

Impurities in inelastic Maxwell models

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Abstract. Transport properties of impurities immersed in a granular gas undergoing homogenous cooling state are studied. The results are obtained from the Boltzmann-Lorentz kinetic equation for inelastic Maxwell models in d dimensions. The kinetic equation is solved by means of the Chapman-Enskog method up to first order in the density gradient of impurities. The mass and heat fluxes associated with impurities are determined and the corresponding transport coefficients are identified. Both transport coefficients (diffusion and Dufour coefficients) are exactly obtained in terms of the coefficients of restitution for the impurity-gas and gas-gas collisions as well as the ratios of mass and diameters. The results are compared with those obtained for inelastic hard spheres in the leading Sonine approximation and by means of Monte Carlo simulations. The comparison shows good agreement between both interaction models, especially in the case of the diffusion coefficient.

1. INTRODUCTION

Granular fluids are usually modelled by an idealized system of smooth hard spheres with inelastic collisions. In the low-density limit, the Boltzmann equation has been conveniently modified to account for the inelasticity of binary collisions and the Navier-Stokes transport coefficients have been computed by solving the corresponding kinetic equation by means of the Chapman-Enskog method [1]. This task has been carried out in the past few years in the case of a monocomponent gas [2] as well as for multicomponent systems [3]. In both cases, as happens for elastic collisions, all the transport coefficients are given in terms of the solutions to linear integral equations which are solved approximately by taking the leading terms in a Sonine polynomial expansion. In spite of this approximation, the kinetic theory results compare quite well with those obtained from numerical solutions of the Boltzmann equation by using the direct simulation Monte Carlo (DSMC) method [4]. The fact that the agreement between kinetic theory and DSMC results even occurs for strong dissipation is a further testimony of the utility of the kinetic theory and the hydrodynamic descriptions for granular fluids beyond the weak dissipation limit.

The main mathematical difficulty in solving the Boltzmann equation for inelastic hard spheres (IHS) comes from the form of the collision rate, which is proportional to the magnitude of the relative velocity of the two colliding particles. In the case of elastic collisions, an alternative to overcome this problem is to consider the repulsive Maxwell potential, for which the collision rate is independent of the relative velocity. This property simplifies the mathematical structure of the Boltzmann collision operator and allows one to get *exact* solutions of the Boltzmann equation for far from equilibrium situations [5]. In the case of inelastic gases, the so-called inelastic Maxwell models (IMM) [6] have been widely used in the past few years as a toy model to characterize the effect of the inelasticity of collisions on the properties of granular gases. The IMM share with elastic Maxwell molecules the property that the collision rate is velocity independent but their scattering rules are the same as for IHS.

Most of the studies performed in the context of IMM have been devoted to homogeneous states, mainly to the analysis of the overpopulated high energy tails [7]. Much less is known for *inhomogeneous* situations, especially for multicomponent systems. One of the few studies considering mixtures of IMM has been carried out by the author [8] in the uniform shear flow problem. The rheological properties (shear and normal stresses) of the mixture have been exactly evaluated in terms of dissipation and parameters of the mixture and surprisingly, the results of IMM show an excellent agreement with those obtained for IHS by means of Grad's approximation and Monte Carlo simulations. This fact stimulates the search for exact solutions for IMM which can be confronted with the results obtained for IHS by using approximate analytical methods and computer simulations.

The goal of this paper is to determine the diffusion coefficient of impurities immersed in a gas of inelastic Maxwell molecules. The gas is in the homogeneous cooling state (HCS), namely, a homogeneous state where the temperature uniformly decreases in time due to collisional cooling. Diffusion is generated in the system by the presence of a

weak concentration gradient, which also induces a heat flux. Both mass and heat fluxes define the relevant transport coefficients of the problem: the diffusion coefficient and the Dufour coefficient. Here, I get explicit expressions for these coefficients by solving the corresponding Boltzmann-Lorentz equation for impurities by means of the Chapman-Enskog method through the first order in the concentration gradient. These transport coefficients are given in terms of the coefficients of restitution for the impurity-gas and gas-gas collisions as well as the masses and diameters of impurities and gas particles. The dependence of these coefficients on the parameters of the system is illustrated and compared with known results derived for IHS [3, 9].

