

TRANSPORT COEFFICIENTS FOR GRANULAR MIXTURES AT LOW DENSITY

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I. INTRODUCTION

- Granular media under rapid flow conditions → hydrodynamic-like type equations.
- Low-density regime: Boltzmann kinetic theory for *inelastic* hard spheres. Chapman-Enskog method: *normal* solution as a perturbation expansion in the hydrodynamic gradients.
- Transport coefficients as functions of the restitution coefficient and other parameters. Issue widely covered for monocomponent systems [Brey, Dufty, Kim and Santos, Phys. Rev. E (1998); Garzó and Dufty, Phys. Rev. E (1999); Garzó and Montanero, Physica A (2002)].
- Real granular systems characterized by some degrees of polydispersity in density and size: *Multicomponent* granular mixtures.

- Previous studies: Jenkins and Mancini, J. Appl. Mech. 1987; Phys. Fluids 1989; Zamankhan, Phys. Rev. E 1995; Arnarson and Willits, Phys. Fluids 1998; 1999.
- Limited to the quasi-elastic limit ($\alpha \simeq 1$). Reference state: Maxwellians at the same temperature. However, many recent studies (theory, simulations, experiments) have shown the *breakdown of energy equipartition*.
- **Motivation**: Determination of transport coefficients by using a kinetic theory which takes into account the effect of temperature differences on them.

2. GRANULAR BINARY MIXTURES. BOLTZMANN EQUATION (BE)

- Binary mixture: $\{m_1, m_2, \sigma_1, \sigma_2, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$.
- Extension of the BE to the multicomponent case: $f_i(\mathbf{r}, \mathbf{v}, t)$ ($i \equiv 1, 2$).

$$(\partial_t + \mathbf{v}_1 \cdot \nabla) f_i(\mathbf{v}_1) = \sum_j J_{ij}[\mathbf{v}_1 | f_i, f_j] .$$

$$J_{ij}[f_i, f_j] = \sigma_{ij}^2 \int d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) [\alpha_{ij}^{-2} f_i(\mathbf{v}'_1) f_j(\mathbf{v}'_2) - f_i(\mathbf{v}_1) f_j(\mathbf{v}_2)] .$$

- Collision rules:

$$\begin{aligned} \mathbf{v}'_1 &= \mathbf{v}_1 - \mu_{ji} (1 + \alpha_{ij}^{-1}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \hat{\boldsymbol{\sigma}}, \\ \mathbf{v}'_2 &= \mathbf{v}_2 + \mu_{ij} (1 + \alpha_{ij}^{-1}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \hat{\boldsymbol{\sigma}}, \end{aligned}$$

where $\mu_{ij} = m_i / (m_i + m_j)$.

- Hydrodynamic fields:

$$\text{local density of species } i \equiv n_i(\mathbf{r}, t) = \int d\mathbf{v}_1 f_i(\mathbf{r}, \mathbf{v}_1, t)$$

$$\text{local flow velocity} \equiv \mathbf{u}(\mathbf{r}, t) = \frac{1}{\rho(\mathbf{r}, t)} \sum_i \int d\mathbf{v}_1 m_i \mathbf{v}_1 f_i(\mathbf{r}, \mathbf{v}_1, t)$$

$$\text{local temperature} \equiv T(\mathbf{r}, t) = \frac{1}{n(\mathbf{r}, t)} \sum_i \int d\mathbf{v}_1 \frac{m_i}{3} [\mathbf{v}_1 - \mathbf{u}(\mathbf{r}, t)]^2 f_i(\mathbf{r}, \mathbf{v}_1, t)$$

- Collision operators $J_{ij}[f_i, f_j]$ conserve the particle number for each species and the total momentum

$$\int d\mathbf{v}_1 J_{ij}[f_i, f_j] = 0, \quad \sum_{i,j} \int d\mathbf{v}_1 m_i \mathbf{v}_1 J_{ij}[f_i, f_j] = 0.$$

- The total energy is not conserved

$$\sum_{i,j} \int d\mathbf{v}_1 \frac{1}{2} m_i v_1^2 J_{ij}[f_i, f_j] = -\frac{3}{2} n T \zeta.$$

- $\zeta \rightarrow$ fractional energy changes per unit time (cooling rate). $\zeta = 0$ if $\alpha = 1$.

- Macroscopic balance equations:

$$\begin{aligned}
 D_t n_i + n_i \nabla \cdot \mathbf{u} + \frac{\nabla \cdot \mathbf{j}_i}{m_i} &= 0 \\
 D_t \mathbf{u} + \rho^{-1} \nabla \mathbf{P} &= 0 \\
 D_t T - \frac{T}{n} \sum_i \frac{\nabla \cdot \mathbf{j}_i}{m_i} + \frac{2}{3n} (\nabla \cdot \mathbf{q} + \mathbf{P} : \nabla \mathbf{u}) &= -\zeta T
 \end{aligned}$$

$$\mathbf{j}_i = \int d\mathbf{v}_1 m_i \mathbf{V} f_i, \quad (\mathbf{V} = \mathbf{v}_1 - \mathbf{u})$$

$$\mathbf{P} = \sum_i \int d\mathbf{v}_1 m_i \mathbf{V} \mathbf{V} f_i$$

$$\mathbf{q} = \sum_i \int d\mathbf{v}_1 \frac{1}{2} m_i V^2 \mathbf{V} f_i$$

- Balance equations become a **closed** set of hydrodynamic equations for $\{n_i, \mathbf{u}, T\}$ once the fluxes and the cooling rate are obtained in terms of $\{n_i, \mathbf{u}, T\}$ and their gradients .

