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## Kinetic models for hard sphere dynamics

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### Abstract

The construction of kinetic models for a practical description of hard sphere dynamics in fluid, amorphous solid, and crystal phases is outlined. The models are constructed to apply for both elastic and dissipative collisions. As an illustration, the Navier–Stokes hydrodynamics and transport coefficients are calculated for rapid flow granular media.

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### 1. Introduction

Perhaps the most fundamental and complete description of dynamical phenomena is that given by the Boltzmann kinetic equation. It is based on nonequilibrium statistical mechanics and applications near equilibrium are in excellent agreement with experiments, for a wide range of simple atomic gases. Applications to states far from equilibrium have occurred primarily in the past 20 years with development of Monte Carlo simulation techniques [1] and analytic studies of closely related kinetic models [2]. The kinetic models are constructed by replacing the Boltzmann collision operator by a mathematically simpler form, constrained to preserve the most important physical properties of the Boltzmann operator. In many cases exact solutions to the latter can be obtained and their comparison with Monte Carlo simulations of the Boltzmann equation show qualitative and even semi-quantitative agreement far from equilibrium [3].

The Boltzmann equation is restricted to low density, and therefore cannot be applied to many interesting phenomena that occur at higher densities: dense fluid transport far from equilibrium, short wavelength structural dynamics, kinetics of freezing, crystal

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elasticity and transport, kinetics of metastable and amorphous states. However, the revised Enskog kinetic theory (RET) provides an appropriate and unique basis for such investigations at high densities [4]. This kinetic theory is restricted to a system of hard spheres, but otherwise has the following remarkable features: asymptotically exact at short times, no a priori limitations on density/space scales, quantitative description of fluid-phase dynamic structure  $S(k, \omega)$ , exact fluid and crystal stationary states with an H-theorem. Recently, the RET has been extended to the case of inelastic hard spheres as model for granular flow [5]. As with the Boltzmann equation its complexity has limited applications to states near equilibrium. Both Monte Carlo techniques [6,7] and kinetic models [5,8,9] have been developed for the RET during the past year, with the potential for applications to the wide range of nonequilibrium phenomena mentioned above. The objective here is to provide an overview of the kinetic model construction and to illustrate its use with an application to transport properties of granular flow. A variant of the kinetic model in Refs. [8,5] with greater quantitative accuracy is presented and used in this calculation.

The RET kinetic equation for the one-particle distribution function,  $f(\mathbf{r}, \mathbf{v}, t)$ , is defined by [4,5]

$$\left( \frac{\partial}{\partial t} + \mathbf{v}_1 \cdot \nabla_1 \right) f(\mathbf{r}_1, \mathbf{v}_1, t) = J_E[\mathbf{r}_1, \mathbf{v}_1 | f(t)], \tag{1}$$

where  $J_E$  is the Enskog collision operator,

$$J_E[\mathbf{r}_1, \mathbf{v}_1 | f(t)] = \sigma^2 \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}) \left\{ \alpha^{-2} f^{(2)}(\mathbf{r}_1, \mathbf{r}_1 - \boldsymbol{\sigma}, \mathbf{v}'_1, \mathbf{v}'_2, t) - f^{(2)}(\mathbf{r}_1, \mathbf{r}_1 + \boldsymbol{\sigma}, \mathbf{v}_1, \mathbf{v}_2, t) \right\}. \tag{2}$$

