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A note on the violation of the Einstein relation in a driven moderately dense granular gas

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Abstract. The Einstein relation for a driven moderately dense granular gas in d dimensions is analyzed in the context of the Enskog kinetic equation. The Enskog equation neglects velocity correlations but retains spatial correlations arising from volume exclusion effects. As expected, there is a breakdown of the Einstein relation $\epsilon = D/(T_0\mu) \neq 1$ relating diffusion D and mobility μ, T_0 being the temperature of the impurity. The kinetic theory results also show that the violation of the Einstein relation is only due to the strong non-Maxwellian behavior of the reference state of the impurity particles. The deviation of ϵ from unity becomes more significant as the solid volume fraction and the inelasticity increase, especially when the system is driven by the action of a Gaussian thermostat. This conclusion qualitatively agrees with some recent simulations of dense gases (Puglisi *et al* 2007 *J. Stat. Mech.* P08016), although the deviations observed in computer simulations are more important than those obtained here from the Enskog kinetic theory. Possible reasons for the quantitative discrepancies between theory and simulations are discussed.

Contents

1. Introduction

The generalization of the fluctuation-response relation to non-equilibrium systems has received considerable attention in the past few years. In this context, granular matter can be considered as a good example of a system that inherently is in a non-equilibrium state. Granular systems are constituted by macroscopic grains that collide inelastically so that the total energy decreases with time. On the other hand, a non-equilibrium steady state (NESS) is reached when the system is heated by the action of an external driving force (thermostat) that does work to compensate for the collisional loss of energy. In these conditions, some attempts to formulate a fluctuation-response theorem based on the introduction of an effective temperature have been made [1]–[4]. However, a complete analysis of the validity of the theorem requires the knowledge of the full dependence of the response and correlation functions on frequency ω [5]. Given that this dependence is quite difficult to evaluate in general, the corresponding limit $\omega \to 0$ is usually considered. In this limit, the classical relation between the coefficients of diffusion D (autocorrelation function) and mobility μ (linear response) is known as the Einstein relation.

The Einstein relation for heated granular fluids has been widely analyzed recently. First, some computer simulation results for dilute systems [6] have shown the validity of the Einstein relation ($\epsilon = D/T_0\mu = 1$) in NESS when the temperature of the bath T is replaced by the temperature of the impurity T_0. This has an interesting consequence in the case of mixtures (where the different species have different temperatures [7]–[9]) since a linear response experiment on a massive intruder or tracer particle to obtain a temperature measurement yields the temperature of the intruder and not the temperature of the surrounding gas. On the other hand, from an analytical point of view, kinetic theory calculations based on the Boltzmann equation have shown the violation of the Einstein relation ($\epsilon \neq 1$) in the free cooling case [10] as well as for driven granular gases [11]. These deviations are in general very small in the driven case (less than 1% when the system is driven by a stochastic thermostat) and are related to non-Gaussian properties of the distribution function of the impurities. This is why such deviations cannot be detected in computer simulations of very dilute gases.

However, a recent computer simulation study of Puglisi *et al* [12] at high densities has provided evidence that the origin of the violation of the Einstein formula is mainly due to spatial and velocity correlations between the particles that are about to collide rather than the deviation from the Maxwell–Boltzmann statistics. These correlations increase as excluded volume and energy dissipation occurring in collisions are increased. The simulation results obtained by Puglisi *et al* [12] motivate the present paper and, as in the case of a dilute gas [11], kinetic theory tools will be used to analyze the effect of density on the possible violation of the Einstein relation. For a moderately dense gas, the Enskog kinetic equation for inelastic hard spheres [13] can be considered as an accurate and practical generalization of the Boltzmann equation. As in the case of elastic collisions, the Enskog equation takes into account spatial correlations through the pair correlation function but neglects velocity correlations (molecular chaos assumption) [14]. Although the latter assumption has been shown to fail for inelastic collisions as the density increases [15]–[17], there is substantial evidence in the literature for the validity of the Enskog theory for densities outside the Boltzmann limit (moderate densities) and values of dissipation beyond the quasielastic limit. This evidence is supported by the good agreement found at the level of macroscopic properties (such as transport coefficients) between the Enskog theory [18]–[20] and simulation [21]–[25] and experimental [26, 27] results. In this context, one can conclude that the Enskog equation provides a unique basis for the description of dynamics across a wide range of densities, length scales, and degrees of dissipation. No other theory with such generality exists.

