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Kinetic model for pair correlations

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The kinetic equations for the single particle distribution function and pair correlation functions are considered for general nonequilibrium states of a low density gas. The formal relationship of the kinetic equations for correlations to the Boltzmann equation is used as the basis for constructing self-consistent kinetic models. The familiar Bhatnagar-Gross-Krook kinetic model for the nonlinear Boltzmann collision operator is extended to kinetic models for the dynamics of correlations at one and two times. The results provide a practical basis for describing both fluctuations and transport phenomena in complex nonequilibrium states.

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I. INTRODUCTION

The nonlinear Boltzmann equation for the one particle distribution function provides an accurate description of transport phenomena in a low density gas. Applications have been limited primarily to states near equilibrium due to the difficulty in solving this equation. However, considerable progress has been made using model kinetic equations obtained by replacing the Boltzmann collision operator with a representative, but more tractable, operator. The simplest of these is a single relaxation time model due to Bhatnagar, Gross, and Krook (BGK model) [1]. The essential qualities of this model are its preservation of the exact equilibrium solution (with an H theorem for asymptotic approach to this solution) and all five conservation laws. The BGK model is still a complex nonlinear, integro-differential kinetic equation for the distribution function, but several exact solutions are now known that provide a rare description of stationary states far from equilibrium [1,2]. Furthermore, this model admits simpler numerical analysis than the Boltzmann equation for a wide class of boundary conditions.

The Boltzmann equation does not provide any direct information about the dynamics of correlations (fluctuations) in the gas, but methods used in its derivation can be extended to obtain kinetic equations for the correlations in the same low density approximation. The most general result is a kinetic equation for a generating functional at low density from which all multipoint correlations can be obtained by functional differentiation [3]. This approach also makes explicit the close relationship of the kinetic equations for correlations to the Boltzmann kinetic equation, and suggests the possibility of formulating BGK models for the correlation function equations as well. The objective here is to indicate how this can be done for the simplest and most important case of pair correlations.

The dynamics of two point correlations at low density is a well-studied problem only for the equilibrium state [4]. Such correlations are described by a linearized Boltzmann collision operator; even here, practical applications are obtained only by introducing a corresponding linearized equilibrium BGK kinetic model. Equilibrium multipoint correlation functions also have been described in terms of the linear and nonlinear Boltzmann operators [5] and applied to steady states close to equilibrium [6]. Ten years ago, there was substantial interest in calculating equal time pair correlations for stationary nonequilibrium states as a test of fluctuation theories away from equilibrium [7]. Most applications were limited to lowest order perturbation about (local) equilibrium, while nonperturbative analyses were based mainly on more macroscopic hydrodynamic descriptions [8]. More recently, interest in pair correlations for nonequilibrium steady states has been revived both by accurate experimental results [9] and a possible association with the concept of self-organized criticality [10]. We address here the problem of describing the dynamics of correlations in the most general nonequilibrium state. The kinetic theory is known and well founded for low density, but practical and accurate approximations are lacking in this general context. The objective here is to provide kinetic models of the BGK type for correlations, such that whenever a solution to the nonlinear Boltzmann-BGK equation can be obtained the correlations can be determined as well. The resulting kinetic model provides a realistic basis for addressing a wide scope of potential applications.

The presentation is organized as follows. Section II has two parts. In the first part the phase space correlation functions are defined, and the kinetic equations for the single particle distribution (nonlinear Boltzmann equation) and the correlation functions are given. These are known results, but their derivation is included in Appendix A for completeness. The analysis is based on an expansion in powers of the ratio of the force range to the mean free path, appropriate for a low density gas of particles with short range interactions [3]. In addition, this derivation gives *all* multipoint correlations at one or two times in terms of the two-point correlations considered in the text. The second part of Sec. II develops the kinetic models for these equations, based on certain fundamental exact functional relationships. The Boltzmann collision operator is a given functional of the distribution function, and the operators characterizing the kinetic equations for the pair correlations can be determined from it by functional differentiation. The properties of this functional reflecting a stationary point and conservation of mass, energy, and momentum are indicated, and the corresponding properties inherited by the kinetic equations for the correlations then are identified as necessary constraints on construction of simple kinetic models. The kinetic equation for equal time correlations has a source term, known as the "noise intensity" (originating from a Langevin model for fluctuations). The relevant exact properties of this source also are identified as constraints for the models. In Sec. III the BGK model for the nonlinear Boltzmann collision operator is introduced and analyzed. A corresponding kinetic model for the pair correlations is proposed, based on the exact functional relationship of all kinetic equations, stationarity, conservation laws, and properties of the noise source. Boundary conditions and the effect of external forces are briefly discussed in Sec. IV. The formal solution to the kinetic equations for the pair correlations is obtained in Sec. V, under the assumption that the Boltzmann-BGK equation has a known stationary solution. More generally, the calculation of correlations for a general nonstationary state follows in a similar way, if the corresponding solution to the Boltzmann-BGK equation is known. Finally, these results are summarized in the last section and some important applications are indicated.

II. KINETIC EQUATIONS AT LOW DENSITY

The system considered is a low density gas of point particles interacting via a short ranged potential. Let $y = \{\mathbf{r}, \mathbf{v}\}$ denote the position and velocity of a point in the single particle phase space. We introduce the microscopic densities

$$\hat{f}(y,t) \equiv \sum_{i=1}^{N} \delta(y - x_i(t)), \tag{2.1}$$

$$\hat{f}(y,t;y',t') \equiv \hat{f}(y,t)\hat{f}(y',t'), \tag{2.2}$$

$$\hat{f}(y_1,y_2,t) \equiv \hat{f}(y_1,t;y_2,t) - \delta(y_1 - y_2)\hat{f}(y_1,t), \tag{2.3}$$

where $x_i(t) \equiv (\mathbf{r}_i(t), \mathbf{v}_i(t))$ is the phase point for particle i at time t. The corresponding *average* phase space densities are the single particle distribution function,

$$f(y,t) \equiv \langle \hat{f}(y,t) \rangle, \tag{2.4}$$

the two particle and two time distribution,

$$f(y,t;y',t') \equiv \langle \hat{f}(y,t;y',t') \rangle, \tag{2.5}$$

and the single time two particle distribution,

$$\begin{aligned} f(y_1,y_2,t) &\equiv \langle \hat{f}(y_1,y_2,t) \rangle \\ &= f(y_1,t;y_2,t) - \delta(y_1 - y_2) f(y_1,t), \end{aligned} \tag{2.6}$$

respectively. The angular brackets denote an average over an ensemble specified at some initial time (taken here to be $t = 0$). Correlations at two phase points and times are defined by

$$\begin{aligned} C(y,t;y',t') &\equiv f(y,t;y',t') - f(y,t)f(y',t') \\ &= \big\langle [\hat{f}(y,t) - \langle \hat{f}(y,t) \rangle] \hat{f}(y',t') \big\rangle. \end{aligned} \tag{2.7}$$

Here and below we choose the convention $t \geq t'$. At low density, and for space and time scales large compared to the force range and collision time, respectively, $f(y,t)$ and $C(y,t;y',t')$ are determined from the kinetic equations [3,11,12] (see Appendix A for a derivation)

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(y,t) = J(y|f(t)), \tag{2.8}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla - \Lambda\right) C(y,t;y',t') = 0. \tag{2.9}$$

The last equation requires specification of the initial data $C(y,t';y,t')$. The analysis in Appendix A also provides a kinetic equation for this equal time correlation function,

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 - \Lambda_1 + \mathbf{v}_2 \cdot \nabla_2 - \Lambda_2\right) C(y_1,t;y_2,t) = B(y_1,y_2|f(t)). \tag{2.10}$$

As expected, Eq. (2.8) for the single particle distribution function is the Boltzmann equation, where $J(y|f(t))$ is the nonlinear Boltzmann collision operator. The kinetic equation for the two time correlation function applies for $t > t'$ and is a generalization of Onsager's regression law for the decay of fluctuations around the nonequilibrium state, $f(y,t)$. It is characterized by a linear operator Λ, which is related to the nonlinear Boltzmann collision operator by

$$\Lambda h(y) = \Lambda(y,t|f,h) = \int dy_1 \, \frac{\delta J(y|f(t))}{\delta f(y_1,t)} h(y_1). \tag{2.11}$$

Since $J(y|f(t))$ is a nonlinear functional of $f(y,t)$, Λ depends on the solution to (2.8), and the solution to (2.9) is therefore a functional of the nonequilibrium distribution. For the special case of Λ operating on the distribution function itself, we have

$$\Lambda(y,t|f,f) \propto J(y|f). \tag{2.12}$$

[The constant of proportionality depends on the form of nonlinearity of $J(y|f)$. For the Boltzmann operator it is 2, while for the BGK model of the next section it is 1.]