3. CHAPMAN-ENSKOG SOLUTION

- **ASSUMPTION**: For long times (much longer than the mean free time) and far away from boundaries (bulk region) the system reaches a **hydrodynamic** regime.
- **Hydrodynamic** regime \leftrightarrow **NORMAL** solution to the BE:

$$f_i(\mathbf{r}, \mathbf{v}_1, t) = f_i(\mathbf{v}_1 | n_i\{\mathbf{r}, t\}, \mathbf{u}(\mathbf{r}, t), T(\mathbf{r}, t)\})$$

- **Chapman-Enskog** method:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \dots$$
$$\epsilon \sim \mathcal{O}(\nabla) : \frac{\text{mean free time}}{\text{hydrodynamic length}}$$

- Since $T(t)$, the **reference state** $f_i^{(0)}$ is not the local equilibrium distribution. Its explicit form is not known.
- **Navier-Stokes** hydrodynamic equations: $f_i^{(1)}$. Microscopic expressions for the **transport coefficients**.

- Some **controversy** about the possibility of going from kinetic theory to hydrodynamics by using the **Chapman-Enskog** method.
- The **time scale** for T is set by the **cooling rate** ζ instead of gradients. This new time scale, T is **much faster** than the usual hydrodynamic scale. Some hydrodynamic excitations decay much slower than T .
- For **large inelasticity** (ζ^{-1} small), **perhaps** there were **no** time scale separation between the hydrodynamic and kinetic contributions to the time evolution of the system \rightarrow **no aging** to hydrodynamics (no normal solution).
- We assume the **validity** of a hydrodynamic description (normal solution) and compare the predictions based on this assumption with **numerical solutions** of the BE.

LOCAL HOMOGENEOUS COOLING STATE

- Spatially **homogeneous** isotropic states:

$$\partial_t f_i^{(0)}(t) = \sum_j J_{ij}[f_i^{(0)}(t), f_j^{(0)}(t)]$$

- **Normal** solution: $f_i^{(0)}(V, t) = n_i v_0(t)^{-3} \Phi_i(V/v_0(t))$, $v_0^2(t) = 2T(t)(m_1 + m_2)/m_1 m_2$.

- The **exact** form of Φ_i is not known. **Sonine** polynomial approximation:

$$\Phi_i(V) \rightarrow \pi^{-3/2} \theta_i^{3/2} e^{-\theta_i V^2} \left[1 + \frac{c_i}{4} \left(\theta_i^2 V^4 - 5\theta_i V^2 + \frac{15}{4} \right) \right], \quad \theta_i = T/(T_i \mu_{ji}).$$

- “**Partial** temperatures ” $T_i(t)$:

$$\frac{3}{2} n_i T_i = \int d\mathbf{v}_1 \frac{1}{2} m_i V_1^2 f_i^{(0)}$$

- **Temperature** of the mixture $T(t) = \sum_i x_i T_i(t)$, $x_i = n_i/n$.

- Cooling rates

$$\zeta_i^{(0)} \equiv -\partial_t \ln T_i, \quad \zeta^{(0)} \equiv -\partial_t \ln T, \quad \zeta^{(0)} = T^{-1} \sum_i x_i T_i \zeta_i^{(0)}.$$

$$\zeta_i^{(0)} = -\frac{2}{3n_i T_i} \sum_j \int d\mathbf{v}_1 \frac{m_i}{2} V_1^2 J_{ij}[\mathbf{f}_i^{(0)}, \mathbf{f}_j^{(0)}]$$