2. Description of the problem

Let us consider a granular gas composed of smooth inelastic disks ($d = 2$) or spheres ($d = 3$) of mass m, diameter σ, and interparticle coefficient of restitution α in a homogeneous state. We assume that, at moderate densities, the velocity distribution function $f(\mathbf{v})$ obeys the Enskog kinetic equation [13]. Due to dissipation in collisions, the gas cools down unless a mechanism of energy input is externally introduced to compensate for collisional cooling. In experiments the energy is typically injected through the boundaries yielding an inhomogeneous steady state. To avoid the complication of strong temperature heterogeneities, it is usual to consider the action of homogeneous external (driving) forces acting locally on each particle. These forces are called thermostats and depend on the state of the system. In this situation, the steady-state Enskog equation reads

$$\mathcal{F}f(\mathbf{v}) = \chi J[\mathbf{v}|f, f], \tag{1}$$

where $J[\mathbf{v}|f, f]$ is the inelastic Boltzmann collision operator, χ denotes the equilibrium configurational pair correlation function evaluated at contact, and $\mathcal{F}$ is an operator representing the effect of the external force. Two types of external force (thermostats) are usually considered: (a) a deterministic force proportional to the particle velocity (Gaussian thermostat), and (b) a white noise external force (stochastic thermostat). The use of these kinds of thermostats has attracted the attention of the granular community in the few past years in studying different problems. In the case of the Gaussian thermostat, $\mathcal{F}$ has the form [28]–[30]

$$\mathcal{F}f(\mathbf{v}) = \frac{1}{2}\zeta\frac{\partial}{\partial\mathbf{v}} \cdot [\mathbf{v}f(\mathbf{v})], \tag{2}$$

where ζ is the cooling rate due to collisions. In the case of the stochastic thermostat, the operator $\mathcal{F}$ has the Fokker–Planck form [31]

$$\mathcal{F}f(\mathbf{v}) = -\frac{1}{2}\frac{T}{m}\zeta\left(\frac{\partial}{\partial\mathbf{v}}\right)^2 f(\mathbf{v}). \tag{3}$$

The exact solution to the Enskog equation (1) is not known, although a good approximation for f in the region of thermal velocities can be obtained from an expansion in Sonine polynomials. For practical purposes, one selects a finite number of terms in the expansion. In the leading order $f(\mathbf{v})$ is given by

$$f(\mathbf{v}) \to n\pi^{-d/2}v_{\mathrm{th}}^{-d}\mathrm{e}^{-v^{*2}}\left[1 + \frac{c}{4}\left(v^{*4} - (d+2)v^{*2} + \frac{d(d+2)}{4}\right)\right], \tag{4}$$

where $\mathbf{v}^* = \mathbf{v}/v_{\mathrm{th}}$, $v_{\mathrm{th}} = \sqrt{2T/m}$ being the thermal velocity. Moreover, c is the fourth cumulant of the velocity distribution function f defined as

$$c = \frac{8}{d(d+2)}\left(\frac{m^2}{4nT^2}\int\mathrm{d}\mathbf{v}\,v^4 f - \frac{d(d+2)}{4}\right). \tag{5}$$

In the approximation (4), cumulants of higher order have been neglected. Inserting equation (4) into the Enskog equation and neglecting non-linear terms in c, one gets the following expression for the cooling rate ζ [31]:

$$\zeta = \frac{\sqrt{2}\pi^{(d-1)/2}}{d\Gamma(d/2)}\chi n\sigma^{d-1}v_{\mathrm{th}}(1-\alpha^2)\left(1 + \frac{3}{32}c\right). \tag{6}$$

The value of c depends on the thermostat used. In the case of the Gaussian thermostat, c is approximately given by [31]

$$c(\alpha) = \frac{32(1-\alpha)(1-2\alpha^2)}{9 + 24d - (41-d)\alpha + 30\alpha^2(1-\alpha)}, \tag{7}$$

while

$$c(\alpha) = \frac{32(1-\alpha)(1-2\alpha^2)}{73 + 56d - 3(35+8d)\alpha + 30\alpha^2(1-\alpha)} \tag{8}$$

for the stochastic thermostat. It is interesting to note that in the homogeneous problem the results obtained with the Gaussian thermostat are completely equivalent to those derived in the free cooling case when one scales the particle velocity with respect to the thermal velocity v_{th} [30]. In addition, although the expressions (6)–(8) have been derived by neglecting non-linear terms in the coefficient c, the estimates (7) and (8) present quite a good agreement with Monte Carlo simulations of the Boltzmann equation [30, 32] for moderate values of dissipation (say for instance, $\alpha \gtrsim 0.5$). However, more recent results [33, 34] for the homogeneous (undriven) cooling state have shown that for very large inelasticity ($\alpha \lesssim 0.5$), the higher order cumulants may not be neglected since they can be of the same order of magnitude as c. The breakdown of the Sonine polynomial expansion is caused by the increasing impact of the overpopulated high energy tail of the velocity distribution f [35].

We assume now that a few impurities or tracer particles of mass m_0 and diameter σ_0 are added to the system. Given that their concentration is very small, the state of

the gas is not affected by the presence of impurities. As a consequence, the velocity distribution function f of the gas still verifies the (homogeneous) Enskog equation (1). Moreover, one can also neglect collisions among impurities themselves versus the impurity–gas collisions, which are characterized by the coefficient of restitution α_0. Diffusion of impurities is generated by a weak concentration gradient ∇n_0 and/or a weak external field $\mathbf{E}$ (e.g. gravity or an electric field) acting only on the impurity particles. Under these conditions, the velocity distribution function $f_0(\mathbf{r}, \mathbf{v}, t)$ of impurities verifies the Enskog–Lorentz equation

$$\partial_t f_0 + \mathbf{v} \cdot \nabla f_0 + \frac{\mathbf{E}}{m_0} \cdot \frac{\partial}{\partial \mathbf{v}} f_0 + \mathcal{F} f_0 = \chi_0 J[\mathbf{v}|f_0, f], \tag{9}$$

