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Dissipative Dynamics for Hard Spheres

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The dynamics for a system of hard spheres with dissipative collisions is described at the levels of statistical mechanics, kinetic theory, and simulation. The Liouville operator(s) and associated binary scattering operators are defined as the generators for time evolution in phase space. The BBGKY hierarchy for reduced distribution functions is given, and an approximate kinetic equation is obtained that extends the revised Enskog theory to dissipative dynamics. A Monte Carlo simulation method to solve this equation is described, extending the Bird method to the dense, dissipative hard-sphere system. A practical kinetic model for theoretical analysis of this equation also is proposed. As an illustration of these results, the kinetic theory and the Monte Carlo simulations are applied to the homogeneous cooling state of rapid granular flow.

KEY WORDS: Granular flow; hard spheres; kinetic theory; hydrodynamics; Monte Carlo; kinetic model; binary scattering operators.

1. INTRODUCTION

The dynamics of hard spheres is conceptually simple but mathematically complicated due to the singular force and the failure of Newton's second law to apply in its usual form. Twenty-five years ago Matthieu Ernst and collaborators presented the first precise discussion of the generator(s) of hard-sphere dynamics.[1] Subsequently, this formalism was the basis for the most penetrating studies of anomalous dynamics in simple fluids (e.g., non-analytic density dependence of transport coefficients, long-time tails, mode coupling). Among these developments was a study of hard-sphere kinetic theory leading to the revised Enskog theory (RET) by van Beijeren and Ernst.[2] This kinetic theory is unique in providing a semiquantitative

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description of the hard-sphere system over all length and times scales, including both fluid and crystal phases. We are very pleased to contribute to this volume in honor of the many contributions to nonequilibrium statistical mechanics by Matthieu, with some extensions of his work on hard spheres to the case of dissipative (energy-nonconserving) dynamics.

Current interest in hard-sphere dynamics with dissipative collisions is due in part to its potential as a model for granular media in rapid flow.[3] Granular media consist of a dense collection of solid particles immersed in gas or liquid. When driven to rapid flows the solid particle collisions dominate the particle–fluid interactions and effects of the surrounding fluid can be neglected. As an idealization, the system can be understood as a collection of hard spheres for which the well-developed methods of nonequilibrium statistical mechanics can be brought to bear. However, as the collisions in granular flows do not conserve energy, it is necessary to consider the modifications of these methods for dissipative dynamics. The objective of our present work is to provide a description of these changes at the levels of statistical mechanics and kinetic theory. We also discuss adaptation to dissipative dynamics of two recently developed practical methods for solving the kinetic equation, Monte Carlo simulation[4] and kinetic models.[5] Analysis of granular flow experiments has typically been in analogy with fluid dynamics (see ref. 6 for a recent overview). However, the basis for a fluid dynamics description, its form, and the dependence of its parameters (e.g., transport coefficients) on density and degree of dissipation remain open questions. The hard-sphere system and associated nonequilibrium statistical mechanics provide the foundation to address all of these questions both qualitatively and quantitatively. For example, a simple kinetic model for dissipative dynamics at low density was used recently to determine precise conditions under which a hydrodynamic description exists and to provide all details of that description.[7] The results below allow extension of that analysis to the more realistic case of higher densities.

Many of the most interesting recent developments have originated from molecular dynamics simulations of the hard-sphere system considered here. The initial preparation in these simulations corresponds to a spatially homogeneous cooling state. However, a variety of spatial structures and phenomena develop at later times (cluster formation, shear, collapse) as a function of the degree of dissipation and particle density.[8-11] Their understanding requires more than a phenomenological hydrodynamic description. The statistical mechanics presented here corresponds faithfully to the simulations[4] and admits a theoretical approach to understanding these

[4] Closely related work has been done by van Noije *et al.*[12]

complex phenomena. The nontrivial mean-field kinetic theory goes beyond the usual Enskog equation with differences that may be significant for the nonlinear evolution of the density during the cluster phase. Similarly, the new Monte Carlo technique for the solution to this equation admits study of inhomogeneous states at finite densities. Finally, the new kinetic model provides a means for practical analytic studies beyond the hydrodynamic level. Some further applications of statistical mechanical methods to the system of inelastic hard spheres are noted in the final section.

