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Statistical mechanics, kinetic theory, and hydrodynamics for rapid granular flow

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Abstract. A system of smooth hard spheres with inelastic collisions is considered as an idealized model to describe rapid granular flow. A non-equilibrium statistical mechanics is formulated for this system, analogous to that for elastic collisions. The associated Liouville equation provides the basis for application of many-body methods such as linear response, kinetic theory, and the derivation of macroscopic hydrodynamic equations. These methods are illustrated for the simplest case of self-diffusion. A Green–Kubo expression for the self-diffusion coefficient is derived and evaluated using an approximate linear kinetic theory. Other recent applications of kinetic theory and kinetic models are reviewed briefly.

1. Introduction

Granular systems have attracted the attention of the physics community in recent years [1], in part because such systems exhibit flow which is strikingly similar to that for normal fluids under many conditions. These conditions include rapid, dilute flow where the dominant transfer of momentum and energy is via successive hard binary collisions of the constituent particles. An important characteristic of such collisions is the loss of kinetic energy. The discussion here will focus on the objective of understanding only the effects of such collisional dissipation by isolating it from other important properties of granular media in an idealized model. Consequently, a successful analysis of the model will not provide a good description of all experiments but it can provide a more complete identification of which qualitative features can be attributed primarily to dissipation. In fact, it is remarkable that there is so much correspondence with real systems in the applications to date.

The idealized model is a system of smooth, hard spheres with inelastic collisions. The collisions are specified in the usual way in terms of the change in relative velocity at contact, but with a decrease in the magnitude of the normal component measured by a positive restitution coefficient, $\alpha \leq 1$. The hard-sphere system with elastic collisions has been studied extensively for both equilibrium and non-equilibrium statistical mechanics, using molecular dynamics simulation and many-body methods. It is tempting to apply these same methods for the case of inelastic collisions and that is indeed what many in the physics community have been attempting during the past five years. Much of the most interesting new information has been obtained by molecular dynamics simulation. The emphasis here will be on complementary theoretical methods being developed and attempts to provide the context for a fluid dynamics description. This brief account is a personal perspective based on the author's work and that of his collaborators; no attempt is made to include the extensive related work of many others in this field.

The starting point is a discussion of the non-equilibrium statistical mechanics for this system to indicate the potential for application of a range of known many-body methods [2]. Subsequently, only a flavour of such applications is provided through a discussion of self-diffusion as the simplest test for hydrodynamics. A more complete description of linear response methods is in progress. Finally, some of the current results from kinetic theory are summarized, including the use of kinetic models for states far from the reference homogeneous state.

2. Statistical mechanics

The system considered is composed of N smooth hard spheres of diameter σ . Their motion consists of free streaming until a given pair i, j is in contact, at which point their relative velocity changes instantaneously according to the inelastic collision rule

$$\tilde{\mathbf{g}}_{ij} = \mathbf{g}_{ij} - (1 + \alpha)\hat{\boldsymbol{\sigma}}(\mathbf{g}_{ij} \cdot \hat{\boldsymbol{\sigma}}). \quad (2.1)$$

Here $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity for particles i and j , and α is the restitution coefficient with values in the range $0 < \alpha \leq 1$ measuring the degree of inelasticity. The special case of elastic spheres is given by $\alpha = 1$. The centre-of-mass velocity is unchanged so the total mass and momentum of the pair is conserved. However, there is an energy loss of $\tilde{E} - E = -(1 - \alpha^2)m(\mathbf{g} \cdot \hat{\boldsymbol{\sigma}})^2/4$ for each collision. The state of the system at time t is completely characterized by the positions and velocities of all spheres at that time and is represented by a point in the associated $6N$ -dimensional phase space, $\Gamma_t \equiv \{\mathbf{q}_1(t), \dots, \mathbf{q}_N(t), \mathbf{v}_1(t), \dots, \mathbf{v}_N(t)\}$. The sequence of free streaming and binary collisions determines uniquely these positions and velocities of the spheres at time t for given initial conditions at $t' < t$. A more complete notation expressing this dependence on initial conditions is $\Gamma_t(\Gamma_{t'})$. Thus, just as in the case of elastic collisions the microdynamics for this system corresponds to a deterministic trajectory in phase space. Observables of interest are represented by the same phase functions as for elastic collisions, $A(\Gamma(t, \Gamma))$, and their average for given statistical initial data at $t = 0$ is defined by

