mathbf{p},t)$, the natural assumption would be to replace $\mathbf{r}_i$ and $\mathbf{p}_i$ in (II.1) by quantum mechanical operators satisfying the customary commutation relations

$$[\mathbf{r}_{i\alpha},\mathbf{r}_{j\beta}] = 0 \,, \; [\mathbf{p}_{i\alpha},\mathbf{p}_{j\beta}] = 0 \,, \quad \text{and} \quad [\mathbf{r}_{i\alpha},\mathbf{p}_{j\beta}] = i\delta_{ij}\delta_{\alpha\beta} \,. \qquad \text{(III.1)}$$

In the above expressions α, β refer to Cartesian components of 3-vectors, and we have used units for which $\hbar$ is unity. Since $\mathbf{r}_i$ and $\mathbf{p}_i$ do not commute, there is an immediate difficulty in trying to define the operator corresponding to f_1. However, Weyl[15] has given a procedure for forming the quantum mechanical operator corresponding to a wide class

[13] E. P. Gross, J. Nuclear Energy, **C2**, 173 (1961).

[14] Yu. L. Klimontovich, Soviet Phys.—JETP **7**, 119 (1958).

[15] H. Weyl, *Theory of Groups and Quantum Mechanics* (Methuen and Company, Ltd., London, England, 1932), p. 275.

of classical functions. Weyl's procedure consists of Fourier expanding the corresponding classical function and then replacing $\mathbf{r}_i$ and $\mathbf{p}_i$ in the exponentials by the relevant quantum mechanical operators. We imagine the system to be enclosed in a box of volume V, so that the δ functions may be expanded as

$$\delta(\mathbf{r}-\mathbf{r}_i) = V^{-1}\sum\nolimits_{\mathbf{k}} \exp[i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_i)]\,, \quad \text{(III.2)}$$

and

$$\delta(\mathbf{p}-\mathbf{p}_i) = (2\pi)^{-3}\int d\mathbf{l}\exp[i\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}_i)]\,, \quad \text{(III.3)}$$

where $\mathbf{k}=2\pi\mathbf{n}/V^{1/3}$ and $\mathbf{n}$ is a vector with integral components.

The classical expression for f_1 is then given by

$$f_1(\mathbf{r},\mathbf{p}) = (2\pi)^{-3}V^{-1}\sum_{i=1}^{N}\sum_{\mathbf{k}}\int d\mathbf{l} \times \exp i[\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_i)+\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}_i)]\,. \quad \text{(III.4)}$$

In the Schrödinger picture $\mathbf{r}_j$ remains the same, and $\mathbf{p}_j$ is replaced by $-i\boldsymbol{\nabla}_j$. The quantum mechanical expression for f_1 can now be written

$$\hat{f}_1(\mathbf{r},\mathbf{p}) = (2\pi)^{-3}V^{-1}\sum_{j=1}^{N}\sum_{\mathbf{k}}\int d\mathbf{l} \times \exp i[\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_j)+\mathbf{l}\cdot(\mathbf{p}+i\boldsymbol{\nabla}_j)]\,. \quad \text{(III.5)}$$

This operator is Hermitian, but it is not positive definite. If we use McCoy's theorem,[16] $\hat{f}_1$ may be written

$$\hat{f}_1(\mathbf{r},\mathbf{p}) = \sum_{j=1}^{N}\hat{f}_1(j)\,, \quad \text{(III.6)}$$

where

$$\hat{f}_1(j) \equiv (2\pi)^{-3}V^{-1}\int d\mathbf{l}\sum_{\mathbf{k}} \times \exp i[\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_j)+\mathbf{l}\cdot(\mathbf{p}+\mathbf{k}/2)] \times \exp(-\mathbf{l}\cdot\boldsymbol{\nabla}_j)\,. \quad \text{(III.7)}$$

Higher order distribution operators can be defined. For example, $\hat{f}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')$ is given by

$$\hat{f}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}') = \sum_{i\neq j}\hat{f}_2(i,j) \quad \text{(III.8)}$$

where

$$\hat{f}_2(i,j) = (2\pi)^{-6}V^{-2}\iint d\mathbf{l}d\mathbf{l}'\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\exp i[\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_i)+\mathbf{k}'\cdot(\mathbf{r}'-\mathbf{r}_j) + \mathbf{l}\cdot(\mathbf{p}+\mathbf{k}/2)+\mathbf{l}'\cdot(\mathbf{p}'+\mathbf{k}'/2)]\exp[-(\mathbf{l}\cdot\boldsymbol{\nabla}_i+\mathbf{l}'\cdot\boldsymbol{\nabla}_j)]\,. \quad \text{(III.9)}$$