2. STATISTICAL MECHANICS AND KINETIC THEORY

The objective of this section is to describe the Liouville formulation for hard-sphere dissipative dynamics and the associated BBGKY hierarchy for reduced distribution functions. The dynamics of a phase function $A(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}, t)$ is defined in terms of the coordinates and velocities $\{\mathbf{r}_\alpha(t), \mathbf{v}_\alpha(t)\}$ as functions of time for $t \geqslant 0$ by

$$A(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}, t) \equiv A(\{\mathbf{r}_\alpha(t), \mathbf{v}_\alpha(t)\}) \tag{1}$$

For hard spheres the particles move along straight lines until they encounter another particle at a separation equal to their diameter, σ. At that point the velocities of the colliding pair change instantaneously, followed by subsequent straight-line motion at their new velocities. Here we limit attention to smooth spheres, for which the relative velocity changes along the line joining the centers of the spheres; more generally, it is possible to consider rough spheres with a tangential change in relative velocity[13] and mixtures of different size particles[14] for a more realistic description. Let $\mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2$ denote the relative velocity for particles 1 and 2. Then the relative velocity after a collision of these two particles, $\tilde{\mathbf{g}}$, is given by

$$\tilde{\mathbf{g}} = \mathbf{g} - (1+\alpha)\,\hat{\boldsymbol{\sigma}}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}}) \tag{2}$$

where α is a constant in the range $0 < \alpha \leqslant 1$. The total momentum of the pair is conserved so that the total energy change on collision is

$$\tilde{E} - E = -(1-\alpha^2)\frac{m}{4}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})^2 \tag{3}$$

This identifies α as the coefficient of restitution, where $\alpha = 1$ corresponds to elastic collisions.

To develop the nonequilibrium statistical mechanics of this system it is necessary to identify the generator for the dynamics. Since the velocity

change occurs instantly, the associated force is singular and a reformulation of Newton's equations of motion is required. Consider the expectation value of the phase function $A(\{\mathbf{r}_\alpha(t), \mathbf{v}_\alpha(t)\})$,

$$\langle A(t)\rangle \equiv \int d\Gamma \rho(\Gamma)\, A(\Gamma(t)) \tag{4}$$

where Γ denotes the N-particle phase point, $\Gamma \leftrightarrow \{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}$, and $\Gamma(t)$ is the evolution of that phase point according to the hard-sphere dynamics at time t. Also, $\rho(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}) = W(\{\mathbf{r}_\alpha\})\, \bar{\rho}(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\})$ is the probability density for the initial state. The right side of this equality makes explicit the fact that all physical states have an overlap function, $W(\{\mathbf{r}_\alpha\})$, which vanishes for any configuration with overlapping spheres and is unity otherwise. The generators for the dynamics, L and $\bar{L}$, are defined by

$$\langle A(t)\rangle \equiv \int d\Gamma \rho(\Gamma)\, e^{Lt} A(\Gamma) = \int d\Gamma (e^{-\bar{L}t}\rho(\Gamma))\, A(\Gamma) \tag{5}$$

The second equality expresses the dynamics in terms of an evolution of the probability density. For conservative, nonsingular forces the two generators are equal, but for nonconservative and/or singular forces they are not equal.

To determine the form of the generators one can proceed in a direct way or consider first collisions for finite forces and take an appropriate hard-sphere limit. The details will be described elsewhere and only the results given here,

$$L = \sum_{\alpha=1}^{N} \mathbf{v}_\alpha \cdot \nabla_\alpha + \tfrac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} T(\alpha, \beta) \tag{6}$$

$$\bar{L} = \sum_{\alpha=1}^{N} \mathbf{v}_\alpha \cdot \nabla_\alpha - \tfrac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta \neq \alpha}^{N} \bar{T}(\alpha, \beta) \tag{7}$$

The first terms on the right sides generate free streaming, while the second terms describe velocity changes. The two binary collision operators $T(\alpha, \beta)$ and $\bar{T}(\alpha, \beta)$ for particles α and β are given by

$$T = -\sigma^2 \int d\Omega\, \Theta(-\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})\, \delta(\mathbf{r}-\boldsymbol{\sigma})(b-1) \tag{8}$$

$$\bar{T} = \sigma^2 \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})[\alpha^{-2}\, \delta(\mathbf{r}-\boldsymbol{\sigma})\, b^{-1} - \delta(\mathbf{r}+\boldsymbol{\sigma})] \tag{9}$$

where $d\Omega$ denotes the solid angle integration for the unit vector $\hat{\boldsymbol{\sigma}}$, $\mathbf{r}$ is the relative position vector of the two particles, and the operators b and b^{-1} are defined by

$$bF(\mathbf{g}) = F(b\mathbf{g}), \qquad b^{-1}F(\mathbf{g}) = F(b^{-1}\mathbf{g}) \tag{10}$$

$$b\mathbf{g} = \mathbf{g} - (1+\alpha)\,\hat{\boldsymbol{\sigma}}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}}), \qquad b^{-1}\mathbf{g} = \mathbf{g} - \alpha^{-1}(1+\alpha)\,\hat{\boldsymbol{\sigma}}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}}) \tag{11}$$

