KINETIC THEORY OF GRANULAR BINARY MIXTURES:

SOME APPLICATIONS

STATISTICAL PHYSICS in EXTREMADURA

European Union

European Regional Development Fund

Vicente Garzó

Departamento de Física, Universidad de Extremadura, Badajoz, Spain

IWNET 2009, August 24-28, Cuernavaca, Mexico

OUTLINE

1. Introduction

2. Granular binary mixtures. *Smooth* inelastic hard spheres: Boltzmann kinetic equation

3. Navier-Stokes hydrodynamics: Some applications

4. Mixtures of inelastic *rough* hard spheres

5. Summary and conclusions

INTRODUCTION

Granular systems are constituted by macroscopic grains that collide inelastically so that the total energy decreases with time.

Behaviour of granular systems under many conditions exhibit a great similarity to ordinary fluids

Rapid flow conditions: hydrodynamic-like type equations.Good example of a system which is inherently in ***non-equilibrium***.

Dominant transfer of momentum and energy is through *binary inelastic* collisions. Subtle modifications of the usual macroscopic balance equations

To isolate collisional dissipation: ***idealized*** microscopic model

Smooth hard spheres
with *inelastic* collisions

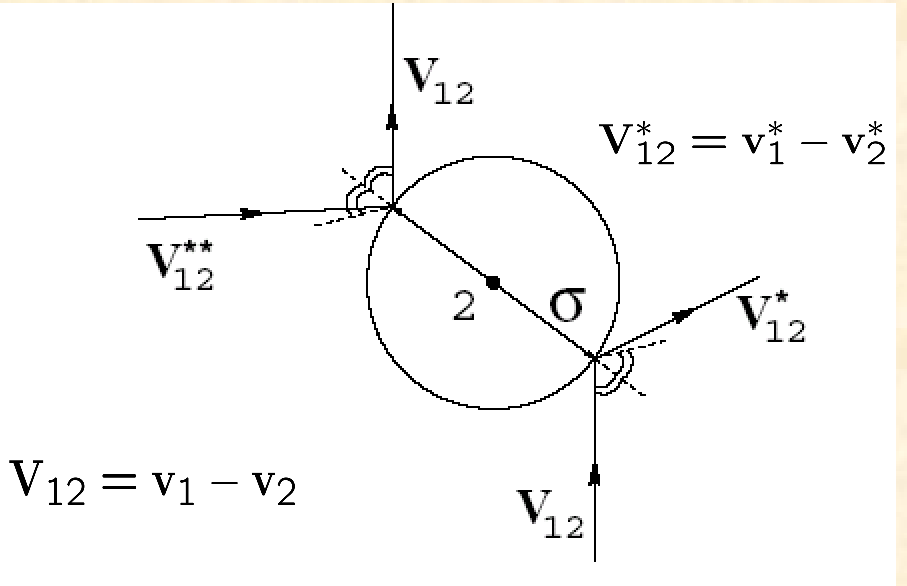


FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

$$\mathbf{V}^*_{12} \cdot \widehat{\boldsymbol{\sigma}} = -\alpha \mathbf{V}_{12} \cdot \widehat{\boldsymbol{\sigma}}$$

Coefficient of restitution

$$0 < \alpha \leq 1$$

Direct collision

$$\mathbf{v}^*_1 = \mathbf{v}_1 - \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}^*_2 = \mathbf{v}_2 + \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

Momentum conservation

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_1^* + \mathbf{v}_2^*$$

Collisional energy change

$$\Delta E = \frac{1}{2} m \left(v_1^{*2} + v_2^{*2} - v_1^2 - v_2^2 \right) = -\frac{m}{4} (1 - \alpha^2)(\mathbf{V}_{12} \cdot \widehat{\boldsymbol{\sigma}})^2$$

Very **simple** model that *captures* many properties of granular flows, especially those associated with dissipation

Nonequilibrium statistical mechanics tools for the (inelastic) hard sphere model

KINETIC DESCRIPTION

One-particle velocity distribution function (vdf)

$$f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}$$ →

Average *number of particles* wich at *t* lie in r+*d*r and move with **v**+*d***v**

Boltzmann kinetic equation

- ***Dilute*** gas (binary collisions)
- ***Molecular chaos*** (no velocity correlations)

$$(\partial_t + \mathbf{v}\cdot\nabla)\, f(\mathbf{v}) = J\left[\mathbf{v}|f(t), f(t)\right]$$

$$J[f,f] = \sigma^{d-1}\int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\left[\alpha^{-2} f(\mathbf{v}_1') f(\mathbf{v}_2') - f(\mathbf{v}_1) f(\mathbf{v}_2)\right]$$

Scattering rules:

$$\mathbf{V}_{12} \equiv \mathbf{g}$$

$$\mathbf{v}_1' = \mathbf{v}_1 - \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \frac{1}{2}\left(1+\alpha^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})\widehat{\boldsymbol{\sigma}}$$

Differences with respect to the usual BE:

Presence of α^{-2} in the gain term and collision rules

Binary granular *mixtures*. Boltzmann description

Mechanical parameters: $\{m_1, m_2, \sigma_1, \sigma_2, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

Extension of the BE to the *multicomponent* case: $f_i(\mathbf{r}, \mathbf{v}, t)$

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

$$J_{ij}[f_i, f_j] = \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathrm{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathrm{g}) \left[\alpha_{ij}^{-2} f_i(\mathbf{v}_1') f_j(\mathbf{v}_2') - f_i(\mathbf{v}_1) f_j(\mathbf{v}_2)\right]$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

Collision rules:

$$\mathbf{v}_1' = \mathbf{v}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot \mathbf{g})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot \mathbf{g})\widehat{\boldsymbol{\sigma}}$$

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

Hydrodynamic fields

$$n_i(\mathbf{r},t) = \int d\mathbf{v} f_i(\mathbf{r},\mathbf{v},t)$$

$$\mathbf{U}(\mathbf{r},t) = \frac{1}{\rho(\mathbf{r},t)}\sum_i \int d\mathbf{v} m_i \mathbf{v} f_i(\mathbf{r},\mathbf{v},t)$$

Granular temperature ←

$$T(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\sum_i \int d\mathbf{v}\frac{m_i}{d}(\mathbf{v}-\mathbf{U})^2 f_i(\mathbf{r},\mathbf{v},t)$$

Boltzmann collision operators $J_{ij}[f_i,f_j]$ *conserve* the particle number of each species and the total momentum

$$\int d\mathbf{v} J_{ij}[\mathbf{v}|f_i, f_j] = 0, \quad \sum_{i=1}^{2}\sum_{j=1}^{2}\int d\mathbf{v} m_i \mathbf{v} J_{ij}[\mathbf{v}|f_i, f_j] = 0$$

but the total energy is ***not*** conserved

$$\sum_{i=1}^{2}\sum_{j=1}^{2} m_i \int d\mathbf{v} V^2 J_{ij}[\mathbf{v}|f_i, f_j] = -dnT\zeta \qquad \mathbf{V} = \mathbf{v} - \mathbf{U}$$

ζ : fractional energy changes per unit time (**cooling rate**)

Macroscopic balance equations

Balance equation for the *partial densities*

$$D_t n_i + n_i \nabla \cdot \mathbf{U} + m_i^{-1} \nabla \cdot \mathbf{j}_i = 0$$

Balance equation for the mean *flow velocity*

$$\rho D_t \mathbf{U} + \nabla \mathsf{P} = 0$$

Balance equation for the granular *temperature*

$$\frac{d}{2} n \left(D_t + \zeta \right) T + \mathsf{P} : \nabla \mathbf{U} + \nabla \cdot \mathbf{q} - \frac{d}{2} T \sum_{i=1}^{2} m_i^{-1} \nabla \cdot \mathbf{j}_i = 0$$

$$D_t = \partial_t + \mathbf{U} \cdot \nabla$$

Mass flux

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

Pressure or stress tensor

$$\mathbf{P} = \sum_{i=1}^{2} m_i \int d\mathbf{v} \, \mathbf{V}\mathbf{V} \, f_i(\mathbf{v})$$

Heat flux

$$\mathbf{q} = \sum_{i=1}^{2} \frac{m_i}{2} \int d\mathbf{v} \, V^2 \mathbf{V} \, f_i(\mathbf{v})$$

CHAPMAN-ENSKOG NORMAL 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.

Normal solution $f_i(\mathbf{r},\mathbf{v};t)=f_i(\mathbf{v}|\{n_i(\mathbf{r},t)\},\mathbf{U}(\mathbf{r},t),T(\mathbf{r},t)\})$

Small spatial gradients: $f_i=f_i^{(0)}+f_i^{(1)}+\cdots$

Some *controversy* about the possibility of going from kinetic theory to hydrodynamics by using the CE method

The **time scale** for *T* is set by the **cooling rate** instead of spatial gradients. This new time scale, *T* is *much faster* than in 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 hydrodynamic and kinetic excitations: **NO AGING** to hydodynamics!!

I assume the validity of a hydrodynamic description and compare with DSMC solutions of the BE

HOMOGENEOUS COOLING STATE
(zeroth-order approximation)

Spatially *homogeneous* isotropic states

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

Partial temperatures $\longrightarrow$ $n_i T_i = \frac{m_i}{d} \int d\mathbf{v}\, v^2 f_i(\mathbf{v})$

Granular temperature $\longrightarrow$ $T = \sum_i x_i T_i, \quad x_i = n_i/n$

Cooling rates for T_i $\longrightarrow \zeta_i = -\partial_t \ln T_i, \quad \zeta = T^{-1} \sum_i x_i T_i \zeta_i$