2. DESCRIPTION OF THE PROBLEM

Let us consider a dilute gas of inelastic Maxwell molecules of mass m , diameter σ , and interparticle coefficient of restitution α . In the low-density regime, its velocity distribution function $f(\mathbf{v})$ obeys the nonlinear Boltzmann equation (BE). We assume that the gas is in the HCS, namely, a homogeneous solution of the BE in which all the time dependence of $f(\mathbf{v}, t)$ is through the granular temperature $T(t)$. In this case, the BE can be written as

$$\frac{1}{2}\zeta\frac{\partial}{\partial\mathbf{v}}\cdot(\mathbf{v}f) = J[\mathbf{v}|f, f], \quad (1)$$

where the Boltzmann collision operator $J[\mathbf{v}|f, f]$ for IMM is

$$J[\mathbf{v}_1|f, f] = \frac{\omega}{n\Omega_d} \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} [\alpha^{-1}f(\mathbf{v}'_1, t)f(\mathbf{v}'_2, t) - f(\mathbf{v}_1, t)f(\mathbf{v}_2, t)]. \quad (2)$$

Here, n is the number density of the gas particles, ω is an effective collision frequency (to be chosen later), $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the total solid angle in d dimensions, and $\hat{\boldsymbol{\sigma}}$ is a unit vector directed along the centers of the two colliding spheres. Upon writing Eq. (1), I have taken into account the balance equation for the temperature $T^{-1}\partial_t T = -\zeta$, where the cooling rate ζ is given by [10]

$$\zeta(\alpha) = \frac{1-\alpha^2}{2d}\omega. \quad (3)$$

The explicit form of the velocity distribution function $f(\mathbf{v}, t)$ is not explicitly known, although its velocity moments can be explicitly computed [10].

We assume now that some impurities of mass m_0 and diameter σ_0 are added to the system. Given that its molar fraction is negligible, the state of the granular gas is not disturbed by the presence of impurities and so the velocity distribution function $f(\mathbf{v}, t)$ obeys the BE (1). Furthermore, collisions among impurities themselves can be neglected versus the impurity-gas collisions, which are characterized by a coefficient of restitution α_0 . As said in the Introduction, I want to determine the transport properties of impurities generated in the system by the presence of a weak concentration gradient ∇x_0 , $x_0 = n_0/n$ being the mole fraction of impurities. Under these conditions, the velocity distribution function $f_0(\mathbf{r}, \mathbf{v}, t)$ of impurities verifies the Boltzmann-Lorentz equation

$$\partial_t f_0 + \mathbf{v} \cdot \nabla f_0 = J[\mathbf{v}|f_0, f], \quad (4)$$

where

$$J[\mathbf{v}_1|f_0, f] = \frac{\omega_0}{n_0\Omega_d} \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} [\alpha_0^{-1}f_0(\mathbf{r}, \mathbf{v}'_1; t)f(\mathbf{r}, \mathbf{v}'_2; t) - f_0(\mathbf{r}, \mathbf{v}_1; t)f(\mathbf{r}, \mathbf{v}_2; t)], \quad (5)$$