The operators $\hat{f}_1$ and $\hat{f}_2$ introduced above are not in a form which is convenient for manipulation. We, therefore, transform them using the method of second quantization. Let $\psi(\mathbf{r})$ be the quantized wave field for the particles. Then, for fermions, ψ and its adjoint $\psi^\dagger$ satisfy the following anticommutation relations:

$$\{\psi(\mathbf{r}),\psi(\mathbf{r}')\}_+ = \{\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')\}_+ = 0\,,$$
$$\text{and}\quad \{\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')\}_+ = \delta(\mathbf{r}-\mathbf{r}')\,, \quad \text{(III.10)}$$

where the spin indices have been suppressed. The operator $\hat{f}_1$ in second-quantized form is then simply

$$\hat{f}_1(\mathbf{r},\mathbf{p}) = \int\psi^\dagger(\mathbf{r}_1)\hat{f}_1(1)\psi(\mathbf{r}_1)d\mathbf{r}_1 \quad \text{(III.11)}$$

$$= (2\pi)^{-3}\int d\mathbf{l}\exp[i\mathbf{p}\cdot\mathbf{l}]\,\psi_\alpha^\dagger(\mathbf{r}+\mathbf{l}/2)\psi_\alpha(\mathbf{r}-\mathbf{l}/2)\,, \quad \text{(III.12)}$$

where repeated indices indicate summation over the index. The operator (III.12) is expressed in the form used by Klimontovich.[10]

Similarly $\hat{f}_2$ may be written as

$$\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}') = (2\pi)^{-6}\iint d\mathbf{l}d\mathbf{l}'\exp i(\mathbf{p}\cdot\mathbf{l}+\mathbf{p}'\cdot\mathbf{l}') \times \psi_\alpha^\dagger(\mathbf{r}+\mathbf{l}/2)\psi_\beta^\dagger(\mathbf{r}'+\mathbf{l}'/2)\psi_\beta(\mathbf{r}'-\mathbf{l}'/2)\psi_\alpha(\mathbf{r}-\mathbf{l}/2)\,, \quad \text{(III.13)}$$

and in general, the N-particle phase space density is expressed by

$$\hat{f}_N(\mathbf{r}',\mathbf{r}^2,\cdots,\mathbf{r}^N;\mathbf{p}',\mathbf{p}^2,\cdots,\mathbf{p}^N) = (2\pi)^{-3N}\int\cdots\int d\mathbf{l}'\cdots d\mathbf{l}^N\exp i\left(\sum_{j=1}^{N}\mathbf{p}^j\cdot\mathbf{l}^j\right)$$
$$\times\,\psi_{\alpha'}^\dagger(\mathbf{r}'+\mathbf{l}'/2)\psi_{\alpha^2}^\dagger(\mathbf{r}^2+\mathbf{l}^2/2)\cdots\psi_{\alpha^N}^\dagger(\mathbf{r}^N+\mathbf{l}^N/2)$$
$$\times\,\psi_{\alpha^N}(\mathbf{r}^N-\mathbf{l}^N/2)\psi_{\alpha^{N-1}}(\mathbf{r}^{N-1}-\mathbf{l}^{N-1}/2)\cdots\psi_{\alpha'}(\mathbf{r}'-\mathbf{l}'/2)\,. \quad \text{(III.14)}$$

[16] N. H. McCoy, Proc. Natl. Acad. Sci. U. S. 18, 674 (1932).

If considerations of spin become important, one may define distribution functions which depend explicitly upon the spin; e.g., one can define

$$\hat{f}_{1\alpha\beta}(\mathbf{r},\mathbf{p}) = (2\pi)^{-3}\int \exp\,[i\mathbf{p}\cdot\mathbf{l}]\,\psi_\alpha^\dagger(\mathbf{r}+1/2) \times \psi_\beta\,(\mathbf{r}-1/2)d\mathbf{l}\,, \tag{III.15}$$

etc.

The relation between the operators $\hat{f}$ and the Wigner distribution functions f_W can now be established directly. Consider the expectation value of $\psi_\alpha{}^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}')$:

$$\langle\psi_\alpha^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}')\rangle \equiv \mathrm{Tr}\,\{\rho\psi_\alpha^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}')\}\,, \tag{III 16}$$

where ρ is the statistical operator which represents the state of the system. The trace can be evaluated conveniently if one makes use of the complete set of states $|x_1\cdots x_N\rangle$, where x_i stands for both coordinates and spin, and $N = 0,1,2,\cdots$. If we make use of the cylic invariance of the trace, we obtain the following expression:

$$\langle\psi_\alpha^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}')\rangle = \sum_N \int\cdots\int dx_1\cdots dx_N \times \langle x_1\cdots x_N|\psi_\beta(\mathbf{r}')\rho\psi_\alpha^\dagger(\mathbf{r})|x_1\cdots x_N\rangle\,, \tag{III.17}$$

where $\int dx$ represents spin summation and space integration. If the well-known expressions,[17]

$$\psi^\dagger(\mathbf{r})|x_1\cdots x_N\rangle = (N+1)^{1/2}|xx_1\cdots x_N\rangle$$

and

$$\langle x_1\cdots x_N|\psi(\mathbf{r}') = (N+1)^{1/2}\rangle x'x_1\cdots x_N| \tag{III.18}$$

are substituted into (III.17), the result is the following expression:

$$\langle\psi_\alpha^\dagger(\mathbf{r})\psi_\beta(\mathbf{r}')\rangle = \sum_N (N+1)\int\cdots\int dx_1\cdots dx_N \times \langle\mathbf{r}'\beta,x_1,\cdots,x_N|\rho|\mathbf{r}\alpha,x_1,\cdots,x_N\rangle \tag{III.19}$$