The equal time correlation function equation (2.10) involves two of these operators, Λ_1 and Λ_2, defined over functions of y_1 and y_2, respectively, and a source term $B(y_1,y_2|f(t))$. To interpret this source term, we first express the nonlinear Boltzmann collision operator in terms of a binary collision kernel $\gamma(y_1, y_2|f(t))$, through the definition

$$\int dy_2\, \gamma(y_1, y_2|f(t)) = J(y_1|f(t)). \tag{2.13}$$

Clearly, $\gamma(y_1, y_2|f(t))$ represents the velocity changes due to a single binary collision; its detailed form is given in Appendix A. The source term $B(y_1, y_2|f(t))$ is related to this collision kernel by

$$B(y_1, y_2|f(t)) = \gamma(y_1, y_2|f(t)) + \delta(y_1 - y_2)J(y_1|f(t)) \\ -(\Lambda_1 + \Lambda_2)\delta(y_1 - y_2)f(y_1, t). \tag{2.14}$$

Further interpretation of this result is given at the end of this section.

For applications, it is often convenient to consider instead of $C(y_1, t; y_2, t)$ a closely related single time pair correlation function, $G(y_1, y_2, t)$, defined by

$$G(y_1, y_2, t) \equiv f(y_1, y_2, t) - f(y_1, t)f(y_2, t) \\ = C(y_1, t; y_2, t) - \delta(y_1 - y_2)f(y_1, t). \tag{2.15}$$

The kinetic equation for $G(y_1, y_2, t)$ follows directly from (2.10) and (2.14),

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 - \Lambda_1 + \mathbf{v}_2 \cdot \nabla_2 - \Lambda_2\right) G(y_1, y_2, t) \\ = \gamma(y_1, y_2|f(t)). \tag{2.16}$$

Equations (2.8)–(2.16) show the close relationship of the kinetic equations for correlations to the nonlinear Boltzmann equation. The kinetic equations for correlations are linear, but depend on the solution to the nonlinear Boltzmann equation; the latter is autonomous and can be solved independently of the correlations. This structure for the equations of transport and correlations is quite general, and extends to systems other than low density gases [12,13]. It will be exploited in the next section to develop a practical kinetic model for a low density gas. Several exact properties of these equations should be preserved by the kinetic model, in addition to the above structural relationship of J, Λ, and B. A first relevant property of $J(y|f(t))$ is its stationary point at the local equilibrium distribution f_l,

$$J(y|f_l(t)) = 0, \tag{2.17}$$

where $f_l(y,t)$ has the form

$$f_l(y,t) = \exp\left(\sum_{\alpha=1}^{5} z_\alpha(\mathbf{r},t)\psi_\alpha(\mathbf{v})\right). \tag{2.18}$$

The five functions $z_\alpha(\mathbf{r},t)$ are arbitrary at this point, and $\psi_\alpha(\mathbf{v})$ are the summational (collisional) invariants of the nonlinear Boltzmann operator,

$$\psi_\alpha(\mathbf{v}) = \{1, \mathbf{v}, v^2\}. \tag{2.19}$$

In fact, (2.17) is a consequence of (2.13) and the property for γ,

$$\gamma(y_1, y_2|f_l) = 0. \tag{2.20}$$

A second essential property of the collision operator follows from the conservation laws,

$$\int d\mathbf{v}\, \psi_\alpha(\mathbf{v})J(y|f(t)) = 0. \tag{2.21}$$

These two properties of the Boltzmann collision operator are inherited by the kinetic equations for correlations via the relationships (2.11) and (2.12),

$$\Lambda(y,t|f_l, f_l) = 0, \tag{2.22}$$

$$\int d\mathbf{v}\psi_\alpha(\mathbf{v})\Lambda(y,t|f,h) = 0. \tag{2.23}$$

Finally, an essential property of the source term $B(y_1, y_2|f(t))$, related to the conservation laws, is the orthogonality condition for the summational invariants,

$$\int d\mathbf{v}_1\psi_\alpha(\mathbf{v}_1)B(y_1, y_2|f(t)) = 0. \tag{2.24}$$

The proof is given in Appendix B.

The above results show the importance of self-consistency in modeling the kinetic equations. The significance of the conservation laws in the kinetic equations for correlations is discussed further in Sec. VI. In the next section, a kinetic model for transport and fluctuations preserving the relevant exact properties is proposed.

For states near equilibrium the source term B has a simple physical interpretation. From (2.20) and (2.17) it follows that for the special case of local equilibrium Eq. (2.14) reduces to

$$B(y_1, y_2|f_l) = -(\Lambda_1 + \Lambda_2)\delta(y_1 - y_2)f_l(y_1, t). \tag{2.25}$$

This is the expected local equilibrium generalization of the fluctuation-dissipation relation derived by Bixon and Zwanzig [14] and by Fox and Uhlenbeck [15], relating the amplitude of "noise" from other degrees of freedom to the equilibrium fluctuations of $\hat{f}$ and the linearized Boltzmann operator (dissipation). The vanishing of the first two terms of (2.14) for the local equilibrium state is a "detailed balance" property of γ for two particle collision effects. In contrast, nonequilibrium states have boundary and initial conditions or external forces leading to distributions that do not satisfy this condition, and additional physical effects arise from the first two terms of (2.14). As illustrated in Sec. V they can lead to very long range correlations not present in the equilibrium state. They are also related to very slow relaxation in fluctuation corrections to the nonlinear Boltzmann equation, but this will not be considered here.

III. BGK MODEL FOR CORRELATIONS

It is clear from the discussion of Sec. II that any kinetic model for the Boltzmann collision operator will also provide a model for Λ, and hence for the two time correlation function $C(y,t;y',t')$ via (2.11). Also, the orthogonality property of B, Eq. (2.24), can be imposed to model the equation for the equal time correlation function. In this section, the simplest kinetic model for the Boltzmann equation is extended to a self-consistent model for the dynamics of correlations using these relationships.

In constructing a simple kinetic model for the Boltzmann collision operator, the primary properties to be preserved are stationarity and the conservation laws, expressed by Eqs. (2.17) and (2.21). The simplest functional that vanishes at f_l is the local, "linear" form,

$$J^{BGK}(y|f(t)) \equiv -\nu\left[f(y,t) - f_l(y,t)\right], \tag{3.1}$$

where ν is a constant collision frequency. (It is straightforward to generalize the analysis of this section to more complex models for which the collision frequency is a function of the local temperature, density, and velocity.) The conservation laws, (2.21), are imposed by choosing the arbitrary functions $z_\alpha(\mathbf{r},t)$ in the local equilibrium distribution to satisfy

$$\int d\mathbf{v}\, \psi_\alpha(\mathbf{v})\left[f(y,t) - f_l(y,t)\right] = 0. \tag{3.2}$$

This provides five equations defining the z_α as functionals of f, $z_\alpha = z_\alpha(\mathbf{r}|f) \equiv z_\alpha(\mathbf{r},t)$. The constant ν is a characteristic collision frequency that can be chosen to fit an exact eigenvalue of the Boltzmann collision operator or some designated transport coefficient. Equations (3.1) and (3.2) define the BGK model collision operator [1], and the resulting model kinetic equation will be referred to as the Boltzmann-BGK equation.