$$\langle A(t) \rangle \equiv \int d\Gamma_0 \rho(\Gamma_0) A(\Gamma_t(\Gamma_0)) \quad (2.2)$$

where $\rho(\Gamma_0)$ is the probability density or ensemble for the initial state, normalized to unity. An equivalent representation of this average is obtained by changing variables to integrate over Γ_t rather than over Γ_0 . This change of variables is possible since trajectories in phase space do not cross, and Γ_0 can be expressed in terms of Γ_t denoted by $\Gamma_t^{-1}(\Gamma_t)$. Then (2.2) becomes

$$\langle A(t) \rangle = \int d\Gamma_t J(\Gamma_0, \Gamma_t) \rho(\Gamma_t^{-1}(\Gamma_t)) A(\Gamma_t) \equiv \int d\Gamma \rho(\Gamma, t) A(\Gamma) \quad (2.3)$$

where $J(\Gamma_0, \Gamma_t)$ is the Jacobian of the transformation. The second equality of (2.3) describes the time evolution through that of the phase-space probability density defined by $\rho(\Gamma, t) \equiv J(\Gamma_t^{-1}(\Gamma), \Gamma) \rho(\Gamma_t^{-1}(\Gamma))$.

For practical purposes it is useful to identify the generators L and \bar{L} for the two representations, defined by

$$A(t) \equiv e^{Lt} A(\Gamma) \quad \rho(\Gamma, t) = e^{-\bar{L}t} \rho(\Gamma). \quad (2.4)$$

These are not the usual generators of Hamilton's equations for continuous forces and are somewhat more complex due to the singular nature of hard spheres. Such generators have been

discussed in detail for the case of elastic collisions and the analysis extends quite naturally to the inelastic case as well [2], with the results

$$L = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_i + \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N T(i, j) \quad \bar{L} = \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_i - \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i}^N \bar{T}(i, j). \quad (2.5)$$

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

$$T(i, j) = -\sigma^2 \int d\Omega \Theta(-\mathbf{g}_{ij} \cdot \hat{\boldsymbol{\sigma}}) (\mathbf{g}_{ij} \cdot \hat{\boldsymbol{\sigma}}) \delta(\mathbf{q}_{ij} - \boldsymbol{\sigma}) (b - 1) \quad (2.6)$$

$$\bar{T}(i, j) = \sigma^2 \int d\Omega \Theta(\mathbf{g}_{ij} \cdot \hat{\boldsymbol{\sigma}}) (\mathbf{g}_{ij} \cdot \hat{\boldsymbol{\sigma}}) [\alpha^{-2} \delta(\mathbf{q}_{ij} - \boldsymbol{\sigma}) b^{-1} - \delta(\mathbf{q}_{ij} + \boldsymbol{\sigma})] \quad (2.7)$$

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 operator b is a substitution operator, $bF(\mathbf{g}_{ij}) = F(b\mathbf{g}_{ij})$, which changes the relative velocity $\mathbf{g}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ into its scattered velocity according to, equation (2.3), $b\mathbf{g}_{ij} = \tilde{\mathbf{g}}_{ij}$.

In terms of this representation for the dynamics, the Liouville equation for the N -particle distribution, $\rho(\Gamma, t)$, is

$$(\partial_t + \bar{L})\rho(\Gamma, t) = 0. \quad (2.8)$$

Similarly, the BBGKY hierarchy for the reduced distribution functions is obtained by partial integration of the Liouville equation over $N - l$ degrees of freedom:

$$(\partial_t + \bar{L}(x_1, \dots, x_l))f^{(l)}(x_1, \dots, x_l, t) = \sum_{i=1}^l \int dx_{l+1} \bar{T}(i, l+1)f^{(l+1)}(x_1, \dots, x_{l+1}, t) \quad (2.9)$$

$$f^{(l)}(x_1, \dots, x_l, t) \equiv N^l \int dx_{l+1} \dots dx_N \rho(\{\mathbf{q}_i, \mathbf{v}_i\}, t) \quad (2.10)$$

where $x_\alpha = \{\mathbf{q}_i, \mathbf{v}_i\}$ denotes the position and velocity for particle i and $\bar{L}(x_1, \dots, x_l)$ is the Liouville operator for a system of l particles.