$$= \langle\mathbf{r}'\beta|\rho_1|\mathbf{r}\alpha\rangle\,, \tag{III.20}$$

which is the one-particle density matrix. We note that if $\mathrm{Tr}\rho = 1$, then ρ_1 has the normalization

$$\int\langle x|\rho_1|x\rangle dx = \langle\hat{N}\rangle\,. \tag{III.21}$$

The expectation value of (III.15), therefore, may be written

$$\langle\hat{f}_1(\mathbf{r},\mathbf{p})\rangle = (2\pi)^{-3}\int d\mathbf{l}\,\exp\,[i\mathbf{p}\cdot\mathbf{l}] \times \sum_\alpha \langle\mathbf{r}-1/2,\alpha|\rho_1|\mathbf{r}+1/2)\alpha\rangle \equiv f_{1W}(\mathbf{r},\mathbf{p})\,. \tag{III.22}$$

Similar arguments show that

$$\langle\hat{f}_N\rangle = f_{NW}\,. \tag{III.23}$$

If the expression for $\hat{f}_2$ is integrated with respect to $\mathbf{r}',\mathbf{p}'$, the result is

$$\int\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')d\mathbf{r}'d\mathbf{p}' = (\hat{N}-1)\hat{f}_1(\mathbf{r},\mathbf{p}) = \hat{f}_1(\mathbf{r},\mathbf{p})(\hat{N}-1)\,, \tag{III.24}$$

where $\hat{N}$, the total particle number operator, is given by

$$\hat{N} = \int\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'\,. \tag{III.25}$$

The operators $\hat{f}_1(\mathbf{r},\mathbf{p})$ and $\hat{f}_1(\mathbf{r}',\mathbf{p}')$ do not commute unless the phase space points $\mathbf{r},\mathbf{p}$ and $\mathbf{r}',\mathbf{p}'$ are the same. The commutator, $[f_1(\mathbf{r},\mathbf{p}),f_1(\mathbf{r}',\mathbf{p}')]$, may be expressed as

$$\begin{aligned}[f_1(\mathbf{r},\mathbf{p}),f_1(\mathbf{r}',\mathbf{p}')] &\equiv C_1(\mathbf{r}-\mathbf{r}',\mathbf{p}-\mathbf{p}')\\ &= (2\pi)^{-6}\int d\mathbf{l}\{\exp i[\mathbf{p}\cdot\mathbf{l}+\mathbf{p}'\cdot(2\mathbf{r}-2\mathbf{r}'-1)]\psi^\dagger(\mathbf{r}+1/2)\psi(2\mathbf{r}'-\mathbf{r}+1/2)\\ &\quad-\exp i[\mathbf{p}\cdot\mathbf{l}+\mathbf{p}'\cdot(2\mathbf{r}'-2\mathbf{r}-1)]\psi^\dagger(2\mathbf{r}'-\mathbf{r}-1/2)\psi(\mathbf{r}-1/2)\}\,.\end{aligned} \tag{III.26}$$

The commutator C_1 is complicated, but can be expressed linearly in terms of $\hat{f}_1$. However, we shall not have explicit need for C_1, so shall not write it in a different form. The lack of commutation of $\hat{f}_1$'s at different points in phase space is a reflection of the uncertainty principle.

As in the classical case, $\hat{f}_2$ can be expressed completely in terms of $\hat{f}_1$. If we write

$$\hat{f}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}') = \hat{f}_1(\mathbf{r},\mathbf{p})\hat{f}_1(\mathbf{r}',\mathbf{p}') + \hat{g}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')\,, \tag{III.27}$$

we find that $\hat{g}_2$ is given by

$$\hat{g}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}') = -(2\pi)^{-6}\exp\,[2i\mathbf{p}'\cdot(\mathbf{r}-\mathbf{r}')]\iint d\mathbf{l}d\mathbf{p}'' \exp i[\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}')-2\mathbf{p}''\cdot(\mathbf{r}-\mathbf{r}')]\hat{f}_1(\mathbf{r}'+1/2,\mathbf{p}'')\,. \tag{III.28}$$

[17] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson & Company, Evanston, Illinois, 1961), p. 139.

For some problems it is convenient to transform $\psi(\mathbf{r})$ to momentum space:

$$\psi(\mathbf{r}) = (2\pi)^{-3/2}\int \exp\,[i\mathbf{p}\cdot\mathbf{r}]\,a_S(\mathbf{p})\chi^{(S)}\,, \quad \text{(III.29)}$$

and

$$\psi^\dagger(\mathbf{r}) = (2\pi)^{-3/2}\int \exp\,[-i\mathbf{p}\cdot\mathbf{r}]\,a_S^\dagger(\mathbf{p})\chi^{(S)\dagger}\,. \quad \text{(III.30)}$$

If (III.29) and (III.30) are used in place of ψ and $\psi^\dagger$ and $\hat{f}_1$, integration over $\mathbf{r}$ can be carried out with the result

$$\int \hat{f}_1(\mathbf{r},\mathbf{p})d\mathbf{r} = \hat{\phi}_1(\mathbf{p}) = a_S^\dagger(\mathbf{p})a_S(\mathbf{p})\,, \quad \text{(III.31)}$$

a result that was to be expected for the momentum space distribution function. The expression which is dual to (III.31) is

$$\int \hat{f}_1(\mathbf{r},\mathbf{p})d\mathbf{p} = \hat{n}_1(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})\,. \quad \text{(III.32)}$$

