

Density Expansion of Quantum Transport Coefficients

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A formal density expansion of transport coefficients expressed in terms of momentum autocorrelation functions is derived for a degenerate quantum gas (Bose-Einstein or Fermi-Dirac statistics) at any frequency and for noncentral as well as central forces. The result to lowest order in density is reduced to the solution of a well-defined quantum two-body problem, and the first density correction is reduced to the solution of a well-defined quantum three-body problem. It is confirmed that at zero frequency one only needs the asymptotic forms of the collision operator to calculate quantum transport coefficients. It is further pointed out that the coefficients of the third- and higher order terms of the density expansion diverge at zero frequency, in analogy with the classical case. A "renormalization" is suggested which, it is believed, leads to a nonanalytic density dependence for quantum gases distinct from the nonanalytic behavior associated with degeneracy statistics.

I. INTRODUCTION

IT is well known that transport coefficients can be expressed in terms of autocorrelation functions.¹⁻³ In particular, autocorrelation functions of momentum operators can be used to calculate self-diffusion coefficients and electrical conductivities. (Other transport coefficients involve correlations of position as well as momenta. The momenta correlation parts are called "kinetic contributions" to the transport coefficient.) By means of such expressions, Mori,⁴ and McLennan and Swenson⁵ have calculated transport coefficients to lowest order in the density for a nondegenerate quantum mechanical gas. (The latter reference contains a comprehensive list of articles on calculations of the electrical conductivity of quantum systems; see Montroll and Ward.⁶)

The purpose of the present article is to derive the formal density expansion of any momentum autocorrelation function for a degenerate quantum-mechanical gas [Bose-Einstein (B.E.) or Fermi-Dirac (F.D.) statistics] in terms of operators which are determined by the dynamics of isolated groups of particles. The results are neither limited to zero frequency, nor to central forces. The result to lowest order, in density, is reduced to the solution of a well-defined quantum two-body problem, and the first-order correction is reduced to the solution of a well-defined quantum three-body problem. This expansion is analogous to the equilibrium virial expansion of a quantum degenerate gas. Our derivation is based on the fact that autocorrelation functions can be exactly expressed in terms of the formal solution of the master equation. Our results then follow by substituting the density expansion

of the quantum master equation.^{7,8} This derivation is, thus, similar to that of the density expansion of classical autocorrelation functions.⁹ Other related discussions of the density expansion of autocorrelation functions for classical systems are to be found in Ref. 10.

The zero-frequency limit of the density expansion of quantum autocorrelation function is examined in Sec. III, where it is pointed out that the coefficients of the third and higher order terms of a density expansion diverge, although the first two terms converge—for a similar reason as in the classical case.^{9,11} A "renormalization" is suggested which, we believe, leads to a nonanalytic density dependence—distinct from the nonanalytic behavior associated with quantum degeneracy statistics. It is also confirmed that at zero frequency one needs only to consider the asymptotic forms of the collision operators in order to calculate transport coefficients—in agreement with Balescu¹² and Swenson.¹³

II. DENSITY EXPANSION OF THE AUTOCORRELATION OF MOMENTUM OPERATORS

Let \mathbf{R}_i and $-i\hbar\partial/\partial\mathbf{R}_i$ denote the vector position and momentum operator, respectively, of particle i in a system of N particles ($N \rightarrow \infty$), and let $V_{ij} \equiv V_{ij}(\mathbf{R}_i - \mathbf{R}_j)$ denote the interaction potential between particles i

⁷ J. Weinstock, Phys. Rev. **136**, A879 (1964).

⁸ J. Weinstock, Phys. Rev. **140**, A98 (1965).

⁹ J. Weinstock, Phys. Rev. **140**, A460 (1965).

