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Classical and Quantum Kinetic Equations with Exact Conservation Laws

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Stationary and dynamic properties of reduced density matrices can be determined from formal or approximate closures of an infinite hierarchy of equations. The local macroscopic conservation laws place weak but important constraints on the reduced density matrices which should be respected by any closure. For pairwise additive forces conditions on the closure of the one- and two-particle equations are obtained that preserve the exact functional dependence of the conserved densities and their fluxes on the reduced density matrices. To illustrate the nature of these conditions, a closure approximation suitable for a quantum gas is given, yielding an extension of the time-dependent Hartree–Fock equations for the dynamics of a nuclear fluid to include collisions.

KEY WORDS: Kinetic theory; conservation law; time-dependent Hartree–Fock.

1. INTRODUCTION

The determination of approximate kinetic equations from the exact hierarchy for the reduced distributions has its origins in the work of Bogoliubov.[4] He postulated that all distribution functions become time-independent functionals of the single-particle distribution after an initial "synchronization" period. This functional relationship provides a formal closure of the hierarchy of equations yielding a kinetic equation for the single-particle distribution function. In particular, Bogoliubov showed that the density expansion of the two-particle functional leads to the Boltzmann equation as a first approximation. The validity of the functional assump-

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[4] Bogoliubov's original work, written in 1946, appears in English translation in ref. 1.

tion and the convergence of its density expansion were clarified only much later with the systematic investigation by Cohen and his collaborators.[5] These studies unveiled a remarkably rich structure of dynamical properties beyond those expected from corresponding equilibrium many-body studies. In contrast to the initial assumptions of Bogoliubov and others, it is now believed that the functional relationship of reduced distribution functions is nonanalytic in most of the controllable parameters (including the density), and that the required separation of time scales does not exist. Nevertheless, the notion of a functional relation as a means for obtaining kinetic equations remains at the heart of both formally exact and approximate methods, although its construction is a more formidable and interesting problem than originally anticipated.

The objective here is to describe an important constraint imposed by local conservation laws on any approximate closure relation.[6] The results below do not indicate a method for constructing such an approximation, but only provide guidance for preservation of some of the most important properties. Attention is limited to a one-component fluid of particles interacting via short-ranged, repulsive, pairwise additive potentials. The notation is chosen to emphasize the structural similarity of classical and quantum problems. Observables of interest are represented by sums of single-particle or two-particle operators. If y denotes such an observable, then its average value at time t is given by

$$\langle y; t\rangle = \operatorname*{Tr}_{1} y(1) f^{(1)}(1; t) + \operatorname*{Tr}_{1,2} y(1, 2) f^{(2)}(1,2; t) \tag{1}$$

Here $y(1)$ and $y(1, 2)$ are the one- and two-particle operators defining y, and $f^{(s)}$ is the reduced density operator for s particles.(3) The traces are defined over one- and two-particle Hilbert spaces, respectively. A complete description of these observables is therefore given by specification of only the two lowest order reduced density operators. These in turn are determined from the quantum BBGKY (Bogoliubov, Born, Green, Kirkwood, Yvon) hierarchy.(3,4)

The microscopic conservation laws are identities relating the local densities to associated fluxes. Each density and flux is represented by an operator of the above form. Let ψ denote the average of one of the local conserved densities and $\boldsymbol{\phi}$ its associated average flux. Then the macroscopic conservation law has the form

$$\frac{\partial}{\partial t} \psi(\mathbf{r} \mid f^{(1)}, f^{(2)}) + \nabla \cdot \boldsymbol{\phi}(\mathbf{r} \mid f^{(1)}, f^{(2)}) = 0 \tag{2}$$

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[5] See ref. 2 for a review with references.

[6] This work was first presented at the 1980 Sanibel Symposium (University of Florida preprint series 80-4, available on request).

where ψ and ϕ are specified time-independent linear functionals of $f^{(1)}$ and $f^{(2)}$. The specific form of these functionals is given in the Appendix. The relationships (2) are the desired constraints on the dynamics of $f^{(1)}$ and $f^{(2)}$, or equivalently, the closure of the hierarchy. The strongest constraint [Eq. (8) below] is required by the energy conservation law.