Thus, b changes functions of the relative velocity to the same function of the scattered relative velocity $b\mathbf{g} = \tilde{\mathbf{g}}$ of Eq. (2). Similarly, b^{-1} generates a function of the inverse velocity with the property $b^{-1}b = 1$. The results (5)–(11) provide a generalization of the hard-sphere dynamics of ref. 1 to include the inelastic collisions case $\alpha < 1$. Conservation of particle number and momentum is assured by the properties

$$\begin{aligned}\int d\mathbf{v}_1\, d\mathbf{v}_2[\psi(\mathbf{v}_1)+\psi(\mathbf{v}_2)]\,\bar{T}\rho(x_1, x_2) \\ = \int d\mathbf{v}_1\, d\mathbf{v}_2\{T[\psi(\mathbf{v}_1)+\psi(\mathbf{v}_2)]\}\,\rho(x_1, x_2) \\ = 0\end{aligned} \tag{12}$$

where $\psi(\mathbf{v}) = 1$ or $\mathbf{v}$.

The N-particle distribution, $\rho(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}, t)$, evolves according to the Liouville equation,

$$(\partial_t + \bar{L})\,\rho(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}, t) = 0 \tag{13}$$

The BBGKY hierarchy for the associated reduced distribution functions follows in the usual way by partial integration over $N-l$ degrees of freedom,

$$\begin{aligned}(\partial_t + \bar{L}(x_1,..., x_l))\, f^{(l)}(x_1,..., x_l, t) \\ = \sum_{\alpha=1}^{l} \int dx_{l+1}\, \bar{T}(\alpha, l+1)\, f^{(l+1)}(x_1,..., x_{l+1}, t)\end{aligned} \tag{14}$$

$$f^{(l)}(x_1,..., x_l, t) \equiv N^l \int dx_{l+1} \cdots dx_N\, \rho(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}, t) \tag{15}$$

where x_α denotes the position and velocity for particle α and $\bar{L}(x_1,..., x_l)$ is the generator of the dynamics for a system of l particles.

As a simple illustration of these results, consider the special state of homogeneous cooling, for which the system is translationally invariant and the dynamics occurs entirely through the time dependence of the temperature, $T(t)$, defined in terms of the average kinetic energy density, by $\langle \hat{e}(\mathbf{r}, t \mid \Gamma) \rangle = \frac{3}{2} n(\mathbf{r}, t)\, k_B T(\mathbf{r}, t)$. The cooling rate is then

$$\partial_t T(t) = -\frac{2}{3nk_B} (1-\alpha^2)\, w(T(t)) \tag{16}$$

where $(1-\alpha^2)\, w(T(t)) \equiv -\langle L\hat{e}(\mathbf{r}, t \mid \Gamma) \rangle$. The right side is easily calculated in terms of the two-particle reduced distribution function $f^{(2)}(x_1, x_2, t)$. To solve this equation it is necessary to know the dependence of w on T, which occurs entirely through this distribution function. Dimensional analysis and symmetry considerations show that for this state it has the form

$$f^{(2)}(x_1, x_2, t) \to n^2 v_0^{-6}(t) \phi^{(2)}(\mathbf{v}_1, \mathbf{v}_2) \tag{17}$$

where the velocities have been scaled to the thermal velocity, $v_0(t) = (2k_B T/m)^{1/2}$. It follows that $w(T(t))$ and $T(t)$ are given by

$$w(T(t)) = \tfrac{1}{8} m(n\sigma)^2 v_0^3(t) \int d\mathbf{v}_1\, d\mathbf{v}_2 \times \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})^3 \phi^{(2)}(\mathbf{v}_1/v_0(t), \mathbf{v}_2/v_0(t)) \tag{18}$$

$$T(t) = T(0)\left(1 + \frac{t}{t_0}\right)^{-2}, \qquad t_0^{-1} = \frac{2}{3}(1-\alpha^2)\, w(T(0))[mnv_0^2(0)]^{-1} \tag{19}$$

where g_c is the equilibrium pair correlation function at contact. Equation (19) is well known from hydrodynamic descriptions of homogeneous cooling,[15] although the derivation here shows it is exact and provides an expression for the time scale valid at all densities and all degrees of dissipation. Further discussion of the homogeneous cooling state is given below.

3. KINETIC EQUATION

A formal kinetic equation for the one particle distribution is obtained if $f^{(2)}(x_1, x_2, t)$ can be expressed as a functional of $f^{(1)}(x_1, t)$. To see how this might be done, consider the class of initial states of the form

$$\rho(\{\mathbf{r}_\alpha, \mathbf{v}_\alpha\}) = W(\{\mathbf{r}_\alpha\}) \prod_{\beta=1}^{N} \phi(x_\beta) \tag{20}$$

where the single-particle function $\phi(x)$ is arbitrary. Then all of the reduced distribution functions are functionals of $\phi(x)$, e.g.,

$$f^{(1)}(x_1, t) = f^{(1)}(x_1, t \mid \phi), \qquad f^{(2)}(x_1, x_2, t) = f^{(2)}(x_1, x_2, t \mid \phi) \tag{21}$$