¹⁰ S. T. Choh and G. E. Uhlenbeck, Navy Theoretical Physics, Contract No. Nonr. 1224 (15), University of Michigan, 1958 (unpublished); J. Weinstock, Phys. Rev. **132**, 454 (1963); **132**, 470 (1963); S. Ono and T. Shizume, J. Phys. Soc. Japan **18**, 29 (1963); M. S. Green and R. A. Piccirelli, Phys. Rev. **132**, 1388 (1963); E. G. D. Cohen, J. Math. Phys. **4**, 183 (1963); R. Zwanzig, Phys. Rev. **129**, 486 (1963); K. Kawasaki and I. Oppenheim, *ibid.* **136**, A1519 (1964); M. H. Ernst, J. R. Dorfman, and E. G. D. Cohen, Physica **31**, 493 (1965); L. S. Garcia-Colin and A. Flores, J. Math. Phys. **7**, 254 (1966).

¹¹ J. Weinstock, Phys. Rev. **132**, 454 (1963); J. R. Dorfman and E. G. D. Cohen, Phys. Letters **16**, 124 (1965); R. Goldman and E. A. Frieman, Bull. Am. Phys. Soc. **11**, 531 (1965).

¹² R. Balescu, Physica **27**, 693 (1961).

¹³ R. J. Swenson, Physica **29**, 1174 (1963).

¹ M. S. Green, J. Chem. Phys. **20**, 1281 (1952); **22**, 398 (1954).

² R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

³ H. Mori, Phys. Rev. **112**, 1289 (1958).

⁴ H. Mori, Phys. Rev. **111**, 694 (1958).

⁵ J. A. McLennan, Jr., and R. J. Swenson, J. Math. Phys. **4**, 1527 (1963).

⁶ E. W. Montroll and J. Ward, Physica **25**, 423 (1959).

and j . The Hamiltonian H of this system is given by

$$\begin{aligned} H &\equiv H_0 + \sum_{1 \leq i < j \leq N} V_{ij}, \\ H_0 &\equiv -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\partial^2}{\partial \mathbf{R}_i^2}. \end{aligned} \quad (1)$$

If we let ψ denote any function of the momenta of the N particles,

$$\psi \equiv \psi \left(-i\hbar \frac{\partial}{\partial \mathbf{R}_1}, -i\hbar \frac{\partial}{\partial \mathbf{R}_2}, \dots, -i\hbar \frac{\partial}{\partial \mathbf{R}_N} \right),$$

then the Laplace transform of the symmetrized auto-correlation of ψ is defined by

$$a(E) \equiv \int_0^\infty dt e^{-Et} \langle \{\psi\psi(t)\} \rangle, \quad (2)$$

$$\langle \{\psi\psi(t)\} \rangle \equiv \text{Tr}[\{\psi\psi(t)\} \rho_{\text{eq}}], \quad (3)$$

$$\{\psi\psi(t)\} \equiv \frac{1}{2}[\psi\psi(t) + \psi(t)\psi],$$

$$\psi(t) \equiv e^{iH/\hbar} \psi e^{-iH/\hbar}, \quad (4)$$

$$\rho_{\text{eq}} \equiv \frac{e^{-\beta H}}{\text{Tr} e^{-\beta H}}, \quad (5)$$

where Tr denotes the trace, β^{-1} denotes the product of Boltzmann's constant with the temperature, and ρ_{eq} is seen to be the normalized equilibrium density matrix of the system. (The more general correlation function $\beta^{-1} \int_0^\infty dt e^{-Et} \int_0^\beta d\lambda \langle \psi(-i\hbar\lambda)\psi(t) \rangle$ will be considered in Sec. IV.)

Since ρ_{eq} commutes with $e^{\pm iH/\hbar}$, and since $\text{Tr} AB = \text{Tr} BA$, we can write (3) as¹⁴:

$$\begin{aligned} \langle \{\psi\psi(t)\} \rangle &= \text{Tr} \{ \psi e^{iH/\hbar} \psi e^{-iH/\hbar} \} \rho_{\text{eq}} \\ &= \text{Tr} \{ \psi e^{-iH/\hbar} \{ \psi \rho_{\text{eq}} \} e^{+iH/\hbar} \} \\ &\equiv \text{Tr} \psi \rho(t), \end{aligned} \quad (6)$$

where we have defined the quantity $\rho(t)$ by

$$\rho(t) \equiv e^{-iH/\hbar} \{ \psi \rho_{\text{eq}} \} e^{+iH/\hbar}, \quad (7)$$

$$\rho(0) \equiv \{ \psi \rho_{\text{eq}} \} \equiv \frac{1}{2} (\psi \rho_{\text{eq}} + \rho_{\text{eq}} \psi). \quad (8)$$

