Letters 15, 618 (1965).
[33]It is to be noted that these values differ slightly from the preliminary values given in Ref. 18.
[34]L. R. Testardi, T. B. Bateman, W. A. Reed, and V. G. Chirba, Phys. Rev. Letters 15, 250 (1965).
[35]F. W. DeWette, L. H. Nosanow, and N. R. Werthamer, Phys. Rev. 162, 824 (1967).
[36]T. R. Koehler, Phys. Rev. Letters 18, 654 (1967); and private communication.
[37]H. Horner, Phys. Rev. Letters 25, 147 (1970).
[38]H. Horner (private communication).
[39]T. R. Koehler and N. R. Werthamer (private communication).
[40]F. I. Fedorov, *Theory of Elastic Waves in Crystals* (Plenum, New York, 1968).
[41]G. Ahlers, Phys. Rev. A 3, 696 (1971).
[42]D. S. Greywall (unpublished).
[43]H. H. Sample and C. A. Swenson, Phys. Rev. 158, 188 (1967).
[44]R. C. Pandorf and D. O. Edwards, Phys. Rev. 169, 222 (1968).
[45]P. N. Henrickson, M. F. Panczyk, S. B. Trickey, and E. D. Adams, Phys. Rev. Letters 23, 518 (1969).
[46]W. C. Thomlinson, Phys. Rev. Letters 23, 1330 (1969).
[47]J. F. Nye, *Physical Properties of Crystals* (Clarendon, Oxford, England, 1957).
[48]H. Horner, Phys. Rev. A 1, 1722 (1970).
[49]J. F. Jarvis, D. Ramm, and H. Meyer, Phys. Rev. 170, 320 (1968).
[50]G. C. Straty and E. D. Adams, Phys. Rev. 169, 232 (1968).
[51]J. H. Hetherington, W. J. Mullin, and L. H. Nosanow, Phys. Rev. 154, 175 (1967).

PHYSICAL REVIEW A VOLUME 3, NUMBER 6 JUNE 1971

Microscopic Method for Calculating Memory Functions in Transport Theory*

Gene F. Mazenko
Department of Physics and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 16 October 1970)

It is shown how the method of thermodynamic Green's functions can be used to approximate the memory function associated with the equilibrium-fluctuation function $S_c(\vec{r}-\vec{r}', \vec{p}\vec{p}', t-t') \equiv \langle [f(\vec{r}\vec{p}t) - \langle f(\vec{r}\ \vec{p}t)\rangle][f(\vec{r}'\vec{p}'t') - \langle f(\vec{r}'\vec{p}'t')\rangle]\rangle$, where $f(\vec{r}\vec{p}t)$ is the phase-space distribution operator. We obtain an approximation for the memory function for a gas, in the low-density limit, that is valid for all distances and times, satisfied various relevant symmetry conditions and sum rules, reduces for long times and distances to the Boltzmann collision operator, and gives results completely consistent with the conservation laws governing the system. We also indicate how these methods can be extended to treat other types of systems.

I. INTRODUCTION

The usefulness of time-dependent correlation functions in describing deviations from equilibrium in many-particle systems is well known. In particular, the equilibrium-fluctuation function for the classical phase-space distribution operator

$$S_c(\vec{r}-\vec{r}', \vec{p}\vec{p}', t-t') \equiv \langle [f(\vec{r}\vec{p}t) - \langle f(\vec{r}\vec{p}t)\rangle][f(\vec{r}'\vec{p}'t) - \langle f(\vec{r}'\vec{p}'t)\rangle]\rangle , \tag{1.1}$$

where

$$f(\vec{r}\vec{p}t) \equiv \sum_{i=1}^{N} \delta(\vec{r}-\vec{r}_i(t))\delta(\vec{p}-\vec{p}_i(t)) , \tag{1.2}$$

describes all information obtained from light- and neutron-scattering experiments,[1,2] gives the linear response of a system to a weak external probe,[2,3] and its space-time Fourier transform contains all information related to linearized hydrodynamics.[4-7] For these reasons, there is considerable interest in developing methods for determining S_c. In order to avoid unphysical secular effects, these methods are usually based on making approximations for the inverse of S_c. This inverse is related to the memory function $\varphi(\vec{r}-\vec{r}', \vec{p}\vec{p}', t-t')$ by the generalized Langevin equation derived formally by Mori[8,9]:

$$\left(\frac{\partial}{\partial t} + \frac{\vec{p}\cdot\nabla_r}{m}\right) S_c(\vec{r}, \vec{p}\vec{p}', t) - \int_0^t d\bar{t} \int d^3\bar{r}\, d^3\bar{p}\, \varphi(\vec{p}\varphi(\vec{r}-\bar{\vec{r}}, \vec{p}\bar{\vec{p}}, t-\bar{t}) S_c(\bar{\vec{r}}, \bar{\vec{p}}, \vec{p}', \bar{t}) = 0 . \tag{1.3}$$

We will be particularly interested in the Fourier-Laplace transform of this equation:

$$\left(z - \frac{\vec{k}\cdot\vec{p}}{m}\right) S_c(\vec{k}, \vec{p}\vec{p}', z) - \int d^3\bar{p}\, \varphi(\vec{k}, \vec{p}\bar{\vec{p}}, z) \times S_c(\vec{k}, \bar{\vec{p}}\vec{p}', z) = -\tilde{S}_c(\vec{k}, \vec{p}\vec{p}') , \tag{1.4}$$

where the complex fluctuation function is defined by

$$S_c(\vec{k}, \vec{p}\vec{p}', z) = i \int d^3r\, e^{-i\vec{k}\cdot\vec{r}} \int_0^{+\infty} dt\, e^{+izt} S_c(\vec{r}, \vec{p}\vec{p}', t) , \tag{1.5}$$

$$\varphi(\vec{k}, \vec{p}\vec{p}', z) = i \int d^3r e^{-i\vec{k}\cdot\vec{r}} \int_0^{+\infty} dt\, e^{+izt} \varphi(\vec{r}, \vec{p}\vec{p}', t) \tag{1.6}$$

for $\mathrm{Im}z > 0$, where $\tilde{S}_c$ is the spatial Fourier transform of the static correlation function $S_c(\vec{k}, \vec{p}\vec{p}', t=0)$. For short times (large z), φ can be approximated through the use of short-time sum rules and symmetry conditions.[10-14] For long times and disturbances varying over "long" distances ($z \to 0$, $\vec{k} \to 0$), φ can be inferred by assuming the validity of linearized hydrodynamics.[4,5] To obtain information about the memory function in the intermediate-time region, the dynamics of the many-particle system must be analyzed.

Recently there have been two independent efforts to calculate φ from a microscopic point of view. Akcazu and Duderstadt[15] and Forster and Martin,[16,17] both working in the limit of a weakly coupled system, have succeeded in deriving equivalent forms for φ. Akcazu and Duderstadt worked with the Mori projection operator technique,[9] while Forster and Martin utilized an analysis of the classical Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equations. Forster and Martin,[16] which we will refer to as FM, have pointed out that the resulting equation for S_c is valid for arbitrary wave numbers and frequencies, is not Markovian, satisfies the relevant short-time sum rules, is completely reversible, and gives results consistent with the thermodynamic properties of the system to the appropriate order in the potential. Furthermore, their results are in complete agreement with linearized hydrodynamics while providing microscopic expressions for the associated transport coefficients.

It is the purpose of this paper to extend this work on the memory function to the case of a real gas by including the effects due to hard cores. We propose to do this by using the method of thermodynamic Green's functions. This method, which has been so successful in describing a wide range of quantum phenomena, offers the possibility of a systematic and self-consistent approach to calculating correlation functions. Self-consistency is extremely important in dealing with transport phenomena in which the thermodynamic derivatives (such as the speed of sound) must be determined to the same accuracy as the dynamical properties of the system. Other advantages of this method are that through the use of diagrammatic techniques we can make approximations from a physical point of view independent of the time scale considered, and, as will be shown in Sec. IV, there exist criteria whereby one can generate these approximations so that they automatically satisfy the conservation laws.

Our aim is not to generate formal relationships that are valid for arbitrary N-particle systems, but to suggest a practical method for performing microscopic calculations. Consequently, the physics relevant to a particular system will be introduced early in the calculation, thereby eliminating irrelevant information. In keeping with this attitude, we will be concerned mainly with a particular approximation: the first nontrivial term in the density expansion. However, these methods, or extensions thereof, are applicable to many other types of systems including plasmas, multicomponent gases, systems with internal degrees of freedom, and also to higher-density systems.

II. CORRELATION FUNCTIONS

We summarize here some definitions and properties of the correlation functions relevant to our discussion.

The equilibrium one- and two-particle Green's functions are defined by the grand-canonical-ensemble averages

$$G(11') = \frac{-i}{\hbar} \langle T(\psi(1)\psi^*(1')) \rangle \equiv \int \frac{d^3p}{(2\pi\hbar)^3} e^{+i\vec{p}\cdot(\vec{r}_1 - \vec{r}_{1'})/\hbar} G(\vec{p}, t_1 - t_{1'}) , \tag{2.1}$$

$$G_2(12, 1'2') = \left(\frac{-i}{\hbar}\right)^2 \langle T(\psi(1)\chi(2)\psi^*(2')\psi^*(1')) \rangle , \tag{2.2}$$

where T represents the Wick time-ordered product, the field operators are in the Heisenberg representation, and $1 = (\vec{r}_1, t_1)$. We are particularly interested in the connected part of the two-particle function, defined as

$$L(12, 1'2') = G_2(12, 1'2') - G(11')G(22') \equiv \int \frac{d^3p d^3p'}{(2\pi\hbar)^3} \frac{d^3k}{(2\pi\hbar)^3} \exp i[\vec{p}\cdot(\vec{r}_1 - \vec{r}_{1'})/\hbar + \vec{p}'\cdot(\vec{r}_2 - \vec{r}_{2'})/\hbar + \vec{k}\cdot\tfrac{1}{2}(\vec{r}_1 + \vec{r}_{1'} - \vec{r}_2 - \vec{r}_{2'})] \times L(\vec{k}, \vec{p}\vec{p}'; t_1 t_2; t_{1'} t_{2'}) . \tag{2.3}$$

In (2.1) and (2.3) we have used the spatial translational invariance of the equilibrium system in defining the transforms.

The properties of the single-particle Green's function are well known.[18] We will concentrate on the properties of L. For reasons pointed out in Sec. IV, we shall be interested in L only for the case in which we set $t_{2'} = t_2 + 0^+$. Suppressing spatial coordinates, we define $L(t_1 t_{1'}; t_2) = L(t_1 t_2; t_{1'} t_2^+)$. This time-contracted quantity is composed of six analytic pieces corresponding to the various time orderings of t_1, $t_{1'}$, and t_2. The analytic properties of L, which satisfy Kubo-Martin-Schwinger (KMS) boundary conditions,[3,19] are described in Appendix A.

In order to relate $L(t_1 t_{1'}; t_2)$ to the quantity $S_c(t_1 - t_2)$ defined by (1.1), we make the additional

time contraction $t_{1'} = t_1 + 0^+$ and introduce the Wigner operator

$$f_{op}(1) \equiv f_{op}(\vec{r}_1, \vec{p}_1, t_1) = \int \frac{d^3\bar{r}}{(2\pi\hbar)^3} e^{-i\vec{p}_1\cdot\vec{\bar{r}}/\hbar} \psi^*(\vec{r}_1 - \tfrac{1}{2}\vec{\bar{r}}, t_1) \times \psi(\vec{r}_1 + \tfrac{1}{2}\vec{\bar{r}}, t_1) . \quad (2.4)$$

We refer to the thermodynamic average of (2.4) as the Wigner function f_W. We can then write, using (2.1)–(2.3),

$$L(\vec{r}_1 - \vec{r}_2, \vec{p}_1\vec{p}_2; t_1 t_1^+; t_2) = (-i/\hbar)^2(2\pi\hbar)^6 \times \langle T\{[f_{op}(1) - \langle f_{op}(1)\rangle][f_{op}(2) - \langle f_{op}(2)\rangle]\}\rangle . \quad (2.5)$$

This quantity is closely related to the quantum-mechanical fluctuation function

$$S(1, 1') = \langle \tfrac{1}{2}\{[f_{op}(1) - \langle f_{op}(1)\rangle], [f_{op}(1') - \langle f_{op}(1')\rangle]\}_+\rangle \equiv \int \frac{d\omega}{2\pi}\frac{d^3k}{(2\pi)^3} e^{-i\omega(t_1 - t_{1'})} \times e^{+i\vec{k}\cdot(\vec{r}_1 - \vec{r}_{1'})} S(\vec{k}, \vec{p}\vec{p}', \omega) \quad (2.6)$$

and dissipation function

$$\chi(1, 1') = \langle (1/2\hbar)[f_{op}(1), f_{op}(1')]_-\rangle \equiv \int \frac{d\omega}{2\pi}\frac{d^3k}{(2\pi)^3} e^{-i\omega(t_1 - t_{1'})} \times e^{+i\vec{k}\cdot(\vec{r}_1 - \vec{r}_{1'})} \chi''(\vec{k}, \vec{p}\vec{p}', \omega) , \quad (2.7)$$

where $[\,,\,]_\pm$ indicates the anticommutator-commutator. We can show, using (A14) to define the analytic pieces of $L(t_1 t_{1'}; t_2)$ and the KMS boundary conditions (A1)–(A4) to relate the Fourier transforms of these analytic pieces, that

$$S(\vec{k}, \vec{p}\vec{p}', \omega) = (-i/\hbar)^2(2\pi\hbar)^{-6} \times L_{1'12}(\vec{k}, \vec{p}\vec{p}', \omega)\tfrac{1}{2}(1 + e^{-\beta\hbar\omega}) , \quad (2.8)$$

$$\chi''(\vec{k}, \vec{p}\vec{p}', \omega) = (-i/\hbar)^2(2\pi\hbar)^{-6} \times L_{1'12}(\vec{k}, \vec{p}\vec{p}', \omega)(\tfrac{1}{2}\hbar)(1 - e^{-\beta\hbar\omega}) , \quad (2.9)$$

where

$$L_{1'12}(\vec{k}, \vec{p}\vec{p}', \omega) \equiv \int \frac{d\epsilon}{2\pi\hbar} L_{1'12}(\vec{k}, \vec{p}\vec{p}', \epsilon\omega) . \quad (2.10)$$