The loss of energy on each binary collision implies a corresponding decrease in the average velocity for each particle in the absence of external driving forces. A characteristic average velocity is defined in terms of the kinetic energy per particle by $v_0^2(t) \equiv 2 \langle \sum_i v_i^2(t) \rangle / 3N$. This definition is chosen such that v_0 becomes the familiar thermal velocity for the case of elastic collisions. Its time dependence can be calculated from (2.3) using the Liouville equation and the explicit form of \bar{L} :

$$\partial_t \ln(v_0(t)) = -v_c(t)\omega^*(t) \quad v_c(t) \equiv n\pi\sigma^2 v_0(t). \quad (2.11)$$

where $v_c\omega^*$ gives the slowing rate of the particles due to inelastic collisions. It is proportional to the collision frequency $v_c(t) \equiv n\pi\sigma^2 v_0(t)$. The remaining dimensionless factor $\omega^*(t)$ depends on the degree of dissipation through the factor $1 - \alpha^2$, and the two-particle reduced distribution function at contact:

$$\omega^*(t) = (1 - \alpha^2) \frac{1}{6v_0^3(t)} \int d\mathbf{v}_1 d\mathbf{v}_2 f^{(2)}(r_{12} = \sigma, \mathbf{v}_1, \mathbf{v}_2, t) g_{12}^3. \quad (2.12)$$

The collisional decrease in velocities will be referred to as ‘cooling’, by analogy to the elastic case where the thermal velocity is proportional to the square root of the temperature. This

effect can be made explicit by introducing the generator for velocity scaling in the Liouville equation:

$$(\partial_t + \mathcal{L})\rho + \sum_{i=1} \nabla_{u_i} \cdot (\mathbf{F}_i \rho) = 0 \quad \mathcal{L}\rho = \bar{L}\rho - \sum_{i=1} \nabla_{v_i} \cdot (\mathbf{F}_i \rho) \quad (2.13)$$

where $\mathbf{F}_i = -v_c(t)\omega^*(t)\mathbf{v}_i$. This trivial rearrangement leads to an interesting interpretation for the dominant effects of inelasticity. It is easily shown that the new generator \mathcal{L} does not change the total kinetic energy and in this respect is similar to that in the case of elastic collisions. Instead, the cooling effect is now represented by an effective Stokes law drag force \mathbf{F}_i on each particle with friction constant $v_c(t)\omega^*(t)$. This representation is particularly instructive for steady shear flow where this drag force acts as an internal thermostat to control viscous heating, allowing close analogy to studies of shear flow for elastic collisions using an externally imposed thermostat for steady states.

The above is a brief and formal description of the tools for application of non-equilibrium statistical mechanics to this system of inelastic hard spheres. Clearly the analogy with the usual statistical mechanics of elastic collisions is close at this operational level. However, the justification for use of the average properties obtained in non-equilibrium statistical mechanics relies on subtle concepts such as mixing which may not have the same implications for systems with inelastic collisions. On the other hand, many of the new features of the latter are similar to those of open systems with elastic collisions (e.g., those driven by non-conservative forces). The approach here is to assume that the usual qualitative properties necessary for statistical mechanics remain valid, and to probe such questions in the context of specific applications for comparison with molecular dynamics and other simulation experiments.

3. Homogeneous cooling state

The average velocity, the collision frequency, and the mean free path $\ell \equiv 1/\pi n\sigma^2$ can be used to define the appropriate dimensionless variables for analysis:

$$s(t, t') \equiv \int_{t'}^t d\tau v_c(\tau) \quad \mathbf{u}_i = \mathbf{v}/v_0(t) \quad \mathbf{r}_i = \mathbf{q}_i/\ell \quad (3.1)$$

$$\rho(\Gamma, t) = (\ell v_0)^{-3N} \rho^* \quad f^{(l)} = (\ell v_0)^{-l} f^{(l)*} \quad \bar{L} = v_c(t)\bar{L}^* \quad (3.2)$$

It is easily verified that the generator \bar{L}^* is time independent and has the same form as \bar{L} in the new variables. The dimensionless Liouville equation becomes

$$(\partial_s + \mathcal{L}^*)\rho^* = 0 \quad \mathcal{L}^*\rho^* \equiv \bar{L}^*\rho^* - \sum_{i=1} \nabla_{u_i} \cdot (\mathbf{F}_i^* \rho^*) \quad (3.3)$$

with $\mathbf{F}_i^* = -\omega^*(t)\mathbf{u}_i$.

