In general, the total kinetic energy in a multicomponent gas of inelastic and rough hard spheres is unequally partitioned among the different degrees of freedom. On the other hand, partial energy equipartition can be reached, in principle, under appropriate combinations of the mechanical parameters of the system. Assuming common values of the coefficients of restitution, in this paper we use kinetic-theory tools to determine the conditions under which the components of a granular mixture in the homogeneous cooling state have the same translational and rotational temperatures as those of a one-component granular gas (mimicry effect). Given the values of the concentrations and the size ratios, the mimicry effect requires the mass ratios to lie inside certain intervals and the smaller spheres to have a larger particle mass density than the bigger spheres. The theoretical predictions for the case of an impurity immersed in a host granular gas are compared against both DSMC and molecular dynamics simulations with a good agreement.

I. INTRODUCTION

Graeme Austin Bird was a gigantic figure in the field of rarefied gas dynamics. He developed an intuitive and original stochastic algorithm—the direct simulation Monte Carlo (DSMC) method—that obtains exact numerical solutions of the Boltzmann equation. The DSMC method boosted a fruitful new area of research with many important applications in science and engineering alike. This technique was later imported into the field of granular gas dynamics (gases of macroscopic particles that undergo collisions where energy is not preserved, i.e., inelastic collisions). Due to the flexibility of the DSMC technique, the adaptation of the method to inelastic collisions is relatively straightforward, even if rotational motion of grains is taken into account. The present work is a sincere tribute to G. A. Bird’s long-lasting influence and accomplishments.

One of the most intriguing phenomena displayed in granular gases (and not present in its molecular gas counterpart, where collisions are elastic) is the absence of energy equipartition among the different degrees of freedom, even in homogeneous and isotropic states. In particular, for systems of mechanically different grains (granular mixtures), the mean kinetic translational and rotational energies of each component are in general different. The lack of energy equipartition is also present in the special cases of monocomponent rough granular gases and smooth granular mixtures.

A simple but realistic way of accounting for the effect of inelasticity on the translational and rotational degrees of freedom is by means of a model of inelastic and rough hard spheres. In this model, collisions between spheres of components $i$ and $j$ are characterized by two independent constant coefficients of normal ($\alpha_{ij}$) and tangential ($\beta_{ij}$) restitution. While the coefficient $0 < \alpha_{ij} \leq 1$ characterizes the decrease in the magnitude of the normal component of the relative velocity of the points at contact of the colliding spheres, the coefficient $-1 \leq \beta_{ij} \leq 1$ takes into account the change of the tangential component of the relative velocity. Except for $\alpha_{ij} = 1$ and either $\beta_{ij} = -1$ (perfectly smooth spheres) or $\beta_{ij} = 1$ (perfectly rough spheres), the total kinetic energy is not conserved in a collision for this model. An interesting feature of the model is that the rotational and translational degrees of freedom of the spheres are coupled through the inelasticity of collisions.

Since the study of energy nonequipartition in gas mixtures of inelastic rough hard spheres is in general quite complex, it is convenient to consider simple nonequilibrium situations in order to gain some insight into more general problems. In this paper, we consider the so-called homogeneous cooling state (HCS), namely a spatially uniform state where the (granular) temperature monotonically decays in time.

As mentioned before, one of the novel features arising from inelasticity is that the partial temperatures (measuring the mean kinetic translational and rotational energies of each component) are in general different. More specifically, for a granular mixture one generally has $T^\text{rot}_{i} \neq T^\text{tr}_{i}$ for any component $i$, and $T^\text{rot}_{i} \neq T^\text{rot}_{j}$ and $T^\text{rot}_{i} \neq T^\text{rot}_{j}$ for any pair $i$ and $j$. Here, $T^\text{tr}_{i}$ and $T^\text{rot}_{i}$ refer to the translational and rotational temperatures, respectively, of component $i$. The HCS conditions for determining the dependence of the temperature ratios $T^\text{rot}_{i}/T^\text{tr}_{i}$, $T^\text{rot}_{j}/T^\text{tr}_{j}$, and $T^\text{rot}_{i}/T^\text{rot}_{j}$ on the set of coefficients of restitution ($\{\alpha_{ij}\}$ and $\{\beta_{ij}\}$), the concentrations, and the mechanical parameters of the mixture (masses, diameters, and moments of inertia) were obtained in Ref. 3 by neglecting (i) correlations between translational and angular velocities and (ii) deviations of the marginal translational velocity distribution from the Maxwellian. In spite of those approximations, the theoretical results for the temperature ratios have been recently shown to present a general good agreement with computer simulations in the tracer limit (a binary mixture where the
concentration of one of the components is negligible).