A corresponding model for the dynamics of the correlations at two different times is obtained directly from (2.11):

$$\begin{aligned}\Lambda^{BGK}h(y) &\equiv \int dy_1 \left(\frac{\delta}{\delta f(y_1,t)} J^{BGK}(y|f(t))\right) h(y_1)\\ &= -\nu\left(h(y) - \int dy_1\, h(y_1)\frac{\delta}{\delta f(y_1,t)} f_l(y,t)\right).\end{aligned} \tag{3.3}$$

The functional dependence of f_l on f occurs entirely through the z_α. Therefore

$$\frac{\delta}{\delta f(y_1,t)} f_l(y,t) = f_l(y,t)\psi_\alpha(\mathbf{v})\frac{\delta}{\delta f(y_1,t)} z_\alpha(\mathbf{r},t). \tag{3.4}$$

A summation convention over repeated greek labels is assumed. To evaluate the functional derivative in (3.4), take the same functional derivative of (3.2) to get

$$\begin{aligned}\delta(\mathbf{r}-\mathbf{r}_1)\psi_\alpha(\mathbf{v}_1) &= \int d\mathbf{v}\, \psi_\alpha(\mathbf{v})\frac{\delta}{\delta f(y_1,t)} f_l(y,t)\\ &= \int d\mathbf{v}\, \psi_\alpha(\mathbf{v}) f_l(y,t)\psi_\beta(\mathbf{v})\\ &\quad\times\frac{\delta}{\delta f(y_1,t)} z_\beta(\mathbf{r},t)\\ &= g_{\alpha\beta}(\mathbf{r},t)\frac{\delta}{\delta f(y_1,t)} z_\beta(\mathbf{r},t),\end{aligned} \tag{3.5}$$

where $g_{\alpha\beta}$ is defined by

$$g_{\alpha\beta}(\mathbf{r},t) = g_{\alpha\beta}(\mathbf{r}|f(t)) \equiv \int d\mathbf{v} f_l(y,t)\psi_\alpha(\mathbf{v})\psi_\beta(\mathbf{v}). \tag{3.6}$$

Inversion of (3.5) for the functional derivative gives

$$\frac{\delta}{\delta f(y_1,t)} z_\alpha(\mathbf{r},t) = \delta(\mathbf{r}-\mathbf{r}_1) g^{-1}_{\alpha\beta}(\mathbf{r},t)\psi_\beta(\mathbf{v}_1) \tag{3.7}$$

and, therefore,

$$\frac{\delta}{\delta f(y_1,t)} f_l(y,t) = f_l(y,t)\delta(\mathbf{r}-\mathbf{r}_1)\psi_\alpha(\mathbf{v}) g^{-1}_{\alpha\beta}(\mathbf{r},t)\psi_\beta(\mathbf{v}_1). \tag{3.8}$$

Finally, use of this result in Eq. (3.3) gives the BGK model for Λ:

$$\Lambda^{BGK}h(y) = -\nu\,(1-P)\,h(y), \tag{3.9}$$

where $P(t)$ is a projection operator defined over functions $X(y)$ by

$$PX(y) = f_l(y,t)\psi_\alpha(\mathbf{v}) g^{-1}_{\alpha\beta}(\mathbf{r},t)\int d\mathbf{v}_1\, \psi_\beta(\mathbf{v}_1) X(\mathbf{r},\mathbf{v}_1). \tag{3.10}$$

This operator is linear with respect to X, but is a nonlinear functional of $f(t)$ through f_l. We notice that from Eq. (3.9) one gets

$$\Lambda^{BGK} f(y,t) = J^{BGK}(y|f(t)), \tag{3.11}$$

which agrees with (2.12). There is a factor of 2 difference in the proportionality constant relative to the Boltzmann result which results from the fact that the Boltzmann-BGK collision operator is highly nonlinear in f (through f_l) whereas the Boltzmann operator is only quadratic in f. This difference does not represent a strong violation of the physics of the Boltzmann description, since the relevant property preserved by the model is that the equation for C can be directly obtained by functional linearization of the equation for f. A more general discussion of this point can be found in Ref. [13].

Next consider the equal time correlations. This requires, in addition to Λ^{BGK}, a model for $B(y_1,y_2|f(t))$. The primary constraint is that imposed by the conservation laws, (2.24). To construct our model we first make the orthogonality of B to the summational invariants explicit by inserting two orthogonal projections in (2.14),

$$\begin{aligned}B(y_1,y_2|f) = (1-P_1)(1-P_2)&\\ \times[\gamma(y_1,y_2|f) + \delta(y_1-y_2)J(y_1|f)&\\ -(\Lambda_1+\Lambda_2)\delta(y_1-y_2)f(y_1)].&\end{aligned} \tag{3.12}$$

This result is still exact. To define the corresponding BGK model for B, we replace J and Λ by J^{BGK} and Λ^{BGK} *and* neglect $(1-P_1)(1-P_2)\gamma(y_1,y_2|f)$, leading to the result

$$\begin{aligned}B^{BGK}(y_1,y_2|f) = \nu(1-P_1)(1-P_2)\delta(y_1-y_2)&\\ \times[f(y_1)+f_l(y_1)],&\end{aligned} \tag{3.13}$$

where use has been made of the property $P_1(1-P_2)f_l(y_2)\delta(y_1-y_2)=0$. While the orthogonality condition is not sufficient to determine B^{BGK} uniquely, the choice (3.13) appears to be the simplest one consistent with the known form near equilibrium, (2.25). It is shown in Sec. V that this choice also yields correct results for correlations in nonequilibrium states.

We have now completed the BGK model for the distribution function and the correlations. Equations (2.8)–(2.10) now become

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f(y,t)=-\nu\left[f(y,t)-f_l(y,t)\right], \tag{3.14}$$

$$\left(\frac{\partial}{\partial t}+\mathcal{L}(t)\right)C(y,t;y',t')=0, \tag{3.15}$$

$$\left(\frac{\partial}{\partial t}+\mathcal{L}_1(t)+\mathcal{L}_2(t)\right)C(y_1,t;y_2,t)$$
$$=\nu(1-P_1)(1-P_2)\delta(y_1-y_2)\left[f(y_1,t)+f_l(y_1,t)\right]. \tag{3.16}$$

To simplify the notation we have introduced the operator

$$\mathcal{L}(t)\equiv\mathbf{v}\cdot\nabla+\nu(1-P). \tag{3.17}$$

The equation for $G(y_1,y_2,t)$ equivalent to (3.16) is obtained from (2.15),

$$\left(\frac{\partial}{\partial t}+\mathcal{L}_1(t)+\mathcal{L}_2(t)\right)G(y_1,y_2,t)$$
$$=\gamma^{BGK}(y_1,y_2|f(t)), \tag{3.18}$$

where γ^{BGK} is defined in terms of B^{BGK} via (2.14),

$$\begin{aligned}B^{BGK}(y_1,y_2|f)=&\ \gamma^{BGK}(y_1,y_2|f)\\&+\delta(y_1-y_2)J^{BGK}(y_1|f)\\&-(\Lambda_1^{BGK}+\Lambda_2^{BGK})\delta(y_1-y_2)f(y_1).\end{aligned} \tag{3.19}$$

More explicitly, $\gamma^{BGK}(y_1,y_2|f(t))$ is found to be

$$\gamma^{BGK}(y_1,y_2|f)=\nu P_1P_2\delta(y_1-y_2)[f(y_1)-f_l(y_1)]. \tag{3.20}$$

Equations (3.14)–(3.16) provide a model for fluctuations and transport in a nonequilibrium gas that is both tractable and realistic. There is no *a priori* restriction to states near equilibrium, so a wide range of problems dealing with the dynamics of correlations in both steady and unsteady nonequilibrium states (including unstable states) can be considered. The equations must be solved sequentially. First, the BGK-Boltzmann equation is solved for given initial and boundary conditions; next, this solution is used to determine the operator $\mathcal{L}$ in Eqs. (3.15) and (3.16). The two time correlation function equation is then solved for $t\geq t'$ in terms of the initial value at $t=t'$. Finally, this initial value is calculated from the solution to (3.16) or (3.18). Since the correlation function equations are linear, their solution is a tractable problem for the kinetic model.

It is well known that the BGK equation retains many of the most important qualitative features of the nonlinear Boltzmann equation, with the obvious quantitative limitations of a single relaxation time model. To explore any additional limitations of this more general model for pair correlations, it is instructive to consider an alternative route to constructing a kinetic model. It is clear from Sec. II that specification of γ completely determines J, Λ, and B. In this way complete consistency with the kinetic theory of Sec. II is maintained. Here, however, we start with a given kinetic model for J and deduce Λ and γ. The reason is, of course, that the BGK model for J is a well-studied and successful model for the distribution function. The price is that the relationship of γ to J in (2.13) is lost. Instead, the BGK model gives

$$\int dy_2\,\gamma^{BGK}(y_1,y_2|f(t))=0. \tag{3.21}$$

In fact, there is no choice of γ consistent with the exact relations (2.13), (2.14), and (2.24), and with the BGK definition (3.1). This is not unexpected since the details of two particle collisions have been replaced in the BGK model for J by an average single relaxation time effect. Consequently, γ^{BGK} also must be understood as an average measure of binary collisions. The illustrations of Sec. V confirm that the relevant properties of γ are retained by γ^{BGK}.