Dividing (2.8) by (2.9), we obtain the fluctuation-dissipation theorem

$$S(\vec{k}, \vec{p}\vec{p}', \omega) = \hbar \coth\tfrac{1}{2}\beta\hbar\omega\, \chi''(\vec{k}, \vec{p}\vec{p}', \omega) . \quad (2.11)$$

In our further analysis we will also be interested in the complex dissipation function (suppressing momenta indices)

$$\chi(z) = 2i\int_0^{+\infty} d(t_1 - t_{1'}) e^{+iz(t_1 - t_{1'})} \chi(t_1 - t_{1'}) = \int \frac{d\omega}{\pi}\frac{\chi''(\omega)}{\omega - z} , \quad (2.12)$$

the complex fluctuation function

$$S(z) = i\int_0^{+\infty} d(t_1 - t_{1'}) e^{+iz(t_1 - t_{1'})} S(t_1 - t_{1'}) = \int \frac{d\omega}{2\pi}\frac{S(\omega)}{\omega - z} , \quad (2.13)$$

and the generalized Kubo function

$$\mathfrak{L}(z) = \frac{\chi(z) - \chi(z=0)}{iz} = \int \frac{d\omega}{\pi i}\frac{\chi''(\omega)}{\omega(\omega - z)} , \quad (2.14)$$

where the transform expressions are only valid for $\mathrm{Im}z > 0$. In the classical limit the trace over energy eigenstates in the thermodynamic average goes over to an average over phase space and $f_{op}(1)$ is mapped onto the phase-space distribution operator $f(1)$. In this limit S clearly reduces to S_c, and combining (2.14) with (2.11), we see that in the classical limit $\mathfrak{L}$ reduces to $-i\beta S_c$.

III. QUANTUM-MECHANICAL LANGEVIN EQUATION

We are interested in finding the quantum analog of the classical Langevin equation (1.4). We do this by investigating the equation of motion satisfied by the spatial Wigner function

$$\langle B_r^U(\vec{R}, t)\rangle = \langle \psi_U^+(\vec{R} + \tfrac{1}{2}\vec{r}, t)\psi_U(\vec{R} - \tfrac{1}{2}\vec{r}, t)\rangle \quad (3.1)$$

in the presence of the external interaction

$$H_{ext}(t) = -\int d^3R\, d^3\bar{r}\, U_{\bar{r}}(\vec{R}, t) B_{\bar{r}}^U(\vec{R}, t) . \quad (3.2)$$

We recognize from (2.4) that the Fourier transform of B over $\vec{r}$ is the Wigner function. The equation of motion for B is given by

$$\frac{\partial\langle B_r^U(\vec{R}, t)\rangle}{\partial t} = \frac{i}{\hbar}\langle [H_T, B_r^U(\vec{R}, t)]_-\rangle , \quad (3.3)$$

where $H_T = H + H_{ext}$ is the total Hamiltonian for the system and H is the internal Hamiltonian

$$H(t_1) = \int d^3r_1 \psi_U^+(1)[(-\hbar^2/2m)\vec{\nabla}_{r_1}^2]\psi_U(1) + \tfrac{1}{2}\int d^3r\, d^3r'\, \psi_U^+(\vec{r}, t_1)\psi_U^+(\vec{r}', t_1) \times V(\vec{r} - \vec{r}')\psi_U(\vec{r}', t_1)\psi_U(\vec{r}, t_1) . \quad (3.4)$$

If we evaluate the commutator involving the kinetic part of H explicitly, and group the external and internal potentials into H_p, we can write

$$\left(\frac{\partial}{\partial t} - \frac{i\hbar}{m}\vec{\nabla}_R\cdot\vec{\nabla}_r\right)\langle B_r^U(\vec{R}, t)\rangle = \frac{i}{\hbar}\langle [H_p, B_r^U(\vec{R}, t)]_-\rangle \equiv Q_r^U(\vec{R}, t) . \quad (3.5)$$

Clearly, the commutator term depends on higher-order correlations. To make progress, we need to make two assumptions. First, we assume we are

interested in processes that are linear in the external potential. We can then expand $\langle B\rangle$ and Q in U and note that the functional derivative of (3.5), evaluated for $U=0$, relates the linear coefficients of U in the expansions of $\langle B\rangle$ and Q. The second assumption we make concerns the resulting quantity $\delta Q/\delta U$. If we assume that Q depends on U only through its dependence on B, we can use the chain rule for functional differentiation and obtain the kinetic equation

$$\left(\frac{\partial}{\partial t}-\frac{i\hbar}{m}\vec{\nabla}_R\cdot\vec{\nabla}_r\right)\left(\frac{\delta B_r^U(\vec{R},t)}{\delta U_{r'}(\vec{R}',t')}\right)_{U=0}$$
$$=\int d^3\bar{r}\,d^3\bar{R}\,d\bar{t}\left(\frac{\delta Q_r^U(\vec{R},t)}{\delta B_{\bar{r}}^U(\vec{\bar{R}},\bar{t})}\right)_{U=0}\left(\frac{\delta B_{\bar{r}}(\vec{\bar{R}},\bar{t})}{\delta U_{r'}(\vec{R}',t')}\right). \tag{3.6}$$

This equation has the form of a Langevin equation for $\delta B/\delta U$ if we note that $\delta Q/\delta B$ must vanish for $\bar{t}>t$ due to causality.

There is one difficulty with this program as we have outlined it. Keldysh[20] and Fujita[21] have pointed out that the assumption that the higher-order correlation functions depend on U only through their dependence on B is not necessarily correct for an arbitrary initial state where independent knowledge of all N reduced distribution functions is required. Consequently, the dependence on U at $t=0$, of a correlation function of order n, cannot be expressed strictly in terms of B. On the other hand, for any arbitrary initial state, after a time greater than the average collision time in the system, the initial correlations between clusters of particles due to the external interaction disappear due to randomization and the functional assumption becomes valid.[21] If we wish to avoid the imprecision of a "waiting time," we must give up the idea of treating an arbitrary initial state, and concentrate on a system in which this randomization process has already taken place in the distant past. More specifically, we consider a system in absolute equilibrium at $t\to-\infty$. We then prescribe the manner in which the system is removed from equilibrium by applying the adiabatic nonlocal external perturbation

$$U_r(\vec{R},t)=U_r(\vec{R})e^{\delta t}\times\begin{cases}1 & \text{for } t<0\\ 0 & \text{for } t>0\end{cases}, \tag{3.7}$$

where $\delta\to 0^+$. We can then specify the initial nonequilibrium state at $t=0$ in terms of H_{ext}. For times greater than zero, the system relaxes back to equilibrium.

If we reconsider (3.5) for this adiabatic external interaction for times greater than zero, the term explicitly proportional to U in Q vanishes. We then Laplace-transform (3.5) over time as in (1.5). If we then take the functional derivative of the resulting equation with respect to the time-independent part of U, use the chain rule on the term proportional to Q, and note from Appendix D that the functional derivative of B with respect to the time-independent part of the adiabatic external potential U is just the Fourier transform of the generalized Kubo function, we find the Langevin equation

$$\left(z-\frac{\vec{k}\cdot\vec{p}}{m}\right)\mathfrak{L}(\vec{k},\vec{p}\vec{p}',z)-\int d^3\bar{p}\;\varphi_Q(\vec{k},\vec{p}\vec{\bar{p}},z)$$
$$\times\mathfrak{L}(\vec{k},\vec{\bar{p}}\vec{p}',z)=i\chi(\vec{k},\vec{p}\vec{p}',z=0), \tag{3.8}$$

where

$$\varphi_Q(\vec{k},\vec{p}\vec{p}',z)=\int_0^{+\infty}d(t_1-t_{1'})\,e^{+iz(t_1-t_{1'})}$$
$$\times\int d^3r\,d^3r'\,e^{+i\vec{p}\cdot\vec{r}/\hbar}e^{+i\vec{p}'\cdot\vec{r}'/\hbar}$$
$$\times\int d^3(\vec{R}-\vec{R}')\,e^{-i\vec{k}\cdot(\vec{R}-\vec{R}')}$$
$$\times\left(\frac{\delta Q_r(\vec{R},t_1)}{\delta\langle B_{r'}(\vec{R}',t_{1'})\rangle}\right). \tag{3.9}$$

It is clear, in the classical limit, where $\mathfrak{L}\to -i\beta S_c$, that (3.8) reduces to the Langevin equation (1.4).

We can understand from this discussion why $S_c(z)$ satisfies a simple kinetic equation. If one writes a Langevin equation for $\chi_c(z)$, one finds there is a problem due to a small k divergence in the associated memory function. Such a divergence is unphysical and tells us that $\chi(z)$ does not satisfy a simple Langevin equation. This problem is treated in some detail in Ref. 17.

We should note that, although we have established the form of the quantum-mechanical Langevin equation, it is difficult, for reasons we discuss in Sec. VI, to make progress with the form for φ given by (3.9). In Sec. IV we describe a more convenient technique for determining the memory function.

IV. GREEN'S-FUNCTION APPROACH TO TRANSPORT

We proceed to investigate a method for determining the Green's function $L(12,1'2')$. This method will enable us to determine the memory function φ_Q.

The basic equations of motion satisfied by L and the associated higher-order Green's functions are in the form of a system of coupled equations that have to be made definite by imposing the proper boundary conditions. Since we work in the equilibrium ensemble, it is the KMS boundary conditions that make these equations of motion definite. Quantum mechanically, these boundary conditions can be built into our equations if we use imaginary-time Green's functions.[22]

In formulating a purely classical theory it is very cumbersome to implement these KMS boundary conditions. This, of course, follows from the fact that the quantum-mechanical quantities are periodic

over an interval $0 \leq t \leq -i\beta\hbar$ that vanishes in the classical limit. The procedure in many classical theories has been to assume that these initial conditions become unimportant after a short time and do not contribute to quantities measured in the so-called kinetic stage. Such randomization assumptions are, of course, applicable only to nonequilibrium situations. Correlations in the equilibrium ensemble can persist for long times since the system is already very near its most random state. Therefore, one is led to errors if these initial correlations are ignored when calculating equilibrium-averaged correlation functions.

If we use the imaginary-time Green's functions, the primary problem is to effect a truncation of the infinite set of coupled equations. To this end, it is extremely useful to introduce a generating functional.[19,23] We do this by perturbing the system through the introduction of an external potential that acts in the imaginary time interval $0 \leq t \leq \tau \equiv -i\beta\hbar$. Writing the operators in the interaction representation for the external disturbance, we define

$$e^{\eta W'} = \mathrm{Tr}[e^{-\beta(H-\mu N)} T(\mathcal{S})] , \tag{4.1}$$

where H and N are the unperturbed Hamiltonian and number operators and η equals $+1$ for bosons and -1 for fermions. $\mathcal{S}$, defined by

$$\mathcal{S} = \exp\left(\frac{-i}{\hbar}\int_0^\tau dt_2 dt_{2'} \int d^3r_2 d^3r_{2'}\, \psi^+(2) U(22')\psi(2')\right), \tag{4.2}$$

is the scattering matrix in the interaction representation. The entire dependence of W' on U is displayed explicitly in $\mathcal{S}$. We can then generate nonequilibrium Green's functions by noting that

$$\begin{aligned} G(11'; U) &= \frac{\delta W'}{\delta U(1'1)} \\ &= (-i/\hbar)\mathrm{Tr}[e^{-\beta(H-\mu N)} T(\mathcal{S}\psi(1)\psi^+(1'))]/ \\ &\qquad \mathrm{Tr}[e^{-\beta(H-\mu N)} T[S]] . \end{aligned} \tag{4.3}$$

This clearly reduces to the equilibrium Green's function when we set $U = 0$. If we take the functional derivative of (4.3) with respect to U and then set $U = 0$, we find that $G(U)$ serves as the generator for the two-particle correlation function L, since

$$\left(\frac{\delta G(11'; U)}{\delta U(2'2)}\right)_{U=0} = \eta L(12, 1'2') . \tag{4.4}$$

In order to make use of (4.4) we must make some statements about $G(U)$. We calculate $G(U)$ through an evaluation of its inverse[24]

$$G^{-1}(1\bar{1})G(\bar{1}1') = \delta(11') . \tag{4.5}$$

It is customary to write

$$G^{-1}(11') = G_0^{-1}(11') - U(11') - \Sigma(11') , \tag{4.6}$$

where G_0^{-1} is the free-particle inverse

$$G_0^{-1}(11') = \left(i\hbar\frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m}\nabla_1^2\right)\delta(1-1') , \tag{4.7}$$

and Σ is the mass operator associated with $G(U)$. There exist methods, either perturbative[25] or by use of equations of motion,[18,19] for determining Σ.