Here,  $f^{(2)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{v}_1, \mathbf{v}_2, t) = \chi[\mathbf{r}_1, \mathbf{r}_2 | n(t)] f(\mathbf{r}_1, \mathbf{v}_1, t) f(\mathbf{r}_2, \mathbf{v}_2, t)$ ,  $\sigma$  is the hard sphere diameter,  $\boldsymbol{\sigma} = \sigma \hat{\boldsymbol{\sigma}}$ ,  $\hat{\boldsymbol{\sigma}}$  being a unit vector,  $\Theta$  is the Heaviside step function, and  $\mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2$ . The primes on the velocities denote the initial values  $\{\mathbf{v}'_1, \mathbf{v}'_2\}$  that lead to  $\{\mathbf{v}_1, \mathbf{v}_2\}$  following a binary collision,  $\mathbf{v}'_1 = \mathbf{v}_1 - \frac{1}{2}(1 + \alpha^{-1})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g})\hat{\boldsymbol{\sigma}}$ ,  $\mathbf{v}'_2 = \mathbf{v}_2 + \frac{1}{2}(1 + \alpha^{-1})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g})\hat{\boldsymbol{\sigma}}$ . The parameter  $\alpha$  is the coefficient of restitution with  $0 < \alpha \leq 1$ , and having the value unity for elastic spheres. Finally,  $\chi[\mathbf{r}, \mathbf{r} + \boldsymbol{\sigma} | n(t)]$  is the equilibrium pair correlation function at contact as a functional of the nonequilibrium density field  $n(\mathbf{r}, t)$  defined by  $n(\mathbf{r}, t) = \int d\mathbf{v} f(\mathbf{r}, \mathbf{v}, t)$ . In principle,  $\chi[n]$  is a functional of  $n$  that can be determined exactly in terms of the equilibrium free energy functional for an inhomogeneous state [10], for which practical approximations are currently available. As a consequence of this dependence of  $\chi[n]$  on  $n$ ,  $J_E[f]$  is a highly non-linear functional of  $f$ . This is an essential feature of the RET that is necessary to admit the broken symmetry crystal phase. Both fluid and crystal equilibrium stationary solutions for  $\alpha = 1$  are Maxwellian velocity distributions, with a local density determined from Eq. (1) which reduces to

$$\nabla \ln n_s(\mathbf{r}) = - \sigma^2 \int d\hat{\boldsymbol{\sigma}} \hat{\boldsymbol{\sigma}} \chi[\mathbf{r}, \mathbf{r} + \boldsymbol{\sigma} | n_s] n_s(\mathbf{r} + \boldsymbol{\sigma}). \tag{3}$$

This can be recognized as the exact first BBGKY hierarchy equation for a stationary state.

The conservation equations for mass, momentum, and energy follow directly from Eq. (1). By multiplying with 1,  $m\mathbf{v}_1$ , and  $m\mathbf{v}_1^2/2$  and integrating over  $\mathbf{v}_1$ ,

$$D_t n + n \nabla \cdot \mathbf{U} = 0, \quad (4)$$

$$D_t U_i + (mn)^{-1} \partial_j P_{ij} = 0, \quad (5)$$

$$D_t T + \frac{2}{3nk_B} (P_{ij} \partial_j U_i + \nabla \cdot \mathbf{q} + (1 - \alpha^2)w) = 0, \quad (6)$$

where  $D_t = \partial_t + \mathbf{U} \cdot \nabla$ ,  $T(\mathbf{r}, t)$  is the temperature, and  $\mathbf{U}(\mathbf{r}, t)$  is the flow velocity. The term  $(1 - \alpha^2)w$  represents energy dissipation in the case of dissipative collisions; its explicit form can be found in [5]. The pressure tensor  $P_{ij}(\mathbf{r}, t)$  and the heat flux  $\mathbf{q}(\mathbf{r}, t)$  have both “kinetic” and “collisional transfer” contributions, i.e.  $P_{ij} = P_{ij}^k + P_{ij}^c$  and  $\mathbf{q} = \mathbf{q}^k + \mathbf{q}^c$ . The kinetic contributions are given by

$$P_{ij}^k(\mathbf{r}, t) = \frac{n}{\beta} \delta_{ij} + \int d\mathbf{v} D_{ij}(\mathbf{V}) f(\mathbf{r}, \mathbf{v}, t), \quad \mathbf{q}^k(\mathbf{r}, t) = \int d\mathbf{v} \mathbf{S}(\mathbf{V}) f(\mathbf{r}, \mathbf{v}, t), \quad (7)$$