And yet, the fact that energy equipartition is in general violated in granular mixtures does not preclude that, under certain conditions, partial or total equipartition might be present. To simplify the analysis, we consider here mixtures with common coefficients of restitution \((\alpha, \beta)\) and reduced moment of inertia \((\kappa)\). Thus, the goal now is to explore whether a particular choice of concentrations, masses, and diameters of the mixture components leads to partial energy equipartition, namely \(T^\text{rot}_i = T^\text{rot}_s\) and \(T^\text{rot}_i = T^\text{rot}_s\) (for all \(i\)), so that the common rotational-to-translational temperature ratio \(T^\text{rot}_i / T^\text{rot}_s\) coincides with that of a one-component gas of inelastic rough hard spheres\(^{11,14}\). We can think of this phenomenon if we imagine that a number of intruder spheres are added to a one-component granular gas and their partial temperatures mimic the corresponding values of the host gas\(^{30,31}\). Our results show that in fact there are regions in the parameter space of an s-component system displaying this mimicry effect. More specifically, for given values of the \(s-1\) concentration parameters and the \(s-1\) diameter ratios, there are \(s-1\) conditions whose solution gives the \(s-1\) mass ratios where partial equipartition (in the sense described before) is possible.

To assess the accuracy of our approximate theoretical predictions, a comparison with computer simulations has also been carried out. In particular, we have numerically solved the Boltzmann kinetic equation via the DSMC method\(^{12}\). In addition, event-driven molecular dynamics (MD) simulations for very dilute systems have also been performed. While the DSMC results assess the reliability of the approximated solution (statistical independence of the translational and angular velocities plus Maxwellian translational distribution), the comparison against MD can be considered as a stringent test of the kinetic equation itself since MD avoids any assumption inherent to kinetic theory (molecular chaos hypothesis). The simulations have been performed in the simple case of a binary mixture \((s=2)\) where one of the components (say \(i=1\)) is present in tracer concentration (i.e., \(n_1/n_2 \to 0\), \(n_i\) being the number density of component \(i\)). This problem is equivalent to that of an impurity or intruder immersed in a granular gas of rough spheres (component 2). This implies that (a) the state of the excess component is not perturbed by the presence of the tracer particles (so that its velocity distribution function \(f_2\) obeys the closed Boltzmann equation for a one-component granular gas) and, additionally, (b) collisions among tracer particles can be neglected in the kinetic equation for the distribution function \(f_1\) (Boltzmann–Lorentz equation). In this limiting case, the three relevant temperature ratios (namely \(T_{1i}^\text{tr} / T_{2i}^\text{tr}\), \(T_{1i}^\text{rot} / T_{2i}^\text{rot}\), and \(T_{2i}^\text{rot} / T_{2i}^\text{tr}\)) are in general functions of \(\alpha, \beta, \kappa\), the mass ratio \(m_1/m_2\), and the diameter ratio \(\sigma_1/\sigma_2\). As we will see, the (approximate) conditions for mimicry (i.e., \(T_{1i}^\text{tr} / T_{2i}^\text{tr} = 1\), \(T_{1i}^\text{rot} / T_{2i}^\text{rot} = T_{2i}^\text{rot} / T_{2i}^\text{tr}\)) turn out to be independent of \(\alpha, \beta, \) and \(\kappa\).

The paper is organized as follows. The kinetic theory for multicomponent granular gases is briefly summarized in Sec. III. Section III deals with the explicit determination of the so-called production rates when the marginal translational distribution is approximated by a Maxwellian distribution. Starting from these general expressions, the conditions for the mimicry effect are obtained in Sec. IV for an s-component mixture and, next, particularized to a binary mixture \((s=2)\). Section V focuses on the comparison between the approximate results and computer simulations performed in the tracer limit for some representative systems. The paper is closed in Sec. VI with a brief discussion of the main results reported here.

II. BOLTZMANN EQUATION FOR GRANULAR MIXTURES OF ROUGH SPHERES

We consider an s-component gas of inelastic rough hard spheres. Particles of component \(i\) have a mass \(m_i\), a diameter \(\sigma_i\), and a moment of inertia \(I_i = \kappa_i m_i \sigma_i^2 / 4\). The reduced moment of inertia \(\kappa_i\) ranges from \(\kappa_i = 0\) (mass concentrated in the center) to \(\kappa_i = \frac{2}{3}\) (mass concentrated in the surface). If the mass of a particle of component \(i\) is uniformly distributed, then \(\kappa_i = \frac{2}{3}\). The inelasticity and roughness of colliding particles are characterized by the set of coefficients of normal \((\alpha_{ij})\) and tangential \((\beta_{ij})\) restitution. Those coefficients of restitution are defined by the collision rule

\[
\sigma \cdot w'_{ij} = -\alpha_{ij} \sigma \cdot w_{ij}, \quad \sigma \times w'_{ij} = -\beta_{ij} \sigma \times w_{ij},
\]

where \(w_{ij}\) and \(w'_{ij}\) are the pre- and post-collisional relative velocities of the points at contact of two colliding spheres of components \(i\) and \(j\), while \(\sigma\) is the unit vector joining their centers. While the coefficient \(\alpha_{ij}\) ranges from \(\alpha_{ij} = 0\) (perfectly inelastic particles) to \(\alpha_{ij} = 1\) (perfectly elastic particles), the coefficient \(\beta_{ij}\) runs from \(\beta_{ij} = -1\) (perfectly smooth particles) to \(\beta_{ij} = 1\) (perfectly rough particles). Except if \(\alpha_{ij} = 1\) and \(|\beta_{ij}| = 1\), kinetic energy is dissipated upon a collision \(ij\).