Clearly

$$\int a_S^\dagger(\mathbf{p})a_S(\mathbf{p})d\mathbf{p} = \int \psi^\dagger(\mathbf{r})\psi(\mathbf{r})d\mathbf{r} = \hat{N}\,. \quad \text{(III.33)}$$

The distribution functions $\hat{f}$ are useful in expressing any classical phase space function as an operator. For example, if $G_1(\mathbf{r},\mathbf{p})$ is any classical one-particle additive phase space function, the classical phase space density g_1 of G_1 may be expressed by

$$g_1(\mathbf{r},\mathbf{p}) = \sum_{i=1}^{N} G_1(\mathbf{r}_i,\mathbf{p}_i)\delta(\mathbf{r}-\mathbf{r}_i)\delta(\mathbf{p}-\mathbf{p}_i)\,. \quad \text{(III.34)}$$

The quantum mechanical density $\hat{g}_1$ corresponding to g_1 is easily shown to be

$$\hat{g}_1(\mathbf{r},\mathbf{p}) = G_1(\mathbf{r},\mathbf{p})\hat{f}_1(\mathbf{r},\mathbf{p})\,. \quad \text{(III.35)}$$

For a two-particle additive phase space quantity $G_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')$, the phase space density $\hat{g}_2(\mathbf{r},\mathbf{p})$ is

$$\hat{g}_2(\mathbf{r},\mathbf{p}) = \iint d\mathbf{r}'d\mathbf{p}'G_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')\,. \quad \text{(III.36)}$$

The total "amounts" of G_1 and G_2 are simply expressed by the operators

$$\hat{G}_1 = \iint d\mathbf{r}d\mathbf{p}G_1(\mathbf{r},\mathbf{p})\hat{f}_1(\mathbf{r},\mathbf{p})\,, \quad \text{(III.37)}$$

and

$$\hat{G}_2 = \iiiint d\mathbf{r}d\mathbf{r}'d\mathbf{p}d\mathbf{p}'G_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')\,. \quad \text{(III.38)}$$

The expectation value of expressions such as (III.37) and (III.38) gives the familiar result of Wigner,

$$\langle \hat{G}_n \rangle = \int G_n f_W d\Omega\,, \quad \text{(III.39)}$$

which states that the average value of any phase space function, G_n is the integral over an appropriate phase space of the product of the classical expression for G_n and the Wigner distribution function.

The particles are assumed to interact through a two-body potential $V(r_{ij})$, and the Hamiltonian (nonrelativistic) is taken to be

$$H = -\frac{1}{2m}\int \psi_\alpha^\dagger(\mathbf{r}_1)\nabla_{r1}^2\psi_\alpha(\mathbf{r}_1)d\mathbf{r}_1 + \frac{1}{2}\iint \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\beta^\dagger(\mathbf{r}_2)V(\mathbf{r}_{12})\psi_\beta(\mathbf{r}_2)\psi_\alpha(\mathbf{r}_1)d\mathbf{r}_1d\mathbf{r}_2\,. \quad \text{(III.40)}$$

Then the equations of motion of the $\hat{f}_n$'s can be inferred from those of ψ and $\psi^\dagger$ which are

$$i\dot{\psi}(\mathbf{r}) \equiv [\psi(\mathbf{r}),H] = -\frac{\nabla^2}{2m}\psi(\mathbf{r}) + \int d\mathbf{r}'\psi^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) \quad \text{(III.41)}$$

and

$$i\dot{\psi}^\dagger(\mathbf{r}) \equiv [\psi^\dagger(\mathbf{r}),H] = \frac{\nabla^2}{2m}\psi^\dagger(\mathbf{r}) - \int d\mathbf{r}'\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\psi(\mathbf{r}')\,. \quad \text{(III.42)}$$

The resulting equation for $\dot{\hat{f}}_1$ is analogous to the first member of the quantum mechanical hierachy, and is given by

$$\dot{\hat{f}}_1(\mathbf{r},\mathbf{p}) + \frac{\mathbf{p}}{m}\cdot\nabla\hat{f}_1(\mathbf{r},\mathbf{p}) = i(2\pi)^{-3}\int\cdots\int d\mathbf{l}d\mathbf{r}'d\mathbf{p}'d\mathbf{p}''\exp\,[i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{l}] \times [V(\mathbf{r}-\mathbf{r}'+\mathbf{l}/2) - V(\mathbf{r}-\mathbf{r}'-\mathbf{l}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}',\mathbf{p}'')\,. \quad \text{(III.43)}$$