where  $\beta \equiv (k_B T)^{-1}$ ,  $D_{ij}(\mathbf{V}) \equiv m(V_i V_j - \frac{1}{3} V^2 \delta_{ij})$ ,  $\mathbf{S}(\mathbf{V}) \equiv (\frac{1}{2} m V^2 - 5/2 \beta) \mathbf{V}$ , and  $\mathbf{V} \equiv \mathbf{v} - \mathbf{U}$ . The divergences of the collisional transfer parts are related to moments of the collision operator,

$$\partial_j P_{ij}^c(\mathbf{r}, t) = - \int d\mathbf{v} m V_i J_E[\mathbf{r}, \mathbf{v} | f(t)], \quad (8)$$

$$\nabla \cdot \mathbf{q}^c(\mathbf{r}, t) = - \int d\mathbf{v} \frac{m}{2} V^2 J_E[\mathbf{r}, \mathbf{v} | f(t)] - P_{ij}^c(\mathbf{r}, t) \partial_j U_i(\mathbf{r}, t) - (1 - \alpha^2) w. \quad (9)$$

The explicit forms for  $\mathbf{q}^c(\mathbf{r}, t)$  and  $P_{ij}^c(\mathbf{r}, t)$  can be obtained directly from these definitions and (2) [5,8] but will not be given here. These equations provide the basis for discussion of transport both near and far from equilibrium, and will be imposed as essential constraints on the construction of any acceptable kinetic model for the RET.

## 2. Kinetic models

A kinetic model for the RET is obtained by replacing the collision operator,  $J_E[\mathbf{r}_1, \mathbf{v}_1 | f(t)]$ , by a simpler, more tractable form while retaining the most important qualitative features of the RET. The primary constraints imposed on the kinetic model are (1) the exact stationary solutions for both fluid and crystal phases in the case of  $\alpha = 1$ , Eq. (3), and (2) the exact conservation laws (4)–(6), including the collisional transfer contributions to the fluxes. As indicated above, the conservation laws follow from moments of the kinetic equation using polynomials constructed from  $\{1, \mathbf{v}, v^2\}$ . To describe this feature of the kinetic equation a projection operator  $\mathcal{P}$  is defined by

$$\mathcal{P}g(\mathbf{v}) = \psi_x(\mathbf{v}) \phi_r(\mathbf{v}) (\psi_x, \phi_r^{-1} g), \quad (10)$$

where  $n\phi_r(\mathbf{v})$  is the local equilibrium distribution,

$$f_r(\mathbf{v}) = n\phi_r(\mathbf{v}) = n \left( \frac{\beta m}{2\pi} \right)^{3/2} \exp(-\beta m V^2/2). \tag{11}$$

The scalar product is defined by  $(\zeta, \zeta) = \int d\mathbf{v} \phi_r(\mathbf{v}) \zeta^*(\mathbf{v}) \zeta(\mathbf{v})$ , and  $\{\psi_\alpha\}$  is the set of orthonormal functions,

$$\psi_\alpha = \left\{ 1, (m\beta)^{1/2} V, \left( \frac{2}{3} \right)^{1/2} \left( \frac{m\beta}{2} V^2 - \frac{3}{2} \right) \right\}. \tag{12}$$

The conservation laws now may be understood as the projection of the kinetic equation into the subspace defined by  $\mathcal{P}$ . Accordingly, the RET collision operator is then decomposed into two parts,  $J_E[f] = \mathcal{P}J_E[f] + (1 - \mathcal{P})J_E[f]$ . The conservation laws require that any kinetic model for  $J_E[f]$  must retain the contribution  $\mathcal{P}J_E[f]$ . The additional requirement of the exact stationary equilibrium solutions imposes only the condition that the second term vanishes at equilibrium. The simplest choice of a kinetic model then would appear to be

$$J_E[f] \rightarrow \mathcal{P}J_E[f] - (1 - \mathcal{P})vf = \mathcal{P}J_E[f] - v(f - f_r), \tag{13}$$

where  $v = v(\mathbf{r}, t)$  is an average local collision frequency, and use has been made of the property  $\mathcal{P}f = f_r$  in the second equality. This is the kinetic model proposed in Ref. [8]. The term  $\mathcal{P}J_E[f]$  vanishes in the low-density limit and this kinetic model reduces for  $\alpha = 1$  to the familiar Bhatnagar–Gross–Krook (BGK) kinetic model for the Boltzmann equation [11].