IV. BOUNDARY CONDITIONS AND EXTERNAL FORCES

The most interesting applications of the BGK equations are to nonequilibrium states. These states can arise from initial conditions, boundary conditions, external forces, or a combination of these. The initial conditions for the distribution function $f(y,0)$ and for the equal time correlation function $C(y_1,0;y_2,0)$ must be given in any problem. The specific form for any external forces, $\mathbf{F}_{ext}(y,t)$, also must be given for all times. The presence of this force leads to a modification of Eqs. (3.14)–(3.16) only through the following replacement everywhere:

$$\mathbf{v}\cdot\nabla\rightarrow\mathbf{v}\cdot\nabla+m^{-1}\nabla_{\mathbf{v}}\cdot\mathbf{F}_{ext}(y,t), \tag{4.1}$$

where m is the mass of a particle. The divergence operator with respect to the velocity variable operates on everything to its right, including F_{ext} in the case of nonconservative forces [16].

Systems driven at the boundaries are represented by local boundary conditions on the distribution function obeying the BGK-Boltzmann equation. The microscopic origins of such conditions are corresponding boundary conditions for the Liouville equation, in particular due to the free streaming operator. A wide class of boundary conditions is given by a linear relationship between the distribution of particles incident on a surface to those emerging from it [17]. For conditions of low density, correlations among particles at the surface can be neglected and the boundary conditions for each of the degrees of freedom are imposed independently. Accordingly, the boundary conditions are attached implicitly to each of the free streaming operators in the Liouville equation. The derivation of the kinetic equations for the reduced distribution functions and the correlation functions in Appendix A is unchanged, but the streaming operators there must be understood to carry appropriate boundary conditions. For the single particle distribution function they can be expressed in the form

$$f(\mathbf{r}\in\Sigma,\mathbf{v}\cdot\hat{\mathbf{n}}>0)=\mathcal{K}f(\mathbf{r}\in\Sigma,\mathbf{v}\cdot\hat{\mathbf{n}}<0), \tag{4.2}$$

where Σ denotes a point on the surface and $\hat{\mathbf{n}}$ is a unit vector normal to the surface and pointing into the region occupied by the gas. In general, physical boundary conditions are local in space, so that the operator $\mathcal{K}$ involves only transformation of velocities. However, some idealized boundary conditions used in computer simulations have nonlocal boundary conditions [18]. The boundary conditions for $C(y,t;y',t')$, considered as a function of y, take the *same* form as Eq. (4.2). In addition, the boundary conditions on $f(y,t)$ affect $C(y,t;y',t')$ as well through the dependence of the operator $\mathcal{L}(t)$ on $f(y,t)$.

The boundary value problem for the BGK-Boltzmann equation is complicated by the nonlinearity of this equation. However, since the nonlinearity appears entirely through the five fields $z_\alpha(\mathbf{r},t)$ [see Eq. (3.2)], the solution can be expressed as a functional of these fields with the boundary conditions made explicit. The fields are then determined by a coupled set of five nonlinear integral equations. While these equations are still formidable, the number of independent variables has been reduced to only space and time. Particularly for geometries of high symmetry (e.g., planar or cylindrical), this representation can be quite useful for both analytical and numerical studies. The corresponding solution to the correlation function equations is much simpler, for given $f(y,t)$, since they are linear. As will be illustrated in the next section, a Green's function solution can be obtained in terms of the boundary value problem for an ideal gas.

V. STEADY STATE CORRELATIONS

Equations (3.15) and (3.16) are linear and their solution can be reduced to quadratures once $f(y,t)$ has been specified, as illustrated below. The difficult part of the problem is therefore (3.14), which is still a highly nonlinear integro-differential equation (due to the functional dependence of f_l on f). Exact solutions for nonequilibrium steady states corresponding to heat and momentum transport have been obtained recently for planar geometries [2] and the results here allow the study of correlations in these far from equilibrium states. To illustrate the analysis of the correlations, we consider such a stationary state and assume that a solution, f_s, to (3.14) has been specified. Then, the operator Λ^{BGK} is time independent and the formal solution to (3.15) is

$$C_s(y,t;y',0)=\int dy_1\,K(y,y_1,t)C(y_1,0;y',0), \tag{5.1}$$

$$K(y,y',t)\equiv\exp\{-\mathcal{L}t\}\,\delta(y-y'). \tag{5.2}$$

Stationarity has been used to choose the initial time $t'=0$. The function $K(y,y',t)$ is only a formal representation of the Green's function as we now understand that the free streaming operator has boundary conditions associated with it. The initial condition in (5.1) is determined from the stationary solution to the equal time correlation function equation, (3.16),

$$\begin{aligned}C_s(y,y')&=C_s(y,0;y',0)\\&=\int_0^\infty d\tau\int dy_1dy_2\,K(y,y_1,\tau)K(y',y_2,\tau)\\&\quad\times B^{BGK}(y_1,y_2|f_s).\end{aligned} \tag{5.3}$$

The parameters of the local equilibrium distribution appearing in the expression of B^{BGK} are now considered known via (3.2) since f_s is assumed known.

The results (5.1) and (5.3) express the correlations in terms of the Green's function $K(y,y',t)$, defined in (5.2), and that is the solution to

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla+\nu\right)K(y,y',t)=\nu f_l(y)\psi_\alpha(\mathbf{v})K_\alpha(\mathbf{r},y',t), \tag{5.4}$$

with the initial condition $K(y,y',0)=\delta(y-y')$. The functions $K_\alpha(\mathbf{r},y',t)$ are defined by

$$K_\alpha(\mathbf{r},y',t)\equiv g^{-1}_{\alpha\beta}(\mathbf{r}|f_l)\int d\mathbf{v}_1\,\psi_\beta(\mathbf{v}_1)K(\mathbf{r},\mathbf{v}_1,y',t). \tag{5.5}$$

The solution to (5.4) can be reduced to the corresponding ideal gas problem as follows. Integration of (5.4) gives

$$\begin{aligned}K(y,y',t)&=K_0(y,y',t)\\&\quad+\nu\int_0^t d\tau\int dy_1\,K_0(y,y_1,t-\tau)f_l(y_1)\\&\quad\times\psi_\alpha(\mathbf{v}_1)K_\alpha(\mathbf{r}_1,y',\tau),\end{aligned} \tag{5.6}$$

where we have introduced

$$K_0(y,y',t)\equiv\exp\left[-\left(\mathbf{v}\cdot\nabla+\nu\right)t\right]\delta(y-y'). \tag{5.7}$$

The remaining set of five functions $K_\alpha(\mathbf{r},y',t)$ is determined by substituting (5.6) into the right side of (5.5) to give

$$\begin{aligned}K_\alpha(\mathbf{r},y',t)&=K_{0\alpha}(\mathbf{r},y',t)\\&\quad+\int_0^t d\tau\int d\mathbf{r}_1 I_{\alpha\beta}(\mathbf{r},\mathbf{r}_1,t-\tau)\\&\quad\times K_\beta(\mathbf{r}_1,y',\tau),\end{aligned} \tag{5.8}$$

with

$$K_{0\alpha}(\mathbf{r},y',t) \equiv g^{-1}_{\alpha\beta}(\mathbf{r}|f_l) \int d\mathbf{v}\, \psi_\beta(\mathbf{v}) K_0(y,y',t) \quad (5.9)$$

and

$$I_{\alpha\beta}(\mathbf{r},\mathbf{r}_1,t) \equiv \nu\, g^{-1}_{\alpha\gamma}(\mathbf{r}|f_l) \int d\mathbf{v} d\mathbf{v}_1\, \psi_\gamma(\mathbf{v}) K_0(y,y_1,t) \times f_l(y_1)\psi_\beta(\mathbf{v}_1). \quad (5.10)$$

The quantities $K_0, K_{0\alpha}$, and $I_{\alpha\beta}$ are determined entirely from the dynamics of an ideal gas (with appropriate boundary conditions) which is a solvable problem in general. The Green's function K is then obtained by integration via (5.6), and the correlation functions via (5.1) and (5.3). The analysis of this section extends to nonstationary states as well without significant difficulty. The problem of calculating the dynamics of the correlations is thus completely solved, once the solution to the BGK-Boltzmann equation has been obtained. To illustrate this analysis and the fact that the BGK model retains a wide scope of physical phenomena, we specialize the above to the equilibrium state and to stationary states near equilibrium.