Substituting (6) into (2), and assuming that the time integration commutes with the trace, we have

$$a(E) = \text{Tr} \psi \int_0^\infty dt e^{-Et} \rho(t). \quad (9)$$

The trace of an operator, however, is identical to the trace of the diagonal part of the operator—in any

representation—so that if D denotes the diagonal part of an operator, then (9) can be written as

$$a(E) = \text{Tr} D \left[\psi \int_0^\infty dt e^{-Et} \rho(t) \right]. \quad (10)$$

Let us choose a momentum representation of symmetrized free-particle states in all that follows. We can denote an eigenfunction of the momentum operators of the N system particles by $|\mathbf{k}\rangle$ so that

$$|\mathbf{k}\rangle = |\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_N\rangle, \quad (11)$$

where \mathbf{k}_j is an eigenvalue of $-i\hbar \partial / \partial \mathbf{R}_j$. We can further choose the eigenfunctions $|\mathbf{k}\rangle$ to be properly symmetrized for Bose-Einstein or Fermi-Dirac statistics so that our formalism can be applied to indistinguishable particles. The diagonal part of any operator A can be expressed in this representation by

$$\begin{aligned} DA &\equiv \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k} | A | \mathbf{k}\rangle \langle \mathbf{k} | \\ &\equiv \sum_{\mathbf{k}} |\mathbf{k}\rangle A_{kk} \langle \mathbf{k} |. \end{aligned} \quad (12)$$

But ψ is a function of momentum operators and, hence, is diagonal in any representation of free-particle states so that (10) becomes

$$a(E) = \text{Tr} \psi \int_0^\infty dt e^{-Et} D \rho(t). \quad (13)$$

We now note that $D\rho(t)$ is the solution of the master equation with initial value $\rho(0) = \{ \psi \rho_{\text{eq}} \}$.^{7,8} An exact expression for the master equation is given in the form of a density expansion in Eq. (48) of Ref. 7 and Eq. (3) of Ref. 8. The latter equation, which is valid for arbitrary initial states [arbitrary $\rho(0)$], is given by

$$\begin{aligned} \frac{\partial D\rho(t)}{\partial t} &= [K'(t) + \sum_{s=1}^{\infty} \beta_s'(t)] \mathbf{O}_D \rho(0) \\ &+ \int_0^t dy [K''(t-y) + \sum_{s=1}^{\infty} \beta_s''(t-y)] D\rho(y), \end{aligned} \quad (14)$$

where primes denote derivatives with respect to arguments and \mathbf{O}_D denotes the off-diagonal part of an operator, i.e., $\mathbf{O}_D \rho(0) \equiv \rho(0) - D\rho(0)$. The quantity $\beta_s(t)$ is defined in Ref. 7 in terms of the Hamiltonian of $(s+1)$ isolated particles. The properties of $\beta_s(t)$ which are of present concern are that it is proportional to the s th power of the particle density and it involves the dynamics of $(s+1)$ particles. The quantity $K(t)$ is also defined in Ref. 7 as a function of the collision operators $\beta_s(t)$. [It is interesting to note here that $K(t)$ is a manifestation of degeneracy statistics and vanishes in a representation of unsymmetrized free particle states.⁷]

¹⁴ U. Fano, Rev. Mod. Phys. **29**, 74 (1957); Phys. Rev. **131**, 259 (1963). In these articles a "Liouville" formalism for quantum statistical mechanics is proposed, and applied to the pressure broadening problem.

Equation (14) can be solved for the Laplace transform of $D\rho(t)$, in terms of the collision operators β_s and K , by multiplying both sides of (14) with e^{-Et} , integrating over t , and making use of the convolution theorem. We thereby obtain

$$\begin{aligned} & \int_0^\infty dt e^{-Et} D\rho(t) \\ &= (E - E^2[\bar{K}(E) + \sum_{s=1}^\infty \bar{\beta}_s(E)])^{-1} \\ & \quad \times (D\rho(0) + E[\bar{K}(E) + \sum_{s=1}^\infty \bar{\beta}_s(E)]\mathbf{O}_{D\rho}(0)), \quad (15) \end{aligned}$$

where $\bar{K}(E)$ and $\bar{\beta}_s(E)$ denote the Laplace transforms of $K(t)$ and $\beta_s(t)$, respectively, and we have used the fact that $\beta_s(0) = \beta_s'(0) = K(0) = K'(0) = 0$.