While the kinetic model defined by (13) satisfies the constraints of exact conservation laws and stationary solutions, the transport coefficients calculated from it are only semi-quantitative. A more quantitative model can be obtained by improving the approximation to  $(1 - \mathcal{P})J_E[f]$ . Following a suggestion by Lutsko [9], it is noted that  $(1 - \mathcal{P})J_E[f]$  does not vanish for  $f = f_r$  as in the approximation above (except for homogeneous temperature and velocity, as required for the stationary solutions). Therefore, this contribution is isolated and the above approximation is applied only to the remainder:  $(1 - \mathcal{P})J_E[f] \rightarrow (1 - \mathcal{P})J_E[f_r] - v(f - f_r)$ . This provides an improved representation of the collision operator, but at the price of complicating its velocity dependence considerably. Further analysis shows that only the projections of  $(1 - \mathcal{P})J_E[f_r]$  onto the two functions  $D_{ij}(\mathbf{V})$  and  $\mathbf{S}(\mathbf{V})$  contribute to the transport coefficients. Thus, a simple velocity dependence is restored by keeping only this part of  $(1 - \mathcal{P})J_E[f_r]$ , an approximation that is exact to first order in the hydrodynamic gradients at  $\alpha = 1$ . The resulting kinetic model is given by

$$\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f = -v(f - f_r) + \mathcal{P}J_E[f] + \beta f_r [D_{ij}A_{ij} + \mathbf{S} \cdot \mathbf{B}]. \tag{14}$$

with

$$A_{ij} = \frac{\beta}{2n} \int d\mathbf{v} D_{ij}(\mathbf{V}) J_E[f_r], \quad \mathbf{B} = \frac{2m\beta^2}{5n} \int d\mathbf{v} \mathbf{S}(\mathbf{V}) J_E[f_r]. \tag{15}$$

The second term on the right-hand side of (14) can be expressed in terms of the exact collisional transfer contributions to the fluxes,

$$\begin{aligned} \mathcal{P}J_E[f] = & -\frac{\beta}{n}f_\ell \left( \frac{m\beta}{3}V^2 - 1 \right) [\nabla \cdot \mathbf{q}^c + P_{ij}^c \partial_j U_i + (1 - \alpha^2)w] \\ & - \frac{\beta}{n}f_\ell V_i \partial_j P_{ij}^c. \end{aligned} \quad (16)$$

The difference between this model and the low-density BGK model are terms on the right-hand side of (14) that are polynomials in the velocity of degree 3, with coefficients that are known functionals of  $f$ . This implies that the velocity dependence of the distribution function can be determined whenever the low-density BGK model can be solved. In addition to the exact conservation laws and stationary states, this model also predicts the same density dependence for the transport coefficients (shear viscosity, bulk viscosity, and thermal conductivity) as that obtained from the RET in the case of  $\alpha = 1$ . The case  $\alpha < 1$  is considered in the next section.

It is instructive to rewrite this equation using the conservation laws and the substitution,  $f = f_\ell + \Delta f$ , to obtain

$$\begin{aligned} \left( \frac{\partial}{\partial t} + (1 - \mathcal{P})\mathbf{v} \cdot \nabla + \nu \right) \Delta f = & -\beta f_\ell D_{ij}(\mathbf{V})(\partial_i U_j - A_{ij}) \\ & -\beta f_\ell \mathbf{S}(\mathbf{V}) \cdot (\nabla \ln T - \mathbf{B}). \end{aligned} \quad (17)$$

Interestingly, Eq. (17) shows no explicit dependence on the dissipation parameter  $\alpha$ . However, this equation only determines  $\Delta f$  as a functional of the hydrodynamic fields. This functional then can be used to calculate the fluxes as functionals of the fields. Finally, the resulting expressions for the fluxes together with the conservation laws provide hydrodynamic equations for the fields. This decoupling of the problem into the solution to a simple equation for the velocity dependence, and equations for the fields is a primary simplifying feature of the kinetic models.