At a kinetic level, all the relevant information is contained in the velocity distribution function \(f_i(v, \omega; t)\) of each component, where we have particularized to homogeneous states. Here, \(v\) and \(\omega\) denote the translational and angular velocities, respectively. From the knowledge of \(f_i\) one can obtain the number density and the so-called translational and rotational (partial) temperatures of component \(i\) as

\[
n_i = \int dv \int d\omega f_i(v, \omega; t),
\]

\[
T_i^\text{tr}(t) = \frac{m_i}{3 n_i} \int dv \int d\omega v^2 f_i(v, \omega; t),
\]

\[
T_i^\text{rot}(t) = \frac{I_i}{3 n_i} \int dv \int d\omega \omega^2 f_i(v, \omega; t).
\]
As a measure of the total kinetic energy per particle, one can define the global temperature as

\[ T = \sum_{i=1}^{s} \frac{n_i}{n} (T_i^{tr} + T_i^{rot}), \]  

(2.3)

where \( n = \sum_{i=1}^{s} n_i \) is the total number density.

In the low density regime \((n_i \sigma_i^3 \ll 1)\), the velocity distribution functions obey a closed set of coupled Boltzmann equations:

\[ \partial_t f_i(\mathbf{v}, \omega; t) = \sum_{j=1}^{s} J_{ij}[\mathbf{v}, \omega; t | f_i, f_j], \]  

(2.4)

where

\[ J_{ij}[\mathbf{v}, \omega; t | f_i, f_j] = \sigma_{ij}^2 \int d\mathbf{v}_2 \int d\omega_2 \int d\tilde{\mathbf{\sigma}} \times \Theta(\mathbf{v}_{12} \cdot \tilde{\mathbf{\sigma}})(\mathbf{v}_{12} \cdot \tilde{\mathbf{\sigma}}) \left[ \frac{1}{\alpha_{ij}^{\prime} \beta_{ij}^{\prime}} f_i(\mathbf{v}_1^{\prime \prime}, \omega_1^{\prime \prime}; t) f_j(\mathbf{v}_2^{\prime \prime}, \omega_2^{\prime \prime}; t) - f_i(\mathbf{v}_1, \omega_1; t) f_j(\mathbf{v}_2, \omega_2; t) \right], \]  

(2.5)

is the collision operator. Here, \( \Theta(x) \) is the Heaviside step function, \( \sigma_{ij} \equiv (\alpha_i + \sigma_j)/2 \), \( \mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2 \) is the relative translational velocity, and the double primes denote precollisional velocities. Note that Eq. (2.4) describes a freely cooling (or undriven) granular gas, so that the total translational velocity, and the double primes denote distribution functions obey a closed set of coupled Boltzmann equations.

\[ \partial_i T_i^{tr} = -\xi_i^{tr} T_i, \]  

\[ \partial_i T_i^{rot} = -\xi_i^{rot} T_i, \]  

(2.6)

with

\[ \xi_i^{tr} = \sum_{j=1}^{s} \xi_{ij}^{tr}, \quad \xi_i^{rot} = \sum_{j=1}^{s} \xi_{ij}^{rot}. \]  

(2.7)

Here,

\[ \xi_i^{tr} \equiv -\frac{m_i}{3 n_i T_i^{tr}} \int d\mathbf{v} \int d\omega \, \mathbf{v}_2^2 J_{ij}[\mathbf{v}, \omega; t | f_i, f_j], \]  

(2.8a)

\[ \xi_i^{rot} \equiv -\frac{I_i}{3 n_i T_i^{rot}} \int d\mathbf{v} \int d\omega \, \mathbf{v}_2^2 J_{ij}[\mathbf{v}, \omega; t | f_i, f_j], \]  

(2.8b)

are energy production rates.

After a certain transient stage, a scaling regime is expected to be reached (the so-called HCS) such that all the time dependence of the distributions \( f_i \) occurs through the total temperature \( T \). This implies \( \partial_i (T_i^{tr}/T) = \partial_i (T_i^{rot}/T) = 0 \) for all \( i \), and hence

\[ \xi_i^{tr} = \cdots = \xi_s^{tr} = \xi_1^{rot} = \cdots = \xi_s^{rot}. \]  

(2.9)

It must be stressed that the energy production rates \( \xi_{ij}^{tr} \) and \( \xi_{ij}^{rot} \) are in general complex functionals of the distribution functions \( f_i \) and \( f_j \), so that the set of Eqs. (2.4) is not closed and Eq. (2.9) cannot be solved exactly, unless an approximate closure is assumed.