If the functional relationship of $f^{(1)}$ to ϕ can be inverted, it can be used to express $f^{(2)}$ as a functional of $f^{(1)}$, i.e., $f^{(2)}(x_1, x_2, t \mid \phi) = G^{(2)}(x_1, x_2, t \mid f^{(1)})$. Substitution of this into the first BBGKY hierarchy equation then gives a formally exact closed kinetic equation,

$$(\partial_t + \mathbf{v}_1 \cdot \nabla_1) f^{(1)}(x_1, t) = \int dx_2 \, \bar{T}(x_1, x_2) \, G^{(2)}(x_1, x_2, t \mid f^{(1)}) \tag{22}$$

This formal analysis provides a useful starting point for obtaining approximate kinetic theories. For example, at low density the dimensionless parameter $n\sigma^3$ is small and an asymptotic expansion of the functional $G^{(2)}(x_1, x_2, t \mid f^{(1)})$ gives the Boltzmann–Bogoliubov equation as a leading approximation. Here, we consider a different approximation that does not imply a limitation to low density. This approximation, the revised Enskog theory (RET), is obtained by using the exact short-time form of the functional $G^{(2)} \to G^{(2)}(x_1, x_2, 0 \mid f^{(1)})$ in Eq. (22). It is remarkable that this functional can be determined exactly in terms of the equilibrium free energy density functional for an inhomogeneous state.[16] This is a consequence of the special choice of initial conditions in Eq. (20), where all spatial correlations arise from the overlap function $W(\{\mathbf{r}_\alpha\})$. More precisely, the functional $G^{(2)}(x_1, x_2, 0 \mid f^{(1)})$ is determined from the second functional derivative of the free energy, which in turn defines the equilibrium pair correlation function, $g_e(\mathbf{r}_1, \mathbf{r}_2 \mid n)$,

$$G^{(2)}(x_1, x_2, 0 \mid f^{(1)}) = g_e(\mathbf{r}_1, \mathbf{r}_2 \mid n) \, f^{(1)}(x_1, t) \, f^{(1)}(x_2, t) \tag{23}$$

The equilibrium pair correlation function is a functional of the nonequilibrium density,

$$n(\mathbf{r}) = \int d\mathbf{v} \, f^{(1)}(x, t) \tag{24}$$

As there are excellent approximations available for the hard-sphere free energy density functional,[17] we will take $g_e(\mathbf{r}_1, \mathbf{r}_2 \mid n)$ as a known functional of n. Substitution of Eq. (23) into Eq. (22) gives the RET, generalized to the case of dissipative dynamics,

$$(\partial_t + \mathbf{v}_1 \cdot \nabla_1) f^{(1)}(x_1, t) = \mathscr{J}(x_1, t \mid f^{(1)}) \tag{25}$$

$$\mathscr{J}(x_1, t \mid f^{(1)}) = \sigma^2 \int d\mathbf{v}_2 \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})[\alpha^{-2} g_c(\mathbf{r}_1, \mathbf{r}_1 - \boldsymbol{\sigma} \mid n)$$
$$\times f^{(1)}(\mathbf{r}_1, b^{-1}\mathbf{v}_1, t)\, f^{(1)}(\mathbf{r}_1 - \boldsymbol{\sigma}, b^{-1}\mathbf{v}_2, t)$$
$$- g_c(\mathbf{r}_1, \mathbf{r}_1 + \boldsymbol{\sigma} \mid n)\, f^{(1)}(\mathbf{r}_1, \mathbf{v}_1, t)\, f^{(1)}(\mathbf{r}_1 + \boldsymbol{\sigma}, \mathbf{v}_2, t)] \tag{26}$$

The RET is a highly nonlinear equation through the dependence on $f^{(1)}$ of $g_c(\mathbf{r}_1, \mathbf{r}_2 \mid n)$. It is this nonlinearity that constitutes Ernst and van Beijeren's *revision* of the earlier kinetic theory of Enskog. This change is essential to admit stationary solutions of Eq. (25) for both fluid and crystal phases[18] in the case of elastic hard spheres. To our knowledge, all previous kinetic theory applications to granular flow have been based on the Boltzmann or Enskog equations.[15, 19] In the present context, this revision from the usual Enskog equation should be significant for a description of the cluster phase following instability of the homogeneous cooling state, since $g_c(\mathbf{r}_1, \mathbf{r}_2 \mid n)$ describes the structure for an inhomogeneous fluid. The RET provides a unique basis for the description of dynamics across the whole range of densities, length scales, and degrees of dissipation. We know of no other theory with such generality.