We now take the functional derivative of (4.5) with respect to $U(2', 2)$ and multiply from the left by G^{-1} to obtain

$$\frac{\delta G(11'; U)}{\delta U(2'2)} = -G(1\bar{3})\left(\frac{\delta G^{-1}(\bar{3}\bar{4})}{\delta U(2'2)}\right) G(\bar{4}1') . \tag{4.8}$$

Computing the derivative of G^{-1} from (4.6) and setting $U = 0$, we have

$$\begin{aligned} L(12, 1'2') &= \eta G(12')G(21') \\ &\quad + \eta\int G(1\bar{3})\left(\frac{\delta\Sigma(\bar{3}\bar{4})}{\delta U(2'2)}\right)_{U=0} G(\bar{4}1') . \end{aligned} \tag{4.9}$$

Then, following arguments similar to those used in Sec. III, we can assume that Σ depends on U only through its dependence on $G(U)$, and we can compute $\delta\Sigma/\delta U$ by the chain rule for differentiation

$$\begin{aligned} \left(\frac{\delta\Sigma(\bar{3}\bar{4})}{\delta U(2'2)}\right)_{U=0} &= \int\left(\frac{\delta\Sigma(\bar{3}\bar{4})}{\delta G(\bar{6}\bar{5})}\right)_{U=0}\left(\frac{\delta G(\bar{6}\bar{5})}{\delta U(2'2)}\right)_{U=0} \\ &= \eta\int\left(\frac{\delta\Sigma(\bar{3}\bar{4})}{\delta G(\bar{6}\bar{5})}\right)_{U=0} L(\bar{6}2, \bar{5}2') . \end{aligned} \tag{4.10}$$

Therefore, we can rewrite (4.9) in the form

$$\begin{aligned} L(12, 1'2') &= \eta G(12')G(21') \\ &\quad + \int G(1\bar{3})G(\bar{4}1')\left(\frac{\delta\Sigma(\bar{3}\bar{4})}{\delta G(\bar{6}\bar{5})}\right)_{U=0} L(\bar{6}2, \bar{5}2') . \end{aligned} \tag{4.11}$$

We can obtain one equation from (4.11) by applying the inverse operator G^{-1} to the 1 variable, and a second equation by applying G^{-1} to the $1'$ variable. On subtracting these equations and substituting for G^{-1} in terms of G_0^{-1} and Σ, we obtain a general kinetic equation for L:

$$\begin{aligned} &[G_0^{-1}(1\bar{1})\delta(1'-\bar{1}') - G_0^{-1}(\bar{1}'1')\delta(1\bar{1})]L(\bar{1}2, \bar{1}'2') \\ &\quad = \eta[\delta(1-2')G(21') - G(12')\delta(2-1')] \\ &\qquad + \int W(1\bar{1}', 1'\bar{1})L(\bar{1}2, \bar{1}'2') , \end{aligned} \tag{4.12}$$

with

$$\begin{aligned} W(12, 1'2') &= \frac{\delta}{\delta G(2'2)} \\ &\quad \times[\Sigma(1\bar{1})G(\bar{1}1') - G(1\bar{1})\Sigma(\bar{1}1')] . \end{aligned} \tag{4.13}$$

The problem of finding a kinetic equation for $L(12, 1'2')$ has thus been reduced to finding an ap-

proximation for the mass operator in terms of the *equilibrium* propagators G.

Equation (4.12) can be put in a form similar to (3.8) after a few simple steps. Using the explicit form for the free-particle inverse and defining the spatial Fourier transform of W in analogy with (2.3), we can take the Fourier transform of (4.12) over space to obtain

$$\left[i\hbar\left(\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_{1'}}\right)-\frac{\vec{p}\cdot\hbar\vec{k}}{m}\right]L(\vec{k},\vec{p}\vec{p}';t_1t_2;t_{1'}t_{2'})=\eta(2\pi\hbar)^3\delta(\vec{p}-\vec{p}')$$
$$\times[G(\vec{p}-\tfrac{1}{2}\hbar\vec{k},t_2-t_{1'})\,\delta(t_1-t_{2'})-G(\vec{p}+\tfrac{1}{2}\hbar\vec{k},t_1-t_{2'})\delta(t_2-t_{1'})]$$
$$+\int W(\vec{k},\vec{p}\bar{\vec{p}};t_1\bar{t}_5;t_{1'}\bar{t}_6)L(\vec{k},\bar{\vec{p}}\vec{p}';\bar{t}_6t_2;\bar{t}_5t_{2'})\ . \quad (4.14)$$

Next, we set $t_{2'}=t_2^*$ and $t_{1'}=t_1^*$, multiply by $(-i\hbar)\times(2\pi\hbar)^{-6}e^{+i\Omega_\nu(t_1-t_2)}$, and integrate over t_1 from 0 to τ to obtain

$$\left(\Omega_\nu-\frac{\vec{p}\circ\vec{k}}{m}\right)\chi(\vec{k},\vec{p}\vec{p}',\Omega_\nu)=\delta(\vec{p}-\vec{p}')\hbar^{-1}(2\pi\hbar)^{-3}[f_W(\vec{p}+\tfrac{1}{2}\hbar\vec{k})-f_W(\vec{p}-\tfrac{1}{2}\hbar\vec{k})]+D(\vec{k},\vec{p}\vec{p}',\Omega_\nu)\ , \quad (4.15)$$

with

$$D(\vec{k},\vec{p}\vec{p}',\Omega_\nu)=-i\hbar(2\pi\hbar)^{-6}\int_0^\tau dt_1\,e^{+i\Omega_\nu(t_1-t_2)}\int W(\vec{k},\vec{p}\bar{\vec{p}};t_1;\bar{t}_5\bar{t}_6)L(\vec{k},\bar{\vec{p}}\vec{p}';\bar{t}_6\bar{t}_5;t_2)\ . \quad (4.16)$$

We have used (2.1) and (2.4) to evaluate $G(p,t=0^-)=-i\eta\hbar^{-1}f_W(p)$, where $f_W(p)$ is the Wigner function evaluated in equilibrium, and we have noted, using (2.5), (2.9), and (A16), that

$$\chi(\vec{k},\vec{p}\vec{p}',\Omega_\nu)=-i\hbar\int_0^\tau dt_1\,e^{+i\Omega_\nu(t_1-t_2)}(2\pi\hbar)^{-6}$$
$$\times L(\vec{k},\vec{p}\vec{p}';t_1t_1^+;t_2)\ , \quad (4.17)$$

with $\Omega_\nu=2\pi\nu/\tau$ $(\nu=0,\pm1,\pm2,\ldots)$.

Equation (4.15) is in the form of a general kinetic equation for χ. Clearly, D is a generalized collision term. It is important to note that (4.15) is not in a closed form for χ. Since the collision term involves the quantities $L(\bar{t}_6\bar{t}_5;t_2)$, the time integrations over $\bar{t}_5$ and $\bar{t}_6$ will in general couple the various time orderings of $L(\bar{t}_6\bar{t}_5;t_2)$. Therefore, we will not assume that D is linear in χ. Instead, we must interpret D as a sum of terms which are linear in χ and $\mathfrak{L}$. We will investigate the structure of (4.16), in detail, in Sec. VI.

In treating systems slightly removed from equilibrium we must include situations in which there are spatial inhomogeneities in the density, energy, etc., which are dispersed through space as the system relaxes to equilibrium. The detailed manner in which these quantities are dispersed is governed by the conservation laws. Therefore, a fundamental constraint on (4.14) is that it be consistent with these conservation laws. Baym and Kadanoff,[23,26] through a detailed analysis of the exact conservation laws for particles, momentum, angular momentum, and energy, have shown that these laws are maintained for any approximate Σ that is derived from a "closed" functional Φ:

$$\Sigma(11')=\frac{\delta\Phi[G,V]}{\delta G(1'1)}\ . \quad (4.18)$$

Through an analysis of the variational properties of Φ and W' it can be shown that Φ and the partition function $(e^{\eta W'})_{U=0}$ are intimately connected.[27,28] Abrikosov, Gor'kov, and Dzyaloshinskii[25] have pointed out that if we select from the set of diagrams in the perturbation-theory expansion for the partition function all of the compact diagrams (diagrams with no self-energy corrections), replace the free propagators by complete Green's functions, and sum the diagrams with a coefficient $1/n$ for each diagram of order n, we obtain Φ. We are therefore able to derive conserving kinetic equations from an approximation to the partition function.

V. LOW-DENSITY SYSTEMS

We will investigate Φ derivable approximations that are valid for a low-density gas. In particular, we seek an expression for Φ that is valid to second order in the density. This requires that we also obtain the partition function correct to second order.

In the perturbation expansion of the partition function each diagram consists of a series of closed loops, with each loop consisting of a hole-particle pair contributing a factor proportional to one order in the density. The procedure is to write down all of the connected diagrams for the partition function[25,28] and to discard all diagrams with either self-energy insertions or with more than two closed loops. We then replace the free propagators with complete Green's functions and put a factor $1/m$ in front of the set of diagrams of order m in the inter-

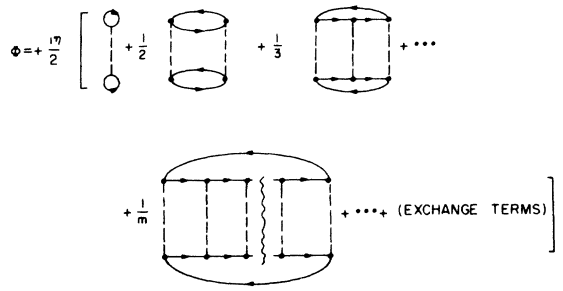

FIG. 1. Diagrammatic representation for the functional Φ in the low-density approximation. Here, and in Figs. 2 and 3, propagators are represented by solid lines and the potential by dashed lines.

action potential. We thus obtain the diagrammatic expression for Φ given in Fig. 1. On taking the functional derivative of Φ with respect to G, it is easy to verify that we obtain $2m$ topologically equivalent terms in the set of diagrams of order m, whence we obtain the graphical expression for Σ given in Fig. 2. In this case there are no factors of $1/m$ and we can sum the infinite set of ladder diagrams by defining the many-particle T matrix in Fig. 3. Combining the diagrams in Figs. 2 and 3, we arrive at our basic approximation for the mass operator

$$\Sigma(11') = i\eta\hbar \int \langle 1\bar{3}\,|\,T\,|\,1'\,\bar{4}\rangle G(\bar{4}\,\bar{3}^{+}) \,, \tag{5.1}$$

where

$$\langle 12|\,T\,|\,1'2'\rangle - \langle 12|\,V_s\,|\,1'2'\rangle$$

$$= i\hbar \int \langle 12|\,T\,|\,\bar{1}\,\bar{2}\rangle G(\bar{1}\,1') G(\bar{2}\,2') V(1'-2') \tag{5.2a}$$

$$= i\hbar V(1-2) \int G(1\,\bar{1}) G(2\,\bar{2}) \langle \bar{1}\,\bar{2}\,|\,T\,|\,1'2'\rangle \,. \tag{5.2b}$$

We have used the symmetrized potential

$$\langle 12|\,V_s\,|\,1'2'\rangle = V(1-2)[\delta(1-1')\delta(2-2') + \eta\delta(1-2')\delta(2-1')] \,, \tag{5.3a}$$

where

$$V(1-2) = V(\vec{r}_1 - \vec{r}_2)\delta(t_1 - t_2) \,. \tag{5.3b}$$

Since we have derived Σ from a functional Φ, we are assured that our approximations will be conserving; on the other hand, this approximation for Σ can be derived in other ways that give greater insight into the physical interpretation of the approximation. Martin and Schwinger[19] have derived (5.1) through an analysis of the hierarchy of equations satisfied by the Green's functions; their basic approximation is for the three-particle Green's function, which they assume can be factored into a product of G's and G_2's in the absence of three-body collisions. Similarly, Kadanoff and Baym[18] point out that in a system in which two particles propagate independently or come together and collide only once, the two-particle Green's function satisfies the Bethe-Goldstone equation

$$G_2(12, 1'2') = G(11')G(22') + \eta G(12')G(21')$$

$$+ i\hbar \int G_2(12, \bar{1}\,\bar{2}) V(\bar{1}-\bar{2}) G(\bar{1}\,1') G(\bar{2}\,2') \,.$$

Kadanoff and Baym have shown that this approximation for G_2 leads directly to the approximation for the mass operator given by (5.1).