### III. MAXWELLIAN APPROXIMATION

In order to determine the production rates \( \xi_{ij}^{tr} \) and \( \xi_{ij}^{rot} \) in terms of the partial temperatures \( T_i^{tr}, T_i^{rot}, T_j^{tr}, \) and \( T_j^{rot} \), we assume that the velocity distributions in Eqs. (2.8) can be approximated by considering that (i) the translational and rotational velocities are statistically independent and (ii) the marginal translational distribution is a Maxwellian function. More specifically,

\[ f_i(\mathbf{v}, \omega) \rightarrow \left( \frac{m_i}{2 \pi T_i^{tr}} \right)^{3/2} \exp \left( -\frac{m_i \mathbf{v}^2}{2 T_i^{tr}} \right) f_i^{rot}(\omega), \]  

(3.1)

where \( f_i^{rot}(\omega) \) is the marginal rotational distribution function. By inserting Eq. (3.1) into Eqs. (2.8), and after some algebra, one obtains the explicit expressions:

\[ m_{ij} \equiv \frac{m_i m_j}{m_i + m_j}, \quad \kappa_{ij} \equiv \kappa_i \kappa_j \frac{m_i + m_j}{\kappa_i m_i + \kappa_j m_j}. \]  

(3.3b)

where we have introduced the quantities

\[ \alpha_{ij} \equiv 1 + \alpha_{ij}, \quad \beta_{ij} \equiv \frac{\kappa_{ij}}{1 + \kappa_{ij}} (1 + \beta_{ij}). \]  

(3.3a)
The temperature ratios are plotted vs the mass ratio $m_1/m_2$ at equal sizes ($\sigma_1/\sigma_2 = 1$). In both cases, $\alpha = 0.8$ and $\beta = 0$. The effective collision frequencies

$$\nu_{ij} \equiv 2\sqrt{2\pi}n_i\sigma_{ij}^2\sqrt{\frac{T_{1}^{\text{rot}}}{m_i} + \frac{T_{i}^{\text{tr}}}{m_j}}, \quad (3.4)$$

In summary, in an $s$-component mixture, insertion of Eqs. (3.2) into Eq. (2.9) provides a closed set of $2s - 1$ coupled algebraic equations for the $2s - 1$ independent temperature ratios, which in general must be solved numerically. Despite the simplicity of the approximation (3.1), numerical results obtained from the DSMC and MD methods for a binary mixture with a tracer component compare very well with the theoretical results derived from Eqs. (3.2).

The parameter space in an $s$-component mixture is made of $s^2 + 5s - 3$ quantities: $s(s + 1)/2$ coefficients of normal restitution, $s(s + 1)/2$ coefficients of tangential restitution, $s - 1$ mole fractions, $s - 1$ mass ratios, $s - 1$ diameter ratios, and $s$ reduced moments of inertia. To illustrate the impact of both mass and size on the temperature ratios, let us consider a binary mixture ($s = 2$) with common coefficients of restitution and common reduced moments of inertia (i.e., $\alpha_{ij} = \alpha$, $\beta_{ij} = \beta$, and $\kappa_i = \kappa$). Without loss of generality we assume that $n_1 \leq n_2$. Otherwise, the size ratio $\sigma_1/\sigma_2$ and the mass ratio $m_1/m_2$ are arbitrary.

Let us first suppose that $m_1/m_2 = 1$ and qualitatively analyze the influence of the diameter ratio $\sigma_1/\sigma_2$ on the component-component temperature ratios $T_1^{\text{rot}}/T_2^{\text{rot}}$ and $T_1^{\text{rot}}/T_2^{\text{rot}}$. According to Eq. (3.3), if $\sigma_1/\sigma_2 < 1$ component 1 collides less frequently than component 2 and hence it dissipates less kinetic energy. Therefore, one may expect $T_1^{\text{rot}}/T_2^{\text{rot}} < 1$ and $T_1^{\text{rot}}/T_2^{\text{rot}} > 1$. The opposite can be expected if $\sigma_1/\sigma_2 > 1$. This qualitative analysis is confirmed by Fig. 1(a) for a representative case, where it can be observed that the temperature ratios $T_1^{\text{rot}}/T_2^{\text{rot}}$ and $T_1^{\text{rot}}/T_2^{\text{rot}}$ monotonically decrease with increasing $\sigma_1/\sigma_2$, regardless of the value of the concentration. As for the influence of the mass ratio (assuming now $\sigma_1/\sigma_2 = 1$), it is less straightforward than the influence of the size ratio. If initially all the temperatures are equal, Eqs. (3.2) and (3.3) show that the more massive particles have a smaller cooling rate. As a consequence, once the asymptotic HCS is reached, one expects the more massive spheres to have a higher temperature. This is confirmed by Fig. 1(b), which shows a monotonic increase of both $T_1^{\text{rot}}/T_2^{\text{rot}}$ and $T_1^{\text{rot}}/T_2^{\text{rot}}$ in Eq. 1(b), with increasing $m_1/m_2$, again with independence of the concentration.