For an isolated system there is no stationary solution to the Liouville equation (2.8) for ρ . However, the additional terms \mathbf{F}_i^* from the velocity scaling in (3.3) admit the possibility of a stationary solution for ρ^* in the dimensionless variables. Such a solution is characterized by $\partial_s \rho^* = 0$. It is readily seen that this implies that $\omega^*(t)$ is time independent. This is a scaling solution in which all the time dependence of ρ occurs only through the scaling of the velocity and its normalization. The detailed velocity dependence is determined by the stationary dimensionless Liouville equation

$$\mathcal{L}^*\rho_{hcs}^* = 0. \quad (3.4)$$

As discussed above, the operator \mathcal{L}^* differs from \bar{L}^* by the generator for scale transformations that increase the velocity. Thus the stationary solution is obtained as a balance between velocity decreasing due to inelastic collisions and this scale transformation. Such a solution is known

as the homogeneous cooling state (HCS), where the additional assumptions of rotational and translational invariance are implied. It is the analogue of the Gibbs state for elastic collisions and reduces to it for $\alpha = 1$; for $\alpha < 1$ the exact solution is not known (it is not simply the Gibbs state with time-dependent velocity scaling).

Some interesting consequences follow from the velocity scaling of the HCS. Since $\omega^*(t)$ becomes time independent, equation (2.11) can be integrated for the explicit time dependence of $v_0(t)$ and the relationship of s to t :

$$v_0(t) = v_0(t') [1 + \omega^* v_c(t')(t - t')]^{-1} = v_0(t') e^{-\omega^* s(t, t')} \quad (3.5)$$

$$s(t, t') = \omega^{*-1} \ln [1 + \omega^* v_c(t')(t - t')]. \quad (3.6)$$

The velocity decrease is algebraic in real time. This time is logarithmically stretched by the dimensionless time s , so the decay becomes exponential, as indicated in the last equality of (3.5). It is important to recognize that $\omega^* \propto (1 - \alpha^2)$ with the result that for weak inelasticity there is a crossover from a logarithmic to a linear relationship between the two times. Knowledge of the time dependence of $v_0(t)$ also implies that for many average properties. For example, if $A(t)$ is a homogeneous function of the velocity, $A(\{xv_1(t), \dots, xv_N(t)\}) = x^p A(\{v_1(t), \dots, v_N(t)\})$, then its average value in the homogeneous cooling state is

$$\langle A(t) \rangle = v_0^p(t) \int d\Gamma \rho_{hcs}^*(\Gamma) A^*(\Gamma) \quad (3.7)$$

where A^* denotes A in terms of the dimensionless velocities. Similarly, fluctuations and time correlation functions for this state have a corresponding simplification. At this point it is appropriate to recognize that there is convincing evidence from both theory and simulation that the HCS is unstable against small spatial perturbations and spontaneous fluctuations. Thus any analysis based on averages in the HCS must be qualified by an appropriate timescale which is short compared to the onset of instability. In many cases of interest the problem of instabilities can be suppressed. On the other hand, the existence of this instability is due solely to the inelasticity of collisions and therefore is of great interest in itself as a signature of collisional dissipation.

