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Energy nonequipartition in multicomponent granular mixtures

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We study nonequipartition of energy in granular fluids composed by an arbitrarily large number of components. We focus on a simple mean field model, based upon a Maxwell collision operator kernel, and predict the temperature ratios for the species. Moreover, we perform direct Monte Carlo simulations in order to verify the predictions.

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I. INTRODUCTION

The equipartition principle states that the total energy of an equilibrium macroscopic system is equally distributed among the degrees of freedom of its components. For instance, in a classical gas mixture, equilibrium statistical mechanics show that equipartition of energy between the components is overwhelmingly more probable than a state characterized by different energies, i.e., the entropy of the system reaches its maximum at the equipartition state [1]. This result ensures the occurrence of energy equipartition at the thermodynamic limit, and allows one to deduce a microscopic expression and interpretation for the thermodynamic temperature; namely, temperature can be defined kinetically as $T_E=(1/Nd)\langle \mathrm{kin}\rangle_E$, where Nd is the number of degrees of freedom in the system, and $\langle \mathrm{kin}\rangle_E$ is an equilibrium average of the kinetic energy. This preliminary discussion shows the central role played by equipartition of energy in the foundations of equilibrium statistical mechanics, and its deep links with fundamental equilibrium concepts such as energy bath or thermal equilibrium.

However, the above kinetic definition may also be applied in nonequilibrium situations, $T_{NE}=(1/Nd)\langle \mathrm{kin}\rangle_{NE}$. This kinetic temperature, which is now defined as an average with a nonequilibrium distribution in phase space, is a less fundamental quantity than the equilibrium temperature, and is equivalent to the average agitation of the particles in the system. By construction, it does not highlight *a priori* equilibrium features like the equipartition principle. Nonetheless, its inclusion in systems where thermodynamics are ill defined may be relevant practically, as this quantity still provides meaningful information about the variance of the velocity distribution and about the local average energy in the system. This approach has been applied during the last years to describe granular fluids, i.e., systems composed of a large number of agitated grains interacting inelastically. The *granular temperature* is then defined kinetically by $T(\mathbf{r},t)=\langle(1/d)(mV^2/2)\rangle$, where $\mathbf{V}=\mathbf{v}-\mathbf{u}(\mathbf{r},t)$ is the random velocity, $\mathbf{u}(\mathbf{r},t)$ is the local mean velocity, and d is the dimension of the system. The average is now performed with the one-particle velocity distribution $f(\mathbf{r},\mathbf{v};t)$. This quantity has been shown to give a relevant description of granular fluids, for instance by paving the way to an hydrodynamic formalism. In contrast, however, the granular temperature exhibits nonequilibrium features, such as an anomalous Fourier law for the energy flux [2], and nonequipartition of energy in granular mixtures. This nonequipartition phenomenon has been first theoretically predicted in the case of binary mixtures by [3], and successfully verified by numerical simulations [4] and experiments [5]. It has also been observed in the case of rough inelastic spheres, where the *translational temperature* and the *rotational temperature* are different. It is important to note here that energy nonequipartition deserves a careful study due to macroscopic consequences such as nonnegligible corrections to the transport coefficients [6], and its role in vertical segregation [7].

In this Brief Report, we introduce a coherent mean field model for low density granular fluids composed by an arbitrary large number of components. This model rests on a detailed analysis for the collision frequencies of the different components, and generalizes Maxwell-like models introduced by Ben-Naim [11] and Marconi [12]. The values for energy nonequipartition are derived analytically in the low inelasticity limit, and are successfully compared with inelastic hard sphere theory and computer simulations.

II. TWO RATE MAXWELL MODEL

In this paper, we consider a binary system composed by smooth inelastic hard spheres (IHSs) in d dimensions, i.e., the interactions are instantaneous when the spheres are in contact and there is no transfer of angular momentum. Moreover, we focus on a system that is and remains spatially homogeneous in order to focus on the homogeneous cooling state. There are K kinds of grains, which are characterized by the following mechanical quantities: their respective mass m_i and diameter σ_i as well as their mutual inelasticity coefficients α_{ij} that describe the energy dissipation during a collision between particles i and j. These different properties discriminate the components, which are described at the macroscopic level by their concentration $x_i=N_i/N$ and partial temperature $T_i\equiv\langle(1/d)(m_iV^2/2)\rangle_i$, where the average is performed over species i. By definition, these macroscopic quantities are constrained by the relations $\Sigma_{i=1}^K x_i=1$ and