where $J[f_0, f]$ is the (inelastic) Boltzmann–Lorentz collision operator and χ_0 represents the equilibrium pair correlation function for impurity–fluid pairs at contact. Given that the gas is in a homogeneous state, it follows that χ_0 is uniform. At a kinetic level, an interesting quantity is the partial temperature of impurities T_0. It is defined as

$$\frac{d}{2} n_0 T_0 = \int d\mathbf{v} \frac{m_0}{2} v^2 f_0(\mathbf{v}), \tag{10}$$

where n_0 is the number density of impurities. The corresponding cooling rate ζ_0 associated with the partial temperature T_0 of impurities is defined as

$$\zeta_0 = -\frac{\chi_0}{d n_0 T_0} \int d\mathbf{v} \, m_0 v^2 J[\mathbf{v}|f_0, f]. \tag{11}$$

In the absence of diffusion (homogeneous steady state), equation (9) becomes

$$\mathcal{F} f_0 = \chi_0 J[\mathbf{v}|f_0, f]. \tag{12}$$

This equation has been widely analyzed by using both types of thermostats [11, 23] for hard spheres ($d = 3$). The results show that the temperatures of the gas (T) and impurities (T_0) are clearly different and so the energy equipartition is broken down. In general, the temperature ratio $\gamma \equiv T_0/T$ presents a complex dependence on the parameters of the problem. The condition for determining the temperature ratio γ is different for each type of thermostat. In the case of the Gaussian thermostat, the temperature ratio is obtained by equating the cooling rates [7, 36]:

$$\zeta = \zeta_0, \tag{13}$$

while for the stochastic thermostat γ is obtained from the condition [23]

$$\frac{\zeta T}{m} = \frac{\zeta_0 T_0}{m_0}. \tag{14}$$

Requirements (13) and (14) lead to a different dependence of the temperature ratio T_0/T on the control parameters, namely, the mass ratio m_0/m, the size ratio σ_0/σ, the coefficients of restitution α and α_0, and the solid volume fraction

$$\phi \equiv \frac{\pi^{d/2}}{2^{d-1} d \Gamma(d/2)} n \sigma^d. \tag{15}$$

In addition to the temperature ratio, an interesting quantity is the fourth cumulant c_0. It is defined as

$$c_0 = \frac{8}{d(d+2)} \left(\frac{m_0^2}{4n_0 T_0^2} \int \mathrm{d}\mathbf{v}\, v^4 f_0 - \frac{d(d+2)}{4} \right). \tag{16}$$

As in the case of the coefficient c, the cumulant c_0 measures the deviation of f_0 from its Maxwellian form

$$f_{0,M}(\mathbf{v}) = n_0 \left(\frac{m_0}{2T_0} \right)^{d/2} \exp\left(-\frac{m_0 v^2}{2T_0} \right). \tag{17}$$

In order to determine the coefficients ζ_0 and c_0 one has to expand the velocity distribution function f_0 in terms of the orthogonal Sonine polynomials. As in the case of the granular gas distribution f, a good estimate of ζ_0 and c_0 can be obtained from the leading Sonine approach to f_0:

$$f_0(\mathbf{v}) \to n_0 \pi^{-d/2} v_{\mathrm{th}}^{-d} \theta^{d/2} \mathrm{e}^{-\theta v^{*2}} \left[1 + \frac{c_0}{4} \left(\theta^2 v^{*4} - (d+2)\theta v^{*2} + \frac{d(d+2)}{4} \right) \right], \tag{18}$$

where $\theta = m_0 T / m T_0$ is the mean square velocity of the gas particles relative to that of impurities. Expressions for ζ_0 and c_0 have been derived in the appendix for an arbitrary number of dimensions d by considering only linear terms in c and c_0. These expressions extend previous results derived in [11] for hard spheres. Once ζ_0 and c_0 are known, the temperature ratio can be obtained from the constraints (13) and (14) for the Gaussian and stochastic thermostats, respectively. To get this explicit dependence, the form of the pair correlation functions χ and χ_0 in terms of the size ratio σ_0/σ and the solid volume fraction ϕ must be given. For a three-dimensional gas $(d=3)$, a good approximation for these functions is [37]

$$\chi = \frac{1 - (1/2)\phi}{(1-\phi)^3}, \tag{19}$$

$$\chi_0 = \frac{1}{1-\phi} + \frac{3}{2} \frac{\sigma_0}{\overline{\sigma}} \frac{\phi}{(1-\phi)^2} + \frac{1}{2} \left(\frac{\sigma_0}{\overline{\sigma}} \right)^2 \frac{\phi^2}{(1-\phi)^3}, \tag{20}$$

where $\overline{\sigma} = (\sigma + \sigma_0)/2$. For a two-dimensional gas $(d=2)$, χ and χ_0 are approximately given by [38]

$$\chi = \frac{1 - (7/16)\phi}{(1-\phi)^2}, \tag{21}$$

$$\chi_0 = \frac{1}{1-\phi} + \frac{9}{16} \frac{\sigma_0}{\overline{\sigma}} \frac{\phi}{(1-\phi)^2}. \tag{22}$$