### 3. Application to granular flow

In this section the kinetic model is applied to obtain expressions for the pressure tensor and heat flux to first order in the spatial gradients of the hydrodynamic fields. In addition, the associated transport coefficients are determined as explicit functions of the dissipation parameter  $\alpha$  and the density. To do so, the distribution function is assumed to have an expansion in the spatial gradients,

$$f = f^{(0)} + \varepsilon f^{(1)} + \dots, \quad (18)$$

where  $\varepsilon$  is a formal “uniformity” parameter (set equal to unity at the end). Use of this expansion in the definitions for the fluxes and the dissipation function  $w$  gives a corresponding expansion for these quantities. Finally, use of these in the hydrodynamic

equations leads to an identification of the time derivatives of the fields as an expansion in the gradients,  $\partial_t = \partial_t^{(0)} + \partial_t^{(1)} + \dots$ . This is the usual Chapman–Enskog method for solving kinetic equations and is discussed in detail in Refs. [12,13]. The problem is more complex here than for the case  $\alpha = 1$  since the reference state about which gradients are considered is not stationary, and the terms from  $\partial_t^{(0)}$  are not zero. To see this, assume that  $A_{ij}$  and  $\mathbf{B}$  are of first order in the gradients (as is verified below). Then to zeroth order in the gradients the kinetic model, Eqs. (14) and (16), becomes

$$\partial_t^{(0)} f^{(0)} = -v(f^{(0)} - f_\ell) - \frac{\beta}{n} f_\ell \left( \frac{m\beta}{3} V^2 - 1 \right) (1 - \alpha^2) w^{(0)}, \tag{19}$$

where  $w^{(0)} = w[f^{(0)}]$ . The conservation equations to this order become

$$\partial_t^{(0)} n = 0, \quad \partial_t^{(0)} \mathbf{U} = 0, \quad \partial_t^{(0)} T = -\frac{2}{3nk_B} (1 - \alpha^2) w^{(0)}. \tag{20}$$

It is straightforward to verify now that the solution to (19) is  $f^{(0)} = f_\ell$ . This is the same result as for a fluid with elastic collisions. It is somewhat surprising since the time derivative of the temperature is no longer zero as in the elastic collisions case. As a consequence, the corresponding solution to the RET to zeroth order in the gradients is complex and has not been determined to date. The simplified form of the kinetic model leads to the local equilibrium distribution as a non-trivial exact result. Monte Carlo simulations of the RET for the homogeneous cooling state confirm that this is a very good approximation [14].

Since the zeroth-order solution is the local equilibrium distribution, the first-order solution can be obtained directly from (17). The term  $(1 - \mathcal{P}) \mathbf{v} \cdot \nabla f^{(1)}$  is of second order and does not contribute. Also, direct evaluation of (15) to first order in the gradients gives

$$A_{ij} = A(\partial_i U_j + \partial_j U_i - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{U}), \quad B_i = B_T \partial_i \ln T + B_n \partial_i \ln n, \tag{21}$$

with the coefficients

$$A = -(1 + \alpha) \frac{1}{15} \pi n^* g_e [1 - \frac{3}{2} (1 - \alpha)], \tag{22}$$

$$B_T = -(1 + \alpha) \frac{1}{5} \pi n^* g_e [1 - \frac{3}{2} (1 + \frac{2}{3} \alpha) (1 - \alpha)], \tag{23}$$

$$B_n = \alpha (1 - \alpha^2) \frac{1}{10} \pi n^* g_e (1 + \frac{1}{2} n \partial_n \ln g_e), \tag{24}$$