Two forms of the macroscopic conservation laws are distinguished, "weak" and "strong." In their weak form the conservation laws simply relate the time derivative of a conserved density to the divergence of a flux, without regard to the dependence of the flux on $f^{(1)}$ or $f^{(2)}$. Most small-parameter expansion methods lead to weak conservation laws, with the Boltzmann equation as an example. The constraints discussed here lead to strong conservation laws, defined to be such that the exact functional dependence of both the densities and fluxes on the distribution functions is preserved. This point of view takes the reduced density matrices as the primary variables for which approximations are made, with all other properties derived from them.

The conservation laws are associated with underlying symmetries of the Galilei group which must be imposed also on the closure relation for self-consistency. Preservation of the conservation laws and symmetries still allows for a wide class of approximations. For example, any representation of the three-particle reduced density operator as a functional of the one- and two-particle density operators is constrained only by symmetry conditions. An example of such a closure is provided in Section 3. The system considered in this example is a gas with two-particle scattering length a such that the dimensionless density na^3 is small. An appropriate closure is introduced which yields a binary collision approximation generalizing the Boltzmann equation to include small space and time scales. This generalization is precisely what is required to extend the conservation laws to their strong form. However, when degeneracy effects are important(3) this binary collision closure does not satisfy the constraints required for the strong form of the conservation laws. The necessary modifications are found to yield mean field corrections to the quantum Boltzmann equation that are identified as Hartree–Fock and random phase contributions.(5) Thus, the requirement of exact conservation laws introduces effects that are not associated with the small parameter na^3. This model is relevant for generalization of the time-dependent Hartree–Fock description of heavy-ion scattering to include collisions. Early attempts to formulate such a kinetic description of heavy-ion scattering led to difficulties with energy conservation.(6) The results here have exact conservation of energy by construction.

In some cases closure may be accomplished in a formally exact manner. For classical mechanics implicit or explicit statements of the relationship of formal collision operators to conservation laws appear in many different contexts (see refs. 7 and 8 for early examples). Conditions on the closure associated with the Schwinger functional method(9) and formal algebraic methods(10) have been given for both quantum and classical field theories. The discussion of conservation laws here complements these by emphasizing the hierarchy rather than a specific method. In this way the linear kinetic theory of correlation functions or Green's functions and the nonlinear kinetic theory for distribution functions can be treated in the same way. Furthermore, it is straightforward to describe quantum and classical mechanics in a notationally similar form. No analysis of the closure problem itself is given here.

2. HIERARCHY AND CONSERVATION LAWS

The reduced density operators $f^{(s)}$ are obtained from a partial trace of the density operator for the complete system over all except those for s degrees of freedom. The density operator is defined for a Hilbert space of both symmetric and antisymmetric states, with a suitable projection for fermions or bosons.(3) The Liouville–von Neumann equation then leads to a hierarchy of equations for the operators $f^{(s)}$. It is sufficient here to consider only the first two equations of this hierarchy,

$$\begin{gathered}\left[\frac{\partial}{\partial t}+L(1)\right]f^{(1)}(1;t)+\operatorname*{Tr}_{2}L_I(1,2)\,f^{(2)}(1,2;t)=0\\ \left[\frac{\partial}{\partial t}+L(1,2)\right]f^{(2)}(1,2;t)+\operatorname*{Tr}_{3}[L_I(1,3)+L_I(2,3)]\,f^{(3)}(1,2,3;t)=0\end{gathered}\tag{3}$$

The Liouville operators $L(1)$ and $L(1,2)$ are defined by

$$\begin{gathered}L(1,2)=L(1)+L(2)+L_I(1,2)\\ L(\alpha)\,A(\alpha)=i[H(\alpha),A(\alpha)]\\ L_I(\alpha,\beta)\,A(\alpha,\beta)=i[V(\alpha,\beta),A(\alpha,\beta)]\end{gathered}\tag{4}$$

where $H(\alpha)$ is the single-particle Hamiltonian and $V(\alpha,\beta)$ is the potential energy operator for the pair of particles (α,β). Units such that $\hbar=1$ have been used.