A. Equilibrium states

For the special case of the equilibrium state $f = f_l = f_e$, the Maxwell-Boltzmann distribution. The source term B^{BGK} given by (3.13) simplifies to

$$B^{BGK}(y_1,y_2|f_e) = (\mathcal{L}_1 + \mathcal{L}_2)\delta(y_1 - y_2) f_e(y_1), \quad (5.11)$$

in agreement with (2.25). Then (5.2) and (5.3) give immediately the expected result for the low density equilibrium correlations,

$$C_e(y;y') = \delta(y-y') f_e(y), \quad (5.12)$$

or, equivalently, $G_e(y,y') = 0$. Next, use of (5.12) in (5.1) gives the two time correlation function as

$$C_e(y,t;y',0) = K(y,y',t) f_e(y'). \quad (5.13)$$

The correlation function $C_e(y,t;y',0)$ and the Green's function $K(y,y',t)$ are the same up to a factor f_e. The Green's function is determined from (5.4)–(5.8), which are easily solved by the Fourier-Laplace transformation

$$\begin{aligned}\tilde{C}_e(\mathbf{k},\mathbf{k}',z;\mathbf{v},\mathbf{v}') &\equiv \int d\mathbf{r}\, d\mathbf{r}'\, e^{i(\mathbf{k}\cdot\mathbf{r}+\mathbf{k}'\cdot\mathbf{r}')} \\ &\quad \times \int_0^\infty dt\, e^{-zt} C_e(y,t;y',0) \\ &\equiv (2\pi)^3 \delta(\mathbf{k}+\mathbf{k}')\tilde{C}_e(\mathbf{k},z|\mathbf{v},\mathbf{v}'), \quad (5.14)\end{aligned}$$

with the result

$$\begin{aligned}\tilde{C}_e(\mathbf{k},z|\mathbf{v},\mathbf{v}') &= R(\mathbf{k},z|\mathbf{v})\delta(\mathbf{v}-\mathbf{v}') f_e(v) \\ &\quad + \frac{\nu}{n} R(\mathbf{k},z|\mathbf{v}) R(\mathbf{k},z|\mathbf{v}') f_e(v) f_e(v') \\ &\quad \times \phi_\alpha(\mathbf{v})\phi_\beta(\mathbf{v}') B^{-1}_{\alpha\beta}(k,z), \quad (5.15)\end{aligned}$$

where

$$R(\mathbf{k},z|\mathbf{v}) \equiv (z + \nu - i\mathbf{k}\cdot\mathbf{v})^{-1}, \quad (5.16)$$

$$B_{\alpha\beta}(k,z) \equiv \delta_{\alpha\beta} - \tilde{I}_{\alpha\beta}(k,z), \quad (5.17)$$

n is the number density of particles, and the functions ϕ_α are linear combinations of the collisional invariants ψ_α. The analytic structure of $\tilde{C}_e$ in the complex z plane determines the complete dynamics of $C_e(y,t;y',0)$. The resolvent $R(\mathbf{k},z|\mathbf{v})$ has a pole at $-\nu + i\mathbf{k}\cdot\mathbf{v}$, representing free particle motion modulated by pure exponential damping. The remaining dynamical behavior is determined from the analytic structure of $B^{-1}_{\alpha\beta}(k,z)$, which is independent of the velocities. The detailed form of this function is given in Appendix C. It gives five simple poles at $z_\alpha(k)$ that vanish as $k \to 0$. A pole at the origin represents a conserved quantity, so at finite k these poles characterize the associated hydrodynamic modes. To lowest order in k the dynamics are equivalent to the linearized Navier-Stokes equations. However, it is possible also to calculate these poles at larger k values as well to define "extended" hydrodynamic modes. It is found that these extended modes exist up to some maximum value of k, corresponding to wavelengths small compared to the mean free path. The real and imaginary parts for the two propagating modes (i.e., sound speed and damping), the heat diffusion mode, and the shear diffusion modes (twofold degenerate) are shown in Fig. 1. In addition to the hydrodynamic modes there are poles and branch points which approach $-\nu$ as $k \to 0$. These determine the "kinetic" modes with lifetimes of the order of ν^{-1} for all k.

This rich dynamics of equilibrium correlations is well studied for the linearized Boltzmann equation using more complex models [19]. In spite of the simplicity of the BGK model, we see that all qualitative features of fluctuations in equilibrium states are preserved and can be analyzed quite simply.

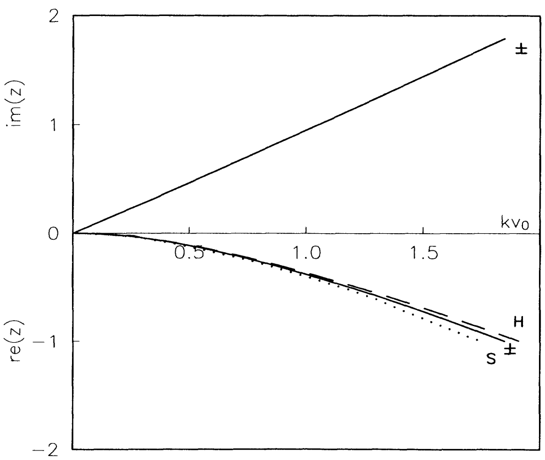

FIG. 1. Real and imaginary parts of the extended hydrodynamic modes from the BGK model (in units of ν).

B. Stationary states near equilibrium

As a second illustration, consider stationary states near equilibrium. More specifically, attention is restricted to the Chapman-Enskog solution to the BGK-Boltzmann equation. This is a "normal" solution for which the space and time dependence of $f(y,t)$ occurs entirely through its dependence on the hydrodynamic fields [i.e., z_α in (3.2)]. The solution is obtained as an expansion in the gradients of these fields and is given to leading order by

$$f_s(y) \to f_l(y)\left[1 - \frac{1}{k_BT\nu}\left(T^{-1}\frac{\partial T}{\partial r_i}S_i(\mathbf{v}) + \frac{\partial u_i}{\partial r_j}D_{ij}(\mathbf{v})\right)\right]. \qquad (5.18)$$

Here $T(\mathbf{r})$ is the temperature, $\mathbf{u}(\mathbf{r})$ is the flow field, and

$$\mathbf{S}(\mathbf{v}) \equiv \mathbf{V}\left(\frac{1}{2}mV^2 - \frac{5}{2}k_BT\right), \qquad (5.19)$$

$$D_{ij}(\mathbf{v}) \equiv m\left(V_iV_j - \frac{1}{3}V^2\delta_{ij}\right), \qquad (5.20)$$

where $\mathbf{V}(\mathbf{r}) \equiv \mathbf{v} - \mathbf{u}(\mathbf{r})$ is the peculiar velocity.

The equal time correlation function can be calculated from (5.3) in the same way as for the equilibrium case above. However, it is somewhat more direct to express C_s in terms of G_s and use the equivalent integral representation for the solution to (3.18),

$$C_s(y_1,y_2) = \delta(y_1 - y_2)f_s(y_1) + \int_0^\infty dt\, e^{-(\mathcal{L}_1+\mathcal{L}_2)t}\gamma(y_1,y_2|f_s). \qquad (5.21)$$

This equation applies to both the Boltzmann description of Sec. II and the BGK model, the difference being in the expressions of $\mathcal{L}$ and γ. The first term has contributions from both the local equilibrium state and the gradients of the hydrodynamic fields. As in the equilibrium case this term is proportional to $\delta(y_1 - y_2)$, representing short ranged correlations in both configuration and velocity space. The second term of (5.21) contains qualitatively different contributions. In particular, there are very long ranged spatial correlations. These arise from the hydrodynamic spectrum of $\mathcal{L}$. To see this more explicitly, we note that to lowest order in the gradients the corresponding eigenvectors are proportional to the summational invariants, ψ_α, so there is a hydrodynamic part of (5.21) arising from the terms

$$\int_0^\infty dt\, e^{-(\mathcal{L}_1+\mathcal{L}_2)t}\delta(\mathbf{r}_1 - \mathbf{r}_2)M_{\alpha\beta}\psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2)f_l(y_1)f_l(y_2) = (\mathcal{L}_1 + \mathcal{L}_2)^{-1}\delta(\mathbf{r}_1 - \mathbf{r}_2)M_{\alpha\beta}\psi_\alpha(\mathbf{v}_1)\psi_\beta(\mathbf{v}_2) \times f_l(y_1)f_l(y_2), \qquad (5.22)$$

$$M_{\alpha\beta}\delta(\mathbf{r}_1 - \mathbf{r}_2) \equiv g_{\alpha\sigma}^{-1}g_{\beta\nu}^{-1}\int d\mathbf{v}_1 d\mathbf{v}_2\psi_\sigma(\mathbf{v}_1)\psi_\nu(\mathbf{v}_2)\gamma(y_1,y_2|f). \qquad (5.23)$$