Obviously, $\chi = \chi_0$ if $\sigma = \sigma_0$. Thus the temperature ratio and the kurtosis c_0 become independent of density for equal-size particles. The dependence of T_0/T on the (common) coefficient of restitution $\alpha = \alpha_0$ is illustrated in figure 1 for $d = 3$ in the case $m_0/m = \sigma_0/\sigma = 0.5$ and for two values of the solid volume fraction ϕ. We consider the two thermostat types discussed before. There is an evident breakdown of the energy equipartition in both thermostat types, especially in the case of the stochastic
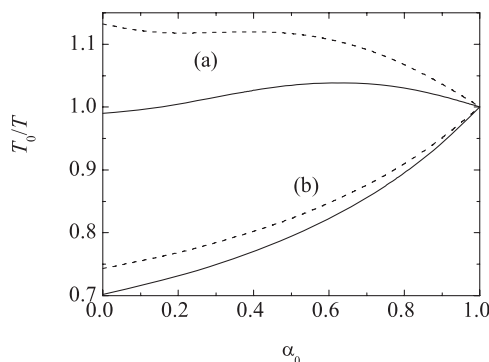
Figure 1. Plot of the temperature ratio T_0/T versus the coefficient of restitution $\alpha = \alpha_0$ for $d = 3$ in the case $m_0/m = \sigma_0/\sigma = 0.5$ for the Gaussian thermostat (a) and the stochastic thermostat (b). The solid lines correspond to a dilute gas ($\phi = 0$) while the dashed lines refer to a moderately dense gas ($\phi = 0.2$).
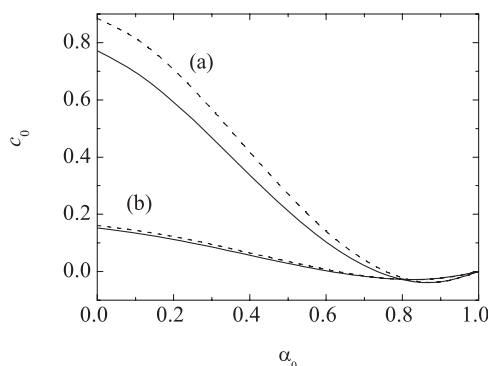

Figure 2. Plot of the coefficient c_0 versus the coefficient of restitution $\alpha = \alpha_0$ for $d = 3$ in the case $m_0/m = \sigma_0/\sigma = 0.5$ for the Gaussian thermostat (a) and the stochastic thermostat (b). The solid lines correspond to a dilute gas ($\phi = 0$) while the dashed lines refer to a moderately dense gas ($\phi = 0.2$).

driving force (3). However, the influence of density is more significant for the Gaussian thermostat than for the stochastic one. The dependence of c_0 on α_0 is plotted in figure 2 for the same cases as were considered in figure 1. It is apparent that for both thermostats the value of c_0 is quite small for not too inelastic systems. This means that in this range of values of α_0 the distribution f_0 of the homogeneous state is quite close to a Maxwellian at the temperature of the impurity particle T_0. However, the magnitude of c_0 increases significantly as the dissipation increases, especially in the case of the Gaussian thermostat. This is a signal of the strong non-Maxwellian behavior of the reference homogeneous state of impurities for quite extreme values of inelasticity. As a consequence, cumulants of higher order than the fourth cumulant c_0 should be considered to assess the deviation of f_0 from its Maxwellian form $f_{0,M}$ for very small values of α and α_0. Finally, with respect to the influence of density, we observe that it is more relevant for the Gaussian thermostat than for the stochastic thermostat, being practically negligible in the latter case.

3. The Einstein relation

The Einstein ratio ϵ is defined as

$$\epsilon = \frac{D}{T_0 \mu}, \tag{23}$$

where D and μ are the diffusion and mobility coefficients, respectively. If the Einstein relation were to hold, one would have $\epsilon = 1$. I want here to analyze the influence of density on ϵ. The transport coefficients D and μ can be determined by solving the (inelastic) Enskog–Lorentz equation (9) by means of the Chapman–Enskog method [39]. In the first order of the expansion, the current of impurities $\mathbf{j}_0$ has the form [11]

$$\mathbf{j}_0 = -D\nabla \ln n_0 + \mu \mathbf{E}. \tag{24}$$

Given that χ and χ_0 are uniform in this problem, it is evident that, when properly scaled, the previous solution obtained in [11] for a dilute gas can be directly translated to the Enskog equation by making the changes $J[f, f] \rightarrow \chi J[f, f]$ and $J[f_0, f] \rightarrow \chi_0 J[f_0, f]$. Technical details on the calculation of D and μ by means of the Chapman–Enskog expansion [39] up to the second Sonine approximation can be found in [11] for inelastic hard spheres ($d = 3$). The extension to an arbitrary number of dimensions is straightforward. Taking into account these results, the dependence of the Einstein ratio ϵ on the parameter space of the problem can be obtained. In the case of the Gaussian thermostat, the result is