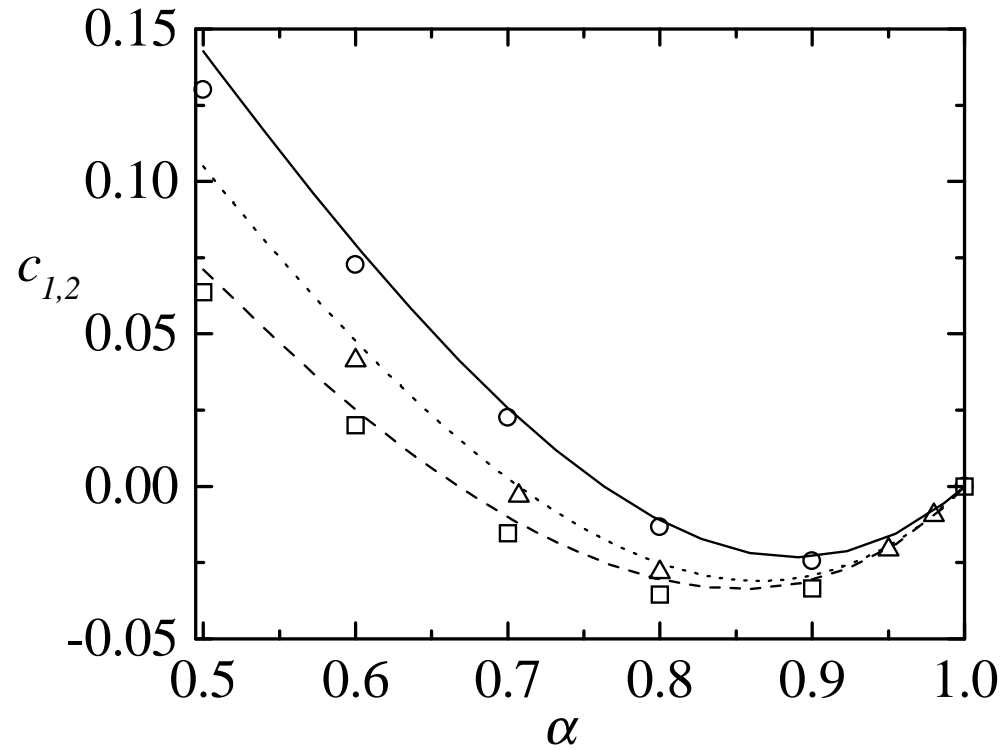
- Temperature ratio $\gamma \equiv T_1(t)/T_2(t)$:

$$\partial_t \ln \gamma = \zeta_2^{(0)} - \zeta_1^{(0)}$$

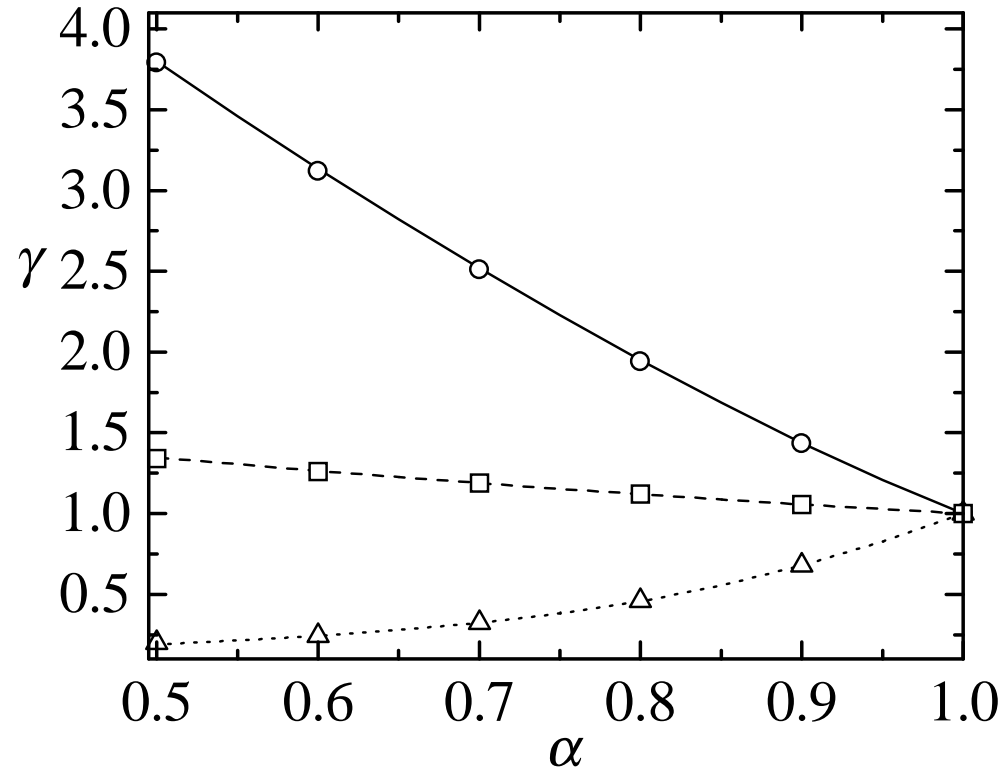
- Since $f_i^{(0)}$ depends on t only through $T(t) \rightarrow$ temperature ratio must be independent of time and so,

$$\zeta_2^{(0)} = \zeta_1^{(0)}.$$

- Garzó and Dufty, Phys. Rev. E (1999); Montanero and Garzó, Granular Matter (2002).



Fourth cumulant for $\sigma_1/\sigma_2 = 1$, $x_1 = \frac{1}{2}$, and $m_1/m_2 = 2$. The solid line refers to c_1 , the dashed line is for c_2 and the dotted line is for the common value in the single gas case. Symbols are DSMC results.