$\zeta = -\partial_t \ln T$ $\longrightarrow$ $T(t) \propto t^{-2}$ Haff's law (1983)

$$\zeta_1 = \zeta_{11} + \zeta_{12}$$

$$\zeta_{11} = -\frac{m_1}{d n_1 T_1} \int d\mathbf{v} v^2 J_{11}[f_1, f_1]$$

→ Zero for *elastic* systems

$$\zeta_{12} = -\frac{m_1}{d n_1 T_1} \int d\mathbf{v} v^2 J_{12}[f_1, f_2]$$

→ *Nonzero* in general for *elastic* systems

If f_i are *Maxwellians* at the same temperature, then **ζ_{12}=0** (elastic case). Detailed balance whereby the energy transfer between species is balanced by energy conservation for this state

The *analog* of the balance detailed state for *inelastic* systems:

Homogeneous cooling state (HCS)

Assumption

Hydrodynamic or ***normal*** state: all the *time* dependence of vdf occurs only through the temperature T(t)

$$f_i(v,t) = n_i v_0^{-d}(t)\Phi_i(v/v_0(t))$$

$$v_0^2(t) \propto T(t)$$

Consequence: ***temperature ratio*** $\gamma = T_1/T_2$ must be ***constant*** (independent of time)

HCS condition: $\partial_t \ln \gamma = \zeta_2 - \zeta_1 \longrightarrow \boxed{\zeta_1 = \zeta_2}$

Elastic collisions: $\zeta_1 = \zeta_2 = 0, \quad T_1 = T_2 = T$

$\downarrow$

Equipartition theorem for classical statistical mechanics

What happens if the collisions are **inelastic** ?

Well-posed *mathematical* problem: one has to solve the BE for the reduced distributions subject to $\zeta_1=\zeta_2$

So far, an ***exact*** solution is not known….

Approximate solution

$$\Phi_i(V^*) \to \left(\frac{\theta_i}{\pi}\right)^{d/2} e^{-\theta_i v^{*2}} \left[1 + \frac{c_i}{4}\left(\theta_i^2 v^{*4} - (d+2)v^{*2} + \frac{d(d+2)}{4}\right)\right]$$

$$v^* = v/v_0, \quad \theta_i = \frac{m_j}{m_i+m_j}\frac{T}{T_i}, \quad i \neq j$$

VG&Dufty PRE **60**, 5706 (1999)

Time evolution of temperature ratio γ. Comparison with Monte Carlo simulations

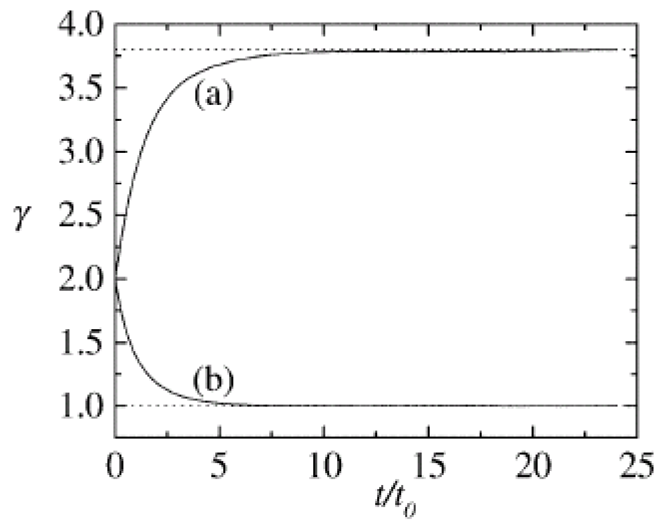


Fig. 1. Time evolution of $\gamma(t) = T_1(t)/T_2(t)$ for $n^* = 0$, $\delta = 2$, $w = 1$, $\mu = 10$, and $\alpha = 0.5$ (a) and $\alpha = 1$ (b). The dotted lines refer to the theoretical predictions. Time is measured in units of $t_0 \equiv \lambda_{11}/v_{01}(0)$

Montanero&VG, Granular Matter **4**, 17 (2002)

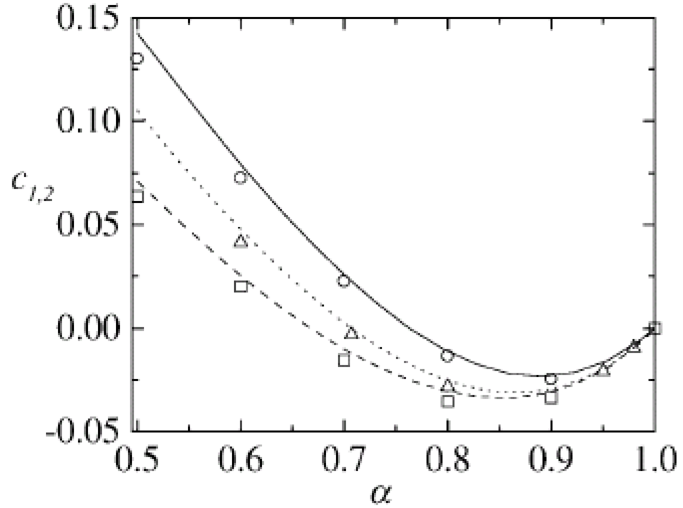


Fig. 2. Plot of the coefficients c_i versus the restitution coefficient α for $n^* = 0$, $\delta = 1$, $w = 1$ and $\mu = 2$. The solid line and the circles refer to c_1 while the dashed line and the squares correspond to c_2. The dotted line and the triangles refer to the common value in the single component case. The lines are the theoretical predictions and the symbols correspond to the simulation results