4. Hydrodynamics and linear response

For the hard-sphere fluid with elastic collisions there is a clear separation of timescales between microscopic (or kinetic) excitations which occur on the timescale of the inverse collision frequency, and longer-timescale hydrodynamic phenomena. Generally, the latter is characterized by timescales of the order of macroscopic spatial disturbances relative to the mean free path. The hydrodynamic excitations dominate at long times as the system approaches a homogeneous state and these timescales become very long compared to all other microscopic excitations. The circumstances are somewhat more complicated for the case of inelastic collisions due to the additional timescale for cooling. The cooling timescale is incorporated in the reference state about which spatial perturbations are considered and occurs for both the microscopic and hydrodynamic excitations. Thus, no matter how rapid the cooling of the reference state, conditions for hydrodynamics still consist of the timescales for spatial perturbations being long compared to all other microscopic perturbations. This distinction between the dynamics of spatial perturbations and the cooling of the reference state has led to some misconceptions about the existence of hydrodynamics for inelastic collisions. However, detailed calculations with kinetic models (see the discussion below) show that the dynamics of the reference state simply changes the timescale from t to s and the separation between microscopic and hydrodynamic excitations is still preserved in these units.

Linear response methods are important and effective many-body tools for the analysis of hydrodynamics and related perturbations of the Gibbs state. Formally, one considers initial states for the Liouville equation that have small deviations from the Gibbs state characterized by the physical variables of interest. The average values of these observables are then calculated from a formal solution to the Liouville equation. In this way it is possible to obtain expressions for the energy and momentum fluxes in the macroscopic balance equations for mass, energy, and momentum, to linear order in the spatial gradients of these systems (Fourier's law for thermal conduction, and Newton's law for viscous dissipation). A similar analysis is possible for inelastic collisions using the HCS as the analogue of the Gibbs reference state. The analysis is somewhat more involved due to the time dependence of the reference state and the details will be presented elsewhere. However, it is possible to illustrate the basic ideas here for the special case of tagged-particle diffusion. In this case an additional particle (with label q_0, v_0) is inserted among the N identical particles and identified for special consideration. The initial distribution for the Liouville equation is taken to be a spatial perturbation of the HCS for the entire system:

$$\rho(0) = \rho_{hcs} [1 + V \delta P(q_0, 0)] \quad (4.1)$$

where $P(x, 0) = \langle \delta(x - q_0) \rangle$ is a given initial probability density for finding the tagged particle at x , and $\delta P(x, 0)$ is its deviation from the uniform probability density in the HCS. The volume factor V is required by normalization of $P(x, 0)$ to unity. Using this initial state a formal solution to the Liouville equation can be found for calculating $P(x, t) = \langle \delta(x - q_0(t)) \rangle$ at later times. Using standard linear response methods and an expansion in small spatial gradients it can be shown that $P(r, t)$ obeys the generalized diffusion equation. The details of the derivation will be given elsewhere and only the result quoted here:

$$\partial_t P(x, t) - D(t) \nabla^2 P(x, t) = 0 \quad D(t) = \frac{1}{3} \int_0^t dt' \langle v_0(t) \cdot v_0(t'); 0 \rangle_{hcs}. \quad (4.2)$$

The function $D(t)$ is given by the time integral of the tagged-particle velocity autocorrelation function, averaged over the initial HCS. This is quite similar to the case of elastic collisions for self-diffusion in the Gibbs state. In that case the correlation function is stationary and depends only on the time difference. Then, $D(t)$ approaches a constant for long times if the velocity autocorrelation function is integrable, and the equation for $P(x, t)$ becomes the diffusion equation for long times. The diffusion equation, with constant diffusion coefficient D , constitutes the hydrodynamic description for this process. It is approached exponentially fast in time for elastic collisions.

The analysis here is somewhat more complex due to the cooling of the reference state. However, this additional time dependence can be removed by use of the dimensionless variables, leading to (again, the details will be given elsewhere)

$$\partial_s P^*(r, s) - D^*(s) \nabla^2 P^*(r, s) = 0 \quad (4.3)$$

$$D^*(s) = \frac{1}{3} \int_0^s d\tau C(\tau) \quad C(\tau) = \int d\Gamma u_0 \cdot e^{-\mathcal{L}^* \tau} (u_0 \rho) \quad (4.4)$$

where $D^*(s) = D(t)/\ell^2 v_c(t)$ and \mathcal{L} is given by (3.4). Thus diffusion is recovered in terms of the variable s rather than t , with the diffusion coefficient given by the Green-Kubo expression

$$D^* = \frac{1}{3} \int_0^\infty d\tau C(\tau). \quad (4.5)$$

Alternatively, diffusion can be discussed in terms of the mean square displacement of the tagged particle obtained in dimensionless form from the second moment of (4.3):

$$M^*(s) \equiv \int dr r^2 P^*(r, t) = \frac{2}{3} \int_0^s d\tau (s - \tau) C(\tau) \rightarrow 2D^* s. \quad (4.6)$$

The last asymptotic result is the Einstein relation giving the diffusion coefficient in terms of the mean square displacement at long times. Here, however, the mean square displacement becomes linear in s rather than t .