$$\epsilon = 1 - \frac{c_0}{2} \frac{\nu_2}{\nu_4 - (3/2)\zeta}, \tag{25}$$

where the collision frequencies ν_2 and ν_4 are explicitly given in the appendix for an arbitrary number of dimensions d. The result for the case of the stochastic thermostat is

$$\epsilon = 1 - \frac{c_0}{2} \frac{\nu_2}{\nu_4}. \tag{26}$$

It is clear that ϵ becomes independent of the density ϕ when $\sigma = \sigma_0$. As in the case of dilute gases [11], equations (25) and (26) show that the violation of the Einstein relation in a heated moderately dense granular gas is basically due to the departures of f_0 from its Maxwellian form $f_{0,M}$. At this level of approximation (second Sonine approximation to the coefficients D and μ), the deviation of f_0 from $f_{0,M}$ is only accounted for by the fourth cumulant c_0. However, the coefficient c_0 depends on the solid volume fraction ϕ through its dependence on the temperature ratio T_0/T. To assess the influence of density on the Einstein ratio ϵ, in figure 3 a plot of ϵ versus the size ratio σ_0/σ is shown for the case of the Gaussian thermostat for $d = 3$ and $\alpha = \alpha_0 = 0.5$ when the impurities have the same mass density as the gas particles (namely, $m_0/m = (\sigma_0/\sigma)^3$). Three different values of the solid volume fraction ϕ have been considered: $\phi = 0$ (dilute gas), $\phi = 0.2$ (moderate dense gas), and $\phi = 0.4$ (quite dense gas). The corresponding plot for the stochastic thermostat has not been included since the deviation of ϵ from 1 is less than 1% for all the cases analyzed. It is apparent that the degree of violation of the Einstein relation is more important when the impurities are lighter and/or smaller than the gas particles, especially for high densities. To confirm this trend, the Einstein ratio has been plotted in figures 4 and 5 as a function of the (common) coefficient of restitution $\alpha = \alpha_0$ for $d = 2$,
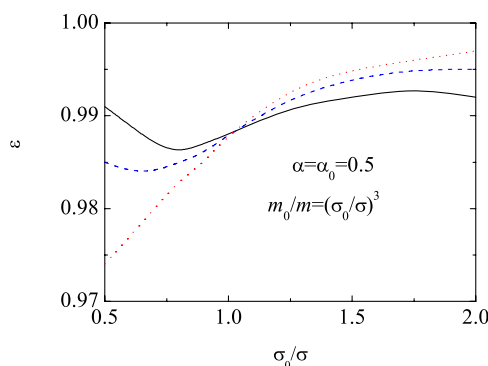
Figure 3. Plot of the Einstein ratio $\epsilon = D/T_0\mu$ versus the size ratio σ_0/σ in the case of the Gaussian thermostat for $d = 3$ and $\alpha = \alpha_0 = 0.5$ when the impurities have the same mass density as the gas particles. Three different values of the solid volume fraction are considered: $\phi = 0$ (solid line), $\phi = 0.2$ (dashed line), and $\phi = 0.4$ (dotted line).
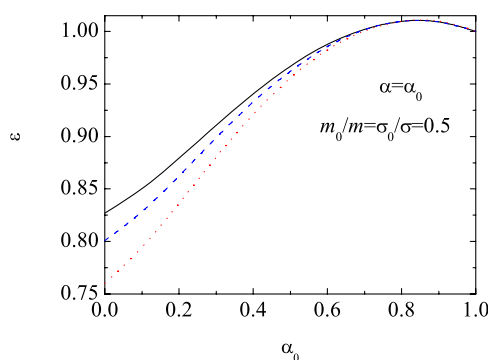

Figure 4. Plot of the Einstein ratio $\epsilon = D/T_0\mu$ versus the coefficient of restitution $\alpha = \alpha_0$ in the case of the Gaussian thermostat for $d = 2$, $m_0/m = \sigma_0/\sigma = 0.5$ and three different values of the solid volume fraction: $\phi = 0$ (solid line), $\phi = 0.2$ (dashed line), and $\phi = 0.4$ (dotted line).

$m_0/m = \sigma_0/\sigma = 0.5$, and for the same values of ϕ as considered before. Figure 4 shows the results obtained by using the Gaussian thermostat and figure 5 refers to the results obtained for the stochastic thermostat. While ϵ is close to 1 in the case of the stochastic thermostat for all the densities considered, significant deviations from unity are observed for the Gaussian thermostat. In this latter case, it is apparent that the degree of violation of the Einstein formula increases with the volume fraction and the inelasticity.