VG&Dufty PRE **60**, 5706 (1999)

Montanero&VG, Granular Matter **4**, 17 (2002)

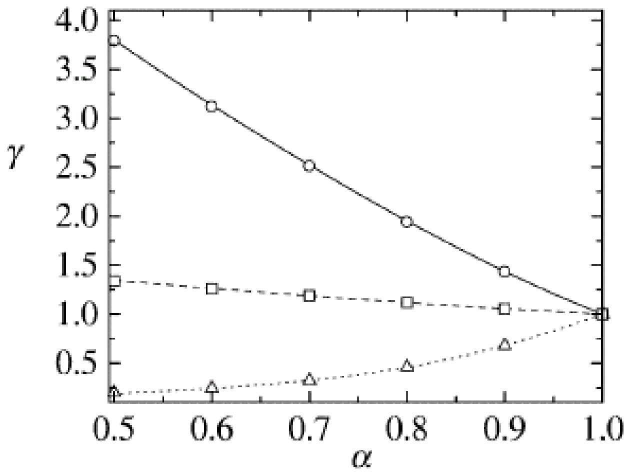


Fig. 4. Plot of the temperature ratio γ versus the restitution coefficient α for $n^* = 0$, $\delta = 2$, $w = 1$ and three different values of the mass ratio: $\mu = 1/10$ (dotted line and triangles), $\mu = 2$ (dashed line and squares) and $\mu = 10$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

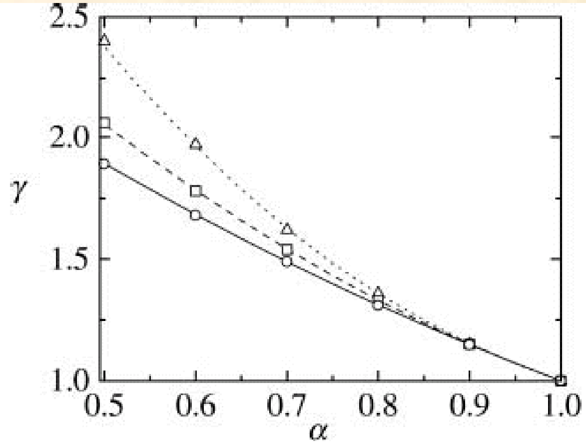


Fig. 5. Plot of the temperature ratio versus the restitution coefficient α for $n^* = 0$, $w = 1$, $\mu = 4$ and three different values of the concentration ratio: $\delta = 1/4$ (dotted line and triangles), $\delta = 1$ (dashed line and squares) and $\delta = 4$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

Comparison with *molecular dynamics* (MD) simulations

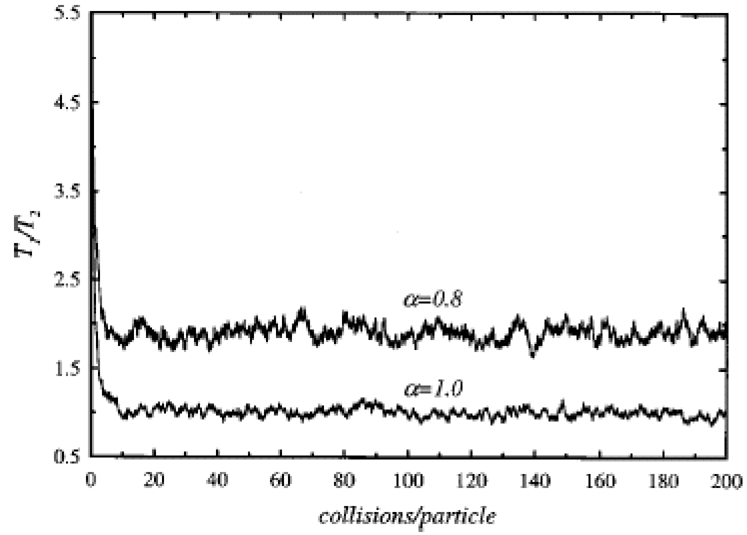


FIG. 1. Time evolution of $\gamma(t)=T_1(t)/T_2(t)$ for $\phi=0.1$, $\sigma_1/\sigma_2=\phi_1/\phi_2=1$, $m_1/m_2=8$, and two values of α: $\alpha=0.8$ and $\alpha=1$.