ω_0 is an effective collision frequency (to be chosen also later) for impurity-gas collisions, and

$$\mathbf{v}'_1 = \mathbf{v}_1 - \frac{m}{m+m_0}(1+\alpha_0^{-1})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})\hat{\boldsymbol{\sigma}}, \quad \mathbf{v}'_2 = \mathbf{v}_2 + \frac{m_0}{m+m_0}(1+\alpha_0^{-1})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})\hat{\boldsymbol{\sigma}}, \quad (6)$$

where $\mathbf{g}_{12} = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity of the colliding pair. The partial temperature of impurities T_0 is defined as

$$\frac{d}{2}n_0T_0 = \int d\mathbf{v} \frac{m_0}{2}v^2 f_0(\mathbf{v}), \quad (7)$$

where n_0 is the number density of impurities. In contrast to what happens for normal fluids, if impurities and gas particles are mechanically different, the partial temperature T_0 can differ from the granular temperature T when

dissipation is present. The failure of energy equipartition in granular fluids has even observed in real experiments [11]. Momentum and energy are not collisional invariants of the Boltzmann-Lorentz collision operator $J[f_0, f]$. Only the number density of impurities is conserved:

$$\partial_t n_0 + \frac{\nabla \cdot \mathbf{j}_0}{m_0} = 0, \quad (8)$$

where the mass flux \mathbf{j}_0 is defined as

$$\mathbf{j}_0 = \int d\mathbf{v} m_0 \mathbf{v} f_0(\mathbf{v}). \quad (9)$$

In the absence of diffusion, impurities are also in HCS and Eq. (4) becomes

$$\frac{1}{2} \zeta_0 \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{v} f_0) = J[\mathbf{v} f_0, f], \quad (10)$$

where use has been made of the relation $T_0^{-1} \partial_t T_0 = -\zeta_0$, where ζ_0 is the cooling rate associated with the partial temperature T_0 of impurities. Its expression is [8]

$$\zeta_0 = \frac{2\omega_0}{d} \mu (1 + \alpha_0) \left[1 - \frac{\mu}{2} (1 + \alpha_0) (1 + \theta) \right], \quad (11)$$

where $\mu = m/(m + m_0)$ and $\theta = m_0 T / m T_0$ is the mean square velocity of gas particles relative to that of impurities. The balance equations for the temperatures T and T_0 lead to the following time evolution equation for the temperature ratio $\gamma \equiv T_0/T$:

$$\gamma^{-1} \partial_t \gamma = \zeta - \zeta_0. \quad (12)$$

The fact that f_0 depends on time only through $T(t)$ necessarily implies that the temperature ratio γ must be independent of time, and so Eq. (12) gives the HCS condition $\zeta(t) = \zeta_0(t)$. The impurity equilibrates to a common HCS with different temperatures for the impurity and gas particles. This implies a breakdown of the energy equipartition.

In order to get the explicit dependence of γ on the parameter space, one still needs to fix the parameters ω and ω_0 . To optimize the agreement with the IHS results, the cooling rates ζ and ζ_0 of IMM given by Eqs. (3) and (11), respectively, are adjusted to be the same as the ones given for IHS [12]. Since ζ and ζ_0 are not exactly known for IHS, one can estimate them by taking their local equilibrium approximations. In this case, the collision frequencies ω and ω_0 are given by

$$\omega = \sqrt{\frac{2}{\pi}} \Omega_d \nu, \quad \omega_0 = \frac{\Omega_d}{\sqrt{\pi}} \left(\frac{\bar{\sigma}}{\sigma} \right)^{d-1} \left(\frac{1 + \theta}{\theta} \right)^{1/2} \nu, \quad (13)$$

where $\bar{\sigma} = (\sigma + \sigma_0)/2$ and $\nu = n \sigma^{d-1} \sqrt{2T/m}$ is an effective collision frequency. With these choices, the dependence of the temperature ratio T_0/T on the parameters of the system given for IMM presents an excellent agreement with the one found for IHS, even for strong dissipation [13].