This latter conclusion qualitatively agrees with the results obtained by Puglisi *et al* [12] from computer simulations since they observe a significant violation of the Einstein formula when excluded volume effects and dissipation are increased. However, at a quantitative level, the deviations observed by Puglisi *et al* [12] are larger than those found here (see figure 3 of [12]). The quantitative disagreement between simulations [12] and the Enskog theory results (25) and (26) could be due to two different and independent factors. First, as noted before in section 2, the expression for the fourth cumulant c_0 used here has been obtained by neglecting cumulants of higher order and considering only
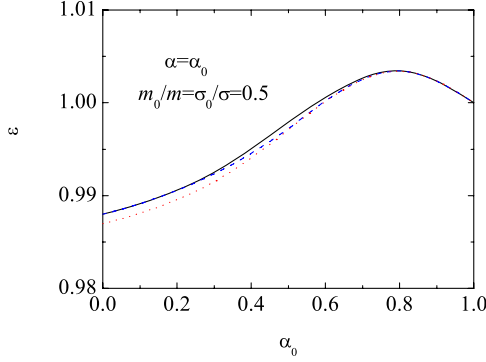
Figure 5. Plot of the Einstein ratio $\epsilon = D/T_0\mu$ versus the coefficient of restitution $\alpha = \alpha_0$ in the case of the stochastic thermostat for $d = 2$, $m_0/m = \sigma_0/\sigma = 0.5$ and three different values of the solid volume fraction: $\phi = 0$ (solid line), $\phi = 0.2$ (dashed line), and $\phi = 0.4$ (dotted line).

linear terms in c and c_0. On the other hand, according to the previous results [33, 34] obtained in the free cooling case for a monocomponent gas, the value of c_0 could change significantly for very strong dissipation when cumulants of higher order were taken into account in the form of the homogeneous distribution. In this context, the estimate of c_0 obtained in this paper could be unreliable for this range of values of inelasticity and so, the quantitative deviations of ϵ from 1 observed in figures 3 and 4 for the Gaussian thermostat when $\alpha_0 \lesssim 0.5$ could be questionable. As a second reason for discrepancy between simulations and theory, one could argue that the velocity correlations (absent in the Enskog equation but present in computer simulations) play a more important role than spatial correlations (excluded volume effects) in the violation of the Einstein formula. In this case, one should correct the Enskog equation by incorporating recollision events ('ring' collisions) that take into account multiparticle collisions.

Finally, since the results derived in this paper hold for a d-dimensional system, it is interesting to investigate the influence of dimensionality on the violation of the Einstein relation. To illustrate this effect, in figure 6 the dependence of the ratio $\epsilon(\phi)/\epsilon(0)$ on the solid volume fraction ϕ is shown for $\alpha = \alpha_0 = 0.5$, $m_0/m = 2$ and $\sigma_0/\sigma = 0.25$ in the case of the Gaussian thermostat. I have considered the physical cases of hard spheres ($d = 3$) and hard disks ($d = 2$). Here, $\epsilon(0)$ corresponds to the value of the Einstein ratio for a dilute gas. Although the qualitative dependences of the ratio $\epsilon(\phi)/\epsilon(0)$ on ϕ are quite similar in the two systems, we observe that the violation of the Einstein ratio is stronger for $d = 3$ than for $d = 2$ for moderate densities. However, this trend changes as density becomes larger.

4. Conclusions

In this paper I have analyzed the validity of the Einstein relation $\epsilon = D/T_0\mu = 1$ for driven moderately d-dimensional dense granular gases in the framework of the Enskog equation. This work extends a previous study carried out by the author [11] in the case of a dilute gas ($\phi = 0$) of inelastic hard spheres ($d = 3$). To achieve a NESS, two types of thermostat (external forces) have been considered: (i) an 'anti-drag' force proportional to the particle velocity (Gaussian force), and (b) a stochastic force, which give frequent
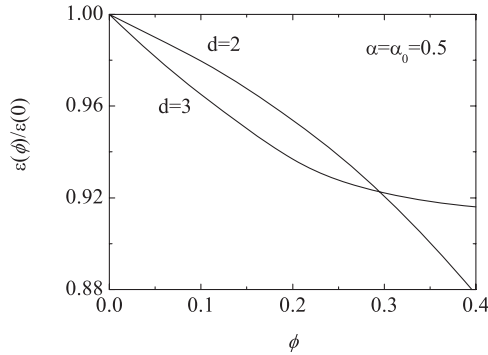
Figure 6. Plot of the ratio $\epsilon(\phi)/\epsilon(0)$ versus the solid volume fraction ϕ for $\alpha = \alpha_0 = 0.5$, $m_0/m = 2$ and $\sigma_0/\sigma = 0.25$ in the case of the Gaussian thermostat for spheres ($d = 3$) and disks ($d = 2$).

kicks to each particle between collisions. The present work has been motivated by recent computer simulation results of Puglisi *et al* [12] where the spatial and velocity correlations between the particles have shown to be the most important ingredient in a strong violation of the Einstein relation. It is shown that $\epsilon \neq 1$, especially in the case of the Gaussian thermostat when the impurity is lighter and/or smaller than particles of the gas. As in the case of a dilute gas [11], the violation of the Einstein relation is connected to the strong non-Maxwellian behavior of the homogeneous velocity distribution function of impurities, which is mainly measured through its fourth cumulant c_0. The results also show that the deviation of the Einstein ratio from 1 is more important as both the density and dissipation increase, which is consistent with the observations made by Puglisi *et al* [12]. However, at a quantitative level, the deviations of the Einstein formula obtained here from the Enskog equation are smaller than those found in computer simulations. As discussed before, this quantitative disagreement between theory and simulation could be due to (i) the possible lack of convergence of the Sonine polynomial expansion for the reference Gaussian driven state, and/or (ii) the influence of velocity correlations which are absent in the Enskog description (molecular chaos hypothesis). With respect to the first source of discrepancy, one perhaps should include cumulants of higher order as well as non-linear terms in c and c_0 to get an accurate estimate of the fourth cumulant c_0 for very small values of the coefficients of restitution α and α_0. However, given that perhaps the absolute value of the higher order cumulants increases with inelasticity, the Sonine expansion could be not relevant in the sense that one would need an infinite number of Sonine coefficients to characterize the reference state. In this case, a possible alternative would be the use of the direct simulation Monte Carlo (DSMC) method [40] to numerically solve the Enskog equation in the homogeneous driven problem. Regarding the influence of velocity correlations, the inclusion of this new ingredient in the Enskog collision operator makes analytic calculations intractable since higher order correlations must be included in the evaluation of the collision integrals. This contrasts with the explicit results reported in this paper, where the transport coefficients D and μ have been explicitly obtained in terms of the parameters of the system (masses, sizes and coefficients of restitution).