Temperature ratio $\gamma = T_1/T_2$ for $\sigma_1/\sigma_2 = 1$, $x_1 = \frac{2}{3}$, and $m_1/m_2 = 0.1$ (solid line) , 2 (dashed line), and 10 (dotted line). Symbols are DSMC results.

NAVIER-STOKES HYDRODYNAMIC EQUATIONS

- **Motivation**: determine the transport coefficients **without limitation** to the degree of dissipation.
- **Chapman-Enskog** method adapted to dissipative collisions. **Two** new features:
 1. Reference state (HCS) is **not** steady.
 2. **New** contributions to the transport due to the temperature differences. **Significant** consequences on the transport coefficients.
- The distribution functions are given by

$$f_i^{(1)} = \mathcal{A}_i \cdot \nabla x_1 + \mathcal{B}_i \cdot \nabla p + \mathcal{C}_i \cdot \nabla T + \mathcal{D}_{i,\alpha\beta} \nabla_\alpha u_\beta$$

- After some efforts....

$$\left(-\zeta^{(0)}T\partial_T + \mathcal{L}_i\right) \mathcal{A}_i + \mathcal{M}_i \mathcal{A}_j = \mathbf{A}_i + \left(\frac{\partial\zeta^{(0)}}{\partial x_1}\right)_{p,T} (p\mathcal{B}_i + T\mathcal{C}_i)$$

$$\left(-\zeta^{(0)}T\partial_T + \mathcal{L}_i - 2\zeta^{(0)}\right) \mathcal{B}_i + \mathcal{M}_i \mathcal{B}_j = \mathbf{B}_i + \frac{T\zeta^{(0)}}{p} \mathcal{C}_i$$

$$\left(-\zeta^{(0)}T\partial_T + \mathcal{L}_i - \frac{1}{2}\zeta^{(0)}\right) \mathcal{C}_i + \mathcal{M}_i \mathcal{C}_j = \mathbf{C}_i - \frac{p\zeta^{(0)}}{2T} \mathcal{B}_i$$

$$\left(-\zeta^{(0)}T\partial_T + \mathcal{L}_i\right) \mathcal{D}_{i,\alpha\beta} + \mathcal{M}_i \mathcal{D}_{j,\alpha\beta} = D_{i,\alpha\beta}$$

- Fluxes and transport coefficients:

$$\mathbf{j}_1^{(1)} = -\frac{m_1 m_2 n^2}{\rho} D \nabla x_1 - \frac{\rho}{p} D_p \nabla p - \frac{\rho_1 \rho_2}{\rho} D' \nabla T, \quad \mathbf{j}_1^{(1)} = -\mathbf{j}_2^{(1)}$$

$$\mathbf{q}^{(1)} = -T^2 D'' \nabla x_1 - L \nabla p - \lambda \nabla T$$

$$P_{\alpha,\beta}^{(1)} = -\eta \left(\nabla_\alpha u_\beta + \nabla_\beta u_\alpha - \frac{2}{3} \delta_{\alpha,\beta} \nabla \cdot \mathbf{u} \right)$$

Transport coefficients:

$$\begin{aligned}
 D &= -\frac{1}{3} \frac{\rho}{m_2 n^2} \int d\mathbf{v} \mathbf{V} \cdot \mathbf{A}_1, & D_p &= -\frac{m_1 p}{3\rho} \int d\mathbf{v} \mathbf{V} \cdot \mathbf{B}_1, & D' &= -\frac{m_1 T}{3\rho} \int d\mathbf{v} \mathbf{V} \cdot \mathbf{C}_1, \\
 D'' &= -\frac{1}{3T^2} \sum_i \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathbf{A}_i, & L &= -\frac{1}{3} \sum_i \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathbf{B}_i, \\
 \lambda &= -\frac{1}{3} \sum_i \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathbf{C}_i, & \eta &= -\frac{1}{10} \sum_i \int d\mathbf{v} m_i V_\alpha V_\beta \mathcal{D}_{i,\alpha\beta}
 \end{aligned}$$

- 7 transport coefficients: $\{D, D_p, D', D'', L, \lambda, \eta\}$
- These transport coefficients have been evaluated in the [leading](#) Sonine approximation [[Garzó and Dufty](#), Phys. Fluids (2002); [Montanero and Garzó](#), Phys. Rev. E (2003)].
- To test the accuracy of the Sonine solution: comparison with numerical solutions of the BE by means of the [direct simulation Monte Carlo](#) (DSMC) method.
- [Parameter space](#): $\{m_1/m_2, \sigma_1/\sigma_2, x_1, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

4. TRACER DIFFUSION COEFFICIENT

- **Tracer** limit: $x_1 \rightarrow 0$. Diffusion of impurities in a granular gas under HCS. The unknown \mathcal{A}_1 obeys a closed integral equation:

$$\left(-\zeta^{(0)}T\partial_T + \mathcal{L}_1\right) \mathcal{A}_1 = - \left(\frac{\partial}{\partial x_1} f_1^{(0)}\right)_{p,T} \mathbf{V}$$