3. TRANSPORT PROPERTIES OF IMPURITIES

The aim of this Section is to get the transport properties (mass and heat fluxes) of impurities in the limit of small concentration gradient ∇x_0 . These fluxes are determined by solving the Boltzmann-Lorentz equation (4) from the Chapman-Enskog method [1] adapted to dissipative systems. Thus, I look for a *normal* solution in which all the space and time dependence of f_0 is through the hydrodynamic fields. In our problem, this means that $f_0(\mathbf{r}, \mathbf{v}, t) = f_0[\mathbf{v}|x_0(t), T(t)]$. The normal solution is generated by expanding f_0 in powers of ∇x_0 as

$$f_0 = f_0^{(0)} + \varepsilon f_0^{(1)} + \dots, \quad (14)$$

where each factor ε corresponds to the implicit factor ∇x_0 . The time derivative is also expanded as $\partial_t = \partial_t^{(0)} + \varepsilon \partial_t^{(1)} + \dots$, where the action of the different operators $\partial_t^{(k)}$ can be obtained from the balance equation (8). They are given by

$$\partial_t^{(0)} x_0 = 0, \quad \partial_t^{(0)} T = -T \zeta, \quad \partial_t^{(k)} x_0 = -\frac{\nabla \cdot \mathbf{j}_0^{(k-1)}}{m_0 n}, \quad \partial_t^{(k)} T = 0, \quad k \geq 1, \quad (15)$$

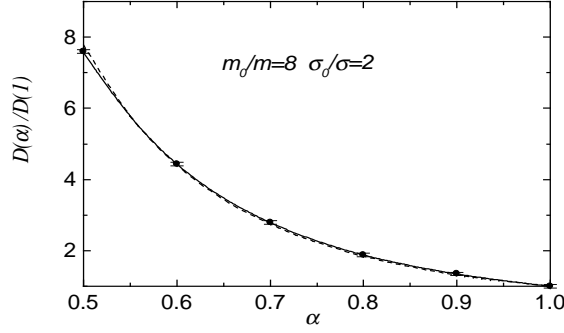


FIGURE 1. Plot of the reduced diffusion coefficient $D(\alpha)/D(1)$ as a function of the coefficient of restitution $\alpha = \alpha_0$ in the three-dimensional case for $\sigma_0/\sigma = 2$ and $m_0/m = 8$. The solid line corresponds to the exact result obtained here for IMM while the dashed line is the result derived for IHS in the second Sonine approximation. The symbols refer to Monte Carlo simulations for IHS.

where

$$\mathbf{j}_0^{(k)} = \int d\mathbf{v} m_0 \mathbf{v} f_0^{(k)}. \quad (16)$$

The zeroth-order approximation $f_0^{(0)}$ is the solution of Eq. (10) but taking into account now the local dependence on the mole fraction x_0 . Since $f_0^{(0)}$ is isotropic, it follows that the flux of impurities vanishes at this order, i.e., $\mathbf{j}_0^{(0)} = \mathbf{0}$, and so $\partial_t^{(1)} x_0 = 0$. To first order in ε , one has the kinetic equation

$$\begin{aligned} \partial_t^{(0)} f_0^{(1)} - J[f_0^{(1)}, f] &= - \left(\partial_t^{(1)} + \mathbf{v}_1 \cdot \nabla \right) f_0^{(0)} \\ &= - \left(\frac{\partial}{\partial x_0} f_0^{(0)} \right) \mathbf{v}_1 \cdot \nabla x_0. \end{aligned} \quad (17)$$

The second equality follows from the balance equations (15) and the space dependence of $f_0^{(0)}$ through x_0 . The mass flux $\mathbf{j}_0^{(1)}$ and the contribution to the heat flux coming from impurities $\mathbf{q}_0^{(1)}$ can be easily obtained from Eq. (17). The heat flux is defined as

$$\mathbf{q}_0^{(1)} = \int d\mathbf{v} \frac{m_0}{2} v^2 \mathbf{v} f_0^{(1)}. \quad (18)$$