Equations (3) do not determine $f^{(1)}$ and $f^{(2)}$, because of the coupling to $f^{(3)}$. However, a closed set of equations is obtained by a closure relation of the form

$$G(1,2;t\,|\,f^{(1)},f^{(2)})=\operatorname*{Tr}_{3}[L_I(1,3)+L_I(2,3)]\,f^{(3)}(1,2,3;t)\tag{5}$$

where $G(1, 2; t \mid \cdot, \cdot)$ is an operator-valued functional for the two-particle Hilbert space. In some cases this replacement can be made as a formally exact construction; in others it only defines an approximation. The functional in general is nonlinear in the reduced density matricies and nonlocal in space and time. Once $G(1, 2; t \mid \cdot, \cdot)$ has been determined, the one- and two-particle density operators can be calculated from (3) without further regard of higher-order density operators. Some general constraints on the choice of G are easily identified. For example, the exact hierarchy is invariant under transformations of the Galilei group, so G must reflect the corresponding symmetry. Also, permutation symmetry requires $G(1, 2; t \mid \cdot, \cdot) = G(2, 1; t \mid \cdot, \cdot)$. Finally, two other conditions follow from Eq. (5) and the definition of $f^{(2)}$,

$$\operatorname*{Tr}_{1,2} G(1, 2; t \mid f^{(1)}, f^{(2)}) = 0 \tag{6}$$

$$\operatorname*{Tr}_{2} G(1, 2; t \mid f^{(1)}, f^{(2)}) = N \operatorname*{Tr}_{3} L_I(1, 3) f^{(2)}(1, 3) \tag{7}$$

The conservation laws for a simple fluid are those for mass, energy, and momentum. The local macroscopic conservation equations are determined from the first two hierarchy equations by writing the average densities in the form of Eq. (1) and differentiating with respect to time. The contributions from $L(\alpha)$ and $L(\alpha, \beta)$ can be transformed to the divergence of an average flux, yielding equations of the forms given in (2). The calculation is straightforward, but lengthy,(11,12) and only an outline is given in the Appendix. The specific form of the densities and fluxes as linear functionals of $f^{(1)}$ and $f^{(2)}$ are also given in the Appendix. The primary observation is that the analysis places only *one* additional constraint on $G(1, 2; t \mid \cdot, \cdot)$ beyond those indicated above,

$$\operatorname*{Tr}_{1,2} u_\phi(\mathbf{r}; 1, 2)\, G(1, 2; t \mid f^{(1)}, f^{(2)}) = 0 \tag{8}$$

where $u_\phi(\mathbf{r}; 1, 2)$ is the potential energy density,

$$u_\phi(\mathbf{r}; 1, 2) = [\delta(\mathbf{r} - \mathbf{q}_1) + \delta(\mathbf{r} - \mathbf{q}_2)]\, V(1, 2) \tag{9}$$

Here $\mathbf{q}_1$ and $\mathbf{q}_2$ are the position operators for particles 1 and 2, and $\mathbf{r}$ is a classical field point. This remarkably simple condition is sufficient to impose the exact conservation laws in their strong form.

3. DEGENERATE QUANTUM GAS

To illustrate the utility of the requirements of the conservation laws and the other constraints of Section 2, a closure approximation suitable for the description of a degenerate quantum gas is described here. It is easily verified that all conditions of the last section are satisfied by a closure approximation of the form

$$G(1, 2; t \,|\, f^{(1)}, f^{(2)}) = -(1 + \mathscr{P}_{12}) \operatorname*{Tr}_{3} L_I(1, 3)\, f^{(3)}(123 \,|\, f^{(1)}, f^{(2)}) \tag{10}$$

where the three-particle reduced density operator is expressed as a functional of $f^{(1)}$ and $f^{(2)}$. The symbol $\mathscr{P}_{12}$ indicates a permutation of the labels 1 and 2 in all operators to its right. It is perhaps easiest to understand the approximation to be considered here by describing the nondegenerate case first. For a low-density gas with two-particle scattering length a and density n the dimensionless quantity na^3 is a small parameter. To lowest order in this parameter only pairwise independent binary collisions contribute and a typical term on the right side of Eq. (10) can be approximated by

$$V(\alpha, \beta)\, f^{(3)}(\alpha\beta\gamma) \rightarrow V(\alpha, \beta)\, f^{(2)}(\alpha, \beta)\, f^{(1)}(\gamma) \tag{11}$$

This approximation results from recognizing that $V(\alpha, \beta)$ requires particles α and β to be within the range a, and consequently the probability of the third particle γ also being in this range is of order na^3. Correlations of γ with either α or β therefore are negligible to lowest order. Use of Eq. (11) in the first two hierarchy equations gives an accurate description of a low-density gas. The equilibrium state is exact to order na^3. The kinetic equation for $f^{(1)}$ reduces to the usual Boltzmann equation if the further restrictions to large space and time scales are imposed. Without these restrictions it is easily verified that the exact conservation laws hold in their strong form. It is also verified that the resulting closed equations for $f^{(1)}$ and $f^{(2)}$ have the symmetry of the Galilei group, including time-reversal invariance. (For large space and time scales, the time-reversed equations lead to the "anti-Boltzmann equation" discussed by Cohen and Berlin.(13)) Equation (11) will be referred to as the binary collision approximation.