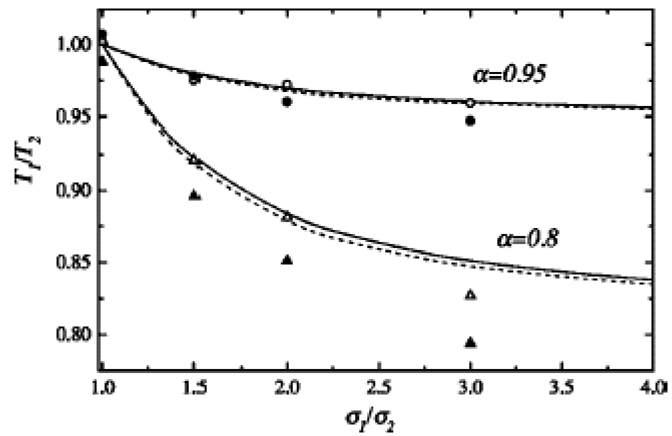


FIG. 3. Plot of the temperature ratio T_1/T_2 as a function of the size ratio σ_1/σ_2 for $m_1/m_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (lines and circles) and $\alpha=0.8$ (lines and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The solid (dashed) lines correspond to $\phi=0.1$ ($\phi=0.2$), while the open (solid) symbols correspond to $\phi=0.1$ ($\phi=0.2$).

Dahl, Hrenya,VG& Dufty, PRE **66**, 041301 (2002)

Breakdown of energy equipartition

Computer simulation studies: Barrat&Trizac GM **4**, 57 (2002); Krouskop&Talbot, PRE **68**, 021304 (2003); Wang *et al*. PRE **68**, 031301 (2003); Brey et al. PRE **73**, 031301 (2006); Schroter *et al*. PRE **74**, 011307 (2006);…….

Real experiments: Wildman&Parker, PRL **88**, 064301 (2002); Feitosa&Menon, PRL **88**, 198301 (2002).

All these results ***confirm*** this new feature in granular mixtures !!

NAVIER-STOKES HYDRODYNAMIC EQUATIONS

Previous studies: Jenkins et al. JAM 1987; PF 1989; Zamankhan, PRE 1995; Arnarson et al. PF 1998; PF 1999; PF 2004; Serero et al. JFM 2006

Limited to the quasielastic limit. They are based on the energy equipartition assumption

Our **motivation**: Determination of the transport coefficients by using a kinetic theory which takes into account the effect of temperature differences on them. **NO limitation** to the degree of dissipation

Constitutive equations

$$\mathbf{j}_1 = -\frac{m_1 m_2 n}{\rho} D \nabla x_1 - \frac{\rho}{p} D_p \nabla p - \frac{\rho}{T} D_T \nabla T$$

$$P_{\gamma\beta} = p\delta_{\gamma\beta} - \eta \left(\nabla_\gamma U_\beta + \nabla_\beta U_\gamma - \frac{2}{d} \nabla \cdot \mathbf{U} \right)$$

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

Seven transport coefficients: $\left\{ D, D_p, D_T, \eta, D'' L, \lambda \right\}$

Transport coefficients given in terms of solutions of coupled linear integral equations. Complex mathematical problem

Sonine polynomial approximation. Only leading terms are usually considered

To test the accuracy of the Sonine solution: comparison with numerical solutions of the BE (DSMC)

Parameter space: $\{m_1/m_2, \sigma_1/\sigma_2, x_1, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

What is the **influence** of energy nonequipartition on ***transport properties*** of the granular mixture?

In particular, the pressure diffusion coefficient

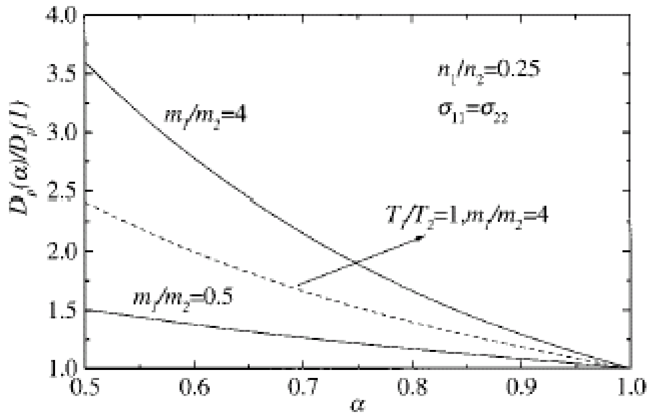


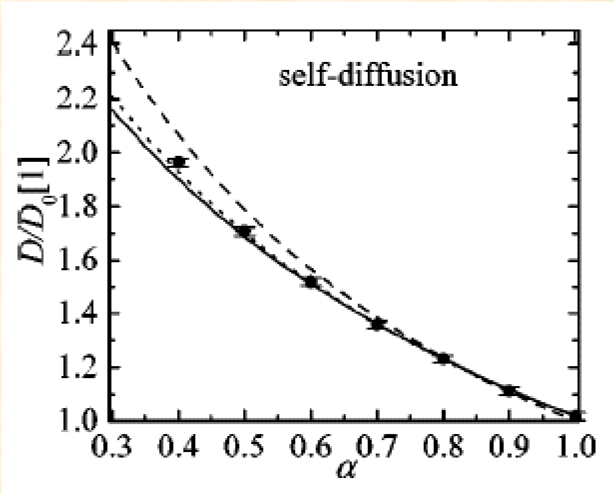
FIG. 1. Plot of the reduced pressure diffusion coefficient $D_p(\alpha)/D_p(1)$ as a function of the restitution coefficient $\alpha=\alpha_{11}=\alpha_{22}=\alpha_{12}$ for $\sigma_{11}=\sigma_{22}=\sigma_{12}$, a concentration ratio $n_1/n_2=0.25$, and two different values of the mass ratio: $m_1/m_2=0.5$ and $m_1/m_2=4$. The dashed line refers to the case $m_1/m_2=4$ by assuming the equality of the partial temperatures $\gamma=T_1/T_2=1$.