For elastic collisions, a fluid dynamics description is based on the local conservation laws for mass, momentum, and energy. In the case of dissipative dynamics energy is no longer conserved. Nevertheless, it is straightforward to obtain the corresponding balance equations for these same variables. The results are

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{U}) = 0 \tag{27}$$

$$\frac{\partial U_i}{\partial t} + \mathbf{U} \cdot \nabla U_i + (nm)^{-1} \partial_j P_{ij} = 0 \tag{28}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot (e\mathbf{U}) + P_{ij}\, \partial_i U_j + \nabla \cdot \mathbf{q} = -(1 - \alpha^2)\, w \tag{29}$$

where n, e, and $\mathbf{U}$ are the number density, internal energy density, and flow velocity, respectively. The pressure tensor P_{ij} and the heat flux $\mathbf{q}$ have both "kinetic" and "collisional transfer" contributions, $P_{ij} = P_{ij}^k + P_{ij}^c$ and $\mathbf{q} = \mathbf{q}^k + \mathbf{q}^c$, given by

$$P_{ij}^k = \int d\mathbf{v}\, m v_i' v_j' f^{(1)}(x, t), \qquad \mathbf{q}^k = \int d\mathbf{v}\, \frac{1}{2} m v'^2 \mathbf{v}' f^{(1)}(x, t) \tag{30}$$

$$P_{ij}^c = \frac{1+\alpha}{4} m\sigma^3 \int d\mathbf{v}_1\, d\mathbf{v}_2 \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})^2 \hat{\sigma}_i \hat{\sigma}_j$$

$$\times \int_0^1 d\lambda\, g_e(\mathbf{r}-(1-\lambda)\,\boldsymbol{\sigma}, \mathbf{r}+\lambda\boldsymbol{\sigma}\,|\,n)$$

$$\times f^{(1)}(\mathbf{r}-(1-\lambda)\,\boldsymbol{\sigma}, \mathbf{v}_1, t)\, f^{(1)}(\mathbf{r}+\lambda\boldsymbol{\sigma}, \mathbf{v}_2, t) \tag{31}$$

$$\mathbf{q}^c = \frac{1+\alpha}{4} m\sigma^3 \int d\mathbf{v}_1\, d\mathbf{v}_2 \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})^2 (\mathbf{G}'\cdot\hat{\boldsymbol{\sigma}})\,\hat{\boldsymbol{\sigma}}$$

$$\times \int_0^1 d\lambda\, g_e(\mathbf{r}-(1-\lambda)\,\boldsymbol{\sigma}, \mathbf{r}+\lambda\boldsymbol{\sigma}\,|\,n)$$

$$\times f^{(1)}(\mathbf{r}-(1-\lambda)\,\boldsymbol{\sigma}, \mathbf{v}_1, t)\, f^{(1)}(\mathbf{r}+\lambda\boldsymbol{\sigma}, \mathbf{v}_2, t) \tag{32}$$

Here $\mathbf{v}' = \mathbf{v} - \mathbf{U}(\mathbf{r}, t)$ is the peculiar velocity and $\mathbf{G}' = \frac{1}{2}(\mathbf{v}_1' + \mathbf{v}_2')$. The collisional transfer contributions vanish at low density, but dominate at high densities. Finally, the source term w in the energy equation describes the dissipation and its expression is

$$w = \frac{m\sigma^2}{8} \int d\mathbf{v}_1\, d\mathbf{v}_2 \int d\Omega\, \Theta(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})^3$$

$$\times g_e(\mathbf{r}, \mathbf{r}+\boldsymbol{\sigma}\,|\,n)\, f^{(1)}(\mathbf{r}, \mathbf{v}_1, t)\, f^{(1)}(\mathbf{r}+\boldsymbol{\sigma}, \mathbf{v}_2, t) \tag{33}$$

which is the RET approximation to (18). These balance equations are an exact consequence of the kinetic equation (25) and provide the basis for a fluid dynamics description of rapid granular flow. A detailed elaboration will be given elsewhere.

4. MONTE CARLO SIMULATION

In the low-density limit the RET for elastic collisions reduces to the Boltzmann–Bogoliubov equation. If the further limitation to length scales large compared to σ is made, then the usual Boltzmann kinetic equation is regained. While analytic solutions to the Boltzmann equation are difficult in general, a numerical Monte Carlo simulation method has been developed over the past 20 years to the point that most low-density gas flows can be addressed quantitatively by this method. It is known as the Bird direct simulation method.[20] Recently, this method has been extended to provide direct simulation of the RET equation.[4] It is difficult to overemphasize the

importance of such a practical tool for study of the hard-sphere system over the full range of densities and space scales, even far from equilibrium. Initial results for a fluid under large shear at high densities have verified the promise of this method.