We now want to calculate the collision kernel W in the T approximation. This involves calculating (4.13) using the mass operator given by (5.1). In carrying out the functional derivatives we need the result

$$\frac{\delta\langle 13|\,T\,|1'4\rangle}{\delta G(2'2)} = i\hbar \int \langle 13|\,T\,|\bar{5}2'\rangle\, G(\bar{5}\,\bar{6}) \langle \bar{6}2|\,T\,|1'4\rangle \,, \tag{5.4}$$

which was obtained by Baym and Kadanoff.[23] The properties of the T matrix are discussed in Appendix B. After performing the various functional derivatives indicated in (4.13), integrating over the time δ functions in T given above Eq. (13.6) in Kadanoff and Baym,[18] using (B7a) and (B7b) that relate T and the Ω matrices, and setting $t_{1'} = t_1^{+}$, we obtain[29]

$$W(12, 1'_{+}2') = i\eta\hbar \int G(\vec{\bar{r}}_4 - \vec{\bar{r}}_5, t_{2'} - t_2)\,[\langle \vec{r}_1\vec{\bar{r}}_3|\,T(t_1 - t_{2'})\,|\vec{r}_{2'}\vec{\bar{r}}_4\rangle \langle \vec{r}_2\vec{r}_5|\,\Omega^R(t_2 - t_1)\,|\vec{r}_1\vec{\bar{r}}_3\rangle$$

$$- \langle \vec{r}_1\vec{\bar{r}}_3|\,\Omega^L(t_1 - t_{2'})\,|\vec{r}_{2'}\vec{\bar{r}}_4\rangle \langle \vec{r}_2\vec{\bar{r}}_5|\,T(t_2 - t_1)\,|\vec{r}_{1'}\vec{\bar{r}}_3\rangle] \,. \tag{5.5}$$

Note that this can also be written

$$W(12, 1'_{+}2') = i\eta\hbar \int G(\vec{\bar{r}}_4 - \vec{\bar{r}}_5, t_{2'} - t_2) \langle \vec{r}_1\vec{\bar{r}}_3|\,\Omega^L(t_1 - t_{2'})\,|\vec{r}_{2'}\vec{\bar{r}}_4\rangle \langle \vec{r}_2\vec{\bar{r}}_5|\,\Omega^R(t_2 - t_1)\,|\vec{r}_{1'}\vec{\bar{r}}_3\rangle\, [V(\vec{r}_1 - \vec{\bar{r}}_3) - V(\vec{r}_{1'} - \vec{\bar{r}}_3)] \,. \tag{5.6}$$

From the definition of the Fourier transform of W over the variables $\vec{r}_1$ and $\vec{r}_{1'}$, we see that setting $\vec{r}_1 = \vec{r}_{1'}$ corresponds here to an integration over the free-momentum index of W in the kinetic equation. It immediately follows that

$$\int d^3p\, W(\vec{k}, \vec{p}\,\vec{p}'; t_1; t_2 t_{2'}) = 0 \,.$$

It is this property that ensures conservation of particle number in the system. We now transform (5.5) over the spatial variables to obtain

$$W(\vec{k},\vec{p}\vec{p}';t_1;t_2t_{2'}) = +i\mu\hbar\int\frac{d^3\bar{p}}{(2\pi\hbar)^3}\,G(\vec{\alpha}_5,t_{2'}-t_2)\,[\langle\vec{\alpha}_1|\,\Omega^R(\vec{\alpha}_6,t_2-t_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\,T(\vec{\alpha}_7,t_1-t_{2'})|\vec{\alpha}_4\rangle$$
$$-\langle\vec{\alpha}_1|\,T(\vec{\alpha}_6,t_2-t_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\,\Omega^L(\vec{\alpha}_7,t_1-t_{2'})|\vec{\alpha}_4\rangle]\,, \qquad (5.7)$$

where

$$\vec{\alpha}_1=\vec{u}+\tfrac{1}{2}\bar{\vec{p}}+\tfrac{1}{2}\hbar\vec{k},\quad \vec{\alpha}_2=\vec{u}-\tfrac{1}{2}\bar{\vec{p}}-\tfrac{1}{2}\hbar\vec{k},\quad \vec{\alpha}_3=\vec{u}-\tfrac{1}{2}\bar{\vec{p}}\,,$$
$$\vec{\alpha}_4=\vec{u}+\tfrac{1}{2}\bar{\vec{p}},\quad \vec{\alpha}_5=\vec{p}+\bar{\vec{p}}+\tfrac{1}{2}\hbar\vec{k},\quad \vec{\alpha}_6=\vec{P}+\bar{\vec{p}}\,, \qquad (5.8)$$
$$\vec{\alpha}_7=\vec{P}+\bar{\vec{p}}+\hbar\vec{k},\quad \vec{P}=\vec{p}+\vec{p}',\quad \vec{u}=\tfrac{1}{2}(\vec{p}-\vec{p}')\,.$$

VI. ANALYTIC CONTINUATION

In this section we will be interested in performing the time integrations in the collision term given by (4.16). We see, in contrast to the theory developed in Sec. III, where we treated only single-time quantities, we now must perform, in a rough manner of speaking, a nontrivial integration in the collision term over the time variable $\bar{t}_2-\bar{t}_{2'}$. We can understand why this extra time variable is involved by considering the work of Kadanoff and Baym[18] on the nonequilibrium Green's functions defined for real times. In dealing with $G(11';U)=G(t_1-t_{1'};\frac{1}{2}(t_1+t_{1'}))$, Kadanoff and Baym found that the variable $\frac{1}{2}(t_1+t_{1'})$ is measured on a macroscopic time scale and is the time that enters into the BBGKY hierarchy of equations. The time $t_1-t_{1'}$, on the other hand, is a microscopic time interval of order $\hbar\beta$. On Fourier-transforming G over $t_1-t_{1'}$ and $\frac{1}{2}(t_1+t_{1'})$, we associate the frequencies $\epsilon/\hbar$ and ω with $t_1-t_{1'}$ and $\frac{1}{2}(t_1+t_{1'})$, respectively. It is not difficult to show, in that case, that ϵ is a measure of the energy of a single particle $\epsilon\approx p^2/2m$, while $\hbar\omega$ is an energy characteristic of an external probe in the system. Consequently, in the two-time formalism, there is an energy parameter available that allows us to conserve the total energy in a collision process $(12)\to(1'2')$ by writing the δ-function condition $\delta(\epsilon_1+\epsilon_2-\epsilon_{1'}-\epsilon_{2'})$. In our diagrams, therefore, we are able to treat collisions in a natural way by conserving the momentum and the total energy as δ-function conditions. Thus, physically, the extra time integration in our expression for D corresponds, in energy space, to an integration over the energy variable ϵ in $L_{ijk}(\vec{k},\vec{p}\vec{p}',\epsilon\omega)$ that arises from the "collision" in the collision term.

In the traditional one-time theories, t_1 and $t_{1'}$ are set equal, thereby removing this energy variable from the problem at the outset. But in such a theory, as developed in Sec. III, we have no convenient method for evaluating the functional derivatives indicated in (3.9). On the other hand, when we maintain the two times in the problem, we do have a convenient way of evaluating the functional derivative $\delta\Sigma/\delta G$. If we maintain the two-times, we have a diagrammatic technique for evaluating Σ in terms of the complete propagators G and our functional derivatives are with respect to these complete propagators. The functional derivatives can therefore be performed in an unambiguous manner. Thus, in the two-time theory, although we do have an extra time integration to carry out in evaluating D, we need this additional time variable if we want to generate approximations for D in an economical way.

In order to evaluate the time integrations in D, we must investigate some general properties of W. We note, in the most general case, that W is of the form (suppressing momentum indices)

$$W(t_1;t_5t_6)=\delta(t_1-t_5)\delta(t_1-t_6)W_0+\delta(t_1-t_5)W_1(t_6-t_5)$$
$$+\delta(t_1-t_6)W_2(t_6-t_5)+Y(t_1;t_5t_6). \qquad (6.1)$$

If we insert (6.1) into (4.14) after setting $t_{2'}=t_2^+$ and $t_{1'}=t_1^+$, we see first that the integrations over the term corresponding to the two-time δ functions are trivial (it is this term that gives rise to the linearized Vlasov or RPA approximation.) Next, if Eqs. (4.14) and (6.1) are to be consistent with the KMS boundary conditions satisfied by $L(t_1t_{1'};t_2)$, $W1$ and W must obey the KMS boundary conditions given by (A15), and $Y(t_2t_{2'};t_1)$ must obey the same KMS boundary conditions as $L(t_2t_{2'};t_1)$. Then, in principle, the program for performing the time integrations and continuing from the discrete index Ω_ν to the complex variable z is straightforward. Since all of the quantities in D obey KMS boundary conditions, we can expand them in a periodic series and perform the time integrations. This leaves us with a set of sums to perform over a discrete Fourier parameter. We can perform these sums by inserting the spectral representations for the various quantities. We can then continue $D(\Omega_\nu)$ to the arbitrary complex variable z by simply setting $\Omega_\nu\to z$. We outline the process here since in practice this calculation is rather tedious.[30]

First we expand W_1, W_2, Y, and L in periodic series, insert these series into (4.16), and carry out the time integrations to obtain

$$D(\Omega_\nu)=W_0\chi(\Omega_\nu)+(-i\hbar)\tau^{-1}(2\pi\hbar)^{-6}$$
$$\times\sum_{\bar{\nu}}\{[W_1(z_{\bar{\nu}}+\Omega_\nu)+W_2(z_{\bar{\nu}})]\,L(z_{\bar{\nu}}+\Omega_\nu,z_{\bar{\nu}})$$
$$+Y(z_{\bar{\nu}}-\Omega_\nu,z_{\bar{\nu}})L(z_{\bar{\nu}},z_{\bar{\nu}}-\Omega_\nu)\}\,. \qquad (6.2)$$

If we now introduce the spectral representations for $W_{1,2}(z)$ given by (A16) and for $Y(z_1,z_2)$ and $L(z_1,z_2)$ given by (A6), we find that $D(\Omega_\nu)$ consists of fifteen sums; nine of the sums are of the form

$$S_{ij}(\Omega_\nu, \epsilon'\omega', \epsilon\omega) = \tau^{-1}\sum_{\bar{\nu}} \Phi_i(z_{\bar{\nu}} - \Omega_\nu, z_{\bar{\nu}}, \epsilon'\omega') \times \Phi_j(z_{\bar{\nu}}, z_{\bar{\nu}} - \Omega_\nu, \epsilon\omega), \quad (6.3a)$$

three of the form

$$S_i'(\Omega_\nu, \omega', \epsilon\omega) = \tau^{-1}\sum_{\bar{\nu}} (z_{\bar{\nu}} + \Omega_\nu - \omega')^{-1} \times \Phi_i(z_{\bar{\nu}} + \Omega_\nu, z_{\bar{\nu}}, \epsilon\omega), \quad (6.3b)$$

and three of the form

$$S_i''(\Omega_\nu, \omega', \epsilon\omega) = \tau^{-1}\sum_{\bar{\nu}} (z_{\bar{\nu}} - \omega')^{-1}\Phi_i(z_{\bar{\nu}} + \Omega_\nu, z_{\bar{\nu}}, \epsilon\omega), \quad (6.3c)$$

where i and j range over 1, 2, and 3. The Φ's are defined in Appendix A. While there is no essential problem in evaluating all of these sums, the complete results are rather cumbersome. We therefore choose to specialize the analysis to the low-density case. Evidently the techniques we develop are applicable to more general cases.

Since we are interested in calculating D to lowest order in the density, we must investigate the density dependences of the quantities

$$\Delta_{ij}(\Omega_\nu, \epsilon'\omega', \epsilon\omega) = Y_j(\epsilon'\omega')L_i(\epsilon\omega)S_{ij}(\Omega_\nu, \epsilon'\omega', \epsilon\omega), \quad (6.4a)$$

$$\Delta_i'(\Omega_\nu, \omega', \epsilon\omega) = W_1(\omega')L_i(\epsilon\omega)S_i'(\Omega_\nu, \omega', \epsilon\omega), \quad (6.4b)$$

$$\Delta_i''(\Omega_\nu, \omega', \epsilon\omega) = W_2(\omega')L_i(\epsilon\omega)S_i''(\Omega_\nu, \omega', \epsilon\omega) \quad (6.4c)$$

that appear as terms in D. As a preliminary we must fix the relationship between the density and the chemical potential. To lowest order in the density n, we have the standard result

$$e^{\beta\mu} = (2\pi\hbar)^3 n (\beta/2\pi m)^{3/2}. \quad (6.5)$$

Next we note, to lowest order in the density, that L has its free-particle value

$$L^0(12, 1'2') = \eta G(12')G(21'). \quad (6.6)$$

We obtain this result from (4.9) if we set $\Sigma = 0$ and use the free-particle single-particle Green's functions. We see directly that $L_{11'2} = L_{1'12}$. Similarly, in the T approximation, we see from inspection of (5.5) that $Y_{22'1}/Y_{2'21} \sim e^{\beta\mu} \sim n$. Therefore, we have from Eqs. (A10)–(A12) that L_1 and L_2 are of higher order in the density than L_3, and similarly Y_1 and Y_2 are of higher order in the density than Y_3.

We can show, in an analysis similar to that in the Appendix of Kadanoff and Baym,[18] that all of the sums are proportional to $e^{\beta\mu}$ and therefore of first order in the density.

Combining our information about the L_i's, Y_j's, and S_{ij}'s, it is clear that the term Δ_{33} is of lower order in the density than any of the other eight combinations. Similarly, since the six sums S_i' and S_i'' are all of the same order in the density, we see, for a dilute gas, that Δ_1' and Δ_2' are negligible compared with Δ_3', and that Δ_1'' and Δ_2'' are negligible compared with Δ_3''. In evaluating D to lowest order in the density, there is considerable simplification since the number of terms reduces from 16 to 4. It should be apparent that we can perform essentially the same type of analysis in treating any type of expansion in a small parameter where the free-particle result is of zeroth order in that parameter. We then evaluate Y to lowest order in this expansion parameter rather than to lowest order in the density.