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$\Sigma_{i=1}^{K} x_i T_i = T$. Conservation of impulsion implies the following collision rule:

$$\mathbf{v}_i^* = \mathbf{v}_i - \frac{m_j}{(m_i+m_j)}(1+\alpha_{ij})\boldsymbol{\epsilon}(\boldsymbol{\epsilon}\cdot\mathbf{v}_{ij}),$$

$$\mathbf{v}_j^* = \mathbf{v}_j + \frac{m_i}{(m_i+m_j)}(1+\alpha_{ij})\boldsymbol{\epsilon}(\boldsymbol{\epsilon}\cdot\mathbf{v}_{ij}), \tag{1}$$

where $\mathbf{v}_{ij}$ and $\mathbf{r}_{ij}$ are, respectively, the relative velocities $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ and positions $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ of the colliding disks i and j. The velocities with asterisks are their postcollisional velocities and $\boldsymbol{\epsilon}$ is the unitary vector along the axis joining the centers of the two colliding spheres. In the low density limit, by assuming that precollisional correlations may be neglected [8], the system is described by a system of K coupled Boltzmann equations. In this paper, we use mean field methods in order to simplify the mathematical structure of the collision operator, by assuming that the collision frequency between particles i and j, i.e., proportional to v_{ij} in the case of hard spheres, is approximated by the mean field quantity $\nu_{ij} = (1/\sqrt{2})\sqrt{T_i/m_i + T_j/m_j}$. Let us stress that this kind of assumption is common in order to build inelastic Maxwell models [9,10,12]. In the case of binary mixtures, a simplified form has been introduced by Ben-Naim and Krapivsky [10], $\nu_{ij} = (1/\sqrt{2})\sqrt{T_i(t) + T_j(t)}$, but it does not describe correctly the mass dependence of the collision frequencies and does not give correct relations in the case of mass-dispersed mixtures. The above assumption leads to a system of K kinetic equations for the velocity distributions f_i:

$$\frac{\partial f_i(\mathbf{v})}{\partial t} = x_i \sigma_i^{d-1}\sqrt{\frac{T_i}{m_i}} K_{ii}[f_i, f_i] + \sum_{j=1, j\neq i}^{K} \frac{x_j}{\sqrt{2}}\sigma_{ij}^{d-1}\sqrt{\frac{T_i}{m_i}+\frac{T_j}{m_j}} K_{ij}[f_i, f_j] \tag{2}$$

where angular integrations have been absorbed into the time scale. We call this model the two-rate Maxwell model (TRMM). The integer i goes from 1 to K, and K_{ij} is defined by

$$K_{ij}[f(\mathbf{v}), g(\mathbf{w})] = \int d\boldsymbol{\epsilon}\, d\mathbf{w} \frac{1}{\alpha_{ij}}[f(\mathbf{v}')g(\mathbf{w}') - f(\mathbf{v})g(\mathbf{w})]. \tag{3}$$

Because of the Maxwell-like structure of the collision operators, this set equation leads to a closed system of equations for the partial temperatures T_i. Straightforward calculations lead to the following expressions:

$$\frac{\partial T_i}{\partial t} = -x_i \sigma_i^{d-1}\sqrt{\frac{T_i}{m_i}}\frac{(1-\alpha_{ii}^2)}{2} T_i(t) + \sum_{j=1, j\neq i}^{K} \frac{x_j}{\sqrt{2}}\sigma_{ij}^{d-1}\sqrt{\frac{T_i}{m_i}+\frac{T_j}{m_j}}\mu_{ji}(1+\alpha_{ij}) \times\{[\mu_{ji}(1+\alpha_{ij}) - 2]T_i + \mu_{ij}(1+\alpha_{ij})T_j\}, \tag{4}$$

where we have introduced the normalized mass ratios $\mu_{ij} = m_i/(m_i+m_j)$. We rewrite this set into a more compact expression after defining the related $\epsilon_{ij} = 1 - \alpha_{ij}$:

$$\frac{\partial T_i}{\partial t} = \sum_{j=1}^{K} x_j \frac{\sigma_{ij}^{d-1}}{\sqrt{2}}\sqrt{\frac{T_i}{m_i}+\frac{T_j}{m_j}}\mu_{ij}(2-\epsilon_{ij}) \times[(-2\mu_{ij} - \mu_{ji}\epsilon_{ij})T_i + (2\mu_{ij} - \mu_{ij}\epsilon_{ij})T_j]. \tag{5}$$