The short-time behaviour of the velocity autocorrelation function can be obtained from the leading term in a cumulant expansion:

$$C(\tau) = \int d\Gamma \mathbf{u}_0 \cdot e^{-\mathcal{L}^* \tau}(\mathbf{u}_0 \rho) \rightarrow C(0)e^{-\gamma s} \quad (4.7)$$

where

$$\gamma = \frac{2}{3} \int d\Gamma \mathbf{u}_0 \cdot \mathcal{L}^*(\mathbf{u}_0 \rho) = \frac{2}{3} \int d\Gamma \mathbf{u}_0 \cdot \bar{L}^*(\mathbf{u}_0 \rho) - \omega^*.$$

If this approximation is assumed to persist at longer times, then $D^*(s)$, $M^*(s)$, and the D^* have the approximations

$$D^*(s) \rightarrow \frac{1}{2\gamma}(1 - e^{-\gamma s}) \quad M^*(s) \rightarrow \gamma^{-1} [s - \gamma^{-1}(1 - e^{-\gamma s})] \quad D^* \rightarrow (2\gamma)^{-1}. \quad (4.8)$$

In the elastic limit these approximations are known to be quite good for all except the highest densities near crystallization. The first equality shows that the approach to hydrodynamics, i.e. diffusion in this case, is exponentially fast in s although logarithmic in real time. Similarly, the mean square displacement shows the crossover from short-time free-particle motion to diffusion on the same timescale.

5. Linear kinetic theory

Linear response theory expresses properties of interest in terms of equilibrium time correlation functions, or for the case of inelastic collisions, HCS time correlation functions. A more accurate evaluation than the cumulant expansion above can be obtained using linear kinetic theory methods. To illustrate this, the velocity autocorrelation function is expressed in terms of an appropriate reduced correlation function and evaluated using a Markov approximation known to be good for elastic collisions. From the definition in (4.3), $C(s)$ is written in the equivalent form

$$C(s) = \int dx_0 \mathbf{u}_0 \cdot \Phi^{(1)}(x_0, s). \quad (5.1)$$

Thus, formally, evaluation of the correlation function is reduced to taking an average in the single-particle phase space of the tagged particle. The single-particle function $\Phi^{(1)}(x_0, s)$ is the first in a set that is similar to the reduced distribution functions of (2.11):

$$\Phi^{(\ell)}(x_0, \dots, x_\ell, s) \equiv N^{\ell-1} \int dx_{\ell+1} \dots dx_n e^{-\mathcal{L}^* \tau} \rho_{hcs}^* \mathbf{u}_0 \equiv U^{(\ell)}(0, \dots, \ell, s) \mathbf{u}_0. \quad (5.2)$$

$\Phi^{(1)}$ obeys the first equation of the same BBGKY hierarchy as in (2.10), which in the reduced variables becomes

$$\partial_s \Phi^{(1)}(\mathbf{u}_0, s) + \omega^* \nabla_{\mathbf{u}_0} \cdot (\mathbf{u}_0 \Phi^{(1)}(\mathbf{u}_0, s)) = \int dx_1 \bar{T}(0, 1) \Phi^{(2)}(x_0, x_1, s). \quad (5.3)$$