The situation is somewhat more complex for a degenerate gas because the thermal de Broglie wavelength λ provides an additional length whereby the density may be scaled. The parameter na^3 is still small for a dilute gas, but the parameter $n\lambda^3$ can be very large at low temperatures. This means the correlation effects associated with Bose–Einstein or Fermi–Dirac statistics can be quite large and must be accounted for. The approximation (11) cannot be correct in this case because it does not account for long-range correlations due to the fact that $f^{(3)}$ is a projection onto properly symmetrized three-particle states. It is convenient to make this property explicit by defining $\bar{f}^{(s)}(1..s)$ as

$$f^{(s)}(1..s) = S(1..s) \frac{1}{s!} \bar{f}^{(s)}(1..s)\, S(1..s) \tag{12}$$

$$= \bar{f}^{(s)}(1..s)\, S(1..s) \tag{13}$$

where $S(1..s)$ is the s-body symmetrization operator

$$S(1..s)=\sum_{P_s}\varepsilon^{P_s}P_s \tag{14}$$

Here P_s denotes a member of the permutation group for s-particles and ε has the value $+1$ for bosons or -1 for fermions. Equation (13) follows from the identity $S^2(1..s)=s!\,S(1..s)$ and the symmetry of $f^{(s)}(1..s)$. The quantity considered on the left side of (11) can be written exactly as

$$V(\alpha,\beta)\,f^{(3)}(\alpha\beta\gamma)=V(\alpha,\beta)\,\bar{f}^{(3)}(\alpha\beta\gamma)\,S(\alpha\beta\gamma) \tag{15}$$

Since the exchange effects are now explicitly displayed in (15), the binary approximation of Eq. (11) can be applied now to $V(\alpha,\beta)\,\bar{f}^{(3)}(\alpha\beta\gamma)$,

$$V(\alpha,\beta)\,\bar{f}^{(3)}(\alpha\beta\gamma)\rightarrow V(\alpha,\beta)\,\bar{f}^{(2)}(\alpha\beta)\,\bar{f}^{(1)}(\gamma) \tag{16}$$

Then, noting that $S(\alpha\beta\gamma)=S(\alpha\beta)[1+P_{\alpha\gamma}+P_{\beta\gamma}]$, where $P_{\alpha\beta}$ is the permutation operator for two-particle states, (15) and (16) yield the approximate closure

$$V(\alpha,\beta)\,f^{(3)}(\alpha\beta\gamma)\rightarrow V(\alpha,\beta)\,f^{(2)}(\alpha\beta)\,f^{(1)}(\gamma)[1+P_{\alpha\gamma}+P_{\beta\gamma}] \tag{17}$$

This result generalizes the binary collision approximation to include degenerate gases.

Before criticizing (17), it is instructive to see its implications for the first two hierarchy equations. The first of Eqs. (3) is of course unchanged. The second becomes

$$\left[\frac{\partial}{\partial t}+L(1)+L(2)+\hat{L}_I(12)\right]g(12)=-\hat{L}_I(12)\,f^{(1)}(1)\,f^{(1)}(2)(1+P_{12}) \tag{18}$$

$$g(12)=f^{(2)}(12)-f^{(1)}(1)\,f^{(1)}(2)(1+P_{12}) \tag{19}$$

where $g(12)$ is the correlated part of $f^{(2)}(12)$, and $\hat{L}_I$ describes an exchange-modified pair interaction,

$$\begin{aligned}\hat{L}_I(12)\,X(12)&=i[\hat{V}(12)\,X(12)-X(12)\,\hat{V}^*(12)]\\ \hat{V}(12)&\equiv[f^+(1)\,f^+(2)-f^{(1)}(1)\,f^{(1)}(2)]\,V(12)\end{aligned} \tag{20}$$