- **First** and **second** Sonine approximations:

$$\mathcal{A}_1 \rightarrow f_{1,M} \left[a_{1,1} \mathbf{V} + a_{1,2} \left(\frac{1}{2} m_1 V^2 - \frac{5}{2} T_1 \right) \mathbf{V} \right],$$

$$f_{1,M} = n_1 (m_1 / 2\pi T_1)^{3/2} \exp\left(-\frac{m_1 v^2}{2T_1}\right)$$

$$a_{1,1} = -\frac{m_1 D}{n_1 T_1}$$

- Diffusion equation

$$\partial_t x_1(\mathbf{r}, t) = D(t) \nabla^2 x_1, \quad D(t) \propto \sqrt{T(t)}$$

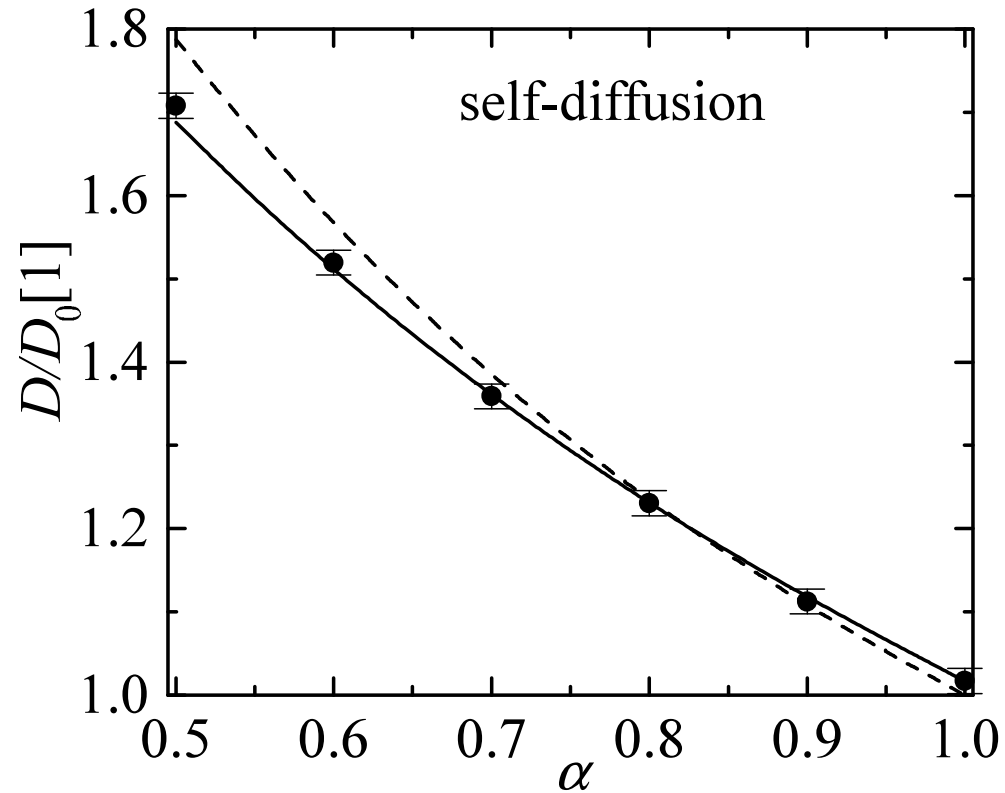
- Time dependence can be eliminated by introducing dimensionless variables:

$$\tau = \int_0^t dt' \nu_0(t'), \quad \mathbf{s} = \frac{\nu_0(t)}{v_0(t)} \mathbf{r}, \quad \nu_0(t) = n_2 \sigma_2^2 v_0(t)$$