The next step consists in introducing the quantities $R_i = T_i/T_1$, which measure the departure from energy equipartition. Obviously, the K quantities R_i, $i = 1, \ldots, K$, are equal to 1 when equipartition takes place, and R_1 is always equal to 1 by construction. We also rescale the time $d\tau = dt\sqrt{T_1(t)/m_1}$, thereby considering a time scale proportional to the average number of collision 1-1 in the system:

$$\begin{aligned}\partial_\tau R_i = &\sum_{j=1}^{K} x_j \frac{\sigma_{ij}^{d-1}}{\sqrt{2}}\sqrt{R_i\frac{m_1}{m_i}+R_j\frac{m_1}{m_j}}\mu_{ji}(2-\epsilon_{ij}) \times[(-2\mu_{ij} - \mu_{ji}\epsilon_{ij})R_i + (2\mu_{ij} - \mu_{ij}\epsilon_{ij})R_j] \\ &- R_i\sum_{j=1}^{K} x_j \frac{\sigma_{1j}^{d-1}}{\sqrt{2}}\sqrt{1+R_j\frac{m_1}{m_j}}\mu_{j1}(2-\epsilon_{1j}) \times[(-2\mu_{1j} - \mu_{j1}\epsilon_{1j}) + (2\mu_{1j} - \mu_{1j}\epsilon_{1j})R_j]\end{aligned} \tag{6}$$

where one verifies that $R_1 = 1$ as imposed by construction. In the following, we are interested in the stationary solutions for small inelasticity parameters. Therefore, we solve Eq. (6) by perturbation methods assuming that the quantities ϵ_{ij} are all small and of the same order of magnitude. The temperature ratios are written under the form $R_j = 1 + \epsilon R_j^1$, where ϵ is a small formal perturbation coefficient. This development is based on the fact that the zeroth order solution of Eq. (6) is $R_j = 1$, $\forall\ j$, which corresponds to equilibrium equipartition of energy. The stationary first order solution of Eq. (6) reads

$$\sum_{j=1}^{K} x_j \frac{2\sigma_{ij}^{d-1}}{\sqrt{2}}\sqrt{\frac{m_1}{m_i}+\frac{m_1}{m_j}}\mu_{ji}[2\mu_{ij}(R_j^1 - R_i^1) - \epsilon_{ij}) - \sum_{j=1}^{K} x_j \frac{2\sigma_{1j}^{d-1}}{\sqrt{2}}\sqrt{1+\frac{m_1}{m_j}}\mu_{j1}[2\mu_{1j}R_j^1 - \epsilon_{1j}) = 0. \tag{7}$$

In a system composed of two components, straightforward calculations lead to the relation

$$\frac{2m_2m_1}{(m_1+m_2)^2}R_2^1 = -\frac{\sigma_{11}^{d-1}}{\sigma_{12}^{d-1}}\sqrt{\frac{m_1}{m_1+m_2}}\frac{x_2}{\sqrt{2}}\epsilon_{22} + \frac{\sigma_{22}^{d-1}}{\sigma_{12}^{d-1}}\sqrt{\frac{m_2}{m_1+m_2}}\frac{x_1}{\sqrt{2}}\epsilon_{11} - \frac{(m_1x_1 - m_2x_2)}{(m_1+m_2)}\epsilon_{12} \tag{8}$$

where $R_1^1 = 0$ by definition. This expression gives the first order deviation to equipartition, in the limit of small inelasticity. Remarkably, solution (8) is exactly equivalent to the solution obtained by Garzo and Dufty [3] from the IHS Boltzmann equation in the low inelasticity limit.

III. ARBITRARY NUMBER OF COMPONENTS

In order to treat systems composed by a large number of species, it is helpful to rewrite Eq. (7) into the canonical form

$$A_i R_i^1 + \sum_{j=2, j\neq i}^{K} B_{ij} R_j^1 = C_i \tag{9}$$

where the coefficients read explicitly

$$A_i = 2x_i \frac{\sigma_{1i}^{d-1}\sqrt{m_1 m_i}}{(m_1+m_i)^{3/2}} + \sum_{j=1, j\neq j}^{K} 2x_j \frac{\sigma_{ij}^{d-1}\sqrt{m_i m_j}}{(m_i+m_j)^{3/2}},$$

$$C_i = \sum_{j=1}^{K} x_j \left(\frac{\sigma_{1j}^{d-1}\sqrt{m_j}}{\sqrt{m_1(m_1+m_j)}}\epsilon_{1j} - \frac{\sigma_{ij}^{d-1}\sqrt{m_j}}{\sqrt{m_i(m_i+m_j)}}\epsilon_{ij} \right),$$

$$B_{ij} = -2x_j \left(\sigma_{ij}^{d-1} \frac{\sqrt{m_i m_j}}{(m_i+m_j)^{3/2}} - \sigma_{1j}^{d-1} \frac{\sqrt{m_1 m_j}}{(m_1+m_j)^{3/2}} \right). \tag{10}$$