The factors $f^+\equiv 1+\varepsilon f^{(1)}$ and $f^{(1)}(1)$ in the modified potential energy operator $\hat{V}$ result from the possible exchange of either one of the pair $(1, 2)$ with any other particle of the fluid, and represents a true many-body effect. [In the language of many-body perturbation theory, the factor $f^+(1)\,f^+(2)$ results from two-particle lines, while $f^{(1)}(1)\,f^{(1)}(2)$ corresponds to two-hole lines.] The equilibrium and nonequilibrium properties of this approximate closure have been studied in some detail in ref. 3. The equilibrium two-particle density matrix agrees with that of Martin and Schwinger's ladder approximation to the Bethe–Salpeter equation for the two-particle Green's function.(14) The corresponding pressure has been compared with the Bethe–Uhlenbeck, Brueckner, and de Domenicis forms using realistic potentials for nuclear matter.(15) A kinetic equation for the one-particle reduced density operator also was obtained in the form of a generalized Uehling–Uhlenbeck equation.

The binary collision approximation (11) leads to a closure of the form given by Eq. (10) and therefore implies the strong conservation laws. However, the degenerate case, (17), cannot be put in this form and does not satisfy the constraints of Section 2 for strong conservation laws. The difficulty can be traced to the use of $S(\alpha\beta\gamma)\,\bar{f}^{(3)}(\alpha\beta\gamma)=\bar{f}^{(3)}(\alpha\beta\gamma)\,S(\alpha\beta\gamma)$ to write Eq. (15), while this symmetry no longer holds after the binary collision approximation (16). This inconsistency is not unexpected, since the binary collision approximation applies to the product $V(\alpha\beta)\,\bar{f}^{(3)}(\alpha\beta\gamma)$ rather than to $\bar{f}^{(3)}(\alpha\beta\gamma)$ alone. It appears, however, that the conservation laws require a more symmetric treatment of $\bar{f}^{(3)}$ that includes additional effects not of the binary collision type. The simplest such closure that contains the binary collision approximation appears to be

$$\begin{aligned} V(\alpha,\beta)\,\bar{f}^{(3)}(\alpha\beta\gamma) \to V(\alpha,\beta)[&\bar{f}^{(2)}(\alpha\beta)\,\bar{f}^{(1)}(\gamma)+\bar{f}^{(2)}(\alpha\gamma)\,\bar{f}^{(1)}(\beta) \\ &+\bar{f}^{(2)}(\gamma\beta)\,\bar{f}^{(1)}(\alpha)-2\bar{f}^{(1)}(\alpha)\,\bar{f}^{(1)}(\beta)\,\bar{f}^{(1)}(\gamma)] \end{aligned} \tag{21}$$

The first term is the binary collision term of Eq. (16), while the second and third terms result from its symmetrization. The last term is required to assure the proper uncorrelated limit when all particles are asymptotically far apart. These additional terms cannot be justified as being of lowest order in na^3, instead, their inclusion is required by the conservation laws, which are now assured by the closure (21).

Use of this closure in (12) gives the revised binary collision approximation,

$$\begin{aligned} V(\alpha,\beta)\,f^{(3)}(\alpha\beta\gamma) \to\; & V(\alpha,\beta)\,f^{(2)}(\alpha\beta)\,f^{(1)}(\gamma)[1+P_{\alpha\gamma}+P_{\beta\gamma}] \\ &+V(\alpha,\beta)\;g(\alpha\gamma)\,f^{(1)}(\beta)[1+P_{\alpha\beta}+P_{\gamma\beta}] \\ &+V(\alpha,\beta)\;g(\beta\gamma)\,f^{(1)}(\alpha)[1+P_{\alpha\beta}+P_{\gamma\alpha}] \end{aligned} \tag{22}$$

The second equation of the hierarchy is found to have a form similar to that of Eq. (18),

$$\begin{aligned} &\left[\frac{\partial}{\partial t}+\bar{L}(1)+\bar{L}(2)+\hat{L}_I(12)\right] g(12) \\ &\qquad = -\hat{L}_I(12)\,f^{(1)}(1)\,f^{(1)}(2)(1+P_{12}) \end{aligned} \tag{23}$$

except that the free-particle operators $L(\alpha)$ have been replaced by mean field operators,

$$\bar{L}(\alpha)\, X(\alpha) = i[\varepsilon_{\mathrm{HF}}(\alpha), X(\alpha)] + \mathscr{H}(\alpha)\, X(\alpha) \tag{24}$$