In the low-density limit the number of sums to be performed reduces from fifteen to three: S_3', S_3'', and S_{33}. We can evaluate these sums using contour integration techniques and find, after some rearrangement,

$$D(\vec{k}, \vec{p}\vec{p}', \Omega_\nu) = \int d^3\bar{p}\, W_0(\vec{k}, \vec{p}\bar{\vec{p}})\chi(\vec{k}, \bar{\vec{p}}\vec{p}', \Omega_\nu) + \int \frac{d\omega_{1'}d\omega_{2'}\,d\omega_1 d\omega_2}{(2\pi)^4} d^3\bar{p} \times \left[E(\omega_{1'}; \omega_2\omega_1, \Omega_\nu)\left(W_2(\vec{k}, \vec{p}\bar{\vec{p}}, \omega_{1'})2\pi\delta(\omega_{2'}) + \frac{Y_3(\vec{k}, \vec{p}\bar{\vec{p}}, \epsilon'\omega')}{\Omega_2 + \omega'}\right)\right.$$
$$\left. - E(\omega_{2'}; \omega_1\omega_2, -\Omega_\nu)\left(W_1(\vec{k}, \vec{p}\bar{\vec{p}}, \omega_{2'})2\pi\delta(\omega_{1'}) - \frac{Y_3(\vec{k}, \vec{p}\bar{\vec{p}}, \epsilon'\omega')}{\Omega_\nu + \omega'}\right)\right] \frac{L_3^0(\vec{k}, \bar{\vec{p}}\vec{p}', \epsilon\omega)}{\Omega_\nu - \omega}, \quad (6.7)$$

where

$$E(\omega_{1'}, \omega_2\omega_1, \Omega_\nu) = \frac{\eta\hbar}{(2\pi\hbar)^6}\left(\frac{f(\omega_{1'}) - f(\omega_1)}{\Omega_\nu + \omega_{1'} - \omega_1} - \frac{f(\omega_{1'}) - f(\omega_2)}{\omega_{1'} - \omega_2}\right), \quad (6.8)$$

$$f(\omega) = e^{-\beta(\omega-\mu)}, \quad (6.9)$$

and we have introduced the variables

$$\hbar\omega_1 = \epsilon + \tfrac{1}{2}\hbar\omega, \qquad \hbar\omega_2 = \epsilon - \tfrac{1}{2}\hbar\omega,$$
$$\hbar\omega_{1'} = \epsilon' + \tfrac{1}{2}\hbar\omega', \qquad \hbar\omega_{2'} = \epsilon' - \tfrac{1}{2}\hbar\omega'.$$

At this point we can analytically continue this expression from the discrete set of points Ω_ν to the nonreal complex variable z, simply by replacing Ω_ν with z.[31]

We now want to specialize our results further to the case of the T-matrix approximation. From

(5.7) we can identify the quantities in (6.1) as

$$W_0(\vec{k},\vec{p}\vec{p}') = \int \frac{d\bar{\omega}}{2\pi}\frac{d^3\bar{p}}{(2\pi\hbar)^3} G^<(\vec{\alpha}_5,\bar{\omega}) \times [{}_s\langle\vec{\alpha}_1|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|V|\vec{\alpha}_4\rangle_s - {}_s\langle\vec{\alpha}_1|V|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\vec{\alpha}_4\rangle_s], \quad (6.10)$$

$$W_1(\vec{k},\vec{p}\vec{p}',t_2-t_{2'}) = +i\eta\int\frac{d^3\bar{p}}{(2\pi\hbar)^3} G(\vec{\alpha}_5,t_{2'}-t_2) \times [{}_s\langle\vec{\alpha}_1\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|T_A(\vec{\alpha}_7,t_2-t_{2'})|\vec{\alpha}_4\rangle - {}_s\langle\vec{\alpha}_1|V|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\Omega_A^L(\vec{\alpha}_7,t_2-t_{2'})|\vec{\alpha}_4\rangle], \quad (6.11)$$

$$W_2(\vec{k},\vec{p}\vec{p}',t_2-t_{2'}) = +i\eta\int\frac{d^3\bar{p}}{(2\pi\hbar)^3} G(\vec{\alpha}_5,t_{2'}-t_2) \times [\langle\vec{\alpha}_1|\Omega_A^R(\vec{\alpha}_6,t_2-t_{2'})|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|V|\vec{\alpha}_4\rangle_s - \langle\vec{\alpha}_1|T_A(\vec{\alpha}_6,t_2-t_{2'})|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\vec{\alpha}_4\rangle_s], \quad (6.12)$$

$$Y(\vec{k},\vec{p}\vec{p}';t_1;t_2t_{2'}) = +i\eta\int\frac{d^3\bar{p}}{(2\pi\hbar)^3} G(\vec{\alpha}_5,t_{2'}-t_2) \times [\langle\vec{\alpha}_1|\Omega_A^R(\vec{\alpha}_6,t_2-t_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|T_A(\vec{\alpha}_7,t_1-t_{2'})|\vec{\alpha}_4\rangle - \langle\vec{\alpha}_1|T_A(\vec{\alpha}_6,t_2-t_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\Omega_A^L(\vec{\alpha}_7,t_1-t_{2'})|\vec{\alpha}_4\rangle], \quad (6.13)$$

where T_A, Ω_A^R, and Ω_A^L are defined by

$$T_A(\vec{P},t_1-t_{1'}) = T(\vec{P},t_1-t_{1'}) - V_s\,\delta(t_1-t_{1'}), \quad (6.14)$$

$$\Omega_A^{L,R}(\vec{P},t_1-t_{1'}) = \Omega^{L,R}(\vec{P},t_1-t_{1'}) - 1_s\,\delta(t_1-t_{1'}) \quad (6.15)$$

and we have introduced the convention $|\vec{p}\rangle_s = |\vec{p}\rangle + \eta|-\vec{p}\rangle$.

In the low-density limit, we are interested in W_1 and W_2 for the cases $t_2 > t_{2'}$ and Y for the ordering $t_{2'} > t_2 > t_1$. After selecting these time orderings, performing the Fourier transformations over time, using the identities (B6), (B9a), and (B9b) and the corresponding identities for the Ω's, and using (6.6) to evaluate L_3 to lowest order in the density, we can rewrite (6.7) in the form

$$D(\vec{k},\vec{p}\vec{p}',z) = \int\frac{d\omega_{1'}d\omega_{2'}d\bar{\omega}}{(2\pi)^3}\frac{d^3\bar{p}}{(2\pi\hbar)^3} G^<(\alpha_5,\bar{\omega})\frac{f(\omega')-f(\omega_{2'})}{z+\omega_{1'}-\omega_{2'}}[{}_s\langle\vec{\alpha}_1|N(\vec{\alpha}_6,\bar{\omega}+\omega_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\Omega_S^R(\vec{\alpha}_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle - \langle\vec{\alpha}_1|\Omega_S^L(\vec{\alpha}_6,\bar{\omega}+\omega_{1'})|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|N(\vec{\alpha}_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle_s]. \quad (6.16)$$

Equation (6.16) gives us an explicit expression for the low-density collision term. We will discuss how to determine the memory function φ from this D in Sec. VII.

VII. QUANTUM-MECHANICAL MEMORY FUNCTION

Having derived the kinetic equation (4.15) and evaluated its collisional part in Sec. VI for the T approximation, we want to compare our results with the quantum-mechanical Langevin equation. To facilitate this comparison, we note, as we will show below, that we can write D as a linear combination of the free-particle dissipation and Kubo functions $\chi^0(z)$ and $\mathfrak{L}^0(z)$:

$$D(\vec{k},\vec{p}\vec{p}',z) = \varphi_Q^{(s)}(\vec{k},\vec{p}\bar{\vec{p}})\chi^0(\vec{k},\bar{\vec{p}}\vec{p}',z) + iz\,\varphi_Q^{(c)}(\vec{k},\vec{p}\bar{\vec{p}},z)\mathfrak{L}^0(\vec{k},\bar{\vec{p}}\vec{p}',z), \quad (7.1)$$

where $\varphi_Q^{(s)}$ and $\varphi_Q^{(c)}$ are functions evaluated below and integration over the barred index is implied. Inserting (7.1) into (4.15) and using (2.14) to express $\chi(z)$ in terms of $\mathfrak{L}(z)$, we find

$$iz\{-i\chi(\vec{k},\vec{p}\vec{p}',z=0) + (z-\vec{k}\cdot\vec{p}/m)\mathfrak{L}(\vec{k},\vec{p}\vec{p}',z) - [\varphi_Q^{(s)}(\vec{k},\vec{p}\bar{\vec{p}}) + \varphi_Q^{(c)}(\vec{k},\vec{p}\bar{\vec{p}}\ z)]\mathfrak{L}(\vec{k},\bar{\vec{p}}\vec{p}',z)\} = \delta(\vec{p}-\vec{p}')(-\beta\vec{k}\cdot\vec{p}/m)F(\vec{k},\vec{p}) + (\vec{k}\cdot\vec{p}/m)\chi(\vec{k},\vec{p}\vec{p}',z=0) + \varphi_Q^{(s)}(\vec{k},\vec{p}\bar{\vec{p}})\chi(\vec{k},\bar{\vec{p}}\vec{p}',z=0), \quad (7.2)$$

where

$$(-\beta\vec{k}\cdot\vec{p}/m)F(\vec{k},\vec{p}) = \hbar^{-1}(2\pi\hbar)^{-3}[f_W(\vec{p}+\tfrac{1}{2}\hbar\vec{k}) - f_W(\vec{p}-\tfrac{1}{2}\hbar\vec{k})]. \quad (7.3)$$

To compare this equation with the Langevin equation we must evaluate the collision term in the Langevin equation to lowest order in the density. This requires replacing $\mathfrak{L}$ with its free-particle value in the collision term of the Langevin equation. We can then eliminate $(z-\vec{k}\cdot\vec{p}/m)\mathfrak{L}$ in (7.2) using (3.8):

$$iz[\varphi_Q(\vec{k},\vec{p}\bar{\vec{p}},z) - \varphi_Q^{(s)}(\vec{k},\vec{p}\bar{\vec{p}}) - \varphi_Q^{(c)}(\vec{k},\vec{p}\bar{\vec{p}},z)]\mathfrak{L}^0(\vec{k},\bar{\vec{p}}\vec{p}',z) = \delta(\vec{p}-\vec{p}')(-\beta\vec{k}\cdot\vec{p}/m)F(\vec{k},\vec{p}) + (\vec{k}\cdot\vec{p}/m)\chi(\vec{k},\vec{p}\vec{p}',z=0) + \varphi_Q^{(s)}(\vec{k},\vec{p}\bar{\vec{p}})\chi(\vec{k},\bar{\vec{p}}\vec{p}',z=0). \quad (7.4)$$

Assuming the φ's are well behaved at $z=0$, we can set $z=0$ in (7.4) to find

$$(\vec{k}\cdot\vec{p}/m)\chi(\vec{k},\vec{p}\,\vec{p}',z=0)+\varphi_Q^{(s)}(\vec{k},\vec{p}\,\bar{\vec{p}})\chi(\vec{k},\bar{\vec{p}}\,\vec{p}',z=0)$$
$$=(\beta\vec{k}\cdot\vec{p}/m)\delta(\vec{p}-\vec{p}')F(\vec{k},\vec{p}), \qquad (7.5)$$

and, comparing (7.5) and (7.4), we can identify

$$\varphi_Q(\vec{k},\vec{p}\,\vec{p}',z)=\varphi_Q^{(s)}(\vec{k},\vec{p}\,\vec{p}')+\varphi_Q^{(c)}(\vec{k},\vec{p}\,\vec{p}',z). \qquad (7.6)$$

Since we have assumed that $\varphi_Q^{(s)}$ and $\varphi_Q^{(c)}$ are known, (7.5) is in the form of an integral equation determining the initial condition $\chi(z=0)$. We are therefore able to determine the intial conditions consistent with the dynamics described by the memory function φ_Q.