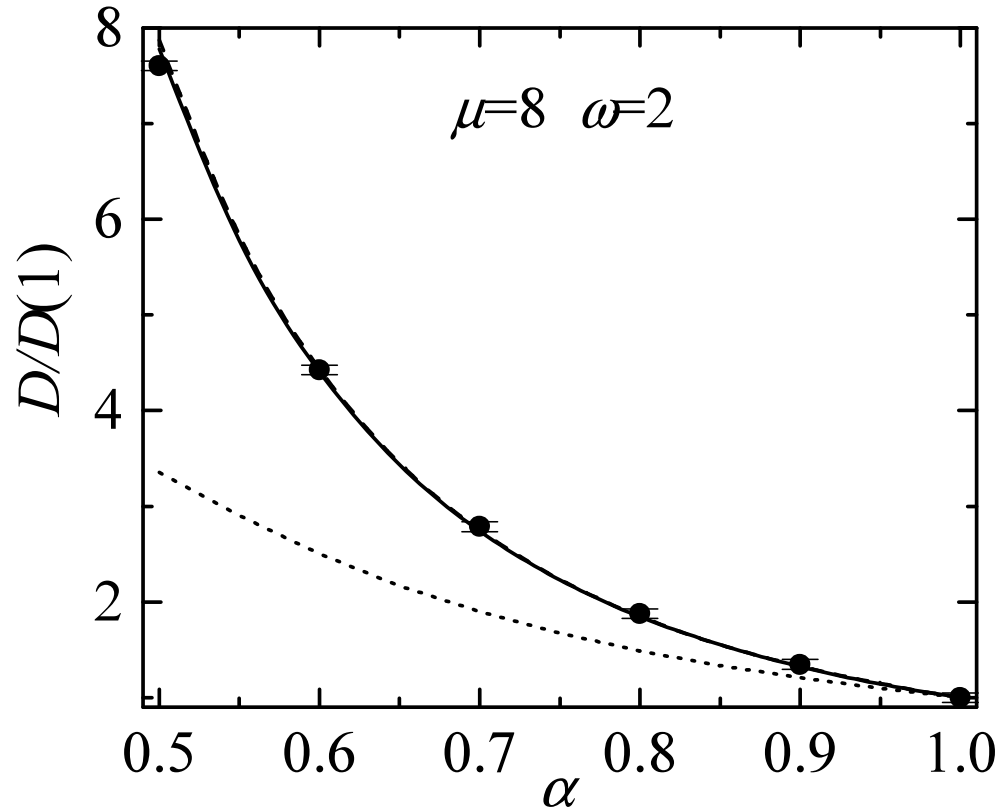
- Mean square deviation of position \mathbf{s} of impurities after a time interval τ is

$$\langle |\mathbf{s}(\tau) - \mathbf{s}(0)|^2 \rangle = 6D^* \tau, \quad D^* = \frac{\nu_0(t) D(t)}{n_2 v_0^2(t)}$$

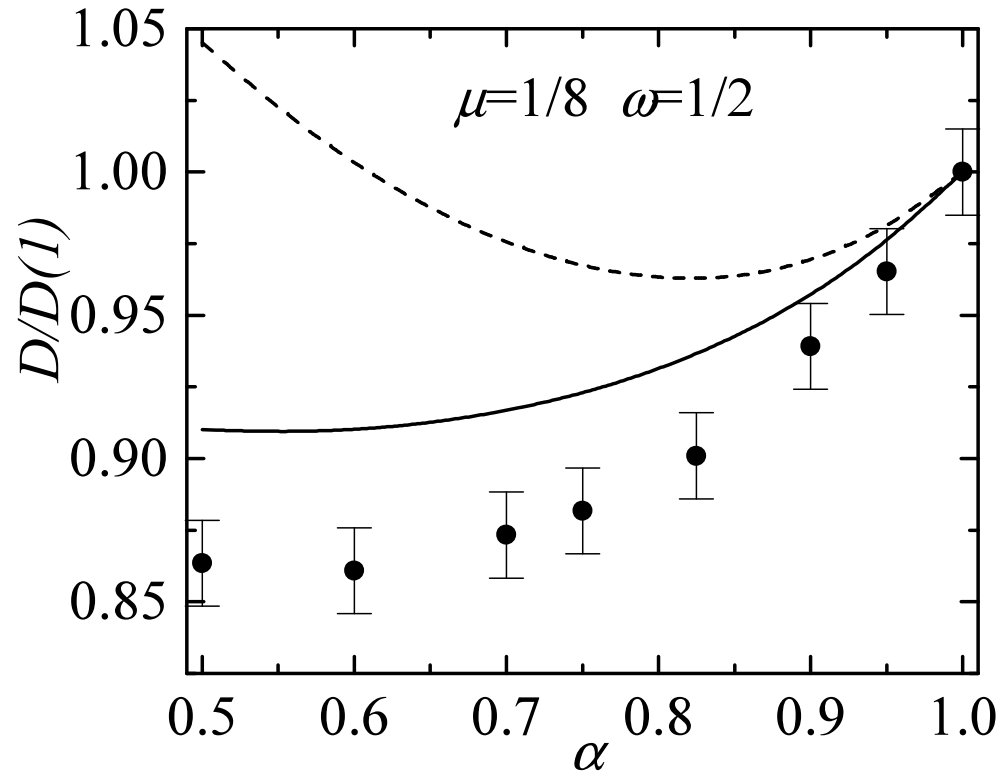
- Einstein form is used to measure D^* from DSMC simulations [Garzó and Montanero, cond-mat/0309639].



First (dashed line) and second (solid line) Sonine approximations for the reduced self-diffusion coefficient $D/D_0[1]$. Here, $D_0[1]$ refers to the first Sonine approximation to the elastic value of D . Symbols are DSMC results.



First (dashed line) and second (solid line) Sonine approximations for the reduced diffusion coefficient $D(\alpha)/D(1)$. Symbols are DSMC results. The dotted line is the first Sonine approximation by assuming $T_1/T_2 = 1$. Here, $D(1)$ refers to the elastic value of D consistently obtained in each approximation.



First (dashed line) and second (solid line) Sonine approximations for the reduced diffusion coefficient $D(\alpha)/D(1)$. Symbols are DSMC results. Here, $D(1)$ refers to the elastic value of D consistently obtained in each approximation.