Here, $\varepsilon_{\mathrm{HF}}(\alpha)$ is the Hartree–Fock Hamiltonian,

$$\varepsilon_{\mathrm{HF}}(\alpha) = H(\alpha) + \operatorname*{Tr}_{\beta} f^{(1)}(\beta)\, V(\alpha\beta)(1 + P_{\alpha\beta}) \tag{25}$$

and $\mathscr{H}(\alpha)$ is the quantum Vlasov operator,

$$\mathscr{H}(\alpha)\, X(\alpha) = i \operatorname*{Tr}_{\beta}[V(\alpha\beta)(1 + P_{\alpha\beta}), f^{(1)}(\alpha)]\, X(\beta) \tag{26}$$

It can be shown(16) that the Vlasov operators generate contributions of the random phase approximation. Thus, the differences between the two binary collision approximations (18) and (23) are Hartree–Fock and random phase renormalization of the free-particle propagation.

The first equation of the hierarchy provides the basis for obtaining a kinetic equation. In terms of $g(12; t)$ it becomes

$$\frac{\partial}{\partial t} f^{(1)}(1; t) + i[\varepsilon_{\mathrm{HF}}(1), f^{(1)}(1; t)] + \operatorname*{Tr}_{2} L_I(1, 2)\, g(1, 2; t) = 0 \tag{27}$$

If correlations are neglected $[g(12; t) = 0]$, the time-dependent Hartree–Fock kinetic equation is obtained. This equation has been applied extensively over the past 10 years to describe heavy-ion collisions (see, e.g., ref. 17). In many cases the effects of dissipation must also be described and several methods have been proposed for the addition of a collision operator to the time-dependent Hartree–Fock equation. As noted in the introduction, there has been some concern about the consistency of collision operators and energy conservation.(6) The closure approximation (23) appears to provide a good model for the desired kinetic equation. It is known that the simple version of this approximation (18) provides an adequate description of the degeneracy effects in nuclear matter.(15) The mean field modifications of this result in (23) assure in addition that the conservation laws are strictly maintained. The detailed form of the collision operator is obtained by solving (23) for $g(12; t)$ as a functional of $f(1; t)$. The procedure parallels closely that of ref. 3, and will be described elsewhere.

4. DISCUSSION

Conservation laws are an essential ingredient for most problems involving macroscopic transport. For example, it would be inconsistent to calculate a transport coefficient from a kinetic theory that did not imply the conservation equation in which the coefficient occurs. This has been a primary problem in attempts to extend the classical dense-gas Enskog kinetic theory of hard spheres to other potential models. For example, a natural generalization for the square-well potential(18) fails to satisfy energy conservation, leading to inconsistencies in the calculation of the bulk viscosity. Although a modification has been developed recently to resolve the difficulty in this particular case,(19) it remains a problem for other potential models. The condition (8) given here provides guidance to a general class of closures that are free of such problems.

Regarding the specific example considered in Section 3, it should be noted that the final result (22) can be obtained directly from the more familiar cluster representation for $\bar{f}^{(3)}(\alpha\beta\gamma; t)$,

$$\begin{aligned}\bar{f}^{(3)}(\alpha\beta\gamma; t) &= \bar{f}^{(1)}(\alpha; t)\,\bar{f}^{(1)}(\beta; t)\,\bar{f}^{(1)}(\gamma; t) + \bar{g}(\alpha\beta; t)\,\bar{f}^{(1)}(\gamma; t)\\ &\quad + \bar{g}(\alpha\gamma; t)\,\bar{f}^{(1)}(\beta; t) + \bar{g}(\beta\gamma; t)\,\bar{f}^{(1)}(\alpha; t) + \bar{g}(\alpha\beta\gamma; t) \qquad (28)\end{aligned}$$