A Fourier decomposition shows that the hydrodynamic spectrum of $\mathcal{L}$ leads to terms proportional to $[\lambda_\alpha(k) + \lambda_\beta(k)]^{-1}$, representing slow algebraic decay in configuration space. The coefficients $M_{\alpha\beta}$ can be easily calculated explicitly for the BGK model for which $\gamma(y_1,y_2|f)$ is found from (3.20),

$$\gamma^{BGK}(y_1,y_2|f_s) = -P_1P_2\delta(y_1 - y_2)f_l(v_1) \times\left[\frac{1}{k_BT}\left(T^{-1}\frac{\partial T}{\partial r_i}S_i(\mathbf{v}_1) + \frac{\partial u_i}{\partial r_j}D_{ij}(\mathbf{v}_1)\right)\right]. \qquad (5.24)$$

The result is

$$M_{\alpha\beta} = -\left[\frac{1}{k_BT}\left(T^{-1}\frac{\partial T}{\partial r_i}S_{\alpha\beta,i} + \frac{\partial u_i}{\partial r_j}D_{\alpha\beta,ij}\right)\right], \qquad (5.25)$$

$$S_{\alpha\beta,i} \equiv g_{\alpha\sigma}^{-1}g_{\beta\nu}^{-1}\int d\mathbf{v}\, f_l(v)\psi_\sigma(\mathbf{v})\psi_\nu(\mathbf{v})S_i(\mathbf{v}), \qquad (5.26)$$

$$D_{\alpha\beta,ij} \equiv g_{\alpha\sigma}^{-1}g_{\beta\nu}^{-1}\int d\mathbf{v}\, f_l(v)\psi_\sigma(\mathbf{v})\psi_\nu(\mathbf{v})D_{ij}(\mathbf{v}), \qquad (5.27)$$

These are *exactly* the same as those obtained from the Boltzmann kinetic theory [20], confirming that the BGK kinetic model retains a correct description of these long range correlations in nonequilibrium states.

VI. DISCUSSION

The objective here has been to describe both transport (single particle distribution) and correlations (at one or two times) in a low density gas. The formal statistical mechanical analysis of the Appendix A, and in earlier references, provides kinetic equations for the analysis of this problem. However, their complexity has limited the scope of applications. Kinetic modeling has proved effective as a means to probe the content of the nonlinear Boltzmann equation in a realistic and practical representation. Here, the simplest BGK model has been extended in a self-consistent way to apply to the kinetic equations that determine pair correlations at one and two times for the same practical objective. All of the important structural relationships of the three types of kinetic equations are preserved by this model. Practicality has been proved in Sec. V by showing how correlations can be determined whenever the Boltzmann-BGK equation can be solved.

To emphasize the broad scope of problems addressed, it is useful to interpret the equations for the correlations. Equations for the correlations at two times have the exact structure of those for linear stability analysis of the Boltzmann equation. Thus analysis of the correlation function equations at two times using this kinetic model provides a practical way of studying unstable as well as stable states. Preservation of the consequences of conservation laws assures that this stability analysis includes the entire field of hydrodynamic stability and bifurcation phenomena. However, it also includes the possibility of exploring the phase space origin of hydrodynamic instabilities, and to study instabilities that do not have a hydrodynamic origin. We do not mean to imply that these difficult problems have been solved, but rather that their scope of analysis has been brought within reasonable control by the kinetic modeling.

The equations for the equal time correlations also involve the linear operator Λ. The self-consistent preservation of conservation laws assures that these equations will have a slowly decaying, long wavelength hydrodynamic spectrum for excitations about nonequilibrium states. It has been proposed [10], and verified perturbatively [7], that equal time correlations in nonequilibrium steady states are of very long range (e.g., algebraic decay). This is somewhat surprising since the equilibrium state of a low density gas has no long range correlations, and the correlations in the nonequilibrium state are expected to be generic: no "tuning" of driving forces or state conditions are required. The nature of such long range correlations far from equilibrium is still largely unexplored. Phenomenological Langevin equations have been analyzed nonperturbatively for special cases, with local equilibrium assumptions about the noise amplitude and dissipative transport matrix that limit their range of validity. In one such example [21], the correlation length for the steady state depends inversely on the driving force, so that study of length scales large compared to the correlation length cannot be done perturbatively near equilibrium. The kinetic models given here, together with several known steady state solutions to the Boltzmann-BGK equation, provide the basis for the study of this problem.

The kinetic theory of transport and correlations presented in Sec. II is obtained in Appendix A to leading order in a density expansion. The pair correlations are determined as functionals of the distribution function $f(y,t)$, which is a solution to the Boltzmann equation. These lowest order correlation functions also determine the first density corrections to the Boltzmann equation. The kinetic equation for the correction, denoted here by $\delta f(y,t)$, is found directly from (A3) for $s=1$ and (A9),

$$\left(\frac{\partial}{\partial t}+\mathbf{v}_1\cdot\nabla-\Lambda_1\right)\delta f(y_1,t)=\int dy_2\,T(1,2)G(y_1,y_2,t). \tag{6.1}$$

Here it is understood that Λ and $G(y_1,y_2,t)$ are computed as functionals of the solution to the nonlinear Boltzmann equation as in Sec. II. The inhomogeneous term on the right side describes sequences of correlated binary collisions ("ring collisions"). The contributions to $G(y_1,y_2,t)$ from the hydrodynamic modes described at the end of the last section are responsible for very slow dynamics in (6.1), which is qualitatively different from that of the Boltzmann equation (e.g., algebraic decay). Further details of these phenomena and the corresponding BGK model for (6.1) will be deferred to future work.

Finally, we mention work in progress for the special case of a steady state representing uniform shear flow. An exact, nontrivial, solution to the Boltzmann-BGK equation is known. However, its stability at large shear rates has not been determined and suggestions of a possible instability have been noted recently [22]. The kinetic model equation (3.15) is an appropriate basis to study this problem without prejudice with regard to a presumed hydrodynamic bifurcation. The question of long range correlations for this same steady state is being studied using the kinetic model equation (3.16). The dominant long wavelength hydrodynamic modes near the steady state involve significant rheological effects that can be calculated for the kinetic model. Similar questions can be raised for steady states with constant heat flux, or combined heat and momentum fluxes, for which exact solutions to the Boltzmann-BGK equation are known. Also, it is possible to obtain nonsteady solutions near equilibrium driven by time dependent boundary conditions. In this case, the correlation functions measure the competition between driven and dissipative dynamics.

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APPENDIX A: CORRELATIONS AT LOW DENSITY

The derivation of the Boltzmann equation from the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy is described in many texts. However, the corresponding analysis of correlations for nonequilibrium states is less extensive and often contradictory. In this appendix the scaling properties of the BBGKY hierarchy for reduced distribution functions at one and two times are exploited to allow a perturbative solution to the entire hierarchy in terms of an expansion parameter that is small at low density [23]. The method applies strictly only for systems of hard spheres, but the same results can be obtained for general short ranged forces by more elaborate methods [3].

The single particle phase space density given in (2.1) can be generalized to a multipoint density according to

$$\hat{f}^{(s)}(y_1,\ldots,y_s,t) \equiv \sum_{i_1\neq i_2\neq\cdots}\cdots\sum_{\cdots\neq i_s}\prod_{\alpha=1}^{s}\delta(y_\alpha - x_{i_\alpha}(t)). \quad (A1)$$

The average of this microscopic density is the s-particle reduced distribution function,

$$f^{(s)}(y_1,\ldots,y_s,t) \equiv \langle \hat{f}^{(s)}(y_1,\ldots,y_s,t)\rangle. \quad (A2)$$

As in the main text, the angle brackets denote an ensemble average over some specified initial ensemble. These functions obey the BBGKY hierarchy. A dimensionless form of this hierarchy is obtained by scaling the space and time with appropriate scales. Here we are interested in length scale large compared to the force range, so the lengths are scaled relative to the mean free path, $\ell_0 \equiv 1/(n\sigma^2)$; also, the time is scaled relative to the mean free time, $t_0 \equiv \ell_0/v_0$. Here, n is the density, σ is the force range, and v_0 is some characteristic velocity. Taking into account the intensive character of the reduced distribution functions in the thermodynamic limit, f^s is scaled with n^s/v_0^{3s}.