Let us, for future convenience, write the formal density expansion of $\bar{K}(E)$ as

$$\bar{K}(E) \equiv \sum_{s=1}^\infty \bar{K}_s(E) \quad (16)$$

such that $\bar{K}_s(E)$ is proportional to the s th power of the density. A formal expression for $\bar{K}_s(E)$ can be obtained from the definition of $\bar{K}(E)$ in Ref. 7. It should be noted (see the Appendix) that

$$\bar{K}_1(E) = 0, \quad (17)$$

i.e., the expansion of $\bar{K}(E)$ begins with second order.

We now substitute (15) and (16) into (13) to obtain the desired result:

$$a(E) = \text{Tr}[\psi(E - E^2 \sum_{s=1}^\infty [\bar{K}_s(E) + \bar{\beta}_s(E)])^{-1} \Phi(E)], \quad (18)$$

where $\Phi(E)$ has been defined by

$$\Phi(E) \equiv D\rho(0) + E \sum_{s=1}^\infty [\bar{K}_s(E) + \bar{\beta}_s(E)]\mathbf{O}_{D\rho}(0), \quad (19)$$

$$D\rho(0) \equiv \frac{1}{2} D(\psi\rho_{\text{eq}} + \rho_{\text{eq}}\psi) = \{\psi D\rho_{\text{eq}}\}, \quad (20)$$

$$\mathbf{O}_{D\rho}(0) = \{\psi \mathbf{O}_{D\rho_{\text{eq}}}\}.$$

Equation (18) is a density expansion of any momentum autocorrelation function at any frequency (replace E by iE). That is, the collision operators $\bar{\beta}_s(E)$ and $\bar{K}_s(E)$ are each proportional to the s th power of the density, and *involve the dynamics of no more than $s+1$ isolated particles*.

Explicit expressions for $\bar{\beta}_1(E)$, $\bar{\beta}_2(E)$, and $\bar{K}_2(E)$ are given, for the readers convenience, in the Appendix. [The operator $\bar{\beta}_s(E)$ is separated from $\bar{K}_s(E)$ in (18) to emphasize that $\bar{\beta}_s(E)$ is a direct quantum analog of a classical $(s+1)$ particle collision operator whereas $\bar{K}_s(E)$

is due to degeneracy statistics and has no classical analog.]

It can be seen from (18) and (19) that $a(E)$ has been expressed as a product of two density expansions. Consequently, to obtain $a(E)$ to a given order in the density one must terminate both summations in (18).

To first order in the density $a(E)$ is simply given by

$$\begin{aligned} a(E) &= \text{Tr} \psi (E - E^2 \bar{\beta}_1(E))^{-1} \{\psi D\rho_{\text{eq}}\} \\ &= \sum_{\mathbf{k}} \psi_{\mathbf{k}\mathbf{k}^2}(\rho_{\text{eq}})_{\mathbf{k}\mathbf{k}} \langle \mathbf{k} | (E - E^2 \bar{\beta}_1(E))^{-1} | \mathbf{k} \rangle, \quad (21) \end{aligned}$$

where \mathbf{k} denotes a symmetrized eigenfunction (for B.E. or F.D. statistics) of momentum operators. Thus, to first order, $a(E)$ is determined by the solution of a well-defined quantum two-body problem. This is, to evaluate $\langle \mathbf{k} | (E - E^2 \bar{\beta}_1(E))^{-1} | \mathbf{k} \rangle$. This has been done by Mori⁴ for Boltzman statistics in the limit of $E=0$. (The sum over \mathbf{k} can frequently, as in Mori's case, be replaced by an integral over momentum.) Equation (21) allows us to calculate lowest order transport coefficients for degenerate gases at finite frequencies as well.