where  $g_e$  is the pair correlation function at contact for a homogeneous fluid and  $n^* = n\sigma^3$ . The equation for  $f^{(1)}$  becomes

$$\begin{aligned} (\partial_t^{(0)} + v) f^{(1)} = & -\beta f_\ell D_{ij}(\mathbf{V}) (1 - 2A) \partial_i U_j \\ & -\beta f_\ell \mathbf{S}(\mathbf{V}) \cdot [(1 - B_T) \nabla \ln T - B_n \nabla \ln n]. \end{aligned} \tag{25}$$

It follows from fluid symmetry that the pressure tensor and heat flux have the forms

$$P_{ij} = p\delta_{ij} - \eta(\partial_i U_j + \partial_j U_i - \frac{2}{3}\delta_{ij}\nabla \cdot \mathbf{U}) - \kappa\delta_{ij}\nabla \cdot \mathbf{U}, \quad (26)$$

$$\mathbf{q} = -\lambda\nabla T - \mu\nabla n, \quad (27)$$

where  $p$  is the hydrostatic pressure,  $\eta$  is the shear viscosity,  $\kappa$  is the bulk viscosity,  $\lambda$  is the thermal conductivity, and  $\mu$  is a transport coefficient that is non-vanishing only for  $\alpha < 1$ . Each of these terms has contributions from the kinetic and collisional transfer parts of the fluxes defined by Eqs. (7)–(9). Equations for the kinetic parts of the pressure tensor and heat flux are obtained directly by integrating (25) after multiplication with  $D_{ij}(\mathbf{V})$  and  $\mathcal{S}(\mathbf{V})$ . The collisional transfer contributions to the fluxes are calculated using the Chapman–Enskog solution for  $f^{(1)}$  in their defining functionals. Since the latter are the same as for the RET, the calculation follows exactly that of Appendix D in Ref. [12] for the Enskog equation, vis-à-vis changes in the Chapman–Enskog form for  $f^{(1)}$ . The analysis is straightforward, leading to the explicit results

$$p = n\beta^{-1}[1 + \frac{1}{3}(1 + \alpha)\pi n^* g_e], \quad (28)$$

$$\eta = \eta^k[1 + (1 + \alpha)\frac{2}{15}\pi n^* g_e] + \frac{3}{5}\kappa, \quad (29)$$

$$\lambda = \lambda^k[1 + (1 + \alpha)\frac{1}{5}\pi n^* g_e] + (3k_B/2m)\kappa, \quad (30)$$

$$\mu = \mu^k[1 + (1 + \alpha)\frac{1}{5}\pi n^* g_e], \quad (31)$$

$$\kappa = (1 + \alpha)\frac{2}{9}n^2\sigma^4 g_e(\pi m/\beta)^{1/2}. \quad (32)$$

The superscript  $k$  denotes the contributions from the kinetic parts of the fluxes,

$$\eta^k = \frac{2}{\beta v(2 - b)}n(1 - 2A), \quad (33)$$

$$\lambda^k = \frac{5k_B}{2m\beta v(1 - 2b)}n(1 - B_T), \quad (34)$$

$$\mu^k = \frac{5}{m\beta^2 v(2 - 3b)}\left[-B_n + b(1 - B_T)(1 - 2b)^{-1}n\partial_n \ln \frac{w^{(0)}}{n}\right]. \quad (35)$$