To get these fluxes, one multiplies both sides of Eq. (17) by $m_0 \mathbf{v}$ and $\frac{1}{2} m_0 v^2 \mathbf{v}$ and integrates over \mathbf{v} . The result for the mass and heat fluxes is, respectively

$$\left(\partial_t^{(0)} + v_d \right) \mathbf{j}_0^{(1)} = -\gamma p \nabla x_0, \quad (19)$$

$$\left(\partial_t^{(0)} + v_q \right) \mathbf{q}_0^{(1)} = -\beta \mathbf{j}_0^{(1)} - \frac{d}{d+2} \frac{pT}{m_0} \left(1 + \frac{c_0}{2} \right) \gamma^2 \nabla x_0, \quad (20)$$

where $p = nT$ is the hydrostatic pressure and

$$c_0 = \frac{8}{d(d+2)} \left[\frac{m_0^2}{4n_0 T_0^2} \int d\mathbf{v} v^4 f_0(\mathbf{v}) - \frac{d(d+2)}{4} \right]. \quad (21)$$

Upon writing Eqs. (19) and (20), use has been made of the collisional moments [13]

$$\int d\mathbf{v} m_0 \mathbf{v} J[f_0^{(1)}, f] = -v_d \mathbf{j}_0^{(1)}, \quad (22)$$

$$\int d\mathbf{v} \frac{m_0}{2} v^2 \mathbf{v} J[f_0^{(1)}, f] = -v_q \mathbf{q}_0^{(1)} - \beta \mathbf{j}_0^{(1)}, \quad (23)$$

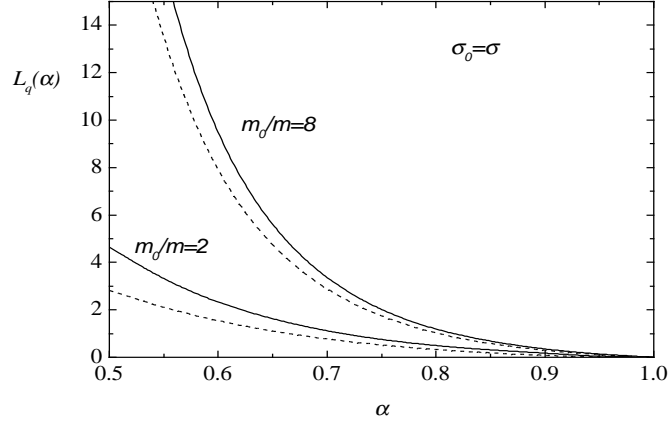


FIGURE 2. Plot of the reduced Dufour coefficient $L_q(\alpha)$ as a function of the coefficient of restitution $\alpha = \alpha_0$ in the three-dimensional case for $\sigma_0 = \sigma$, and two different values of the mass ratio: $m_0/m = 2$ and $m_0/m = 8$. The solid lines correspond to the exact results obtained here for IMM while the dashed lines are the results derived for IHS in the first Sonine approximation.

where

$$v_d = \frac{\Omega_d}{\sqrt{\pi}d} \left(\frac{\bar{\sigma}}{\sigma} \right)^{d-1} \mu \left(\frac{1+\theta}{\theta} \right)^{1/2} v, \quad (24)$$

$$v_q = -\frac{v_d}{d+2} \{ \mu(1+\alpha_0) [d+8-3\mu(1+\alpha_0)] - 3(d+2) \}, \quad (25)$$

$$\beta = -\frac{v_d T}{2} \frac{\mu(1+\alpha_0) [d-3\mu(1+\alpha_0)+2]}{m}. \quad (26)$$

The mass and heat fluxes have the forms

$$\mathbf{j}_0^{(1)} = -m_0 D \nabla x_0, \quad (27)$$

$$\mathbf{q}_0^{(1)} = -T^2 D_q \nabla x_0, \quad (28)$$

where D is the diffusion coefficient and D_q is a cross transport coefficient measuring energy transport due to diffusion of impurities. Dimensional analysis requires that $D \propto T^{1/2}$ and $D_q \propto T^{-1/2}$. Consequently,

$$\partial_t^{(0)} \mathbf{j}_0^{(1)} = -\zeta T \partial_T \mathbf{j}_0^{(1)} = \frac{m_0}{2} \zeta D \nabla x_0, \quad \partial_t^{(0)} \mathbf{q}_0^{(1)} = -\zeta T \partial_T \mathbf{q}_0^{(1)} = \frac{3}{2} \zeta T^2 D_q \nabla x_0. \quad (29)$$