Typically, the bigger spheres are also the heavier ones and, therefore, whether the ratios $T_1^{\text{rot}}/T_2^{\text{rot}}$ and $T_1^{\text{rot}}/T_2^{\text{rot}}$ are smaller or larger than unity results from the competition between both mechanisms exemplified by Fig. 1. Thus, it might be possible that a certain coupling between $\sigma_1/\sigma_2$ and $m_1/m_2$ leads to $T_1^{\text{rot}}/T_2^{\text{rot}} = 1$ and $T_1^{\text{rot}}/T_2^{\text{rot}} = 1$. As mentioned in Sec. IV this is what we refer to as the mimicry effect.

IV. MIMICRY EFFECT

Let us consider again an $s$-component mixture particularized to the case of equal coefficients of restitution and reduced moments of inertia, i.e., $\alpha_{ij} = \alpha$, $\beta_{ij} = \beta$, and $\kappa_i = \kappa$. The question we want to address is under which conditions the mixture exhibits partial equipartition in the sense that $T_1^{\text{rot}} = T_2^{\text{rot}}$ and $T_1^{\text{rot}} = T_2^{\text{rot}}$, even though $T_1^{\text{tr}} \neq T_2^{\text{tr}}$, the ratio $T_1^{\text{rot}}/T_2^{\text{rot}}$ being the same as that of a one-component granular gas.\[11,14\] If that is the case, we can say that the mixture mimics a one-component gas in the above sense.

By setting $T_1^{\text{rot}} = T_2^{\text{rot}}$ and $T_1^{\text{rot}} = T_2^{\text{rot}}$ in Eqs. (3.2), one obtains

$$\xi_{ij}^{\text{tr}} = X_{ij}\sqrt{T_1^{\text{rot}}F_1^{\text{rot}}(\theta)}, \quad (4.1a)$$

$$\xi_{ij}^{\text{rot}} = X_{ij}\sqrt{T_1^{\text{rot}}F_1^{\text{rot}}(\theta)}, \quad (4.1b)$$
where \( \theta \equiv T_{\text{rot}}/T_{\text{tr}} \) and

\[
X_{ij} = \frac{4\sqrt{2\pi}}{3} \sqrt{m_{ij}n_1\sigma_{ij}^2} m_1, \tag{4.2a}
\]

\[
F_{\text{tr}}(\theta) = \overline{\alpha}(2 - \overline{\alpha}) + \overline{\beta}(2 - \overline{\beta}) - \frac{\overline{\beta}^2}{\kappa} \theta, \tag{4.2b}
\]

\[
F_{\text{rot}}(\theta) = \frac{\overline{\beta}}{\kappa^2 \theta} \left[ (2\kappa - \overline{\beta})\theta - \overline{\beta}^2 \right]. \tag{4.2c}
\]

Here, according to Eqs. (4.3), \( \overline{\alpha} = 1 + \alpha \) and \( \overline{\beta} = (1 + \beta)/\kappa \). It is noteworthy that in the factorizations (4.1) the quantity \( X_{ij} \), which is the same in \( \xi_{ij}^r \) and \( \xi_{ij}^\alpha \), depends only on the concentrations, masses, and diameters of the spheres. In contrast, the functions \( F_{\text{tr}}(\theta) \) and \( F_{\text{rot}}(\theta) \) only depend on the temperature ratio \( \theta \) and the mechanical parameters \( \alpha, \beta, \) and \( \kappa \).

The HCS conditions (2.9) decouple into

\[
X_1 = \cdots = X_s, \quad X_i = \sum_{j=1}^s X_{ij}, \tag{4.3}
\]

and \( F_{\text{tr}}(\theta) = F_{\text{rot}}(\theta) \). From the latter equality, one easily gets

\[
\theta = \sqrt{1 + h^2} + h, \tag{4.4a}
\]

\[
h = \frac{(1 + \kappa)^2}{2\kappa(1 + \beta)^2} \left[ 1 - \alpha^2 - (1 - \beta^2)\frac{1 - \kappa}{1 + \kappa} \right]. \tag{4.4b}
\]

For a general \( s \)-component mixture, Eq. (4.3) gives \( s - 1 \) conditions for the \( 3(s - 1) \) density, mass, and diameter ratios. In the particular case of a binary mixture (\( s = 2 \)), the single condition on \( n_1/n_2, m_1/m_2, \) and \( \sigma_1/\sigma_2 \) is

\[
\frac{n_1}{n_2} = \frac{(1 + \sigma_1/\sigma_2)^2 \sqrt{m_1/m_2} - 4 \sqrt{m_1+m_2}}{(1 + \sigma_2/\sigma_1)^2 \sqrt{m_1/m_2} - 4 \sqrt{m_1+m_2}} \tag{4.5}
\]

Equation (4.5) is equivalent to a quadratic equation for \( \sigma_1/\sigma_2 \) and a quartic equation for \( m_1/m_2 \).