To second order in the density $a(E)$ is given, according to (18), by

$$\begin{aligned} a(E) &= \text{Tr} \psi (E - E^2 [\bar{\beta}_1(E) + \bar{\beta}_2(E) + \bar{K}_2(E)])^{-1} \\ & \quad \times (\{\psi D\rho_{\text{eq}}\} + E \bar{\beta}_1(E) \{\psi \mathbf{O}_{D\rho_{\text{eq}}}\}). \quad (22) \end{aligned}$$

Equation (22) shows that the calculation of quantum transport coefficients [of the form (2)] to second order in the density reduces to the solution of a well-defined quantum three-body problem. Namely, to evaluate

$$\begin{aligned} C(2) &\equiv (E - E^2 [\bar{\beta}_1(E) + \bar{\beta}_2(E) + \bar{K}_2(E)])^{-1} \\ & \quad \times (\{\psi D\rho_{\text{eq}}\} + E \bar{\beta}_1(E) \{\psi \mathbf{O}_{D\rho_{\text{eq}}}\}), \quad (23) \end{aligned}$$

which obviously satisfies

$$\begin{aligned} & (E - E^2 [\bar{\beta}_1(E) + \bar{\beta}_2(E) + \bar{K}_2(E)])^{-1} C(2) \\ &= \{\psi D\rho_{\text{eq}}\} + E \bar{\beta}_1(E) \{\psi \mathbf{O}_{D\rho_{\text{eq}}}\}. \quad (24) \end{aligned}$$

To third and higher order in the density there occurs a divergence¹⁵ at $E=0$ which we shall discuss in Sec. III. For sufficiently large E , however, the series in (18) can be terminated above second order.

III. ZERO-FREQUENCY DIFFICULTY

The purpose of this section is to point out that the coefficients of the third and higher order terms in the density expansion of quantum transport coefficients have a divergence at zero frequency. Our purpose is not to completely resolve this difficulty, but to show where it comes from, and to suggest a path for future investigations.

Let us, then, consider the zero-frequency limit

¹⁵ J. Weinstock, Phys. Rev. Letters **17**, 130 (1966).

of (18):

$$a(0) = \text{Tr} \psi \left(-\lim_{E \rightarrow 0} E^2 \sum_{s=1}^{\infty} [\bar{K}_s(E) + \bar{\beta}_s(E)]^{-1} \Phi(0) \right). \quad (25)$$

This can be written in terms of asymptotic time-dependent collision operators by noting, since $\beta(0) = \beta'(0) = K(0) = K'(0) = 0$, that

$$\begin{aligned} \lim_{E \rightarrow 0} E^n \sum_{s=1}^{\infty} [\bar{K}_s(E) + \bar{\beta}_s(E)] \\ = \lim_{E \rightarrow 0} \int_0^{\infty} dt e^{-Et} \sum_{s=1}^{\infty} \frac{d^n}{dt^n} [K_s(t) + \beta_s(t)] \\ = \lim_{t \rightarrow \infty} \sum_{s=1}^{\infty} \frac{d^{n-1}}{dt^{n-1}} [K_s(t) + \beta_s(t)], \quad (n=1, 2), \end{aligned} \quad (26)$$

so that (25) becomes

$$a(0) = \text{Tr} \psi \left(-\lim_{t \rightarrow \infty} \sum_{s=1}^{\infty} [K_s'(t) + \beta_s'(t)]^{-1} \Phi(0) \right), \quad (27)$$

$$\Phi(0) = \{\psi D \rho_{\text{eq}}\} + \lim_{t \rightarrow \infty} \sum_{s=1}^{\infty} [K_s(t) + \beta_s(t)] \{\psi \mathbf{O}_{D \rho_{\text{eq}}}\},$$

or

$$a(0) = \text{Tr} \int_0^{\infty} dt \psi \left[\exp(t \lim_{t \rightarrow \infty} \sum_{s=1}^{\infty} [K_s'(t) + \beta_s'(t)]) \right] \Phi(0). \quad (28)$$

Equations (25), (27), and (28) are equivalent expressions for $a(0)$. [The relaxation form (28) demonstrates that the asymptotic collision operators must be negative definite. This can be recognized as an underlying assumption generally made in nonequilibrium statistical mechanics which has never been proven to all orders, and which is easily lost sight of when autocorrelations are written in E space, as in (25).] An immediate consequence of (27) or (28) is that one only needs the asymptotic forms of the collision operators $\beta_s'(t)$, $K_s'(t)$, $\beta_s(t)$, and $K_s(t)$ to calculate quantum transport coefficients. Related results have been previously established by Balescu¹² and Swenson¹³ for the asymptotic operators in the formal interaction potential expansion of transport coefficients.