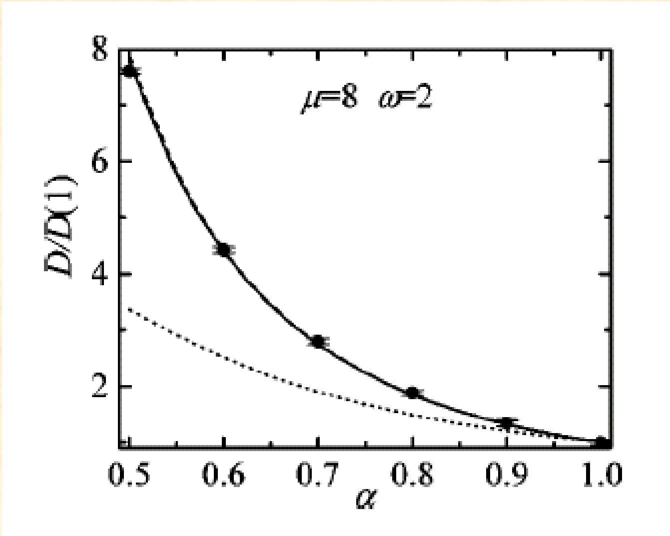
VG&Dufty, Phys.Fluids **14**, 1476 (2002)

IWNET 2009, August 24-28, Cuernavaca, Mexico

COMPARISON WITH MONTE CARLO SIMULATIONS

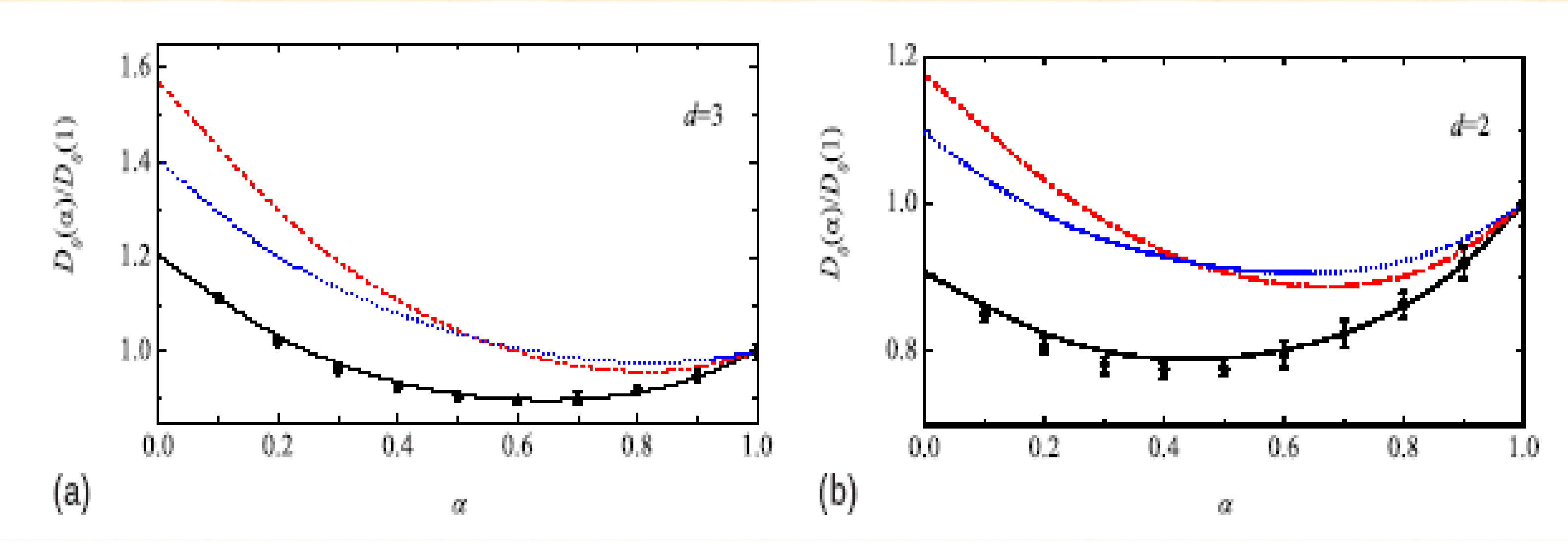
Tracer diffusion coefficient: Diffusion of impurities in granular gas ($x_1 \to 0$)