Consequently, the whole dynamical problem is reduced to the inversion of the matrix $\mathbf{M}$ defined by

$$M_{ij} = A_j \delta_{ij} + B_{ij}. \tag{11}$$

Unfortunately, this problem is not trivial in practice when the system is composed of a large number K of components (inversion of a $K-1$ matrix) and leads to analytical but intractable expressions for the R_j. In the following, we prefer to focus on a particular case which enormously simplifies the inversion of Eq. (9) and whose solutions R_j have a simple analytical form; namely, we consider a system where all particles have the same mass $m_j=m$ and the same diameter $\sigma_{ij}=\sigma$, but whose inelasticities ϵ_{ij} vary. Remarkably, in that case, all the nondiagonal terms B_{ij} vanish exactly, $B_{ij}=0$, so that the general solution of Eq. (10) reads

$$R_i^1 = \sum_{j=1}^{K} x_j(\epsilon_{1j} - \epsilon_{ij}). \tag{12}$$

This solution is instructive for several reasons. First, it is an expression for nonequipartition of energy in multicomponent mixtures. Equation (12) clearly shows that the system behaves qualitatively in the same way as in a binary inelastic mixture, namely, the partial temperatures T_i do not asymptotically reach the same value, but they remain proportional in the long time limit. This behavior justifies the derivation of granular hydrodynamics for complex mixtures (see [13] for binary mixtures). Another nice feature of Eq. (12) comes from its very simple expression, which allows us to recover the solution (8) when $K=2$, and which is easily generalized when the system is composed of an infinite number of species, namely, when there is a continuum of inelasticities in the system. In that case, instead of the concentrations x_i used in order to characterize the components, we use the concentration density $\rho(\iota)$, which represents the density of species ι. The probability normalization reads

$$\int d\iota\, \rho(\iota) = 1. \tag{13}$$

Relation (12) generalizes into

$$R(\iota) = \int d\iota' \rho(\iota')(\epsilon_{r\iota'} - \epsilon_{\iota\iota'}) \tag{14}$$

where r is the arbitrarily chosen reference species to which the temperatures are compared, $R(\iota)=T(\iota)/T(r)$.

We verify the validity of (12) by performing two kinds of computer simulations for the multicomponent mixture. The latter were performed for particles whose masses and diameters are equal, $m_i=1$ $\sigma_i=1$ in order to compare the results with (12). First, we make direct simulation Monte Carlo (DSMC) simulations of the set of kinetic equations (2), namely, we apply the standard DSMC algorithm, where the probability of collisions of a pair is taken to be proportional to $\sqrt{T_i+T_j}$. In the simulations, we considered a system composed of a large number $K=50$ of components. Moreover, each species is composed of the same number of particles,