Use has been made of the properties  $w^{(0)} \propto T^{3/2}$  and  $v \propto T^{1/2}$ , as follows from dimensional analysis for hard spheres. The coefficients  $b = 2\beta(1 - \alpha^2)w^{(0)}/3nv$ ,  $A$ ,  $B_T$ , and  $B_n$  are independent of  $T$ . These results differ from those obtained in Ref. [5] using the simple model (13) only by the density and  $\alpha$  dependence of the kinetic parts of the transport coefficients arising from  $A$ ,  $B_T$ , and  $B_n$ . As an illustration, Fig. 1 shows the density dependence of the transport coefficients obtained at  $\alpha = 0.7$  relative to their values at  $\alpha = 1$  ( $\mu$  has been normalized to  $T\lambda/n$  since it vanishes at  $\alpha = 1$ ). The transport coefficients are positive over the entire range of densities for  $0 < \alpha \leq 1$ , except for  $\mu$  which can become negative at the unphysical values of  $\alpha \sim 0$  and for densities near crystallization. In these calculations we have chosen  $v = \frac{16}{5}\sqrt{\pi}n\sigma^2 g_e(\beta m)^{-1/2}$  which assures the correct Enskog viscosity for  $\alpha = 1$ . This leads to the value  $b = \frac{5}{12}(1 - \alpha^2)$ .

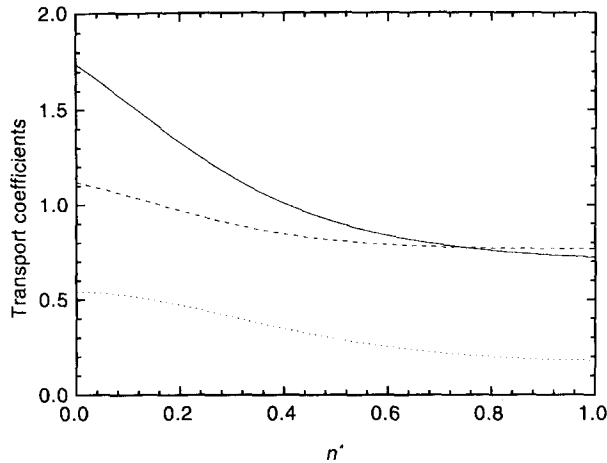


Fig. 1. Density dependence of the reduced transport coefficients  $\lambda(n, \alpha)/\lambda(n, 1)$  (—),  $\eta(n, \alpha)/\eta(n, 1)$  (---), and  $n\mu(n, \alpha)/T\lambda(n, 1)$  (···), at  $\alpha = 0.7$ .

Also, the pair correlation function at contact has been approximated by the Carnahan–Starling form  $g_e \rightarrow (1 - \frac{1}{12}\pi n^*) / (1 - \frac{1}{6}\pi n^*)^3$ .

#### 4. Discussion

The RET kinetic equation for hard spheres has the potential to describe a wide range of dynamical phenomena over the full range of fluid and crystal densities, for phenomena at all wavelengths near and far from equilibrium. This generality is compromised by the practical difficulties confronted in solving the equation for a particular application. Newly developed Monte Carlo simulation methods [5,6] provide a means to explore the content of this kinetic theory in qualitatively different directions than have been considered before. Here, we have described a method of kinetic modeling with the same potential for new applications and exploration. The form of the kinetic models is such that explicit solution for the velocity dependence of the distribution function is often possible as a functional of the five hydrodynamic fields. The latter obey self-consistent non-linear integral equations obtained from the kinetic model, still difficult to solve in general, but considerably more accessible to analytic and numerical approximation.

The example provided here for a system of hard spheres with inelastic collisions is non-trivial since even the reference homogeneous cooling state is not known for the RET. This makes even the determination of properties near equilibrium difficult, such as evaluation of transport coefficients. The kinetic model described here gives the same transport properties as the RET (in the usual first Sonine approximation) for elastic spheres and allows their determination for inelastic spheres with no additional difficulty. These results yield a “Navier–Stokes” level formulation of a hydrodynamic



description of idealized granular flow suitable for comparison with both Monte Carlo and molecular dynamics simulations. For example, the critical wave vectors for long wavelength instabilities can be described over the entire density- $\alpha$  parameter space. Also, the conditions for the existence and dominance of a hydrodynamic description can be determined from an analysis of the spectrum of microscopic excitations as well. A more complete description of the kinetic model, applications to shear flow and granular flow, and comparisons with Monte Carlo simulations will be given elsewhere.

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