If we substitute $\hat{f}_2$ given by (III.27) and (III.28) into (III.43), we find

$$\dot{\hat{f}}_1(\mathbf{r},\mathbf{p}) + \frac{\mathbf{p}}{m}\cdot\nabla\hat{f}_1(\mathbf{r},\mathbf{p}) = i(2\pi)^{-3}\int\cdots\int d\mathbf{l}d\mathbf{r}'d\mathbf{p}'d\mathbf{p}'' \exp[i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{l}]\,[V(\mathbf{r}-\mathbf{r}'+\mathbf{l}/2) - V(\mathbf{r}-\mathbf{r}'-\mathbf{l}/2)]\hat{f}_1(\mathbf{r},\mathbf{p}')\hat{f}_1(\mathbf{r}',\mathbf{p}'') + Q\hat{f}_1, \quad \text{(III.44)}$$

where

$$Q\hat{f}_1 = i(2\pi)^{-3}\int\cdots\int d\mathbf{l}d\mathbf{r}'d\mathbf{p}'d\mathbf{p}''\exp[i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{l}] \times [V(\mathbf{r}-\mathbf{r}'+\mathbf{l}/2) - V(\mathbf{r}-\mathbf{r}'-\mathbf{l}/2)] \times \hat{g}_2(\mathbf{r},\mathbf{r}',\mathbf{p}',\mathbf{p}''), \quad \text{(III.45)}$$

which may be reduced to the following expression:

$$Q\hat{f}_1 = -i(2\pi)^{-3}\iint d\mathbf{r}'d\mathbf{p}'\exp[-2i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}'] \times [V(2\mathbf{r}') - V(0)]\hat{f}_1(\mathbf{r},\mathbf{p}'). \quad \text{(III.46)}$$

Since $\hat{f}_1$ is Hermitian, and $V(\mathbf{r}) = V(-\mathbf{r})$, it follows that $Q\hat{f}_1$ is skew-Hermitian:

$$(Q\hat{f}_1)^\dagger = -Q\hat{f}_1. \quad \text{(III.47)}$$

Therefore, if we add the Hermitian conjugate of (III.44) to (III.44) and divide by two, we obtain the simple result

$$\dot{\hat{f}}_1 + (\mathbf{p}/m)\cdot\nabla\hat{f}_1 = 2^{-1}(2\pi)^{-3}i\int\cdots\int d\mathbf{l}d\mathbf{r}'d\mathbf{p}'d\mathbf{p}'' \exp[i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{l}]\,[V(\mathbf{r}-\mathbf{r}'+\mathbf{l}/2) - V(\mathbf{r}-\mathbf{r}'-\mathbf{l}/2)] \times \{\hat{f}_1(\mathbf{r},\mathbf{p}'),\hat{f}_1(\mathbf{r}',\mathbf{p}'')\}_+. \quad \text{(III.48)}$$

Equation (III.48) is analogous to the classical expression, equation (II.11), and is quite simple in form considering the complexity of the operators involved. We may consider Eq. (III.48) as an expression for the Heisenberg operator $\hat{f}_1(\mathbf{r},\mathbf{p},t)$, in which case $\dot{\hat{f}}_1$ is interpreted as $\partial\hat{f}_1/\partial t$. Since we can express $\hat{f}_1(\mathbf{r},\mathbf{p},0)$ in the form

$$\hat{f}_1(\mathbf{r},\mathbf{p},0) = (2\pi)^{-3}\int d\mathbf{p}'\exp[i\mathbf{p}'\cdot\mathbf{r}] \times a_s^\dagger(\mathbf{p}+\mathbf{p}'/2)a_s(\mathbf{p}-\mathbf{p}'/2), \quad \text{(III.49)}$$

we can, in principle, solve Eq. (III.48) as an initial value problem. The average value $\langle\hat{f}_1(\mathbf{r},\mathbf{p},t)\rangle$ is determined by the initial distribution function.

IV. QUANTUM THEORY: PARTICLES AND ELECTROMAGNETIC FIELD

We shall next generalize the results obtained to include a system of Fermions interacting with an electromagnetic field. The interaction Hamiltonian will be taken to be the sum of an instantaneous Coulomb part and a particle-transverse photon part. The transverse vector potential $\mathbf{A}(\mathbf{r})$ may be expanded as follows:

$$\mathbf{A}(\mathbf{r}) = (2\pi)^{-3/2}\int d\mathbf{k}(2|\mathbf{k}|)^{-1/2} \times \sum_{m=1}^{2}\{a_m(\mathbf{k})\mathcal{E}^{(m)}(\mathbf{k})\exp[i\mathbf{k}\cdot\mathbf{r}] + a_m^\dagger(\mathbf{k})\mathcal{E}^{(m)*}(\mathbf{k})\exp[-i\mathbf{k}\cdot\mathbf{r}] \quad \text{(IV.1)}$$

where $a_m(\mathbf{k})$ and $a_m^\dagger(\mathbf{k})$ are destruction and creation operators for transverse photons satisfying the commutation relations

$$[a_m(\mathbf{k}),a_n(\mathbf{k}')] = [a_m^\dagger(\mathbf{k}),a_n^\dagger(\mathbf{k}')] = 0, \quad \text{(IV.2)}$$

and

$$[a_m(\mathbf{k}),a_n^\dagger(\mathbf{k}')] = \delta_{mn}\delta(\mathbf{k}-\mathbf{k}').$$