The above scaling is particularly helpful for the special case of hard sphere interactions. Collisions between hard spheres yield finite momentum transfer in infinitesimal times since the force is singular. The BBGKY hierarchy takes on a different form for hard spheres, whereby the singular forces are replaced by binary scattering operators [11]. The resulting dimensionless BBGKY hierarchy has the form

$$\left(\frac{\partial}{\partial t} + \sum_{i=1}^{s}\mathbf{v}_i\cdot\nabla_i - \alpha^2\sum_{i<j}^{s}T(i,j)\right)f^{(s)}(y_1,\ldots,y_s,t) = \sum_{i=1}^{s}\int dy_{s+1}\,T(i,s+1)f^{(s+1)}(y_1,\ldots,y_{s+1},t). \quad (A3)$$

Here $T(i,j)$ is an operator describing the scattering of the pair of particles $\{i,j\}$,

$$T(i,j) = \int d\hat{\mathbf{r}}\,\Theta(\mathbf{r}\cdot\mathbf{g}_{ij})\hat{\mathbf{r}}\cdot\mathbf{g}_{ij} \times\left[\delta(\mathbf{r}_{ij}-\alpha\hat{\mathbf{r}})b_{ij} - \delta(\mathbf{r}_{ij}+\alpha\hat{\mathbf{r}})\right], \quad (A4)$$

where $d\hat{\mathbf{r}}$ denotes a two dimensional solid angle integration over the sphere for particles at contact. Also, $\mathbf{g}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity, $\hat{\mathbf{r}}$ is a unit vector along $\mathbf{r}_{ij}$, and b_{ij} is the scattering operator defined for any function $X(\mathbf{v}_i,\mathbf{v}_j)$ by

$$b_{ij}X(\mathbf{v}_i,\mathbf{v}_j) \equiv X(\mathbf{v}_i',\mathbf{v}_j'). \quad (A5)$$

The scattered velocities are $\mathbf{v}_i' \equiv \mathbf{v}_i - (\mathbf{g}_{ij}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}$ and $\mathbf{v}_j' \equiv \mathbf{v}_j + (\mathbf{g}_{ij}\cdot\hat{\mathbf{r}})\hat{\mathbf{r}}$.

Equations (A3) and (A4) depend on the single dimensionless parameter $\alpha \equiv \sigma/\ell_0 = n\sigma^3$, the ratio of the force range to the mean free path. This parameter is small at low density, suggesting an expansion for the solutions to (A3) as a power series in α. Without loss of generality, the residual α dependence of $T(i,j)$ is suppressed and we look for solutions of the form

$$f^{(s)}(y_1,\ldots,y_s,t) = \sum_{n=0}^{\infty}\alpha^{2n}f_n^{(s)}(y_1,\ldots,y_s,t). \quad (A6)$$

Substituting (A6) into (A4) and equating coefficients gives the kinetic equations determining the coefficients $f_n^{(s)}$. To zeroth order in α the solutions are found to be

$$f_0^{(s)}(y_1,\ldots,y_s,t) = \prod_{i=1}^{s}f_0^{(1)}(y_i,t), \quad (A7)$$

where $f_0^{(1)}(y,t)$ is the solution to the kinetic equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1\right)f_0^{(1)}(y_1,t) = \int dy_2\,T(1,2)f_0^{(1)}(y_1,t)f_0^{(1)}(y_2,t). \quad (A8)$$

The solutions to order α^2 are

$$f_1^{(2)}(y_1,y_2,t) = f_0^{(1)}(y_1,t)f_1^{(1)}(y_2,t) + f_0^{(1)}(y_2,t)f_1^{(1)}(y_1,t) + G_1(y_1,y_2,t) \quad (A9)$$

and

$$f_1^{(s)}(y_1,\ldots,y_s,t) = \sum_{j=1}^{s}\prod_{i\neq j}^{s}f_0^{(1)}(y_i,t)f_1^{(1)}(y_j,t) + \sum_{i<j}^{s}\prod_{k\neq i,j}^{s}f_0^{(1)}(y_k,t)G_1(y_i,y_j,t), \quad (A10)$$

for $s \geq 3$. The functions $f_1^{(1)}$ and G_1 are solutions to

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1 - \lambda_1\right)f_1^{(1)}(y_1,t) = \int dy_2\,T(1,2)G_1(y_1,y_2,t), \quad (A11)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1 - \lambda_1 + \mathbf{v}_2\cdot\nabla_2 - \lambda_2\right)G_1(y_1,y_2,t) = T(1,2)f_0^{(1)}(y_1,t)f_0^{(1)}(y_2,t). \quad (A12)$$

Here λ_1 is the operator defined over functions of y_1 by

$$\lambda_1 h(y_1) \equiv \int dy_2\, T(1,2)[f_0^{(1)}(y_1,t)h(y_2) + h(y_1)f_0^{(1)}(y_2,t)]. \tag{A13}$$

These results give an exact solution to the entire hierarchy to order α^2, with reduced distribution functions of any number of particles determined as a sum of products of single particle functions $f_0^{(1)}(y_1,t)$ and $f_1^{(1)}(y_1,t)$ and the pair function $G_1(y_1,y_2,t)$. The single particle functions are simply the first two terms in the α expansion of $f^{(1)}$; the pair function is the leading contribution to the density expansion of $G(y_1,y_2,t)$ in (2.15).

The Boltzmann limit follows from *both* low density *and* neglect of spatial variations over the force range during collision. This requires neglect of the remaining α dependence in (A4) for $T(i,j)$. Then, the kinetic equations (A8) and (A12) become

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1\right) f_0^{(1)}(y_1,t) = J(y_1|f_0^{(1)}(t)), \tag{A14}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1 - \Lambda_1 + \mathbf{v}_2\cdot\nabla_2 - \Lambda_2\right) G_1(y_1,y_2,t) = T_0(1,2)f_0^{(1)}(y_1,t)f_0^{(1)}(y_2,t). \tag{A15}$$

These are the same as Eqs. (2.8) and (2.16), with the identifications

$$J(y_1|f_0^{(1)}(t)) \equiv \int dy_2\, T_0(1,2)f_0^{(1)}(y_1,t)f_0^{(1)}(y_2,t), \tag{A16}$$

$$\Lambda_1 h(y_1) \equiv \int dy_2\, T_0(1,2)[f_0^{(1)}(y_1,t)h(y_2) + h(y_1)f_0^{(1)}(y_2,t)], \tag{A17}$$

$$\gamma(y_1,y_2|f_0^{(1)}) = T_0(1,2)f_0^{(1)}(y_1,t)f_0^{(1)}(y_2,t), \tag{A18}$$

$$T_0(i,j) \equiv \delta(\mathbf{r}_{ij}) \int d\hat{\mathbf{r}}\, \Theta(\mathbf{r}\cdot\mathbf{g}_{ij})\, \hat{\mathbf{r}}\cdot\mathbf{g}_{ij}\,(b_{ij}-1). \tag{A19}$$

The right side of (A16) is recognized as the nonlinear Boltzmann collision operator for hard spheres, so $f_0^{(1)}$ is indeed the solution to the Boltzmann equation. Equation (2.10) for $C(y,t;y',t)$ follows directly from (A19) and the definition (2.15), with $B(y,y'|f)$ given by (2.14).