In this section, this new Monte Carlo simulation method is extended further to include dissipative collisions. There are two parts to the simulation in each unit time step, free streaming followed by a (possible) collision. The volume of the system is divided into cells of dimension smaller than the mean free path, and N particles are introduced at $t = 0$ with positions and velocities sampled statistically from a specified initial distribution function. The distribution of particles is calculated at $t = \tau$, with τ much smaller than the mean free time, as follows. First the particles are displaced by $\{\Delta \mathbf{r}_\alpha = \mathbf{v}_\alpha \tau\}$. For each particle α a sphere of radius σ is drawn around it. A point on each sphere is selected at random, the cell associated with that point identified, and a particle β in that cell is chosen at random. In this way N pairs of particles are identified as candidates for a binary collision. The collision for a pair (α, β) is accepted with probability $\omega_{\alpha\beta}$ equal to the RET collision rate times the time interval τ,

$$\omega_{\alpha\beta} = 4\pi\sigma^2 \Theta(\mathbf{g}_{\alpha\beta} \cdot \hat{\boldsymbol{\sigma}})(\mathbf{g}_{\alpha\beta} \cdot \hat{\boldsymbol{\sigma}})\, g_c(\mathbf{r}_\alpha, \mathbf{r}_\alpha + \boldsymbol{\sigma} \mid n)\, n_\beta \tau \tag{34}$$

Here $\mathbf{g}_{\alpha\beta} = \mathbf{v}_\alpha - \mathbf{v}_\beta$ and n_β is the density in cell β [in general $g_c(\mathbf{r}_\alpha, \mathbf{r}_\alpha + \boldsymbol{\sigma} \mid n)$ depends on the densities of all cells]. If the collision is accepted, the velocity of particle α is changed by the direct scattering relation, Eq. (2), to $\tilde{\mathbf{v}}_\alpha = \mathbf{v}_\alpha - \frac{1}{2}(1 + \alpha)\, \hat{\boldsymbol{\sigma}}(\mathbf{g}_{\alpha\beta} \cdot \hat{\boldsymbol{\sigma}})$. If the collision is rejected, there is no change in the velocity. The process is then repeated for each subsequent time step. In practice there are some variations of the above for better efficiency.

This method provides the complete one particle distribution function (coarse grained over the cells), from which all relevant physical observables can be computed as averages. The more detailed information from the distribution function itself is also useful, as illustrated in the last section for the homogeneous cooling state of rapid granular flow.

5. KINETIC MODEL

Almost all analytic studies of the RET have been restricted to states near equilibrium. Even in the low-density Boltzmann limit there is very little known about solutions far from equilibrium. However, it has proven very fruitful to consider closely related, but more practical, kinetic equations that retain the relevant physical and mathematical properties of the Boltzmann equation (see ref. 21 for a review). Such kinetic equations are called kinetic models. Recently, it has been shown how this concept of

kinetic modeling can be applied to the RET with elastic collisions to study states far from equilibrium at high densities.[5] In this section, we present the corresponding kinetic model for the RET with dissipative dynamics.

The basic idea of a kinetic model is to impose maximum simplicity while preserving the essential exact properties of the RET. These include the exact equilibrium states (both fluid and crystal) and the exact conservation laws. This is accomplished by representing the collision operator $\mathscr{J}$ as an expansion in a complete set of polynomials with a scalar product weighted with respect to a local equilibrium distribution. The contribution from the subspace spanned by 1, $\mathbf{v}$, and v^2 is retained exactly, while the contribution from the orthogonal subspace is approximated by a single relaxation time. The details will be described elsewhere and only the result given here:

$$\begin{aligned}(\partial_t + \mathbf{v}\cdot\nabla) f^{(1)}(x,t) &= -\nu[f^{(1)}(x,t) - f_l(x,t)] \\ &\quad - \frac{1}{k_B T n} f_l(x,t)\{v_i' \partial_j P_{ij}^c + \psi(v')[\nabla\cdot\mathbf{q}^c + P_{ij}^c \partial_i U_j + (1-\alpha^2) w]\}\end{aligned} \tag{35}$$

where $\psi(v) = mv^2/3k_B T - 1$ and f_l is the local equilibrium distribution,

$$f_l(x,t) = n(\mathbf{r},t)\left(\frac{1}{\pi v_0}\right)^{3/2} e^{-(v'/v_0)^2}, \qquad v_0 = v_0(\mathbf{r},t) \equiv [2k_B T(\mathbf{r},t)/m]^{1/2} \tag{36}$$

Also, $\nu(n(\mathbf{r},t), T(\mathbf{r},t))$ is the collision frequency. It can be chosen to optimize agreement between the kinetic model and some specific property of interest, such as a transport coefficient. A specific example is introduced in the next section.