The momentum $\mathbf{\Pi}$ conjugate to $\mathbf{A}$ is given by

$$\mathbf{\Pi}(\mathbf{r}) = i(2\pi)^{-3/2}\int d\mathbf{k}(|\mathbf{k}|/2)^{1/2} \times \sum_{m=1}^{2}\{-a_m(\mathbf{k})\mathcal{E}^{(m)}(\mathbf{k})\exp[i\mathbf{k}\cdot\mathbf{r}] + a_m^\dagger(\mathbf{k})\mathcal{E}^{(m)*}(\mathbf{k})\exp[-i\mathbf{k}\cdot\mathbf{r}]\} \quad \text{(IV.3)}$$

The components of $\mathbf{A}$ and $\mathbf{\Pi}$ satisfy the commutation relations

$$[A_l(\mathbf{k}),A_m(\mathbf{k}')] = [A_l^\dagger(\mathbf{k}),A_m^\dagger(\mathbf{k}')] = [\Pi_l(\mathbf{k}),\Pi_m(\mathbf{k}')] = [\Pi_l^\dagger(\mathbf{k}),\Pi_m^\dagger(\mathbf{k}')] = 0$$

and

$$[A_l(\mathbf{k}),\Pi_m(\mathbf{k}')] = i\delta_{lm}\delta(\mathbf{k}-\mathbf{k}'). \quad \text{(IV.4)}$$

The Hamiltonian for the interacting system can be expressed as follows:

$$H = H_0 + H_I, \quad \text{(IV.5)}$$

where

$$H_0 = -\frac{1}{2m}\int\psi^\dagger(\mathbf{r})\nabla^2\psi(\mathbf{r})d\mathbf{r} + \int[2\pi c^2\Pi^2(\mathbf{r}) + \frac{1}{8\pi}(\nabla\times\mathbf{A}(\mathbf{r}))^2]d\mathbf{r} \quad \text{(IV.6)}$$

and

$$H_I = \frac{ie}{2mc}\int\psi^\dagger(\mathbf{r})\mathbf{A}(\mathbf{r})\cdot\nabla\psi(\mathbf{r})d\mathbf{r} - \frac{ie}{2mc}\int\nabla\psi^\dagger(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})\psi(\mathbf{r})d\mathbf{r} + \frac{e^2}{2mc^2}\int\mathbf{A}^2(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r})d\mathbf{r} + \frac{1}{2}\iint\psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\psi_\beta(\mathbf{r}')\psi_\alpha(\mathbf{r})d\mathbf{r}d\mathbf{r}' - \frac{1}{4\pi c}\iint\nabla\cdot\mathbf{A}(\mathbf{r})V(\mathbf{r}-\mathbf{r}')\nabla\cdot\mathbf{J}(\mathbf{r}')d\mathbf{r}d\mathbf{r}'. \quad \text{(IV.7)}$$

In the above expression $V(\mathbf{r})$ is the Coulomb energy $e^2/|\mathbf{r}|$, and $\mathbf{J}(\mathbf{r})$ is the total current density operator

$$\mathbf{J}(\mathbf{r}) = -(e/2m)\psi^\dagger(\mathbf{r})[i\nabla + (e/c)\mathbf{A}(\mathbf{r})]\psi(\mathbf{r}) + \text{H.c.} \tag{IV.8}$$

The last term is necessary in order that the Hamiltonian lead to the correct equations of motion for $\mathbf{A}(\mathbf{r})$.[18] The transversality condition on $\mathbf{A}(\mathbf{r})$ is reflected in the supplementary condition for admissible states which in the transverse gauge is expressed by

$$\nabla\cdot\mathbf{A}(\mathbf{r})^+|\rangle = 0\,, \tag{IV.9}$$

where the + sign indicates that we retain only the part of the operator having destruction operators. The phase space operators $\hat{f}_1$, etc. are defined in terms of $\psi^\dagger$ and ψ as in Sec. III. It is possible to introduce phase space operators for the transverse photons as has been done by Osborn and Klevans[19] in their treatment of photon transport. The one-photon phase space density operator $\hat{g}_1(\mathbf{r},\mathbf{k})$ may be defined by

$$\hat{g}_1(\mathbf{r},\mathbf{k}) = (2\pi)^{-3}\int d\mathbf{l}\exp[i\mathbf{l}\cdot\mathbf{r}] \times a_m^\dagger(\mathbf{k}+\mathbf{l}/2)a_m(\mathbf{k}-\mathbf{l}/2)\,, \tag{IV.10}$$

with analogous expressions for higher order functions. It is not possible to express the equations of motion of $\hat{f}_1$ and $\hat{g}_1$ solely in terms of $\hat{f}_1$ and $\hat{g}_1$ since terms linear in $a_m(a_m^\dagger)$ appear in the Hamiltonian. Therefore, we shall not consider further the interesting properties of photon density functions.