Finally, it must be noted that the theoretical results derived here have been obtained by considering the second Sonine approximation to the Chapman–Enskog solution. Exact

results can be obtained if one considers the inelastic Maxwell model (IMM) for a dilute gas. This model has been widely used by several authors as a toy model to characterize the influence of the inelasticity of collisions of the physical properties of the granular fluids. The fact the collision rate for the IMM is velocity independent allows one to exactly compute the transport coefficients of the system. In particular, the coefficients D and μ have been evaluated [41] from the Chapman–Enskog method for undriven systems. The extension of such calculations to driven systems is straightforward. Thus, in the case of the Gaussian thermostat, one gets

$$D = \frac{n_0 T_0}{m_0}\left(\nu_D - \frac{1}{2}\zeta\right)^{-1}, \qquad \mu = \frac{n_0}{m_0}\left(\nu_D - \frac{1}{2}\zeta\right)^{-1}, \tag{27}$$

while

$$D = \frac{n_0 T_0}{m_0 \nu_D}, \qquad \mu = \frac{n_0}{m_0 \nu_D} \tag{28}$$

in the case of the stochastic thermostat. Here,

$$\nu_D = \frac{w_0}{d}\frac{m}{m + m_0}(1 + \alpha_0), \qquad \zeta = \frac{w}{2d}(1 - \alpha^2), \tag{29}$$

where w and w_0 are effective collision frequencies of the model. According to equations (27) and (28), $\epsilon = D/T_0\mu = 1$ for both thermostats so the Einstein relation holds for the inelastic Maxwell model in any number of dimensions. This conclusion agrees with previous independent results obtained for $d = 1$ [3, 42], $d = 2$ [12] and $d = 3$ [4].

Acknowledgments

Appendix. Expressions for ζ_0, c_0, ν_2 and ν_4

The explicit expressions for the partial cooling rate ζ_0, the kurtosis c_0 and the collision frequencies ν_2 and ν_4 are displayed in this appendix for an arbitrary number of dimensions d. In order to get these expressions, we consider the leading Sonine approximations (4) for the granular gas distribution f and (18) for the impurity distribution f_0. The cooling rate ζ_0 can be obtained by following the same mathematical steps as were used before in previous papers [11, 36]. The final expression can be written as

$$\zeta_0 = \lambda_{00} + \lambda_{01}c_0 + \lambda_{02}c, \tag{A.1}$$

where

$$\lambda_{00} = \frac{4\pi^{(d-1)/2}}{d\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M\left(\frac{1+\theta}{\theta}\right)^{1/2}(1+\alpha_0)\left[1 - \frac{M}{2}(1+\alpha_0)(1+\theta)\right], \tag{A.2}$$

$$\lambda_{01} = \frac{\pi^{(d-1)/2}}{8d\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M\frac{(1+\theta)^{-3/2}}{\theta^{1/2}}(1+\alpha_0)\left[2(3+4\theta) - 3M(1+\alpha_0)(1+\theta)\right], \tag{A.3}$$

$$\lambda_{02} = -\frac{\pi^{(d-1)/2}}{8d\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M\left(\frac{1+\theta}{\theta}\right)^{-3/2}(1+\alpha_0)\left[2 + 3M(1+\alpha_0)(1+\theta)\right]. \tag{A.4}$$

Here, $\theta = m_0 T/m T_0$ and $M = m/(m + m_0)$.

In order to get the coefficient c_0, one substitutes equations (4) and (18) into the Enskog–Lorentz equation (12), multiplies it by v^4 and integrates over the velocity. After some algebra and neglecting non-linear terms in c and c_0, the result in the case of the Gaussian thermostat is

$$c_0 = -\frac{\lambda_{00} + \lambda_{02}c + (2/(d(d+2)))M_0^{-2}\theta^2 (\Omega_{00} + \Omega_{02}c)}{(1/2)\lambda_{00} + \lambda_{01} + (2/(d(d+2)))M_0^{-2}\theta^2\Omega_{01}}, \tag{A.5}$$

while

$$c_0 = -\frac{\lambda_{00} + \lambda_{02}c + (2/(d(d+2)))M_0^{-2}\theta^2 (\Omega_{00} + \Omega_{02}c)}{\lambda_{01} + (2/(d(d+2)))M_0^{-2}\theta^2\Omega_{01}} \tag{A.6}$$