The analysis of correlations at two times can be accomplished in a similar way. Define the two time distribution function

$$h^{(s+1)}(y_1,\ldots,y_s,t;y',t') \equiv \langle \hat{f}^{(s)}(y_1,\ldots,y_s;t)\hat{f}^{(1)}(y',t')\rangle, \tag{A20}$$

where $\hat{f}^{(s)}$ is still given by (A1). The two time correlation of the text is related to $h^{(2)}$ by

$$C(y,t;y',t') = h^{(2)}(y,t;y',t') - f^{(1)}(y,t)f^{(1)}(y',t'). \tag{A21}$$

The two time distribution functions $h^{(s)}$ obey the same BBGKY hierarchy (A3) for $t > t'$. A solution in powers of α can be obtained from an expansion for $h^{(s)}$ analogous to (A6),

$$h^{(s+1)}(y_1,\ldots,y_s,t;y',t') = \sum_{n=0}^{\infty} \alpha^{2n} h_n^{(s+1)}(y_1,\ldots,y_s,t;y',t'). \tag{A22}$$

The solution up to order α^2 is

$$h_0^{(s+1)}(y_1,\ldots,y_s,t;y',t') = f_0^{(1)}(y',t')f_0^{(s)}(y_1,\ldots,y_s,t), \tag{A23}$$

$$h_1^{(2)}(y_1,t;y',t') = f_0^{(1)}(y_1,t)f_1^{(1)}(y',t') + f_1^{(1)}(y_1,t)f_0^{(1)}(y',t'), \tag{A24}$$

and

$$h_1^{(s+1)}(y_1,\ldots,y_s,t;y',t') = f_0^{(s)}(y_1,\ldots,y_s,t)f_1^{(1)}(y',t') + f_1^{(s)}(y_1,\ldots,y_s,t)f_0^{(1)}(y',t') + \sum_{i=1}^{s}\prod_{j\neq i}^{s} f_0^{(1)}(y_j,t)C_1(y_i,t;y',t'), \tag{A25}$$

for $s \geq 2$, where $f_0^{(s)}$ and $f_1^{(s)}$ are the same as determined above, and C_1 obeys the equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla - \lambda\right) C_1(y,t;y',t') = 0, \tag{A26}$$

for $t > t'$. The operator λ is given by (A13) and reduces to Λ in the Boltzmann limit. Furthermore, substitution of (A25) into (A21) shows that $C_1(y,t;y',t')$ is the first nonvanishing contribution to $C(y,t;y',t')$, so that (A26) becomes the same as (2.9). This completes the derivation of all low density kinetic equations for transport and pair correlations at one and two times.

APPENDIX B: PROOF OF ORTHOGONALITY CONDITIONS

The orthogonality conditions (2.24) for B play a dominant role in the kinetic model for the equal time correlation function. The proof of these conditions is sketched here for completeness. The definition of B in (2.14) leads to

$$\begin{aligned}\int d\mathbf{v}_1\psi_\alpha(\mathbf{v}_1)B(y_1,y_2|f(t)) = \int d\mathbf{v}_1\psi_\alpha(\mathbf{v}_1)\gamma(y_1,y_2|f(t)) + \psi_\alpha(\mathbf{v}_2)\delta(\mathbf{r}_1-\mathbf{r}_2)J(y_2|f(t))\\ -\Lambda_2\delta(\mathbf{r}_1-\mathbf{r}_2)\psi_\alpha(\mathbf{v}_2)f(y_2,t),\end{aligned} \tag{B1}$$

where use has been made of (2.23). From (A19) we note that $T_0(1,2)$ has the form $T_0(1,2) = \delta(\mathbf{r}_1-\mathbf{r}_2)t(\mathbf{v}_1,\mathbf{v}_2)$. Consequently, expressing γ, J, and Λ in terms of $T_0(1,2)$, (B1) can be written as

$$\begin{aligned}\int d\mathbf{v}_1\psi_\alpha(\mathbf{v}_1)B(y_1,y_2|f(t)) = \delta(\mathbf{r}_1-\mathbf{r}_2)\left[\int d\mathbf{v}_1[\psi_\alpha(\mathbf{v}_1)+\psi_\alpha(\mathbf{v}_2)]t(1,2)f(y_1,t)f(y_2,t)\right.\\ \left. - \int d\mathbf{v}_1 t(1,2)f(y_1,t)f(y_2,t)[\psi_\alpha(\mathbf{v}_1)+\psi_\alpha(\mathbf{v}_2)]\right].\end{aligned} \tag{B2}$$

Since $[\psi_\alpha(\mathbf{v}_1)+\psi_\alpha(\mathbf{v}_2)]$ is a summational invariant and unchanged by $t(\mathbf{v}_1,\mathbf{v}_2)$ the two integrals on the right side of (B2) are equal and cancel, giving the desired result (2.24).

APPENDIX C: EQUILIBRIUM EXCITATIONS

The solution to the correlation function equation is given in terms of the matrix $B_{\alpha\beta} = \delta_{\alpha\beta} - I_{\alpha\beta}$, (5.17), which determines the hydrodynamic poles. The matrix $I_{\alpha\beta}$ is obtained from the Fourier-Laplace transform of (5.10), specialized to the equilibrium state

$$\tilde{I}_{\alpha\beta}(k,z) = \nu g^{-1}_{\alpha\gamma}\int d\mathbf{v} f_e(\mathbf{v})R(\mathbf{k},z|\mathbf{v})\psi_\gamma(\mathbf{v})\psi_\beta(\mathbf{v}), \tag{C1}$$

where $R(\mathbf{k},z|\mathbf{v})$ is given by (5.16). Further analysis is simplified by choosing the summational invariants $\psi_\alpha(\mathbf{v})$ to be an orthonormal set constructed from linear combinations of those in (2.19),

$$\phi_\alpha(\mathbf{v}) = \left\{1, \left(\frac{2}{3}\right)^{1/2}\left(\frac{mv^2}{2k_BT}-\frac{3}{2}\right), \left(\frac{m}{k_BT}\right)^{1/2}v_1, \left(\frac{m}{k_BT}\right)^{1/2}v_2, \left(\frac{m}{k_BT}\right)^{1/2}v_3\right\}, \tag{C2}$$

where $v_1 \equiv \hat{\mathbf{k}}\cdot\mathbf{v}$ is the component of $\mathbf{v}$ along $\mathbf{k}$, and v_2 and v_3 are the orthogonal transverse components. With this choice $g_{\alpha\beta} = n\delta_{\alpha\beta}$ and (C1) reduces to

$$\tilde{I}_{\alpha\beta}(k,z) = \frac{i\nu}{kv_0}A_{\alpha\beta}(x). \tag{C3}$$

Here $x \equiv (z+\nu)/ikv_0$, $v_0 \equiv (2k_BT/m)^{1/2}$, and $A_{\alpha\beta}(x)$ is a symmetric matrix, whose elements are given in terms of the complex probability integral,

$$Z(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dv\,\frac{\exp -v^2}{v-x}, \tag{C4}$$

by

$$(A_{\alpha\beta}) = \begin{pmatrix} Z & (\frac{2}{3})^{1/2}[x+(x^2-\frac{1}{2})Z] & \sqrt{2}(1+xZ) & 0 & 0\\ A_{12} & \frac{2}{3}[Z+(\frac{3}{2})^{1/2}(x^2-\frac{1}{2})A_{12}] & \sqrt{2}xA_{12} & 0 & 0\\ A_{13} & A_{23} & \sqrt{2}xA_{13} & 0 & 0\\ 0 & 0 & 0 & Z & 0\\ 0 & 0 & 0 & 0 & Z \end{pmatrix}. \tag{C5}$$

Since $\tilde{I}_{\alpha\beta}$ is analytic for $\mathrm{Re}(z) \neq -\nu$, the singularities of $B^{-1}_{\alpha\beta}(k,z)$ leading to hydrodynamic modes are associated with values of z for which

$$D(k,z) \equiv \det(B_{\alpha\beta}) \equiv \det(\delta_{\alpha\beta} - \tilde{I}_{\alpha\beta}) = 0. \qquad \text{(C6)}$$

This equation has been solved numerically looking for solutions $z = z(k)$ such that $z(0) = 0$. In fact, due to the structure of the matrix A_{ij}, Eq. (C6) factorizes into two independent equations. One of them is

$$\left(1 - \frac{i\nu Z}{kv_0}\right)^2 = 0. \qquad \text{(C7)}$$

It is easily verified that the twofold degenerate solution of this equation, $z_s(k)$, does not have an imaginary part and that there is a limiting value of k, $k_s^* = \sqrt{\pi}\nu/v_0$, where Eq. (C7) no longer has a solution. Besides, z_s is a decreasing function of k and $z_s(k_s^*) = -\nu$. These are the shear modes, and to lowest order in k one gets the Navier-Stokes expression $z_s = -\eta k^2$, where η is the kinematic viscosity.

The other equation coming from Eq. (C6) leads to two solutions which are each others' complex conjugate and to another real solution. These are the two sound modes, $z_\pm(k)$, and the heat mode, $z_H(k)$, respectively. To Navier-Stokes order, $z_\pm = \pm ick - \Gamma k^2$ and $z_H = -D_T k^2$, where c is the sound velocity, Γ is the sound damping constant, and D_T is the thermal diffusivity. For the BGK model, $\eta = \Gamma = D_T$, in agreement with what is observed in Fig. 1. The sound modes and the heat mode also present limiting values of k. From our numerical analysis we have found $k_\pm^* \simeq 1.85\nu/v_0$ and $k_H^* \simeq 1.91\nu/v_0$, corresponding to $z_\pm = z_H = -\nu$.

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