In the above expressions we behave introduced the granular temperature $T(\mathbf{r},t)$. This has proven to be a very useful concept in the description of granular flow. Here it has no association with the equilibrium of two systems in contact, but is simply a measure of the average kinetic energy through the definition given above (16), or equivalently,

$$e(\mathbf{r},t) = \tfrac{3}{2} n(\mathbf{r},t) k_B T(\mathbf{r},t) = \int d\mathbf{v}\, \tfrac{1}{2} m v'^2 f^{(1)}(x,t) \tag{37}$$

The collisional transfer contributions to the fluxes are defined as in Eqs. (31) and (32). The first term on the right side of Eq. (35) is a single-relaxation-time model, while the last term is necessary for the collisional transfer contributions to the local conservation laws. In the limit $\alpha = 1$ this model agrees with that of ref. 5, while in the limit of low density and small

dissipation it agrees with that of ref. 7. An example of its application to granular flow is given in the next section.

6. HOMOGENEOUS COOLING STATE

The special, idealized state of homogeneous cooling has been noted at the end of Section 2. The system is spatially uniform and the dynamics occurs entirely through the time dependence of the temperature, $T(t)$. It is interesting to note that in this case the dependence of Eq. (25) on density can be scaled out by a proper choice of units. Consequently, the distribution function for the homogeneous cooling state is completely determined by the low density Boltzmann equation alone. Equations (27) and (28) are satisfied identically, and the energy equation (29) gives (16)–(19), except that $w(T(t))$ is given by the Enskog approximation (33). The distribution function, $f^{(1)}(x, t) = nv_0^{-3}(t)\,\phi(v/v_0(t))$, is determined from the kinetic equation (25). The solution for $\alpha = 1$ is a Maxwellian as expected, but for $\alpha < 1$ the solution is qualitatively different from a Maxwellian. This can be seen from a perturbation expansion in powers of $(1-\alpha)$ valid for weakly dissipative dynamics. If α differs significantly from unity, the solution to (25) is not known. If one considers the corresponding solution to the kinetic model of Section 5, it is easily seen that a Maxwellian is obtained for all values of α. Although, as mentioned above, this is not exactly the case for the RET, the kinetic model may still be useful for most of the physical situations. To test this assumption, we have performed numerical Monte Carlo simulations using the method described in Section 4 to compute the distribution function for the homogeneous cooling state. The results show that the distribution function for thermal velocities ($v \lesssim 2v_0$) can be approximated very accurately by a Maxwellian, even for relatively small values of the restitution coefficient. On the other hand, there exists a slight overpopulation of high-energy particles. For instance, at $\alpha = 0.7$, the fraction of particles with $v \geqslant 3v_0$ is about 16% larger than the Maxwellian value. These results support using the kinetic model even for conditions of large dissipation. A detailed description of the Monte Carlo simulation results, including tests of the velocity scaling law, deviations from Maxwellian, and the dependence of the cooling rate $t_0(\alpha)$ on α, can be found in ref. 22.

To describe the stability of the homogeneous cooling state and the dynamics of states close to it, a modified Chapman–Enskog expansion can be performed. The distribution function is represented as an expansion in powers of hydrodynamic gradients around the reference state of homogeneous cooling. The results at first order in the gradients can be used to calculate the heat and momentum fluxes as functions of these gradients. This provides the constitutive equations to construct the Navier–Stokes-order

hydrodynamics for granular flow from Eqs. (27)–(29). Since the homogenous cooling state is known for the kinetic model, the Chapman–Enskog solution can be determined exactly to Navier–Stokes order. The resulting fluxes are found to be

$$P_{ij}=\left(p-\frac{1-\alpha}{2}p^c\right)\delta_{ij} -\eta(\alpha)\left(\partial_i U_j+\partial_j U_i-\frac{2}{3}\delta_{ij}\,\nabla\cdot\mathbf{U}\right)-\kappa(\alpha)\,\delta_{ij}\,\nabla\cdot\mathbf{U} \tag{38}$$

$$\mathbf{q}=-\lambda(\alpha)\,\nabla T-\mu(\alpha)\,\nabla n \tag{39}$$

These are quite similar to the results for elastic collisions, with some important differences. The form (38) differs by an additional contribution that effectively reduces the hydrostatic pressure. Also, (39) differs from Fourier's law by the term proportional to the density gradient, with an associated new transport coefficient, $\mu(\alpha)$. The shear viscosity $\eta(\alpha)$, bulk viscosity $\kappa(\alpha)$, thermal conductivity $\lambda(\alpha)$, and the new transport coefficient $\mu(\alpha)$ are given by

$$\eta(\alpha)=\eta^{(0)}(\alpha)\left[g_c^{-1}+(1+\alpha)\frac{2}{15}\pi n^*\right]+\frac{3}{5}\kappa(\alpha) \tag{40}$$

$$\lambda(\alpha)=\lambda^{(0)}(\alpha)\left[g_c^{-1}+(1+\alpha)\frac{1}{5}\pi n^*\right]+\frac{3k_B}{2m}\kappa(\alpha) \tag{41}$$