VG&Montanero, PRE **69**, 021301 (2004)

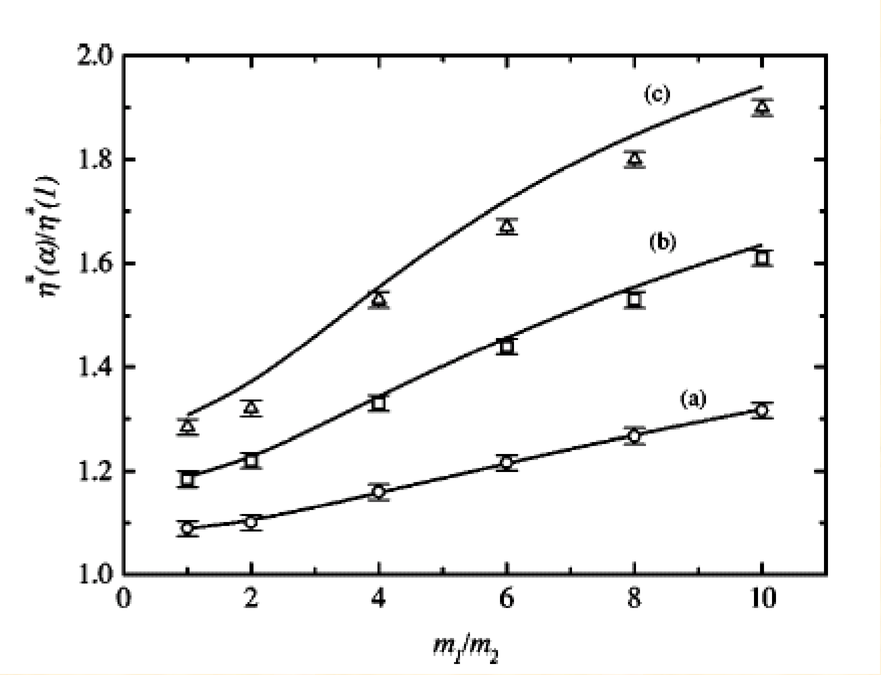
$$m_1/m_2 = \frac{1}{8}, \quad \sigma_1/\sigma_2 = \frac{1}{2}$$

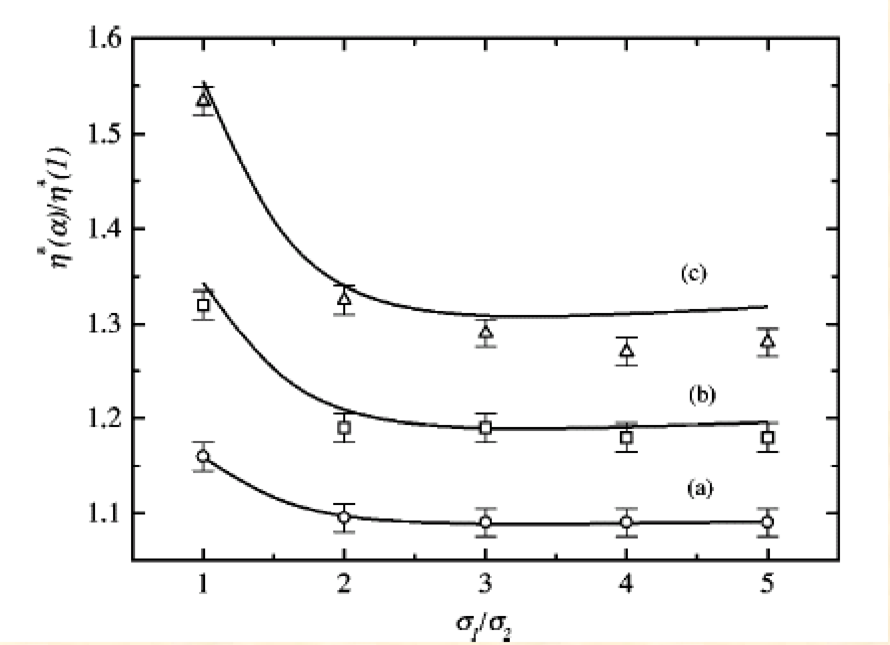


VG&Vega Reyes, PRE **79**, 041303 (2009)

VG, Vega Reyes&Montanero, J.Fluid Mech. **623**, 387 (2009)

Shear viscosity coefficient





Montanero&VG, PRE **67**, 021308 (2003)

Previous results support the validity of hydrodynamics to describe granular fluids. However, some care is warranted in extending properties of ordinary fluids to those with *inelastic* collisions

For example,…

For elastic collisions, response to an external force of an impurity immersed in a granular gas (mobility coefficient) is proportional to the diffusion coefficient

Einstein relation (fluctuation-dissipation theorem)

Einstein relation in a *driven* granular gas

Granular gas is heated by an external driving force (thermostat) that does work on the system to compensate for the collisional loss of energy: NESS