5. SHEAR VISCOSITY COEFFICIENT

- From a computational point of view, it is difficult to measure this coefficient.
- Strategy: (Driven) uniform shear flow

$$n_i = \text{const}, \quad \nabla T = 0, \quad u_{i,x} = ay, \quad a = \text{constant shear rate}$$

- Ordinary fluid (elastic collisions): $T(t)$ due to viscous heating. Average collision frequency $\nu(t) \propto \sqrt{T(t)}$ (hard spheres). Thus, $a^* = a/\nu(t) \rightarrow 0$ and one can measure the Navier-Stokes shear viscosity η in the long time limit [Naitoh and Ono, J. Chem. Phys. (1979); Montanero and Santos, Phys. Rev. E (1996)]

$$\frac{\nu}{nT}\eta = - \lim_{t \rightarrow \infty} \frac{P_{xy}^*}{a^*}, \quad P_{xy}^* = P_{xy}/nT$$

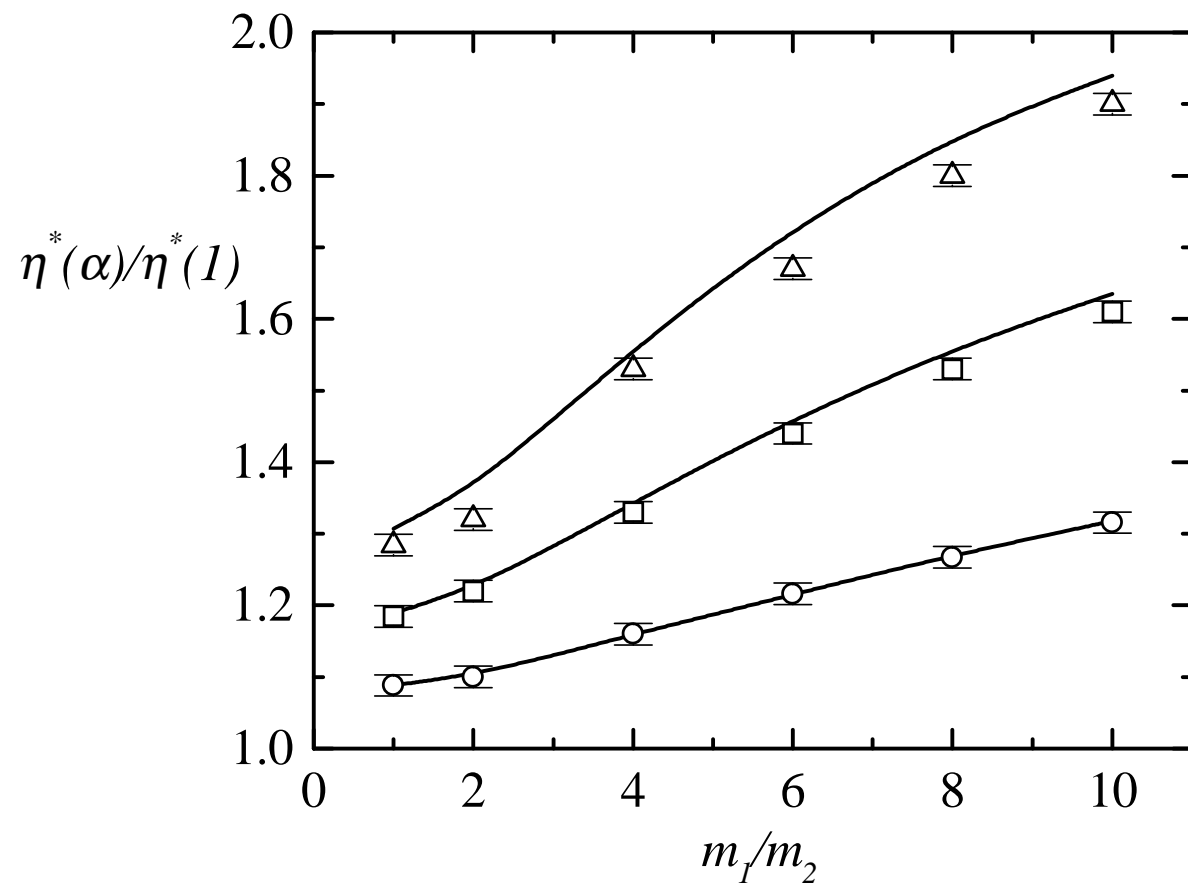
- Granular fluid (inelastic collisions): Energy sink in the balance equation for T :