Figure 2 plots the values of \( m_1/m_2 \) vs \( \sigma_1/\sigma_2 \) exhibiting the mimicry effect for two extreme concentrations, i.e., \( n_1/n_2 \to 0 \) (tracer limit) and \( n_1/n_2 = 1 \) (equimolar mixture). The curves corresponding to intermediate concentrations lie in the region between those two lines. A weak influence of the concentration can be observed, except if \( \sigma_1/\sigma_2 \) is very large. Given a value of \( n_1/n_2 \), the locus \( m_1/m_2 \) vs \( \sigma_1/\sigma_2 \) splits the plane into two regions. In the points below the locus curve, \( T_{\text{tr}}^1 < T_{\text{rot}}^1 \) and \( T_{\text{tr}}^1 < T_{\text{rot}}^2 \) as a consequence of the competition between the size and mass effects previously discussed in connection with Fig. 1. Alternatively, \( T_{\text{tr}}^1 > T_{\text{rot}}^1 \) and \( T_{\text{tr}}^1 > T_{\text{rot}}^2 \) in the points above the locus curve. It is interesting to note that the curve representing equal particle mass density, \( m_1/m_2 = (\sigma_1/\sigma_2)^3 \), lies below the mimicry curve if \( \sigma_1 < \sigma_2 \) and above it if \( \sigma_1 > \sigma_2 \). Thus, if the mass density of both types of spheres is the same, the bigger spheres have a larger (translational or rotational) temperature than the smaller spheres. On the other hand, the mimicry effect requires the bigger spheres to be less dense than the smaller spheres.

In the special tracer limit (\( n_1/n_2 \to 0 \)), the quartic equation for the mass ratio reduces to a quadratic equation whose solution is

\[
\frac{m_1}{m_2} = \frac{1}{2} \left[ \sqrt{1 + \frac{1}{2} \left( 1 + \frac{\sigma_1}{\sigma_2} \right)^4} - 1 \right]. \tag{4.6}
\]

In this tracer limit, \( m_1/m_2 \) has a lower bound \( \mu_-(0) = \sqrt{3}/2 - 1/2 \approx 0.11 \) (corresponding to \( \sigma_1/\sigma_2 \to 0 \)) but it does not have any upper bound. However, for finite concentration (\( n_1/n_2 \neq 0 \)), an additional finite upper bound (corresponding to \( \sigma_1/\sigma_2 \to \infty \) exists, namely

\[
\mu_-(n_1/n_2) \leq m_1/m_2 \leq \mu_+(n_1/n_2), \tag{4.7}
\]

\[
\mu_-(x) = \frac{2\sqrt{2}\sqrt{3 + x - x^2} - x - 4}{8 - x^2}, \quad \mu_+(x) = \frac{1}{\mu_-(x-1)}.
\]

The dependence of \( \mu_-(n_1/n_2) \) and \( \mu_+(n_1/n_2) \) on the concentration parameter \( n_1/n_2 \) is shown in Fig. 2. We observe that \( \mu_-(n_1/n_2) \) presents a very weak dependence on the concentration. On the other hand, \( \mu_+(n_1/n_2) \) increases rapidly as one approaches the tracer limit, diverging at \( n_1/n_2 = 0 \). The mimicry effect is possible only inside the shaded region of Fig. 2 outside of that region, Eq. (4.5) fails to provide physical solutions for \( \sigma_1/\sigma_2 \).

Since the mimicry conditions (4.3) are independent of the values of \( \alpha, \beta, \) and \( \kappa \), they are the same conditions for equipartition in the smooth-sphere case (\( \beta = -1 \), where
only the translational temperatures are relevant. In the rough-sphere case, however, full equipartition is not fulfilled since $T_{tr}$ and $T_{rot}$ are, in general, different. A complete energy equipartition (i.e., $T_{tr} = T_{rot}$) is achieved if $E_{tr}(1) = E_{rot}(1)$, i.e., $a^2(1 + \kappa) = b^2(1 - \kappa) + 2\kappa$.

V. COMPARISON WITH COMPUTER SIMULATIONS

The theoretical predictions discussed in Sec. IV for the mimicry effect are based on the simple ansatz (3.1). On the other hand, previous results show that statistical correlations between the translational and angular velocities, as well as cumulants of the translational distribution, can be observed. Therefore, it is important to assess the reliability of the theoretical results based on Eq. (3.1) by comparison with computer simulations.

For the sake simplicity, we consider here an intruder (component 1) immersed in a one-component granular gas (component 2). This is equivalent to a binary mixture in the tracer limit ($n_1/n_2 \rightarrow 0$). In addition, $\alpha_{12} = \alpha_{22} = \alpha$, $\beta_{12} = \beta_{22} = \beta$, and $\kappa_1 = \kappa_2 = \kappa$. Two representative cases are studied: a small intruder ($\sigma_1/\sigma_2 = 1/2$) and a big intruder ($\sigma_1/\sigma_2 = 2$). The masses of the intruders are taken as the values for which, according to Eq. (4.6), a mimicry effect is expected. More specifically, $m_1/m_2 = \frac{113}{28} - \frac{1}{2} \simeq 0.440$ and $m_1/m_2 = \frac{22}{15} - \frac{1}{2} \simeq 2.721$ for $\sigma_1/\sigma_2 = 1/2$ and $\sigma_1/\sigma_2 = 2$, respectively. Thus, the small intruder is $(m_1/\sigma_1^2)/(m_2/\sigma_2^2) = 3.52$ times denser than a particle of the host gas, while the big intruder is $(m_2/\sigma_2^2)/(m_1/\sigma_1^2) = 2.94$ times less dense than a particle of the host gas.