Here $\bar{g}(\alpha\beta; t) = \bar{f}^{(2)}(\alpha\beta; t) - \bar{f}^{(1)}(\alpha; t)\,\bar{f}^{(1)}(\beta; t)$. If the three-particle correlation function $\bar{g}(\alpha\beta\gamma; t)$ is neglected, then the approximate closure (21) is regained. This approximation has been used to discuss classical kinetic equations both for plasmas(20) and for neutral fluids.(21) Its extension to the degenerate quantum domain is straightforward, leading to (23), which describes a wealth of quantum effects that are difficult to obtain by more standard many-body methods. We are not aware of any detailed analysis of the resulting equations and we hope to present the equilibrium solutions for $\bar{f}^{(1)}$ and $\bar{f}^{(2)}$ as well as the associated kinetic equation elsewhere. The primary point of importance here, however, is that the closure approximation was not obtained by the simple neglect of $g(\alpha\beta\gamma; t)$ in (28). This would be hard to justify on the basis of a systematic expansion in the small parameter na^3. Instead, we attempted to retain the dominant effects to order na^3 in Eq. (17) and found that the constraints imposed by the conservation laws required inclusion of the additional terms in (22). In this sense, the discussion here provides some justification or interpretation of the neglect of $\bar{g}(\alpha\beta\gamma; t)$ in (28) for degenerate fluids. These additional terms also survive in the nondegenerate limit, leading to Vlasov mean field corrections in the classical binary collision kinetic equation.[7]

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[7] It is possible to weaken (22) such that only the exchange parts of the last two terms on the right side are retained. This would still maintain the conservation laws for the degenerate case, and the simple binary collision approximation (17) would be recovered in the nondegenerate limit. However, this weakened version of (22) appears somewhat contrived, and we prefer to consider (22) as the natural extension of the binary collision approximation with exact conservation laws.

The problem of energy conservation from quantum kinetic equations with three-particle collisions also has been studied recently.$^{(22,23)}$ However, only the case of a nondegenerate, spatially homogeneous state was considered. The analysis in these references would be considerably simplified using the general conditions described here. For example, inspection of Eqs. (28)–(30) of ref. 22 is sufficient to see that condition (8) is satisfied, and thus to conclude that energy conservation holds without further computation.

APPENDIX

For a simple fluid the local conserved densities are those associated with mass, momentum, and energy,

$$\begin{aligned}
\rho(\mathbf{r}) &= \sum_{i=1}^{N} m\,\delta(\mathbf{r}-\mathbf{r}_i) \\
\mathbf{p}(\mathbf{r}) &= \sum_{i=1}^{N} [\mathbf{p}_i, \delta(\mathbf{r}-\mathbf{r}_i)]_+ \\
u(\mathbf{r}) &= \sum_{i=1}^{N} (4m)^{-1} [p_i^2, \delta(\mathbf{r}-\mathbf{r}_i)]_+ + \sum_{i\neq j}\sum V(ij)\,\delta(\mathbf{r}-\mathbf{r}_i)
\end{aligned} \tag{A.1}$$

Here r_i and p_i denote the position and momentum operators, respectively, for the ith particle, and the bracket $[\ ,\ ]_+$ denotes the anticommutator. The average values for these densities are obtained by a trace over all degrees of freedom weighted by the N-particle density operator. Since the above are all sums of single-particle and two-particle operators, the results can be expressed in the form (1),

$$\begin{aligned}
\langle \rho(\mathbf{r}); t\rangle &= \operatorname*{Tr}_{1} m\,\delta(\mathbf{r}-\mathbf{r}_1)\, f^{(1)}(1; t) \\
\langle \mathbf{p}(\mathbf{r}); t\rangle &= \operatorname*{Tr}_{1} [\mathbf{p}_1, \delta(\mathbf{r}-\mathbf{r}_1)]_+ f^{(1)}(1; t) \\
\langle u(\mathbf{r}); t\rangle &= \operatorname*{Tr}_{1} (4m)^{-1} [p_1^2, \delta(\mathbf{r}-\mathbf{r}_1)]_+ f^{(1)}(1; t) \\
&\quad + \operatorname*{Tr}_{1,2} V(12)\,\delta(\mathbf{r}-\mathbf{r}_1)\, f^{(2)}(12; t)
\end{aligned} \tag{A.2}$$

This identifies the functionals defining the average conserved densities.