for the stochastic thermostat. In equations (A.5) and (A.6), $M_0 = m_0/(m + m_0)$ and the quantities

$$\Omega_{00} = \frac{\pi^{(d-1)/2}}{\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M_0^2 M \frac{(1+\theta)^{-1/2}}{\theta^{5/2}}(1+\alpha_0)$$
$$\times \left\{-2\left[d+3+(d+2)\theta\right] + M(1+\alpha_0)(1+\theta)\left(11+d+\frac{d^2+5d+6}{d+3}\theta\right)\right.$$
$$\left.- 8M^2(1+\alpha_0)^2(1+\theta)^2 + 2M^3(1+\alpha_0)^3(1+\theta)^3\right\}, \tag{A.7}$$

$$\Omega_{01} = \frac{\pi^{(d-1)/2}}{16\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M_0^2 M \frac{(1+\theta)^{-5/2}}{\theta^{5/2}}(1+\alpha_0)$$
$$\times \left\{-2\left[45+15d+(114+39d)\theta+(88+32d)\theta^2+(16+8d)\theta^3\right]\right.$$
$$+ 3M(1+\alpha_0)(1+\theta)\left[55+5d+9(10+d)\theta+4(8+d)\theta^2\right]$$
$$\left.- 24M^2(1+\alpha_0)^2(1+\theta)^2(5+4\theta) + 30M^3(1+\alpha_0)^3(1+\theta)^3\right\}, \tag{A.8}$$

$$\Omega_{02} = \frac{\pi^{(d-1)/2}}{16\Gamma(d/2)}\chi_0 n\overline{\sigma}^{d-1}v_{\text{th}}M_0^2 M \frac{(1+\theta)^{-5/2}}{\theta^{1/2}}(1+\alpha_0)$$
$$\times \left\{2\left[d-1+(d+2)\theta\right] + 3M(1+\alpha_0)(1+\theta)\left[d-1+(d+2)\theta\right]\right.$$
$$\left.- 24M^2(1+\alpha_0)^2(1+\theta)^2 + 30M^3(1+\alpha_0)^3(1+\theta)^3\right\}, \tag{A.9}$$

have been introduced. Equations (A.2)–(A.4) and (A.7)–(A.9) are consistent with the results [7, 11] obtained for hard spheres $(d = 3)$. Once the coefficient c_0 is given in terms of $\gamma = M_0/M\theta$, the parameters of the mixture and the solid volume fraction, the temperature ratio γ can be explicitly obtained by numerically solving the condition (13) for the Gaussian thermostat or the condition (14) for the stochastic thermostat.

Finally, the collision frequencies ν_2 and ν_4 are given by

$$\nu_2 = \frac{\pi^{(d-1)/2}}{d\Gamma\left(d/2\right)} n\overline{\sigma}^{d-1} v_{\text{th}}\chi_0 M(1+\alpha_0)[\theta(1+\theta)]^{-1/2}, \tag{A.10}$$

$$\nu_4 = \frac{\pi^{(d-1)/2}}{d(d+2)\Gamma\left(d/2\right)} n\overline{\sigma}^{d-1} v_{\text{th}}\chi_0 M(1+\alpha_0)\left(\frac{\theta}{1+\theta}\right)^{3/2}\left[A - (d+2)\frac{1+\theta}{\theta}B\right], \tag{A.11}$$

where

$$
\begin{aligned}
A &= 2M^2\left(\frac{1+\theta}{\theta}\right)^2\left(2\alpha_0^2 - \frac{d+3}{2}\alpha_0 + d+1\right)[d+5+(d+2)\theta] \\
&\quad - M(1+\theta)\Big\{\beta\theta^{-2}[(d+5)+(d+2)\theta][(11+d)\alpha_{12}-5d-7] \\
&\quad - \theta^{-1}[20+d(15-7\alpha_0)+d^2(1-\alpha_0)-28\alpha_0] - (d+2)^2(1-\alpha_0)\Big\} \\
&\quad + 3(d+3)\beta^2\theta^{-2}[d+5+(d+2)\theta] + 2\beta\theta^{-1}[24+11d+d^2+(d+2)^2\theta] \\
&\quad + (d+2)\theta^{-1}[d+3+(d+8)\theta] - (d+2)(1+\theta)\theta^{-2}[d+3+(d+2)\theta], \\
B &= (d+2)(1+2\beta) + M(1+\theta)\left\{(d+2)(1-\alpha_0) - [(11+d)\alpha_0-5d-7]\beta\theta^{-1}\right\} \\
&\quad + 3(d+3)\beta^2\theta^{-1} + 2M^2\left(2\alpha_0^2 - \frac{d+3}{2}\alpha_0 + d+1\right)\theta^{-1}(1+\theta)^2 \\
&\quad - (d+2)\theta^{-1}(1+\theta). \tag{A.12}
\end{aligned}
$$

Here, $\beta = M_0 - M\theta = M_0(1-\gamma^{-1})$. For $d=3$, equations (A.10) and (A.11) coincide with those previously reported [11] for hard spheres.

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