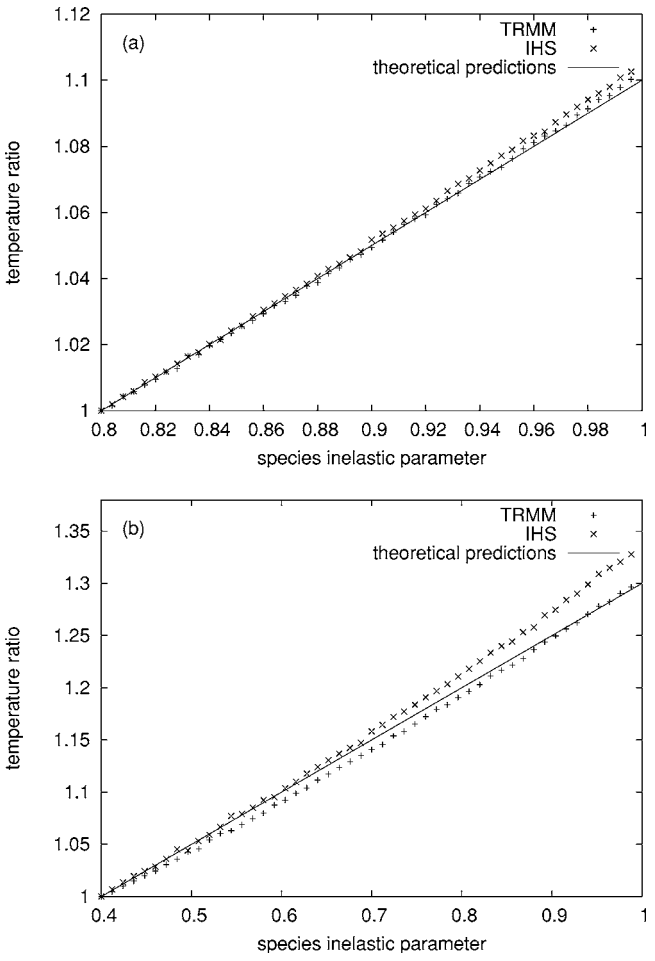

FIG. 1. Asymptotic temperature ratio, as a function of the inelasticity of each species, in a system where $\alpha_{min}=0.8$ (a) and $\alpha_{min}=0.4$ (b). The solid line corresponds to the theoretical predictions (15), while the data points correspond to DSMC simulations of TRMM and IHS.

$N_i=N_j$. This implies that the concentrations are equal to $x_i=\frac{1}{50}$. The species are discriminated by their inelasticities α_{ii}, which are all assumed to be different, and we chose the reference component to be the one with the lowest inelasticity: $\alpha_{11}<\alpha_{ii}$, $i>1$. This arbitrary choice suggests that the quantities R_i should be $\geqslant 1$ in the long time limit, given the fact that other components dissipate less energy than the reference component does. One should note, however, that the choice for the cross inelasticities α_{ij} can still be arbitrarily chosen provided they respect the symmetry relation $\alpha_{ij}=\alpha_{ji}$. For the sake of clarity, we choose for the cross inelasticities $\alpha_{ij}=(\alpha_i+\alpha_j)/2$. This simplification allows us to characterize each species i by their sole inelasticity α_{ii} instead of the vectorial quantity $(\alpha_{1i},\ldots,\alpha_{ii},\ldots,\alpha_{Ni})$, but it should be verified experimentally. It simplifies Eq. (12) into

$$R_j^1=\frac{1}{K}\sum_{n=1}^{K}\frac{1}{2}(\epsilon_1+\epsilon_n-\epsilon_j-\epsilon_n)=\frac{1}{2}(\epsilon_1-\epsilon_j). \qquad (15)$$

In the following simulations, we define a minimum and a maximum inelasticity in the system, α_{min} and α_{max}, respectively. By definition, we choose $\alpha_{11}=\alpha_{min}$. Then, we fill uniformly the interval $[\alpha_{min},\alpha_{max}]$, i.e., $\alpha_{ii}=\alpha_{min}+(i-1)\delta\alpha$, where the quantity $\delta\alpha$ is defined by $\delta\alpha=(\alpha_{max}-\alpha_{in})/50$. Let us stress that this uniform distribution in the interval $[\alpha_{min},\alpha_{max}]$ is an arbitrary choice, and that more general compositions can be considered without any analytical nor computational additional difficulty. In this work, we also perform DSMC simulations of the true set of inelastic Boltzmann equations for the same mixture, where no approximation is made to simplify the collision operator, thereby testing the validity of the TRMM. In Fig. 1, we present results in the small inelastic limit $\alpha_{min}=0.8$, which show an excellent agreement with Eq. (15), and in the high inelasticity limit $\alpha_{min}=0.4$, for which only small discrepancies from the predictions may occur, i.e., deviations do not exceed 15%.

IV. CONCLUSION

In this paper, we have focused on the nonequipartition of energy in inelastic gases composed of a large number of species. We have used mean field approximations, in order to simplify the set of Boltzmann equations, and to focus on an analytically tractable problem. By doing so, we have defined the two-rate Maxwell model, which we have solved formally in the small inelasticity limit, thereby deriving the explicit values for energy nonequipartition in systems where components have the same mass and diameter. These predictions have been verified by simulations for systems composed of 50 components, that show that the TRMM is a relevant model, even in very inelastic systems. At this point, it is important to note that the influence of the shape of the velocity distributions has not been taken into account by the mean field modeling. This is due to the Maxwell-like kernel of the collision operators, which leads to a closed set of equations for the partial temperatures, thereby neglecting the influence of higher velocity moments [14]. Nonetheless, this influence is usually weak and has no quantitative effect when the system is weakly inelastic. That was shown in the small inelasticity limit, both by the DSMC simulation results and by analytical comparisons with the exact inelastic Boltzmann equation. As a consequence, the TRMM is an ideal candidate in order to apprehend more complex phenomena in granular mixtures, such as hydrodynamics for a large number of components, or the detailed study of systems composed of a continuum species.

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