To identify the memory function to lowest order in the density, therefore, we need only show that the collision term (6.16) can be written in the form of (7.1). Before we can express D in that form, we must write down explicit expressions for $\chi^0(z)$ and $\mathcal{L}^0(z)$. This can be accomplished by setting $D=0$ in (4.15), giving

$$\chi^0(\vec{k},\vec{p}\,\vec{p}',z)=-\beta\frac{\vec{k}\cdot\vec{p}}{m}\frac{\delta(\vec{p}-\vec{p}')F^0(\vec{p},\vec{k})}{z-\vec{k}\cdot\vec{p}/m}, \qquad (7.7)$$

and from (2.14) we have

$$\mathcal{L}^0(\vec{k},\vec{p}\,\vec{p}',z)=\frac{i\beta F^0(\vec{p},\vec{k})}{z-\vec{k}\cdot\vec{p}/m}. \qquad (7.8)$$

We see from (7.7) and (7.8) that the expression for D must be written in a form such that it is proportional to $(\vec{k}\cdot\vec{p}'/m-z)^{-1}$ and, from (7.1), that the coefficient of this factor, when $z=0$, must be related to the (s) part of the memory function. If we note the identity

$$\frac{1}{z+\omega_{1'}-\omega_{2'}}=\frac{-\vec{k}\cdot\vec{p}'/m}{(z-\vec{k}\cdot\vec{p}'/m)(\omega_{1'}-\omega_{2'})}+\frac{z(\vec{k}\cdot\vec{p}'/m+\omega_{1'}-\omega_{2'})}{(\omega_{1'}-\omega_{2'})(z-\vec{k}\cdot\vec{p}'/m)(z+\omega_{1'}-\omega_{2'})}, \qquad (7.9)$$

we can then combine (6.16) and (7.9) to identify

$$\varphi_Q^{(s)}(\vec{k},\vec{p}\,\vec{p}')F^0(\vec{p}',\vec{k})=\int\frac{d\omega_{1'}d\omega_{2'}d\bar{\omega}}{(2\pi)^3}\frac{d^3\bar{p}}{(2\pi\hbar)^3}\beta^{-1}\frac{f(\omega_{1'})-f(\omega_{2'})}{\omega_{1'}-\omega_{2'}}G^<(\vec{\alpha}_5,\hbar\bar{\omega})$$
$$\times[{}_s\langle\vec{\alpha}_1|N(\vec{\alpha}_6,\bar{\omega}+\omega_1)\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\Omega_>^R(\vec{\alpha}_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle-\langle\vec{\alpha}_1|\Omega_>^L(\vec{\alpha}_6,\bar{\omega}+\omega_{1'})|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|N(\vec{\alpha}_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle_s], \qquad (7.10)$$

$$\varphi_Q^{(c)}(\vec{k},\vec{p}\,\vec{p}',z)F^0(\vec{p}',\vec{k})=\int\frac{d\omega_{1'}d\omega_{2'}d\bar{\omega}}{(2\pi)^3}\frac{d^3\bar{p}}{(2\pi\hbar)^0}\beta^{-1}\frac{f(\omega_{1'})-f(\omega_{2'})}{\omega_{2'}-\omega_{1'}}G^<(\alpha_5,\hbar\bar{\omega})\frac{\vec{k}\cdot\vec{p}'/m+\omega_{1'}-\omega_{2'}}{z+\omega_{1'}-\omega_{2'}}$$
$$\times[{}_s\langle\vec{\alpha}_1|N(\vec{\alpha}_6,\bar{\omega}+\omega_1)|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|\Omega_>^R(\vec{\alpha}_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle-\langle\vec{\alpha}_1|\Omega_>^L(\vec{\alpha}_6,\bar{\omega}+\omega_{1'})|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3|N(\alpha_7,\bar{\omega}+\omega_{2'})|\vec{\alpha}_4\rangle_s]. \qquad (7.11)$$

If we combine the Langevin equation with (7.5), (7.10), and (7.11), we have a realistic set of equations to use in investigating low-density quantum systems. For simplicity we will restrict the rest of our analysis to the classical limit of this set of equations.

VIII. CLASSICAL MEMORY FUNCTION

In the classical limit, F reduces to the Maxwellian

$$\lim_{\hbar\to 0}F(\vec{k},\vec{p})=f_0(p)=n(\beta/2\pi m)^{3/2}e^{-\beta p^2/2m} \qquad (8.1)$$

and we can decouple the momentum and spatial coordinates in the static correlation function

$$\chi_c(\vec{k},\vec{p}\vec{p}',z=0)=\beta\tilde{S}_c(\vec{k},\vec{p}\vec{p}')$$
$$=\beta f_0(p)\delta(\vec{p}-\vec{p}')+\beta h(k)f_0(p)f_0(p'), \qquad (8.2)$$

where

$$h(k)=c(k)/[1-nc(k)]=\int d^3r\,[g(r)-1]e^{+i\vec{k}\cdot\vec{r}}, \qquad (8.3)$$

$g(r)$ is the equilibrium pair-correlation function

$$n^2g(|\vec{r}-\vec{r}'|)=\left\langle\sum_{i\neq j}^{N}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r}'-\vec{r}_j)\right\rangle, \qquad (8.4)$$

and $c(k)$ is the Fourier transform of the direct pair-correlation function. We see that we can use (8.1)–(8.3) in (7.5) to solve for $\varphi^{(s)}$ in terms of the direct pair-correlation function. We find

$$\varphi^{(s)}(\vec{k},\vec{p})=-(\vec{k}\cdot\vec{p}/m)c(k)f_0(p). \qquad (8.5)$$

Comparing (8.5) with Eq. (1.8b) in FM, we see that $\varphi^{(s)}$ corresponds to what they call the static part of the memory function. We have foreseen this in our choice of superscripts. Correspondingly, we will call $\varphi^{(c)}$ the collisional part of the memory function.

Note that the condition (8.5) serves as a decisive check on the classical limit of (7.10).

As a first step in performing the classical limit for the static term, we substitute for Ω and N in (7.10) the expressions given by (B5), (B8a), and (B8b), and do the integrations over $\omega_{1'}$, $\omega_{2'}$, and $\bar{\omega}$. We obtain

$$\varphi^{(s)}(\vec{k},\vec{p}\vec{p}')f_0(p')=\lim_{\hbar\to 0}\Big\{-n^2\Big(\frac{\beta}{2\pi m}\Big)^3\hbar^{-1}(2\pi\hbar)^6\int\frac{d^3\bar{p}}{(2\pi\hbar)^3}\sum_{i,j}A(E_i-E_j,\vec{\alpha}_8)$$
$$\times\exp\Big[-\beta\Big(\frac{E_i+E_j}{2}+\frac{\vec{\alpha}_8^2}{4m}\Big)\Big]_s\langle\vec{\alpha}_1|E_j\rangle\langle E_j|[V,\rho]_-|E_i\rangle\langle E_i|\vec{\alpha}_4\rangle_s\Big\}\ , \qquad (8.6)$$

where

$$A(E,\vec{\alpha})=\frac{2\beta^{-1}\sinh[\frac{1}{2}\beta(\hbar\vec{k}\cdot\vec{\alpha}/2m+E)]}{\hbar\vec{k}\cdot\vec{\alpha}/2m+E}\ ,$$

$$\vec{\alpha}_8=\vec{P}+\bar{\vec{p}}+\tfrac{1}{2}\hbar\vec{k}\ .$$

We have also introduced the operator

$$\rho=(2\pi\hbar)^{-6}|\vec{\alpha}_2\rangle\langle\vec{\alpha}_3| \qquad (8.7)$$

and used (6.5) to eliminate the chemical potential and Eq. (1.18) of Kadanoff and Baym[18] to evaluate $G^<$. It is clear, in taking the classical limit, that we must transfer our attention from operators acting on the quantum-mechanical Hilbert space spanned by the complete set of energy eigenkets to operators acting on the quantum-mechanical generalization of phase space. As an intermediate step we must change from the energy representation $|E_j\rangle$ to the momentum representation $|\vec{p}\rangle$. For any function $R(E)$ with a well-defined power-series expansion in E, we can write the identities

$$R(E_i)\langle E_i|B_{op}|E_j\rangle=\langle E_i|R(H)B_{op}|E_j\rangle\ , \qquad (8.8)$$

$$R(E_i-E_j)\langle E_i|B_{op}|E_j\rangle=\langle E_i|R(-\hbar L_Q)B_{op}|E_j\rangle\ , \qquad (8.9)$$

where $|E_i\rangle$ is an eigenstate of the Hamiltonian H, and L_Q is the "super" operator defined by $\hbar L_Q=-[H,\ ]_-$, where we take the commutator of the Hamiltonian and the operators standing at the right of L_Q in a matrix element. While it is possible to introduce extended notation to treat such quantities, it will be necessary here only to bracket the operators upon which L_Q operates. We therefore define

$$\hbar L_Q\{A_{op}\}B_{op}=-[H,A_{op}]_-B_{op}\ . \qquad (8.10)$$

Using these definitions, we can remove any reference to the particular eigenstates E_i or E_j in (8.6) except for the sums over complete sets of states. We can replace these sums with complete sets of momentum eigenkets. Equation (8.6) can then be written

$$\varphi^{(s)}(\vec{k},\vec{p}\vec{p}')f_0(p')=\lim_{\hbar\to 0}\Big[-n^2\Big(\frac{\beta}{2\pi m}\Big)^3\int d^3\bar{p}\,d^3\bar{p}'\,\frac{d^3k'}{(2\pi)^3}\,e^{-\beta\vec{\alpha}_8^2/4m}(2\pi\hbar)^3\langle\bar{\vec{p}}'+\tfrac{1}{2}\hbar\vec{k}'|e^{-\beta H/2}\rho' e^{-\beta H/2}|\bar{\vec{p}}'-\tfrac{1}{2}\hbar\vec{k}'\rangle$$
$$\times(2\pi\hbar)^3\langle\bar{\vec{p}}'-\tfrac{1}{2}\hbar\vec{k}'|A(\hbar L_Q,\vec{\alpha}_8)\{\hbar^{-1}[V,\rho]_-\}|\bar{\vec{p}}'+\tfrac{1}{2}\hbar\vec{k}'\rangle\Big]\ , \qquad (8.11)$$

where we have defined the operator

$$\rho'=(2\pi\hbar)^{-6}|\vec{\alpha}_4\rangle_{s\,s}\langle\vec{\alpha}_1|\ . \qquad (8.12)$$

We see from Appendix C that (8.11) has the form of a product of Wigner equivalents. In taking the classical limit, therefore, we need only replace a Wigner equivalent with its classical value. Wigner[32] has shown, for example, that if we expand in powers of $\hbar$, we obtain

$$(e^{-\beta H/2})_W(\vec{r},\vec{p})=\exp\{-\beta[p^2/2m+\tfrac{1}{2}V(r)]\}[1+O(\hbar^2)]\ .$$

Similarly, in this limit, we find

$$\lim_{\hbar\to 0}(L_Q)_W(\vec{r},\vec{p})=i[H,\ ]_{PB}\equiv L(\vec{r},\vec{p})$$
$$=-2i\vec{p}\cdot\vec{\nabla}_r/m+i\vec{\nabla}_r V(r)\cdot\vec{\nabla}_p\ , \qquad (8.13)$$

where L is the Liouville operator for the relative motion of a two-particle system. In most cases the replacement of a Wigner equivalent by its classical limit is obvious and we will not dwell on this point here. Using the rule (C2) for taking the Wigner equivalent of a product of operators, we readily find, after doing some trivial integrations,

$$\varphi^{(s)}(\vec{k},\vec{p}\vec{p}')f_0(p')=-in^2(\beta/2\pi m)^3\int d^3\bar{p}\,d^3r\,\nabla_r^j V(r)$$
$$\times e^{-\beta V(r)}e^{-\beta(\vec{P}+\bar{\vec{p}})^2/4m}$$

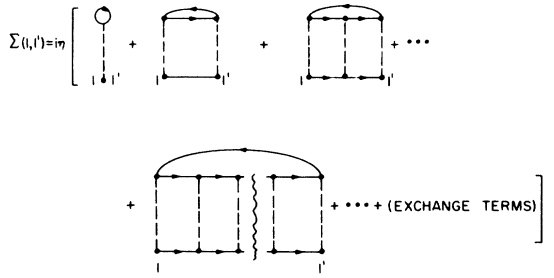

FIG. 2. Diagrammatic representation of the low-density mass operator [$1\cdot 1'$ is to be interpreted as a space-time δ function $\delta(1-1')$].

$$\times\left[e^{-i\vec{k}\cdot\vec{r}}e^{-\beta(\vec{u}+\vec{\bar{p}}/2)^2/m}\nabla_p^j\delta(\vec{\bar{p}})\right.$$

$$\left.-e^{-\beta\vec{\bar{p}}^2/4m}\nabla_p^j\delta(\vec{p}-\vec{p}')\right], \quad (8.14)$$

where we sum over j. Since the second term is odd under the interchange $\vec{r}\to-\vec{r}$, it vanishes, and, if we note in the low-density limit that $g(r)=c(r)+1=e^{-\beta V(r)}$, we find, after several integrations by parts, that (8.14) has the desired form given by (8.5).

We should mention that in evaluating the classical limit of the Wigner equivalent of ρ', the exchange terms (terms proportional to η) vanish. These terms have oscillatory factors that give zero contribution in the classical limit. It is important to note that if we had entirely ignored exchange effects, our analysis would have lost terms proportional to factors like $\eta\langle-\vec{\alpha}_1|-\vec{\alpha}_4\rangle\eta$. Since the two η's cancel, such terms do not necessarily depend on the statistics of the system. We find that these terms are nonzero in the classical limit.

We can perform the limit as $\hbar$ goes to zero in the collision term [(7.11)] in much the same manner as in the static term. The equation for $\varphi^{(c)}$ analogous to (8.11) reads

$$\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z)f_0(p')=\lim_{\hbar\to0}\left[-n^2\left(\frac{\beta}{2\pi m}\right)^3\hbar^{-1}\int d^3\bar{p}\,d^3\bar{p}'\,\frac{d^3k'}{(2\pi)^3}\,e^{-\beta\vec{\alpha}_8^2/4m}\langle\vec{\bar{p}}'+\tfrac{1}{2}\hbar\vec{k}'|\,e^{-\beta H/2}[V,\rho']\,e^{-\beta H/2}|\vec{\bar{p}}'-\tfrac{1}{2}\hbar\vec{k}'\rangle\right.$$

$$\left.\times\langle\vec{\bar{p}}'-\tfrac{1}{2}\hbar\vec{k}'|\,A'(\hbar L_Q,z,\vec{k}\cdot\vec{\alpha}_8/2m)\{[V,\rho]_-\}\,|\vec{\bar{p}}'+\tfrac{1}{2}\hbar\vec{k}'\rangle\right], \quad (8.15)$$

where

$$A'(E,z,\gamma)=\frac{2\beta^{-1}\sinh[\frac{1}{2}\beta(\hbar\gamma+E)]}{(\hbar\gamma+E)(\hbar z-\hbar\gamma+E)}$$

and ρ and ρ' are defined by (8.7) and (8.12). In deriving this equation we have made use of the identities related to (B9a) and (B9b). Since this is again in the form of a product of Wigner equivalents we can pass to the classical limit directly. We find, after some simple manipulations,

$$\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z)f_0(p')=n^2(\beta/\pi m)^3\nabla_p^l\nabla_{p'}^j\int d^3\alpha\,d^3r\,d^3\bar{p}\,e^{-\beta\vec{\alpha}^2/m}e^{-\beta\vec{\bar{p}}^2/m}$$

$$\times g(r)\nabla_r^j V(r)[e^{+i\vec{k}\cdot\vec{r}/2}\delta(\vec{\alpha}-\vec{p}'+\vec{\bar{p}})-e^{-i\vec{k}\cdot\vec{r}/2}\delta(\vec{\alpha}-\vec{p}'-\vec{\bar{p}})]$$

$$\times[z-\vec{k}\cdot\vec{\alpha}/m+L(\vec{r},\vec{\bar{p}})]^{-1}\nabla_r^l V(r)\,e^{-i\vec{k}\cdot\vec{r}/2}\,\delta(\vec{p}-\vec{\alpha}-\vec{\bar{p}}), \quad (8.16)$$

where the sum over l and j is implied. Equation (8.16) is the primary result of this paper. We have obtained an explicit microscopic form for the classical memory function correct to lowest order in the density. We discuss the properties of this function in Sec. IX.