The utility of (25) or (27) as a density expansion depends on whether or not the limit can be interchanged with the sum,

$$\lim_{t \rightarrow \infty} \sum_{s=1}^{\infty} [K_s'(t) + \beta_s'(t)] = \sum_{s=1}^{\infty} [K_s'(\infty) + \beta_s'(\infty)], \quad (29)$$

and this requires that $\beta_s'(\infty)$ and $K_s'(\infty)$ exist. In the classical case⁹ it was shown that $\beta_s'(\infty)$ does not exist for $s \geq 3$, although $\beta_1'(\infty)$ and $\beta_2'(\infty)$ do exist. The same

difficulty obtains for the quantum case. In fact, it has been demonstrated¹⁵ that

$$\beta_s'(t) = O(\ln t), \quad (t \rightarrow \infty), \quad (30)$$

when $\beta_s'(t)$ operates on a function of momenta only. There is no corresponding difficulty with the terms $[K_s(\infty) + \beta_s(\infty)] \{\psi \mathbf{O}_{D \rho_{\text{eq}}}\}$ in $\Phi(0)$, it can be shown, since $\mathbf{O}_{D \rho_{\text{eq}}}$ vanishes as soon as all the $(s+1)$ particles of K_s and β_s separate from each other, whereas the growth of $K_s(t)$ and $\beta_s(t)$ with t comes from configurations in which these $s+1$ particles are all separated. The divergence difficulty can be circumvented, analogous to the classical limit, by expanding $\sum_{s=3}^{\infty} \beta_s'(t)$ back into two-body t matrices (quantum binary-collision operators) and then partially resumming the resultant terms into convergent groups. Thus if $R_s^{(m)}(t)$ denotes the m th-order term in the t -matrix expansion of $\beta_s'(t)$ —see Ref. 7 for this expansion—then

$$\sum_{s=3}^{\infty} \beta_s'(t) = \sum_{m=1}^{\infty} \left(\sum_{s=3}^{\infty} R_s^{(m)}(t) \right) \quad (31)$$

and it can be shown that $\sum_{s=3}^{\infty} R_s^{(1)}(t)$ converges to a logarithmic dependence on the density. The logarithmic dependence, as in the classical case, occurs because the effect of this kind of “renormalization” is to cut off the growth of $\beta_s'(t)$ with t at approximately a mean free time $[R_s^{(1)}(t) \propto (\text{mean free time})^{s-2}]$. The details of this “renormalization,” which shall be reserved for a future paper, is analogous to what has been done for the classical limit of self-diffusion and the electron-gas problem.^{9,16}

A word of caution should be interjected here since although this kind of “renormalization” leads to a convergent result it may not be physically significant when the de Broglie wavelength is greater than a mean free path. In such a circumstance the resummation should include terms from the t -matrix expansion of $\sum_{s=4}^{\infty} K_s'(t)$. This has not yet been investigated.

IV. THE GENERAL MOMENTUM CORRELATION FUNCTION

For some transport coefficients, the imaginary part of the symmetric part of the conductivity tensor, for example, it is necessary to consider the more general correlation function

$$a(E) \equiv \beta^{-1} \int_0^{\infty} dt e^{-Et} \int_0^{\beta} d\lambda \langle \psi(-i\hbar\lambda) \psi(t) \rangle, \quad (32)$$

which is somewhat more complicated than the correlation function defined by Eq. (2). By taking advantage

¹⁶ K. Kawasaki and I. Oppenheim, Phys. Rev. **139**, A1763 (1965); J. van Leeuwen and A. Weyland (unpublished).