In the simulations, the values of the coefficient of tangential restitution are $\beta = -0.75$, $-0.25$, $0.25$, $0.75$ (DSMC) and $\beta = -0.5$, $0$, $0.5$, $1$ (MD), while the coefficient of normal restitution in both sorts of simulation is chosen as $\alpha = 0.9$. Figure 4 displays the simulation values of the three independent temperature ratios $T_{tr}^1/T_{tr}^2$ and $T_{rot}^1/T_{rot}^2$ (panel (a)), $T_{rot}^1/T_{tr}^1$, and $T_{rot}^2/T_{tr}^2$ (panel (b)). One can observe from Fig. 4(a) that the translational temperatures of both the small and big intruders are indeed very close to that of the host gas. The larger deviation of $T_{tr}^1/T_{tr}^2$ from unity (about 5%) appears at $\beta = 1$, but even in that case $T_{tr}^1$ is practically the same for the small and big intruders. As a complement, Fig. 4(b) exhibits a rather good collapse of the rotational-to-translational temperature ratio for the small and big intruders and the host gas. On the other hand, the simulation data show

![FIG. 3. Plot of $\mu_-(n_1/n_2)$ (lower curve) and $\mu_+(n_1/n_2)$ (upper curve) vs the concentration parameter $n_1/n_2$. The mimicry effect is possible only in the region $\mu_-(n_1/n_2) \leq m_1/m_2 \leq \mu_+(n_1/n_2)$.](image.png)

![FIG. 4. Plot of the simulation results for (a) $T_{tr}^1/T_{tr}^2$ and (b) $T_{rot}^1/T_{rot}^2$ (i = 1, 2) vs the coefficient of tangential restitution $\beta$ at $\alpha = 0.9$ and $\kappa = \frac{1}{2}$. In panels (a) and (b) the (red) down triangles correspond to a small intruder with $\sigma_1/\sigma_2 = 1/2$ and $m_1/m_2 = 0.440$, while the (blue) up triangles correspond to a big intruder with $\sigma_1/\sigma_2 = 2$ and $m_1/m_2 = 2.721$. In panel (b) the (black) circles represent DSMC data and the open symbols at $\beta = -0.5, 0, 0.5, 1$ represent MD data. The error bars are of similar size as the symbols.](image.png)
VI. DISCUSSION

It is well known that in a multicomponent gas of inelastic and rough hard spheres the total kinetic energy is not equally partitioned among the different degrees of freedom. This implies that the translational and rotational temperatures associated with each component are in general different.

It is of physical interest to find regions of the system’s parameter space where a certain degree of energy equipartition shows up (effect that we denote as mimicry). Here, we have focused on the HCS of systems with common values of the coefficients of normal and tangential restitution (i.e., $\alpha_{ij} = \alpha$, $\beta_{ij} = \beta$), as well as of the reduced moment of inertia (i.e., $\kappa_i = \kappa$), and have addressed the question of whether all the components of the mixture mimic a one-component system in the sense that they adopt the same rotational and translational temperatures as the latter.

From a simple approximation, where (i) the statistical correlations between the translational and angular velocities are neglected and (ii) the marginal translational distribution function is approximated by a Maxwellian, we have determined the conditions (3.3) for the mimicry effect. Interestingly, those approximate conditions are “universal” in the sense that they are independent of the values of $\alpha$, $\beta$, and $\kappa$. In fact, they are the same conditions as for equipartition in the case of smooth spheres ($\beta = -1$). For a mixture with an arbitrary number of components, and given the mole fractions and the diameter ratios, those conditions provide the mass ratios for which mimicry is present. In the particular case of a binary mixture, there is a single condition given by Eq. (A.2). As can be seen from Fig. 4, the mass ratio has lower and upper bounds, which depend on the concentration. This means that if the mass ratio is outside of the above interval, no mimicry effect is possible, no matter the value of the size ratio.

To assess the theoretical predictions, computer simulations have been carried out in the tracer (or impurity) limit, where the mimicry condition becomes quite simple, as can be seen from Eq. (4.10). Both DSMC and MD simulations present a good agreement with the theoretical results, as shown in Fig. 4. While the DSMC results gauge the reliability of the assumptions (i) and (ii) described in the preceding paragraph, the MD results go beyond that, since they are free from the molecular chaos assumption. Therefore, the agreement between the kinetic theory approximations and the MD data can be considered as a relevant result of the present paper.

The simplicity of the theoretical analysis for mimicry carried out in this work is heavily based on the assumption that the coefficients of normal and tangential restitution and the reduced moment of inertia of the impurity are the same as those of the particles of the host gas. This seems to be at odds with the fact that the mimicry effect requires the smaller spheres to have a higher particle mass density than the bigger spheres. A way of circumventing this problem is by tailoring the impurity particles with a nonuniform mass distribution made of three concentric shells, so that the external shell is made of the same material as that of the host particles. This is worked out in the Appendix.