IX. PROPERTIES OF CLASSICAL MEMORY FUNCTION

First we note that our approximate memory function satisfies the symmetry conditions

$$\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z)=-\varphi^{(c)}(-\vec{k},\vec{p}\vec{p}',-z)$$

$$=[\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z^*)], \quad (9.1)$$

$$\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z)f_0(p')=\varphi^{(c)}(\vec{k},\vec{p}'\vec{p},z)f_0(p). \quad (9.2)$$

As Forster and Martin[16,17] have pointed out, these symmetries guarantee, with the Langevin equation, that $S(\vec{k},\vec{p}\vec{p}',\omega)$ is invariant under translations, rotations, parity, and time reversal.

Next we investigate the validity of our approximation in the time intervals for which we have information. For short times ($z\to\infty$), $S(\vec{k},\vec{p}\vec{p}',z)$ can be calculated from sum rules.[13] These sum rules imply large z conditions on φ,[17]

$$\lim_{z\to\infty}\varphi(\vec{k},\vec{p}\vec{p}',z)=\varphi^{(s)}(\vec{k},\vec{p}), \quad (9.3)$$

$$\lim_{z\to\infty}z\varphi^{(c)}(\vec{k},\vec{p}\vec{p}',z)f_0(p')=n\beta^{-1}\int d^3r\,g(r)[\nabla_r^i\nabla_r^j V(r)]\nabla_p^i\nabla_{p'}^j[f_0(p)\delta(\vec{p}-\vec{p}')]$$

$$-\beta^{-1}\int d^3r\cos(\vec{k}\cdot\vec{r})[g(r)\nabla_r^i\nabla_r^j V(r)+\beta^{-1}\nabla_r^i\nabla_r^j c(r)]\nabla_p^i\nabla_{p'}^j[f_0(p)f_0(p')]. \quad (9.4)$$

In the low-density limit where $g(r)=c(r)+1=e^{-\beta V(r)}$, we see our memory function satisfies both sum rules and gives the correct short-time behavior.

In the limit of long times and wavelengths we expect our results to be in agreement with the Boltzmann equation (although our analysis should elimi-

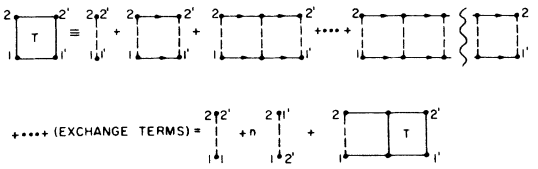

FIG. 3. Diagrammatic definition of the many-body T matrix.

nate the defects in that equation). We find, in this limit, as $\vec{k} \to 0$, $z = +i\delta$, and $\delta \to 0^+$, that $\varphi^{(s)} \to 0$, and, after a calculation similar in spirit to the work of Zwanzig,[33] that $\varphi^{(c)}(\vec{k}, \vec{p}\vec{p}', z) f_0(p')$ reduces to i times the linearized Boltzmann collision operator.[34] If we set $\varphi(\vec{k}, \vec{p}\vec{p}', z) = \varphi(0, \vec{p}\vec{p}', i0^+)$ in the Langevin equation before solving the equation, our results will be in complete agreement with the Boltzmann equation. We know, however, that the Boltzmann equation has the defect that the thermodynamic parameters (for example, the speed of sound) have their free-particle values. If we first solve the Langevin equation and then take the limits of small $\vec{k}$ and z, we find that there are finite contributions from $\varphi^{(s)}$ that have been lost in the Boltzmann-equation analysis and which shift the thermodynamic parameters from their free-particle values to their correct low-density values.

The conservation laws must be satisfied in many-particle systems for all times. We note that the Langevin equation and the associated memory function we have derived are completely consistent with the conservation laws governing particle number, momentum, and energy. Unfortunately, a formulation of the appropriate conservation equations requires more development than we can give here. We intend to give a full discussion of the connection between our results and the conservation laws in a future publication.

We also want to point out that if we expand our approximate memory function to lowest order in the potential and introduce the Fourier transform of the potential, we obtain precisely the form for the memory function obtained by Forster and Martin [their Eq. (1.8c)].

X. DISCUSSION

We have succeeded in deriving an expression for the memory function for a low-density system. We have treated both the quantum-mechanical and classical cases and have taken the classical limit in a natural and unambiguous manner. The validity of our results in the classical limit are reinforced by the analysis of the general properties of our classical memory function in Sec. IX. The corresponding kinetic equation forms the basis for a self-consistent treatment of transport in a low-density system. We believe that the technique presented here for handling the kinetic equation (4.12) can have broad applications. Using the basic methods outlined in Secs. VI and VII, it appears that we can derive expressions for the memory function for any system with an expansion parameter. These memory functions could then serve as models for systems lacking a small parameter.

We should point out that after the memory function is obtained, the solution of the Langevin equation still remains a formidable task. This is so because of the coupling of the momentum variables in the collision term. Accordingly, we will investigate solutions of the Langevin equation associated with the approximate memory function (8.16) in a future publication.

ACKNOWLEDGMENTS

I would like to thank Professor K. U. Ingard for his advice and encouragement and Professor P. C. Martin for a number of enlightening discussions. I would also like to thank Dr. C. Krischer and G. Paul for reading the manuscript and making many valuable suggestions concerning the form of the paper.

APPENDIX A: ANALYTIC PROPERTIES OF CORRELATION FUNCTIONS

We consider a three-time quantity

$$A(t_1 t_{1'}; t_2) = A(t - t_{1'}; \tfrac{1}{2}(t_1 + t_{1'}) - t_2) \tag{A1}$$

obeying the KMS boundary conditions

$$A(t_1 t_{1'}; t_2)\big|_{t_1 = 0} = \eta e^{\beta\mu} A(t_1 t_{1'}; t_2)\big|_{t_1 = \tau}, \tag{A2}$$

$$A(t_1 t_{1'}; t_2)\big|_{t_{1'} = 0} = \eta e^{-\beta\mu} A(t_1 t_{1'}; t_2)\big|_{t_{1'} = \tau}, \tag{A3}$$

$$A(t_1 t_{1'}; t_2)\big|_{t_2 = 0} = A(t_1 t_{1'}; t_2)\big|_{t_2 = \tau}, \tag{A4}$$

where $\tau = -i\beta\hbar$ and $\eta = +1$ for bosons and -1 for fermions. It is well established[18,19,24] that the most convenient method of dealing with such quantities is to expand them in Fourier series over the imaginary time interval $0 \le t \le \tau$:

$$A(t_1 t_{1'}; t_2) = \tau^{-2} \sum_{\nu_1, \nu_2} e^{-i z_{\nu_1} t_1} e^{+i z_{\nu_2} t_{1'}} \times e^{+i(z_{\nu_1} - z_{\nu_2}) t_2} A(z_{\nu_1}, z_{\nu_2}), \tag{A5}$$

where $z_\nu = \pi\nu/\tau + \mu/\hbar$. This sum is taken to run over all even integers for Bose statistics and over odd integers for Fermi statistics. This series can then be inverted to give a dispersion relation for the Fourier coefficients:

$$A(z_{\nu_1}, z_{\nu_2}) = \int \frac{d\epsilon}{2\pi\hbar} \frac{d\omega}{2\pi} \sum_{i=1}^{3} A_i(\epsilon, \omega) \Phi_i(z_{\nu_1}, z_{\nu_2}, \epsilon\omega), \tag{A6}$$

where

$$\Phi_1(z_1, z_2, \epsilon\omega) = (z_2 - \epsilon/\hbar + \tfrac{1}{2}\omega)^{-1} (z_1 - z_2 - \omega)^{-1}, \tag{A7}$$

$$\Phi_2(z_1, z_2, \epsilon\omega) = (z_1 - \epsilon/\hbar - \tfrac{1}{2}\omega)^{-1}\,(z_1 - z_2 - \omega)^{-1}\,, \tag{A8}$$

$$\Phi_3(z_1, z_2, \epsilon\omega) = (z_2 - \epsilon/\hbar + \tfrac{1}{2}\omega)^{-1}\,(z_1 - \epsilon/\hbar - \tfrac{1}{2}\omega)^{-1}\,, \tag{A9}$$

and the A_i's are defined by

$$A_1(\epsilon\omega) = (e^{-\beta\hbar\omega} - 1)\,A_{11'2}(\epsilon, \omega)\,, \tag{A10}$$

$$A_2(\epsilon, \omega) = (1 - e^{-\beta\hbar\omega})\,A_{1'12}(\epsilon, \omega)\,, \tag{A11}$$

$$A_3(\epsilon, \omega) = A_{11'2}(\epsilon, \omega)\,(1 - \eta e^{-\beta(\epsilon+\hbar\omega/2-\mu)}) + A_{1'12}(\epsilon, \omega)\,(1 - \eta e^{\beta(\epsilon-\hbar\omega/2-\mu)})\,, \tag{A12}$$

where the A_{ijk}'s are the Fourier transforms

$$A_{ijk}(t_1 t_{1'}; t_2) = \int \frac{d\epsilon}{2\pi\hbar}\,\frac{d\omega}{2\pi}\,e^{-i\epsilon(t_1 - t_1')/\hbar} \times e^{-i\omega(t_1 + t_1'/2 - t_2)}\,A_{ijk}(\epsilon, \omega) \tag{A13}$$

of the analytic pieces of $A(t_1 t_{1'}; t_2)$,

$$A(t_1 t_{1'}; t_2) = \sum_{i,j,k} \epsilon_{ijk}\,A_{ijk}(t_1 t_{1'}; t_2) \times \theta(t_i - t_j)\,\theta(t_i - t_k)\,\theta(t_j - t_k)\,, \tag{A14}$$

and where i, j, and k run over 1, 1', and 2, $\epsilon_{ijk} = 1$ if $i \neq j \neq k$ and zero otherwise, and θ is the unit-step function. The dispersion relation (A6) can be continued to arbitrary z_1 and z_2 using a procedure developed by Baym and Mermin.[31]

For reference we note that two-time quantities, like $G(11')$, obey the KMS boundary conditions

$$B(t_1 - t_{1'})\,\big|_{t_1 = 0} = \eta e^{\beta\mu}\,B(t_1 - t_{1'})\,\big|_{t_1 = \tau}\,, \tag{A15}$$

and have the corresponding spectral representation

$$B(z_\nu) = \tau^{-1}\int_0^\tau dt_1\,e^{+i z_\nu(t_1 - t_{1'})}B(t_1 - t_{1'}) = \int \frac{d\omega}{2\pi}\,\frac{\beta(\omega)}{z_\nu - \omega}\,, \tag{A16}$$

where

$$B(\omega) = B^{>}(\omega) - B^{<}(\omega) \tag{A17}$$

and the $B^{\gtrless}(\omega)$ are the Fourier transforms of the analytic pieces of $B(t)$.