The conservation laws and associated fluxes are obtained by differentiation of (A.2) with respect to time and use of the hierarchy equations (3). To illustrate the calculation, we consider only the energy density,

$$\begin{aligned}\frac{\partial}{\partial t}\langle u(r); t\rangle = {} & \underset{1}{\mathrm{Tr}}(4m)^{-1}\,[p_1^2, \delta(\mathbf{r}-\mathbf{r}_1)]_+\,\{L(1)\,f^{(1)}(1)\\ & + \underset{2}{\mathrm{Tr}}\,L_I(12)\,f^{(2)}(12)\}\\ & + \underset{1,2}{\mathrm{Tr}}\,V(12)\,\delta(\mathbf{r}-\mathbf{r}_1)\{L(12)\,f^{(2)}(12) + G(12; t\,|\,f^{(2)}, f^{(1)})\}\end{aligned} \tag{A.3}$$

By the cyclic property of the trace, the L operators can be shifted to operate on the phase functions rather than the reduced density operators. Simplifications occur since $L(1)$ vanishes when operating on any function of the momentum only, while $L_I(12)$ vanishes when operating on a function of the coordinate only,

$$\begin{aligned}\frac{\partial}{\partial t}\langle u(\mathbf{r}); t\rangle = {} & -\underset{1}{\mathrm{Tr}}(4m)^{-1}\,[p_1^2, L(1)\,\delta(\mathbf{r}-\mathbf{r}_1)]_+\,f^{(1)}(1)\\ & -\underset{1,2}{\mathrm{Tr}}(4m)^{-1}\,[L_I(1,2)\,p_1^2, \delta(\mathbf{r}-\mathbf{r}_1)]_+\,f^{(2)}(12)\\ & -\underset{1,2}{\mathrm{Tr}}\{[L(1)+L(2)]\,V(12)\,\delta(\mathbf{r}-\mathbf{r}_1)\}\,f^{(2)}(12)\\ & +\underset{1,2}{\mathrm{Tr}}\,u_\phi(\mathbf{r}; 12)\,G(12; t\,|\,f^{(2)}, f^{(1)})\end{aligned} \tag{A.4}$$

where u_ϕ is defined in Eq. (9). The first three terms can be expressed as the gradient of a flux with the identities

$$\begin{aligned}L(1)\,\delta(\mathbf{r}-\mathbf{r}_1) &= -(2m)^{-1}\,\nabla_r\cdot[\mathbf{p}_1, \delta(\mathbf{r}-\mathbf{r}_1)]_+\\ \delta(\mathbf{r}-\mathbf{r}_1)-\delta(\mathbf{r}-\mathbf{r}_2) &= \frac{\partial}{\partial r_\beta}\int_0^1 ds\,(\mathbf{r}_1-\mathbf{r}_2)_\beta\,\delta(\mathbf{r}-\mathbf{r}_1-s(\mathbf{r}_2-\mathbf{r}_1)) \qquad \text{(A.5)}\\ &\equiv -\frac{\partial}{\partial r_\beta}\Delta_\beta(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2)\end{aligned}$$

Then Eq. (A.4) becomes

$$\frac{\partial}{\partial t}\langle u(\mathbf{r}); t\rangle + \frac{\partial}{\partial r_\beta}\langle s_\beta(\mathbf{r}); t\rangle = \underset{1,2}{\mathrm{Tr}}\,u_\phi(\mathbf{r}; 12)\,G(12; t\,|\,f^{(2)}, f^{(1)}) \tag{A.6}$$

where the average energy flux $\langle s_\beta(\mathbf{r}); t\rangle$ is found to be

$$\begin{aligned}\langle s_\beta(\mathbf{r}); t\rangle = {} & \underset{1}{\mathrm{Tr}}(8m^2)^{-1}\,[p_1^2, [p_{1\beta}, \delta(\mathbf{r}-\mathbf{r}_1)]_+]_+\,f^{(1)}(1)\\ & + \underset{1,2}{\mathrm{Tr}}(8m)^{-1}\,\{[V(12), [p_{1\alpha}, \delta(\mathbf{r}-\mathbf{r}_1)]_+]_+\\ & + [(p_1+p_2)_\beta, F_\beta(12)]_+\,\Delta_\alpha(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2)\}\,f^{(2)}(12)\end{aligned} \tag{A.7}$$

Here $\mathbf{F}(12)$ is the force associated with the potential $V(12)$. The local average conservation law for energy is now obtained by noting that the right side of (A.6) vanishes for the exact hierarchy [right side of Eq. (5)]; similarly, any approximate closure must satisfy the condition given by Eq. (8).

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