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Appendix: Tailoring the moment of inertia and mass of a sphere

Consider a sphere of mass $m_1$ and radius $R_1 = 4\sigma_1$ with a nonuniform radial distribution of mass. More specifically, we assume that the sphere is made of an inner core of density $\rho_A$ and radius $R_A$, a spherical shell of density $\rho_B$ and radii $R_A$ and $R_B$, and finally an outer spherical shell of density $\rho_2$ and radii $R_B$ and $R_1$ [see Fig. 5(a)]. The total mass of the sphere is

$$m_1 = \frac{4\pi}{3} \left[ \rho_A R_A^3 + \rho_B (R_B^3 - R_A^3) + \rho_2 (R_1^3 - R_B^3) \right],$$

(A.1)

so that the average density is

$$\rho_1 = \frac{\frac{4\pi}{3} R_1^3}{m_1} = \rho_A z_A^3 + \rho_B (z_B^3 - z_A^3) + \rho_2 (1 - z_B^3),$$

(A.2)

where $z_A \equiv R_A/R_1$ and $z_B \equiv R_B/R_1$. Note that $0 < z_A < z_B < 1$. Equation (A.2) expresses $\rho_1$ as a weighted...
average of \( \rho_A, \rho_B, \) and \( \rho_2. \) Obviously, \( \min\{\rho_A, \rho_B, \rho_2\} \leq \rho_1 \leq \max\{\rho_A, \rho_B, \rho_2\}. \)

The moment of inertia of a spherical shell of density \( \rho_B \) and radii \( R_A \) and \( R_B \) is \( \frac{2}{5} \rho_B (R_B^2 - R_A^2). \) Thus, the moment of inertia of our sphere is

\[
I_1 = \frac{8\pi}{15} \left[ \rho_A R_A^5 + \rho_B (R_B^2 - R_A^2) \rho_2 (R_1^2 - R_B^2) \right],
\]

its reduced value being

\[
\kappa = \frac{I_1}{m_1 R_1^2} = \frac{2}{5} \left[ \frac{\rho_A}{\rho_1} z_A^5 + \frac{\rho_B}{\rho_1} (z_B^5 - z_A^5) + \frac{\rho_2}{\rho_1} (1 - z_B^5) \right].
\]

Therefore, given \( \rho_A/\rho_1, \rho_B/\rho_1, \rho_2/\rho_1, \) and \( \kappa, \) Eqs. (A.2) and (A.4) allow one to obtain \( z_A \) and \( z_B. \)

Henceforth, we assume that the particle mimics a sphere with a uniform mass distribution, i.e., \( \kappa = \frac{2}{5}. \) In that case, Eqs. (A.2) and (A.4) can be rewritten as

\[
1 = Y_{BA} z_B^3 - Y_{BA} z_A^3 = Y_{BA} z_B^5 - Y_{BA} z_A^5,
\]

where

\[
Y_{BA} \equiv \frac{\rho_B - \rho_2}{\rho_1 - \rho_2}, \quad Y_{BA} \equiv \frac{\rho_B - \rho_A}{\rho_1 - \rho_2}. \]

It can be checked that the condition \( 0 < z_A < z_B < 1 \) implies \( 1 < Y_{BA} < 1 + Y_{BA}, \) which yields \( \rho_A < \rho_1 < \rho_B \) and \( \rho_B < \rho_1 < \rho_A \) for \( \rho_1 > \rho_B \) and \( \rho_1 < \rho_B, \) respectively. For the sake of simplicity, let us choose the same density for the inner core and the outer shell, i.e., \( \rho_A = \rho_B. \) In that case, \( Y_{BA} = Y_{BA} = Y \) and Eq. (A.5) yields

\[
1 = z_B^3 - z_A^3 = z_B^5 - z_A^5.
\]

In particular, if \( Y = 2 \) the solution is \( z_A = 0.605907, \)
\( z_B = 0.897293. \)

In the case of a (big) intruder with \( \sigma_1/\sigma_2 = 2 \) and \( m_1/m_2 = 2.721 \) [see Fig. (a)], then \( \rho_1/\rho_2 = m_1 \sigma_2^2/\sigma_2^2 = 0.34 \) and \( (1 - \rho_1/\rho_2)^{-1} = 1.52, \) so it is possible to choose \( Y = 2. \) In such a case, the density of the middle shell is \( \rho_B/\rho_2 = 1 - 2\rho_1/\rho_2 = 0.32. \)

Alternatively, for a (small) intruder with \( \sigma_1/\sigma_2 = \frac{1}{2} \) and \( m_1/m_2 = 0.440 \) [see Fig. (b)], \( \rho_1/\rho_2 = m_1 \sigma_2^2/\sigma_2^2 = 3.52. \) If we again choose \( Y = 2, \) the density of the middle shell is \( \rho_B/\rho_2 = 2\rho_1/\rho_2 - 1 = 6.04. \)

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