Apart from terms involving $\nabla\cdot\mathbf{A}(\mathbf{r})$, whose expectation value for admissible states is zero, the equation of motion for $\hat{f}_1(\mathbf{r},\mathbf{p})$ is given by

$$\begin{aligned}
&\dot{\hat{f}}_1(\mathbf{r},\mathbf{p}) + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{r}}\hat{f}_1(\mathbf{r},\mathbf{p}) - \frac{e}{2(2\pi)^3mc}\iint d\mathbf{k}d\mathbf{p}'\exp[i\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')][\mathbf{A}(\mathbf{r}+\mathbf{k}/2)+\mathbf{A}(\mathbf{r}-\mathbf{k}/2)]\cdot\frac{\partial}{\partial\mathbf{r}}\hat{f}_1(\mathbf{r},\mathbf{p}')\\
&+\frac{ie}{(2\pi)^3mc}\iint d\mathbf{k}d\mathbf{p}'\exp[i\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')]\mathbf{p}\cdot[\mathbf{A}(\mathbf{r}+\mathbf{k}/2)-\mathbf{A}(\mathbf{r}-\mathbf{k}/2)]\hat{f}_1(\mathbf{r},\mathbf{p}')\\
&-\frac{ie^2}{2(2\pi)^3mc^2}\iint d\mathbf{k}d\mathbf{p}'\exp[i\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')][\mathbf{A}^2(\mathbf{r}+\mathbf{k}/2)-\mathbf{A}^2(\mathbf{r}-\mathbf{k}/2)]\hat{f}_1(\mathbf{r},\mathbf{p}')\\
&=\frac{i}{(2\pi)^3}\int\cdots\int d\mathbf{k}d\mathbf{r}'d\mathbf{p}'d\mathbf{p}''\exp[i\mathbf{k}\cdot(\mathbf{p}-\mathbf{p}')][V(\mathbf{r}-\mathbf{r}'+\mathbf{k}/2)-V(\mathbf{r}-\mathbf{r}'-\mathbf{k}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}',\mathbf{p}'')\,.
\end{aligned} \tag{IV.11}$$

The operator $\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}',\mathbf{p}'')$ in the above equation can again be replaced by $\frac{1}{2}\{\hat{f}_1(\mathbf{r},\mathbf{p}'),\hat{f}_1(\mathbf{r}',\mathbf{p}'')\}_+$. The second member of the hierarchy is somewhat more complicated than the first, but it involves nothing new in principle and is given by

$$\begin{aligned}
&\dot{\hat{f}}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}') + \frac{\mathbf{p}}{m}\cdot\frac{\partial}{\partial\mathbf{r}}\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}') + \frac{\mathbf{p}'}{m}\cdot\frac{\partial}{\partial\mathbf{r}'}\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}') - \frac{e^2}{2\pi(2)^3mc}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}'')]\\
&\times[\mathbf{A}(\mathbf{r}+\mathbf{l}/2)+\mathbf{A}(\mathbf{r}-\mathbf{l}/2)]\cdot\frac{\partial}{\partial\mathbf{r}}\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}'',\mathbf{p}') - \frac{e^2}{2(2\pi)^3mc}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}'-\mathbf{p}'')]\\
&\times[\mathbf{A}(\mathbf{r}'+\mathbf{l}/2)+\mathbf{A}(\mathbf{r}'-\mathbf{l}/2)]\cdot\frac{\partial}{\partial\mathbf{r}'}\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}'') + \frac{ie}{(2\pi)^3mc}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}'')]\mathbf{p}\cdot\\
&\times[\mathbf{A}(\mathbf{r}+\mathbf{l}/2)-\mathbf{A}(\mathbf{r}-\mathbf{l}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}'',\mathbf{p}') + \frac{ie}{(2\pi)^3mc}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}'-\mathbf{p}'')]\mathbf{p}'\\
&\times[\mathbf{A}(\mathbf{r}'+\mathbf{l}/2)-\mathbf{A}(\mathbf{r}'-\mathbf{l}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}'') - \frac{ie^2}{2(2\pi)^3mc^2}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}'')]\\
&\times[\mathbf{A}^2(\mathbf{r}+\mathbf{l}/2)-\mathbf{A}^2(\mathbf{r}-\mathbf{l}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}'',\mathbf{p}') - \frac{ie^2}{2(2\pi)^3mc^2}\iint d\mathbf{l}d\mathbf{p}''\exp[i\mathbf{l}\cdot(\mathbf{p}'-\mathbf{p}'')]\\
&\times[\mathbf{A}^2(\mathbf{r}'+\mathbf{l}/2)-\mathbf{A}^2(\mathbf{r}'-\mathbf{l}/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}'') - \frac{i}{(2\pi)^6}\int\cdots\int d\mathbf{l}d\mathbf{l}'d\mathbf{p}''d\mathbf{p}'''\exp i[\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}'')+\mathbf{l}'\cdot(\mathbf{p}'-\mathbf{p}''')]\\
&\times[V(\mathbf{r}-\mathbf{r}'+\mathbf{l}/2-\mathbf{l}'/2)-V(\mathbf{r}-\mathbf{r}'-\mathbf{l}/2+\mathbf{l}'/2)]\hat{f}_2(\mathbf{r},\mathbf{r}',\mathbf{p}'',\mathbf{p}''') = \frac{i}{(2\pi)^3}\int\cdots\int d\mathbf{l}d\mathbf{r}''d\mathbf{p}''d\mathbf{p}'''\\
&\times\{\exp[i\mathbf{l}\cdot(\mathbf{p}-\mathbf{p}''')][V(\mathbf{r}-\mathbf{r}''+\mathbf{l}/2)-V(\mathbf{r}-\mathbf{r}''-\mathbf{l}/2)]\hat{f}_3(\mathbf{r},\mathbf{r}',\mathbf{r}'',\mathbf{p}''',\mathbf{p}',\mathbf{p}'')+\exp[i\mathbf{l}\cdot(\mathbf{p}'-\mathbf{p}''')]\\
&\times[V(\mathbf{r}'-\mathbf{r}''+\mathbf{l}/2)-V(\mathbf{r}'-\mathbf{r}''-\mathbf{l}/2)]\hat{f}_3(\mathbf{r},\mathbf{r}',\mathbf{r}'',\mathbf{p},\mathbf{p}''',\mathbf{p}'')\,.
\end{aligned} \tag{IV.12}$$

[18] The authors are indebted to Dr. S. Nakai for valuable discussions and suggestions regarding this point.