Here it has been recognized that $\Phi^{(1)}$ is independent of the tagged particle's position due to homogeneity of the reference HCS. A closed 'kinetic equation' is obtained if $\Phi^{(2)}$ can be expressed in terms of $\Phi^{(1)}$. To see how this is possible, note that both $\Phi^{(1)}$ and $\Phi^{(2)}$ are

formally linear maps of \mathbf{u}_0 , as indicated in the second equality of (5.2). Assuming that $U^{(1)}$ is invertible, a linear relationship between $\Phi^{(2)}$ and $\Phi^{(1)}$ is obtained:

$$\Phi^{(2)}(s) = U^{(2)}(s) [U^{(1)}(s)]^{-1} \Phi^{(1)}(s). \quad (5.4)$$

Substitution of this result into (5.3) gives the desired kinetic equation:

$$\partial_s \Phi^{(1)}(\mathbf{u}_0, s) + \omega^* \nabla_{\mathbf{u}_0} \cdot (\mathbf{u}_0 \Phi^{(1)}(\mathbf{u}_0, s)) = I(\mathbf{u}_0, s | \Phi^{(1)}) \quad (5.5)$$

with the ‘collision operator’

$$I(\mathbf{u}_0, s | \bullet) \equiv \int dx_1 \bar{T}(0, 1) U^{(2)}(1, 2, s) [U^{(1)}(1, s)]^{-1} \bullet. \quad (5.6)$$

Of course, this linear kinetic theory representation is still very formal since the operators $U^{(1)}$ and $U^{(2)}$ entail analysis of the many-body problem. However, it is an appropriate starting point for introducing approximations. For example, density expansions of these operators can be performed for practical descriptions of dilute gases. Here, a Markovian approximation is used. This assumes that the collision operator is approximately independent of time and therefore can be evaluated at $s = 0$. In this limit $U^{(1)}$ and $U^{(2)}$ are simply related to the reduced distribution function for the HCS and the collision operator becomes

$$I(\mathbf{u}_0 | \bullet) \equiv I(\mathbf{u}_0, s = 0 | \bullet) \equiv \int dx_1 \bar{T}(1, 2) f_{hcs}^{*(2)}(x_0, x_1) [f_{hcs}^{*(1)}(x_0)]^{-1} \bullet. \quad (5.7)$$

For the special case of elastic collisions this approximation gives the familiar Enskog–Lorentz kinetic equation for a dense gas. The diffusion coefficient is now given by

$$D^* = \frac{1}{3} \int d\mathbf{u}_0 \mathbf{u}_0 \cdot \mathbf{A}(\mathbf{u}_0) \quad (5.8)$$

where \mathbf{A} is the solution to the linear integral equation

$$-\omega^* \nabla_{\mathbf{u}_0} \cdot (\mathbf{u}_0 \mathbf{A}) + I(\mathbf{u}_0 | \mathbf{A}) = \mathbf{u}_0 f_{hcs}^{*(1)}. \quad (5.9)$$

These results are quite analogous to those from the kinetic theory for elastic collisions, and polynomial expansion methods for solving such integral equations apply here as well. An additional difficulty is encountered here, however, since the collision operator depends explicitly on $f_{hcs}^{*(2)}$ and $f_{hcs}^{*(1)}$ which are not known. If it is assumed that velocity correlations in $f_{hcs}^{*(2)}$ can be neglected, the problem reduces to a determination of $f_{hcs}^{*(1)}$ only. This has been accomplished using a polynomial expansion of the Boltzmann equation [3, 4] and can be taken as known to a good approximation. Recently, the results (5.8) and (5.9) with this neglect of velocity correlations have been obtained from a Chapman–Enskog solution to the Enskog–Lorentz equation, and the integral equation evaluated in a leading-order polynomial expansion [5]. The corresponding results of the cumulant expansion are regained in this way and have been shown to agree well with direct Monte Carlo simulation of the Enskog–Lorentz equation and molecular dynamics simulations over a wide range of values for the restitution coefficient α . A more detailed description of both the kinetic and diffusive excitations has been obtained for a heavy tagged particle using the Boltzmann–Lorentz kinetic equation to derive a corresponding Fokker–Planck equation [6]. The exact solution to the latter can be given if one wishes to discuss in detail the transition of a given initial perturbation to the long-time diffusive limit. Again, excellent agreement is obtained in comparison with both Monte Carlo simulation of the kinetic equation (confirming the Fokker–Planck limit) and with molecular dynamics (confirming the kinetic equation) [7].