of commutation within the trace, however, we find that

$$\langle \psi(-i\hbar\lambda)\psi(t) \rangle = \text{Tr}\psi\rho_\lambda(t), \quad (33)$$

where

$$\rho_\lambda(t) \equiv e^{itH/\hbar}\rho_\lambda(0)e^{-itH/\hbar}, \quad (34)$$

$$\rho_\lambda(0) \equiv e^{-\lambda H}\rho_{\text{eq}}\psi e^{\lambda H}. \quad (35)$$

We can now substitute (33) into (32), interchange the order of integration, and follow the steps of Sec. II to obtain

$$a(E) = \beta^{-1} \int_0^\beta d\lambda \text{Tr}\{\psi(E - E^2[\bar{K}(E) + \sum_{s=1}^\infty \beta_s(E)])^{-1} \\ \times (D\rho_\lambda(0) + E[\bar{K}(E) + \sum_{s=1}^\infty \beta_s(E)]\mathbf{O}_{D\rho_\lambda(0)})\}. \quad (36)$$

Comparing (36) with (18) it is seen that the more general case introduces an additional complication of the off-diagonal elements of the equilibrium ensemble since, in (36), we have

$$D\rho_\lambda(0) = D e^{-\lambda H}\rho_{\text{eq}}\psi e^{\lambda H},$$

whereas in (18) we have

$$D\rho(0) = \{\psi D\rho_{\text{eq}}\}.$$

APPENDIX

Formulas for $\bar{\beta}_1(E)$ and $\bar{\beta}_2(E)$ can be obtained by combining Eqs. (31), (A1), and (A5) of Ref. 7:

$$\bar{\beta}_1(E) \equiv \sum_{i < j > N} D t_{ij} g_0(E), \quad (A1)$$

$$\bar{\beta}_2(E) \equiv \sum_{i < j < k > N} D [g_{ijk} - g_0 - (t_{ij} + t_{ik} + t_{jk})g_0 \\ - (t_{ij}t_{ik} + t_{ij}t_{jk} + t_{ik}t_{ij} \\ + t_{ik}t_{jk} + t_{jk}t_{ij} + t_{jk}t_{ik})g_0], \quad (A2)$$

where t_{ij} , g_0 and g_{ijk} are given by

$$t_{ij} \equiv (iL_N^0 + iL_{ij} + E)^{-1}(iL_N^0 + E)^{-1}, \quad (A3)$$

$$g_0 \equiv (iL_N^0 + E)^{-1}, \quad (A4)$$

$$g_{ijk} \equiv (iL_N^0 + iL_{ij} + iL_{ik} + iL_{jk} + E)^{-1}, \quad (A5)$$

and L_N^0 and L_{ij} are quantum-mechanical Liouville operators defined, with f denoting any function on which L_N^0 and L_{ij} operate, by

$$L_N^0 f \equiv \hbar^{-1}[H_N^0, f] \equiv \hbar^{-1}(H_N^0 f - f H_N^0), \quad (A6)$$

$$L_{ij} f \equiv \hbar^{-1}[V_{ij}, f] \equiv \hbar^{-1}(V_{ij} f - f V_{ij}). \quad (A7)$$

It is thus seen that g_0 is the resolvent operator for free particles, g_{ijk} is the resolvent operator for three interacting particles, and t_{ij} (the two-body t matrix) involves the resolvent operator for two interacting particles. The important point to note is that $\bar{\beta}_1(E)$ involves the solution of a two-body problem and $\bar{\beta}_2(E)$ involves the solution of a three-body problem in an explicit manner.

The first term in the density expansion of $\bar{K}(E)$ can be obtained by combining Eqs. (47), (45), and (A1) of Ref. 7:

$$\bar{K}(E) = D \sum_{i < j} t_{ij} \mathbf{O}_D \sum'_{k < m} t_{km} g_0 \\ + \text{higher order terms in density}, \quad (A8)$$

where the prime on the sum over $k < m$ denotes that we omit all terms for which $km = ij$.

It is seen, from (A8), that the first term in the expansion of $\bar{K}(E)$ involves the solution of a two-body problem, but is of second order in the density. This term, as previously noted, is a manifestation of degeneracy statistics and vanishes in a representation of unsymmetrized planewave states.