[19] R. K. Osborn and E. H. Klevans, Ann. Phys. **15**, 105 (1961).

The above equations of the hierarchy are coupled with those of the electromagnetic field

$$(1/c^2)\ddot{\mathbf{A}}(\mathbf{r}) - \nabla^2\mathbf{A}(\mathbf{r}) = \frac{4\pi}{c}\mathbf{J}_T(\mathbf{r}), \quad \text{(IV.13)}$$

where

$$\mathbf{J}_T(\mathbf{r}) = \mathbf{J}(\mathbf{r}) + \frac{1}{4\pi e^2}\int \frac{\partial}{\partial \mathbf{r}'} V(\mathbf{r}-\mathbf{r}')\cdot\frac{\partial}{\partial \mathbf{r}'}\mathbf{J}(\mathbf{r}')d\mathbf{r}', \quad \text{(IV.14)}$$

and

$$\mathbf{J}(\mathbf{r}) = \frac{e}{m}\int\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r})\right)\hat{f}_1(\mathbf{r},\mathbf{p})d\mathbf{p}. \quad \text{(IV.15)}$$

The above equations constitute an alternate formulation of quantum electrodynamics in which bilinear products of the particle field operators have been eliminated in favor of phase space distribution functions. The field equations have the form of a generalized magnetohydrodynamics and indeed may be used as the starting point for the investigation of transport phenomena in quantum fluids.

The expectation values formed from these equations no longer satisfy closed sets of equations. In addition to the Wigner distribution $\langle\hat{f}\rangle$ and the average field $\langle\mathbf{A}(\mathbf{r})\rangle$, there arise Green's functions of the types $\langle\mathbf{A}(\mathbf{r})\mathbf{A}(\mathbf{r}')\rangle$, $\langle\hat{f}(\mathrm{x})\hat{f}(\mathrm{x}')\rangle$, and $\langle\hat{f}(\mathrm{x})\mathbf{A}(\mathbf{r}')\rangle$. Theories of irreversibility may be constructed if one makes various statistical assumptions concerning the structure of these Green's functions.

REVIEWS OF MODERN PHYSICS VOLUME 34, NUMBER 4 OCTOBER 1962

On the Stability of Molecules in the Thomas-Fermi Theory

EDWARD TELLER
University of California, Berkeley, California

THE Thomas-Fermi model has been used in approximating the properties of molecules.[1] On the other hand, Sheldon[2] finds no stable equilibrium in a calculation applying the Thomas-Fermi-Dirac model to the N_2 molecule. At the end of his paper, Sheldon gives arguments to support the view that similar calculations will not give rise to stable molecular binding. In the following a proof is given that statistical models cannot give rise to lower energies in the molecular state than obtained for the separated atoms. The proof applies to the stability of both neutral molecules and under certain conditions to positive molecular ions.

Consider first a fixed positive-charge distribution in space and an equal amount of negative charges carried by an electron gas which obeys the Thomas-Fermi equation

$$\Delta\varphi = \varphi^{3/2} - \rho_+. \quad (1)$$

Here $-e\varphi$ is the potential energy of the electrons measured in appropriate units which have been so adjusted as to eliminate numerical coefficients in the Thomas-Fermi equation. The term ρ_+ represents the positive charge density measured in appropriate units. This positive charge density is zero except within the spatial extension of the nuclei of the molecule in question. These locations are fixed and have been chosen without regard to the stability of the configuration. The proof is simpler if we do not consider the nuclei as point charges and do not introduce any singularities. This, of course, happens to correspond to physical reality. For the time being we shall consider neutral molecules. The potential φ and the quantity $\varphi^{3/2}$ are positive, and since ρ_+ is restricted to a finite region in space, φ approaches zero at great distances as $1/r^4$. This behavior is the same as for neutral atoms and is due to the fact that for $1/r^4$ both sides of (1) approach zero with the same power, namely, $1/r^6$.

Let us now add to the positive-charge distribution an infinitesimal additional positive charge near one location. This additional charge distribution shall be designated by ζ. Let us also introduce a corresponding electron distribution so as to keep the system strictly neutral. Then we can prove the following

[1] A summary can be found in the seventh chapter of the book by P. Gombás, *Die Statistische Theorie des Atoms und ihre Anwendungen* (Springer-Verlag, Berlin, 1949). Also S. Flügge, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1956), Vol. 36, p. 108.

[2] J. W. Sheldon, Phys. Rev. 99, 1291 (1955).