APPENDIX B: PROPERTIES OF T MATRIX

Many important properties of the T matrix are discussed by Kadanoff and Baym[18] (referred to here as KB); we will only discuss a few simple properties valid for low-density systems. We start with Eq. (13.17) in KB written in a matrix notation in the radial indices:

$$T(\vec{P}, z_\nu) = V_s + T(\vec{P}, z_\nu)\,(\hbar z_\nu - \vec{P}^2/4m - K)^{-1}\,V\,, \tag{B1}$$

where K is the relative kinetic-energy operator ($K|\vec{p}\rangle = \vec{p}^2/m\,|\vec{p}\rangle$). Note that in our definition of T we have maintained the exchange effects in the inhomogeneous term V_s. Our expression for Σ given by (4.1) differs in this respect from (13.23) of KB. We can then formally invert (B1) to find

$$T(\vec{P}, z_\nu) = V_s + V_s\,(\hbar z_\nu - \vec{P}^2/4m - H)^{-1}\,V\,, \tag{B2}$$

where $H = K + V$ is the relative two-particle Hamiltonian. If we insert a complete set of energy eigenstates[35] (on which H is diagonal), we can rewrite (B2) as

$$T(\vec{P}, z_\nu) = V_s + V_s\textstyle\sum_i |E_i\rangle\langle E_i|\,V(\hbar z_\nu - \vec{P}^2/4m - E_i)^{-1}\,. \tag{B3}$$

It then follows, from (13.9) of KB, that the spectral function associated with T has the form, in the low-density limit,

$$T^{>}(\vec{P}, \omega) = V_s N(\vec{P}, \omega)V = VN(\vec{P}, \omega)V_s\,, \tag{B4}$$

where

$$N(\vec{P}, \omega) = \textstyle\sum_i |E_i\rangle\langle E_i|\,(2\pi)\,\delta(\hbar\omega - \vec{P}^2/4m - E_i)\,. \tag{B5}$$

Note the sum rule on N:

$$\int \frac{d(\hbar\omega)}{2\pi}\,N(\vec{P}, \omega) = 1\,. \tag{B6}$$

We will find it convenient to introduce the auxiliary quantities $\Omega^{L,R}$ defined by

$$\langle \vec{r}_1\vec{r}_2|\,T(t_1 - t_{1'})\,|\vec{r}_{1'}\vec{r}_{2'}\rangle = V(\vec{r}_1 - \vec{r}_2)\,\langle \vec{r}_1\vec{r}_2|\,\Omega^L(t_1 - t_{1'})\,|\vec{r}_{1'}\vec{r}_{2'}\rangle\,, \tag{B7a}$$

$$\langle \vec{r}_1\vec{r}_2|\,T(t_1 - t_{1'})\,|\vec{r}_{1'}\vec{r}_{2'}\rangle = \langle \vec{r}_1\vec{r}_2|\,\Omega^R(t_1 - t_{1'})\,|\vec{r}_{1'}\vec{r}_{2'}\rangle\,V(\vec{r}_{1'} - \vec{r}_{2'})\,. \tag{B7b}$$

The analytic properties of the Ω's follow directly from the properties of T. We can show that in the low-density limit, in analogy with (B4),

$$\Omega^R_{>}(\vec{P}, \omega) = V_s N(\vec{P}, \omega)\,, \tag{B8a}$$

$$\Omega^L_{>}(\vec{P}, \omega) = N(\vec{P}, \omega)V_s\,. \tag{B8b}$$

Finally, we can prove a useful identity from (B4) if we note that the potential operator can be written $V = H - K$. We have

$$T^{>}(\vec{P}, \omega) = (H - K)N(\vec{P}, \omega)V_s = (\hbar\omega - \vec{P}^2/4m - K)\,\Omega^L_{>}(\vec{P}, \omega)\,, \tag{B9a}$$

$$T^{>}(\vec{P}, \omega) = \Omega^R_{>}(\vec{P}, \omega)\,(\hbar\omega - \vec{P}^2/4m - K)\,, \tag{B9b}$$

and we can write similar identities for Ω^L and Ω^R in terms of N.

APPENDIX C: WIGNER EQUIVALENTS

In our short discussion of Wigner equivalents we follow Imre *et al.*,[36] where many more details are given.

Corresponding to a quantum operator $A(\vec{R}, \vec{P})$, we define a function $A_W(\vec{r}, \vec{p})$ by

$$A_W(\vec{r}, \vec{p}) = \hbar^3 \int d^3k\,e^{-i\vec{k}\cdot\vec{r}}\langle \vec{p} - \tfrac{1}{2}\hbar\vec{k}|\,A\,|\vec{p} + \tfrac{1}{2}\hbar\vec{k}\rangle\,. \tag{C1}$$

A_W is called the Wigner equivalent of A. The Wigner equivalent of a product of operator AB is given by

$$(AB)_W(\vec{r},\vec{p}) = A_W(\vec{r},\vec{p})\, e^{\hbar\Lambda/2i} B_W(\vec{r},\vec{p}) , \qquad \text{(C2a)}$$

$$(AB)_W(\vec{r},\vec{p}) = B_W(\vec{r},\vec{p})\, e^{-\hbar\Lambda/2i} A_W(\vec{r},\vec{p}) , \qquad \text{(C2b)}$$

where Λ is the Poisson bracket operator

$$\Lambda = \overleftarrow{\nabla}_p \cdot \overrightarrow{\nabla}_r - \overleftarrow{\nabla}_r \cdot \overrightarrow{\nabla}_p .$$

As a simple example, consider the classical limit of the Wigner equivalent of the commutator of two operators. If the operators A and B are such that their Wigner equivalents have well-defined classical limits, $A_W \to A_c$ and $B_W \to B_c$, then

$$\lim_{\hbar\to 0} i\hbar^{-1}([A,B]_-)_W(\vec{r},\vec{p})$$

$$= \lim_{\hbar\to 0} i\hbar^{-1} A_W(\vec{r},\vec{p})\,(e^{\hbar\Lambda/2i} - e^{-\hbar\Lambda/2i}) B_W(\vec{r},\vec{p})$$

$$= A_c(\vec{r},\vec{p})\,\Lambda B_c(\vec{r},\vec{p}) = [A_c, B_c]_{PB}(\vec{r},\vec{p}) . \qquad \text{(C3)}$$

APPENDIX D: RESPONSE TO ADIABATIC EXTERNAL POTENTIAL

We are interested in the linear response of a system taken out of equilibrium at $t \to -\infty$ by the adiabatic external potential given by (3.2) and (3.7). Kadanoff and Martin[4] and Martin[37] have treated such a system. Using their results, we find that the linear change in the spatial Wigner function (3.1) is given by

$$B_r^U(\vec{R},z) = \int_0^{+\infty} dt\, e^{+izt} [B_r^U(\vec{R},t) - B_r^U(\vec{R},t)|_{U=0}]$$

$$= \int d^3r'\, d^3R'\, d^3p\, d^3p'\, e^{+i\vec{p}\cdot\vec{r}/\hbar}\, e^{+i\vec{p}'\cdot\vec{r}'/\hbar}$$

$$\times \mathfrak{L}(\vec{R}-\vec{R}',\vec{p},\vec{p}',z) U_{r'}(\vec{R}') , \qquad \text{(D1)}$$

where $\mathfrak{L}$ is the generalized Kubo function defined by (2.14). We also find that the linear change in the spatial Wigner function at $t=0$ is given by

$$\delta B_r^U(\vec{R},t=0) = \int d^3R'\, d^3r'\, d^3p\, d^3p'\, e^{+i\vec{p}\cdot\vec{r}/\hbar}\, e^{+i\vec{p}'\cdot\vec{r}'/\hbar}$$

$$\times \chi(\vec{R}-\vec{R}',\vec{p},\vec{p}',z=0)\, U_{r'}(\vec{R}') . \qquad \text{(D2)}$$

To compute the change in the Wigner function, which has a well-defined classical limit, we need only Fourier-transform (D1) and (D2) over $\vec{r}$ and observe that the effective coupling is over the momentum-dependent external potential

$$U(\vec{p},\vec{R}) = \int d^3r'\, e^{+i\vec{p}\cdot\vec{r}'/\hbar}\, U_{r'}(\vec{R}) . \qquad \text{(D3)}$$

---

*Work supported by U. S. Navy, Office of Naval Research, under Contract No. N00014-67-A-0204-0019.

[1]L. Van Hove, Phys. Rev. 95, 249 (1954).
[2]P. C. Martin, in *Many-Body Physics*, edited by C. DeWitt and R. Balian (Gordon and Breach, New York, 1968).
[3]R. Kubo, J. Phys. Soc. Japan 12, 570 (1957).
[4]L. P. Kadanoff and P. C. Martin, Ann. Phys. (N. Y.) 24, 419 (1963).
[5]R. D. Mountain, Rev. Mod. Phys. 38, 205 (1966).
[6]M. S. Green, J. Chem. Phys. 20, 1280 (1952); 22, 398 (1954).
[7]H. Mori, Phys. Rev. 112, 1829 (1958); Progr. Theoret. Phys. (Kyoto) 28, 763 (1962).
[8]R. Zwanzig, Phys. Rev. 124, 983 (1961).
[9]H. Mori, Progr. Theoret. Phys. (Kyoto) 33, 423 (1965).
[10]A. Rahman, Phys. Rev. 136, A405 (1964).
[11]M. Nelkin and S. Ranganathan, Phys. Rev. 164, 222 (1967).
[12]B. J. Berne, J. P. Boon, and S. A. Rice, J. Chem. Phys. 45, 1086 (1966).
[13]D. Forster, P. C. Martin, and S. Yip, Phys. Rev. 170, 155 (1968); 170, 160 (1968).
[14]J. L. Lebowitz, J. K. Percus, and J. Sykes, Phys. Rev. 188, 487 (1969).
[15]A. Z. Akcasu and J. J. Duderstadt, Phys. Rev. 188, 479 (1969).
[16]D. Forster and P. C. Martin, Phys. Rev. A 2, 1575 (1970).
[17]D. Forster, Ph. D. dissertation (Harvard University, 1969) (unpublished).
[18]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962). We follow the notation of these authors when possible.
[19]P. C. Martin and J. Schwinger, Phys. Rev. 115, 1342 (1959).
[20]L. V. Keldysh, Zh. Eksperim. i Teor. Fiz. 47, 1515 (1964) [Sov. Phys. JETP 20, 1018 (1965)].
[21]S. Fujita, J. Math. Phys. 6, 1877 (1965).
[22]The use of imaginary-time Green's functions is purely a mathematical convenience. There exist other techniques whereby one can deal strictly with real-time quantities. Unfortunately these methods do not build the KMS boundary conditions into the analysis and are more convenient for strictly nonequilibrium problems. See J. Schwinger, J. Math. Phys. 2, 407 (1961); V. Korenman, Ann. Phys. (N. Y.) 39, 72 (1966); and Ref. 20.
[23]G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961). We draw heavily from this work in Sec. IV.
[24]There are integrations implied over the barred indices running over all space and over the time interval $0 \le t \le \tau$.
[25]A. Abrikosov, L. Gor'kov, and J. Dzyaloshinskii, *Field Theory Methods in Quantum Statistical Mechanics* (Prentice-Hall, Englewood Cliffs, N. J., 1963).
[26]G. Baym, Phys. Rev. 127, 1391 (1962).
[27]J. M. Luttinger and J. C. Ward, Phys. Rev. 118,

1417 (1960).
[28]V. Ambegaoker, in *Astrophysics and the Many-Body Problem*, edited by K. W. Ford (Benjamin, New York, 1963).
[29]N. D. Mermin, Ann. Phys. (N. Y.) 18, 421 (1962); 18, 454 (1962). Mermin has derived an equation similar to (4.54) in treating the problem of the gas-liquid phase transition.
[30]For another approach to this type of continuation see G. M. Elishberg, Zh. Eksperim. i Teor. Fiz. 41, 1241 (1961) [Sov. Phys. JETP 14, 886 (1962)].
[31]G. Baym and N. D. Mermin, J. Math. Phys. 2, 232 (1961).
[32]E. Wigner, Phys. Rev. 40, 749 (1932).
[33]R. Zwanzig, Phys. Rev. 129, 486 (1963).
[34]G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics* (American Mathematical Society, Providence, R. I., 1963).
[35]We label the energy eigenvalues and states by the index i for convenience. We do not need to analyze the spectrum in detail and consequently need not distinguish between continuum and bound states.
[36]K. Imre, E. Ozizmir, M. Rosenbaum, and P. F. Zweifel, J. Math. Phys. 8, 5 (1967).
[37]P. C. Martin, in *Statistical Mechanics of Equilibrium and Non-Equilibrium*, edited by J. Meixner (North-Holland Amsterdam, 1965).

PHYSICAL REVIEW A VOLUME 3, NUMBER 6 JUNE 1971

Statistical Mechanics of the XY Model. III*

Eytan Barouch†
Department of Mathematics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
and
Barry M. McCoy
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11790
(Received 16 November 1970)

We continue the considerations of the first paper in this series by studying the time dependence of the spin-correlation functions in response to a step-function change in the external magnetic field. We find that these correlation functions exhibit nonergodic behavior.

I. INTRODUCTION

In a previous paper[1] we studied[2] time-dependent properties of the z-direction magnetization of the one-dimensional XY model. In particular, we considered an XY model in thermal equilibrium at temperature T in the presence of an external magnetic field H_1. At time $t=0$ the field is changed to some other value H_2, and $M_z(t)$ was computed. The most interesting aspect of $M_z(t)$ is that if $H_2=0$, then

$$\lim M_z(t) \neq 0 \quad \text{as } t \to \infty \,. \tag{1.1}$$

However, for all values of T, M_z is zero when the model is in thermal equilibrium. Therefore we concluded that (at least when $H_2=0$) the magnetization of this model does not exhibit ergodic behavior. This property was first discovered by Mazur[3] using results obtained by Niemeijer,[4] and further elaborated by Katsura, Horiguchi, and Suzuki.[5]

In this paper we continue the exploration of the nonergodic features of this system by examining the spin-correlation functions. After formulating the problem in Sec. II, we study, in Sec. III, the long-time behavior of $\rho_{zz}(R, t, T)$. We find that for any value of H_2,

$$\lim \rho_{zz}(R, t, T_1) \neq \rho_{zz}(R, 0, T_2) \quad \text{as } t \to \infty \tag{1.2}$$

for any T_2. In other words the $t \to \infty$ limit of ρ_{zz} is not a correlation function of the XY model in thermal equilibrium. Furthermore, in Sec. IV, we study the limit

$$\lim_{R\to\infty} \lim_{t\to\infty} \rho_{xx}(R, t, T)$$

and find that the long-range order[2] exhibited by ρ_{xx} at $t=0$ totally disappears.

II. FORMULATION

Let c_i, $c_i^\dagger$ be the Fermi operators defined by (2.3) of I. Define the operators

$$A_i = c_i^\dagger + c_i \,, \tag{2.1}$$