$$\partial_t T = -\frac{2}{3n} a P_{xy} + (-\zeta T)$$

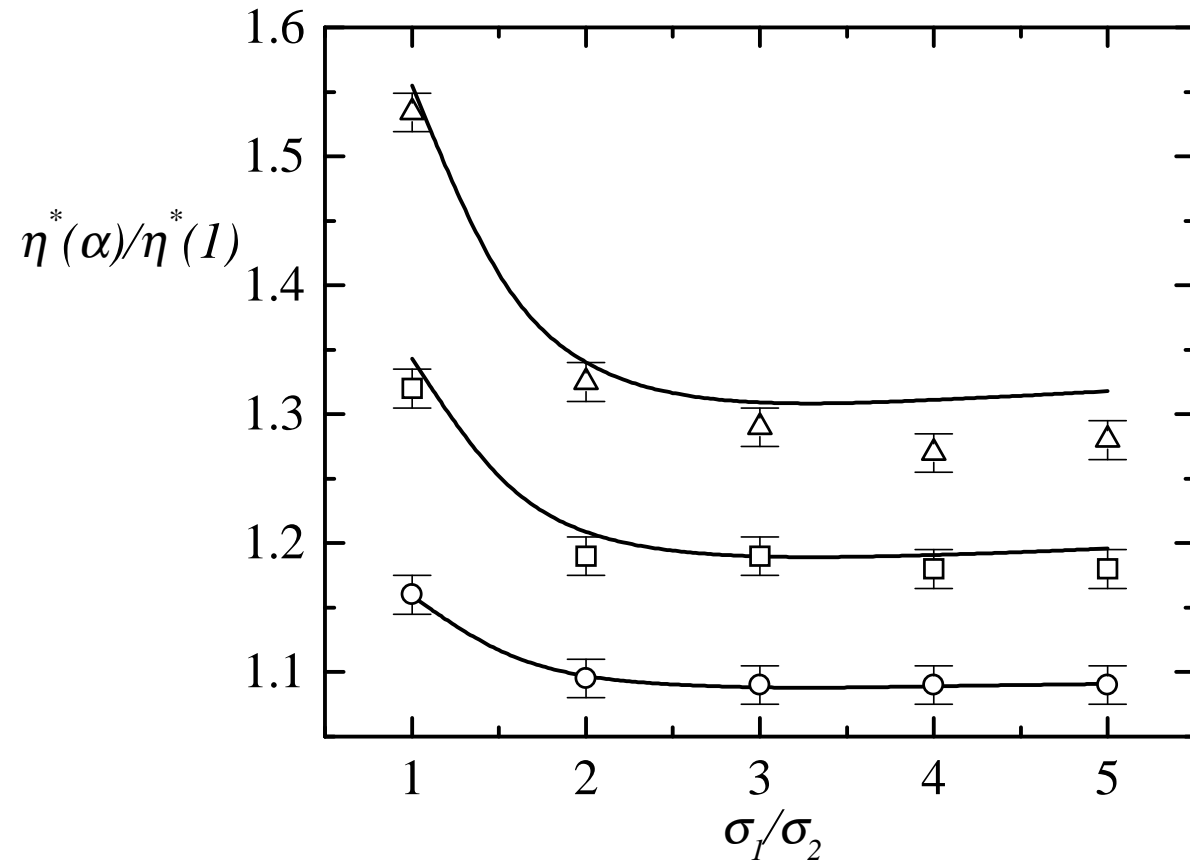
- Is it possible to “frustrate” the cooling effects so that the viscous heating is still able to heat the system, as in the elastic case? Thus, one can identify the shear viscosity coefficient when $a^* \rightarrow 0$.
- Granular fluid is excited by an external energy source that exactly compensates for the collisional loss:

$$\mathbf{F}_i^{\text{exc}} = \frac{1}{2} m_i \zeta \mathbf{V}$$

- Shear viscosity for a heated granular binary mixture η calculated in the first Sonine approximation. It slightly differs from the one obtained in the freely cooling case.



Reduced viscosity coefficient $\eta^*(\alpha)/\eta^*(1)$ versus mass ratio for $\sigma_1/\sigma_2 = x_1/x_2 = 1$ and $\alpha = 0.9$ (circles), 0.8 (squares), and 0.7 (triangles).



Reduced viscosity coefficient $\eta^*(\alpha)/\eta^*(1)$ versus size ratio for $m_1/m_2 = 4$, $x_1/x_2 = 1$ and $\alpha = 0.9$ (circles), 0.8 (squares), and 0.7 (triangles).

6. CONCLUSIONS

- **Hydrodynamic** equations for a binary mixture of inelastic hard spheres have been derived from the **Boltzmann** kinetic theory. A **normal** solution is obtained via the **Chapman-Enskog method** for states near the *local* HCS.
- **Seven** relevant transport coefficients. They are given in terms of the solution of a set of coupled linear integral equations, which can be approximately solved by making an expansion in **Sonine polynomials**. All these coefficients are functions of the restitution coefficients as well as the masses, sizes, and composition.
- The analytical results are compared with those obtained from **numerical** solutions of the Boltzmann equation by means of the **DSMC** method in the cases of the **diffusion** coefficient and the **shear viscosity** coefficient.
- In general, the comparison shows an **excellent agreement** between theory and simulation over a wide range of values of the parameters of the problem. This good agreement can be seen as an evidence of the **validity** of hydrodynamics to describe some states of granular fluids.