$$\mu(\alpha)=\mu^{(0)}(\alpha)\left[g_c^{-1}+(1+\alpha)\frac{1}{5}\pi n^*\right] \tag{42}$$

$$\kappa(\alpha)=\frac{1+\alpha}{2}\kappa_E \tag{43}$$

Here κ_E is the Enskog value for the bulk viscosity at $\alpha=1$ and $n^*\equiv n\sigma^3$. Also, quantities with a superscript zero denote their low-density values,

$$\frac{\eta^{(0)}(\alpha)}{\eta^{(0)}(1)}=\left[1-\frac{5c}{24}(1-\alpha^2)\right]^{-1} \tag{44}$$

$$\frac{\lambda^{(0)}(\alpha)}{\lambda^{(0)}(1)}=\left[1-\frac{5c}{6}(1-\alpha^2)\right]^{-1} \tag{45}$$

$$\frac{\mu^{(0)}(\alpha)}{\lambda^{(0)}(1)}=\frac{5c}{12}(1-\alpha^2)\left[1-\frac{5c}{8}(1-\alpha^2)\right]^{-1}\left[1-\frac{5c}{6}(1-\alpha^2)\right]^{-1} \times T(n^{-1}+g_c^{-1}\,\partial_n g_c) \tag{46}$$

with $\eta^{(0)}(1) = ng_c/\beta v$ and $\lambda^{(0)}(1) = 5k_B ng_c/2m\beta v$. The choice for the collision frequency has been such as to assure the correct low-density limit for the shear viscosity, $v = (16/5c)\, ng_c\sigma^2(\pi k_B T/m)^{1/2}$, where $c \simeq 1.016$. These results illustrate how the kinetic model provides a practical means to derive hydrodynamic equations for inelastic collisions that are appropriate for both high densities and possibly strong dissipation, with explicit expressions for the parameters of these equations. Similar expressions have been obtained by Lun *et al.*[19] from an approximate analysis of the Enskog equation on the assumption of weak dissipation.

The transport coefficients are positive for $0 < \alpha \leqslant 1$. However, linearization of the hydrodynamic equations around the homogeneous cooling state shows a long-wavelength instability. As a consequence a small density perturbation grows in time and it is expected that this is a precursor of the transition to cluster formation. It is not clear to what extent the late-stage cluster phase can be described at a hydrodynamic level. The Monte Carlo simulations of ref. 22 confirm that this phenomenon can be studied at the level of the kinetic theory given here. Furthermore, at small α (large dissipation) a "collapse" occurs and this certainly will require description at the kinetic level. Both the kinetic model and the Monte Carlo simulation method should provide instructive information complementary to the molecular dynamics simulations.

7. DISCUSSION

In this brief presentation several successful methods of nonequilibrium statistical mechanics have been extended for application to systems with dissipative dynamics. Only the basic tools have been provided, along with an indication of their potential for more specific applications. Some of these applications can be summarized as follows:

- The identification of the generators for dissipative hard sphere dynamics and the associated Liouville equation allows application of formal linear response methods to problems such as granular flow. For example, it is possible to identify corresponding Green–Kubo expressions for transport coefficients. Such expressions are appropriate representations for application of theoretical many-body approximations and for controlled molecular dynamics simulations.

- The simplest such realistic many-body approximation is the revised Enskog kinetic theory described here. Applications of this equation to specific physical conditions constitutes a first-order problem for controlled analysis of the qualitative features in granular flow. Its extension to more realistic scattering processes such as rough and irregular particles is complex

but straightforward. Development of kinetic theory beyond the Enskog approximation for elastic spheres is quite advanced for both the distribution function and fluctuations. This has lead to the discovery and understanding of qualitatively different phenomena, such as algebraic decay of correlations in both space and time. The associated mode coupling mechanism can be formulated for inelastic spheres as well from the Liouville formalism of Section 2.

- The proposal given here for an efficient Monte Carlo simulation method to solve the RET has great potential for exploration of complex flows, based on the corresponding success at low density for elastic collisions. Of particular interest is the simulation of highly inhomogeneous states where significant differences from the Enskog theory are expected. This is a developing field whose limitations are not yet identified.

- Theoretical studies of the RET are an essential complement to the numerical Monte Carlo simulations, for interpretation and analysis. At low density and for elastic collisions this complement has been provided by kinetic models such as the BGK model. Here we have proposed its generalization to both higher densities and dissipative collisions. One of the key practical advantages of the kinetic model over the RET is the relative ease of applying it to boundary-driven flows. For example, an exact solution is possible in the case of uniform shear flow.

In summary, it appears there is significant potential for application of methods from the nonequilibrium statistical mechanics of hard spheres to systems with dissipative dynamics. This potential refers both to establishing a firm and clear basis for a macroscopic description and to quantitative methods for analysis.

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