Inserting Eqs. (29) into Eqs. (19) and (20), respectively, the transport coefficients D and D_q can be easily identified from (27) and (28). The result is

$$D = \frac{p}{m_0 v} \frac{\gamma}{v_d^* - \frac{1}{2} \zeta^*}, \quad (30)$$

$$D_q = \frac{n}{m_0 v} \frac{(m_0/m) \beta^* D^* - \frac{d+2}{2} (1 + \frac{c_0}{2}) \gamma^2}{\frac{3}{2} \zeta^* - v_q^*}. \quad (31)$$

Here, $v_d^* = v_d/v$, $\beta^* = \beta m/(T v)$, $v_q^* = v_q/v$, and $\zeta^* = \zeta/v$.

A useful way of characterizing the heat transport in a mixture due to a concentration gradient is through the Dufour coefficient. In our problem, the (dimensionless) Dufour coefficient L_q is defined by the relation

$$\mathbf{J}_q \equiv \mathbf{q}_0^{(1)} - \frac{d+2}{2} T \frac{\mathbf{j}_0^{(1)}}{m_0} = -\frac{n T^2}{m_0 v} L_q \nabla x_0. \quad (32)$$

The coefficient L_q can be easily written in terms of the coefficients D and D_q as

$$L_q = \frac{m_0 v}{p} \left(T D_q - \frac{d+2}{d} D \right). \quad (33)$$

In the elastic case ($\alpha = \alpha_0 = 1$), $\zeta = 0$, $T_0 = T$, and as expected $L_q = 0$. Figures 1 and 2 show the dependence of the reduced coefficients $D(\alpha)/D(1)$ and $L_q(\alpha)$, respectively, on the (common) coefficient of restitution $\alpha = \alpha_0$ for different systems. Here, $D(1)$ is the elastic value of the diffusion coefficient. In the case of the diffusion coefficient, it is apparent that the results for IMM and IHS are practically indistinguishable over the whole range of values of α studied. Moreover, both theories present an excellent agreement with Monte Carlo simulations. More discrepancies between IMM and IHS are found in the case of the Dufour coefficient L_q , especially with increasing dissipation. However, at a qualitative level, the IMM predictions compare well with the ones derived for IHS.

4. CONCLUDING REMARKS

Diffusion of impurities in a dilute granular gas of IMM undergoing HCS has been analyzed. The relevant transport coefficients of the problem (diffusion and Dufour coefficients) have been determined from a Chapman-Enskog solution [1] of the Boltzmann-Lorentz equation up to first order in the concentration gradient. The expressions (30), (31), and (33) derived here for the diffusion D and Dufour L_q coefficients are *exact* (within the context of IMM) and constitute the main goal of this paper. This contrasts with the previous results derived for IHS [3, 9], where the coefficients D and L_q were obtained by considering the leading terms in a Sonine polynomial expansion of the velocity distribution function of impurities. To make contact with the results reported for IHS, the collision frequencies ω and ω_0 (which can be seen as free parameters of the model) need to be chosen. Here, I have taken these frequencies to reproduce the cooling rates ζ and ζ_0 of IHS in the local equilibrium approximation. With this choice, the comparison with known results for IHS shows that in general, the IMM predictions are reasonably good for not too large dissipation, especially for the diffusion coefficient which is related to a first-degree velocity moment of the velocity distribution function. In the case of the Dufour coefficient, although the IMM capture qualitatively well the trends obtained for IHS, the disagreement between both interaction potentials is more significant than the one found for the diffusion coefficient D . In this sense, more discrepancies between IMM and IHS are expected when one considers higher degree velocity moments.

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