6. Non-linear kinetic theory

The derivation of the Boltzmann equation and related kinetic equations such as the revised Enskog equation for the reduced distribution function $f^{(1)}$ has been considered in great detail over the past forty years. While important fundamental questions remain about the precise context in which these equations are valid [1], their accuracy for practical applications is well established. The arguments leading to these equations would appear to hold as well for inelastic collisions with some important exceptions (e.g., the phenomena of inelastic collapse). To date there appears to be no specific evidence that the Boltzmann and Enskog equations have any more limited scope for inelastic collisions than for elastic collisions, and they have provided the basis for most information available about transport processes in granular media. As for elastic collisions, explicit solutions to these equations have been studied primarily for states close to the homogeneous state (equilibrium or HCS, respectively). A partial list of some recent applications for hydrodynamics is provided for an overview:

- The Boltzmann equation has been solved approximately for the HCS using a polynomial expansion about a Maxwellian [3,4]. Monte Carlo simulation of the Boltzmann equation confirms the velocity scaling and form of the distribution function obtained in this approximation [8], except for very large velocities. The asymptotic form for large velocities has been discussed as well [4]. For the HCS, the Boltzmann and Enskog solutions are simply related.
- The Chapman–Enskog method has been generalized to solve the Boltzmann equation to leading order in spatial gradients relative to the HCS [9]. In this way the hydrodynamic equations for a dilute inelastic gas have been derived to Navier–Stokes order and the transport coefficients determined as explicit functions of the restitution coefficient. For dense gases a similar analysis has been performed on the basis of the Enskog kinetic equation [10]. The viscosity following from this analysis has been compared with that from Monte Carlo simulation at low density showing good agreement over a wide range of values for the restitution coefficient, confirming the validity of the Chapman–Enskog method for inelastic collisions.
- Monte Carlo simulation of the Boltzmann equation has been used to study the stability of the HCS. It has been shown that the initial stage of the instability can be described accurately by the hydrodynamic equations derived from the Boltzmann equation [11].
- The single-particle distribution functions for a binary mixture of inelastic particles with different size, mass, concentration, and inelasticities has been determined for the HCS from the corresponding Boltzmann equation using a polynomial expansion [12]. An interesting new feature for mixtures is the necessity of different ‘temperatures’ (defined from the thermal velocity in the usual way, $v_0^2 = 2k_B T/m$, for each species). There is no analogue of this for elastic collisions. Its consequences for transport in mixtures are under investigation [14].

Access to more complex states is possible through Monte Carlo simulation [13] of the Boltzmann or Enskog equations, and by kinetic models based on these equations [6]. The kinetic models provide an excellent prediction of the transport coefficients for states near equilibrium, yet are tractable as well in some cases far from equilibrium. At low density the kinetic model has the form,

$$(\partial_t + \mathbf{v} \cdot \nabla) f + \nabla_v \cdot (\mathbf{F} f) = -\nu(f - f_{hcs})$$

where $\mathbf{F} = -\nu_c \omega \mathbf{v}$ is the drag force of (2.13), introduced there to represent the cooling effects of inelastic collisions and having the same role here. The adjustable parameter ν

is available to fit some chosen property of the Boltzmann equation (such as the viscosity). This kinetic model is almost the same as the BGK model used for the Boltzmann equation with elastic collisions, in the presence of a thermostat. In fact, if f_{hcs} is approximated by a local equilibrium distribution the analogy is complete: the isolated gas of inelastic particles is equivalent to a gas of elastic particles in the presence of a thermostat. An example where this observation is particularly useful is a simple gas in uniform shear flow whose velocity field is given by $u_x = ay$, $u_y = u_z = 0$. For elastic collisions an external thermostat $F_{ext} = -\lambda v$ is introduced to compensate for viscous heating and allow a steady state. There have been extensive studies of the rheology of this flow using both Monte Carlo and kinetic model methods. For inelastic collisions no external thermostat is required. Instead, the cooling force $F = -v_c \omega v$ has the same effect of compensating for viscous heating to give the steady state. Formally, the known results for elastic collisions can be transferred to the inelastic case by the simple correspondence $\lambda \leftrightarrow v_c \omega$ [2]. Predictions of the rheology for steady shear flow for the inelastic case based on the above kinetic model have been shown to be in very good agreement with Monte Carlo simulation [15]. Similar results based on the Enskog equation for a dense gas have been obtained, again in good agreement with simulation [16]. These and other applications of kinetic models far from equilibrium provide strong support for their use where the underlying kinetic equation becomes intractable.

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