MD simulations (Srebro&Levine PRL, 2004; Barrat et al. Physica A, 2004; Shokef et al. PRE, 2006; Puglisi et al. JSTAT, 2007) have proposed a ***modified*** Einstein relation

$$\epsilon = \frac{D}{T_0 \chi} = 1$$

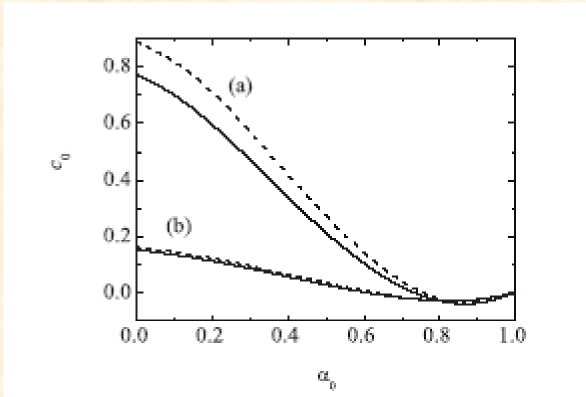
MD simulations do not detect deviations of ε from unity
(validity of the modified Einstein form)

Kinetic theory calculations

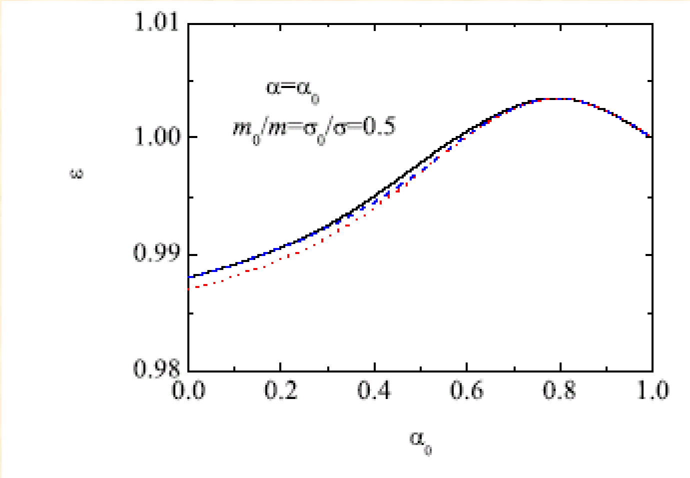
$$\epsilon = 1 - \frac{c_0}{2}\frac{\nu_2}{\nu_4}$$

Non-Maxwellian behavior of the reference state

Second Sonine approximation



Modified Einstein relation is ***not*** exactly verified but….



VG, JSTAT P05007 (2008)

Deviations from unity are smaller than 2% !!

The Einstein relation holds exactly for IMM

(VG&Astillero, J. Stat. Phys. **118**, 935 (2003))

Onsager's reciprocal relations in granular gases

Language of LIT

$$\mathbf{j}_i = -\sum_j L_{ij}(\nabla\mu_j/T)_T - L_{iq}(\nabla T/T^2) - C_p\nabla p,$$

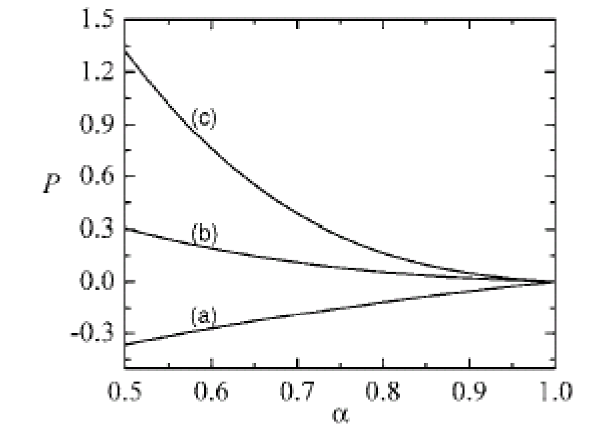
$$\mathbf{J}_q = -L_{qq}\nabla T - \sum_i L_{qi}(\nabla\mu_j/T)_T - C_p'\nabla p$$

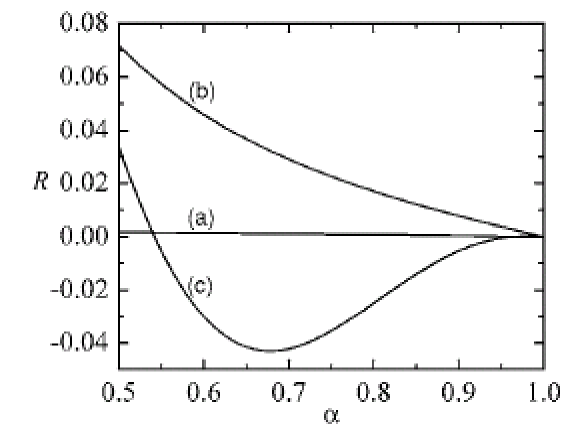
Ordinary fluids: $L_{ij} = L_{ji}, L_{iq} = L_{qi}, C_p = C_p' = 0$

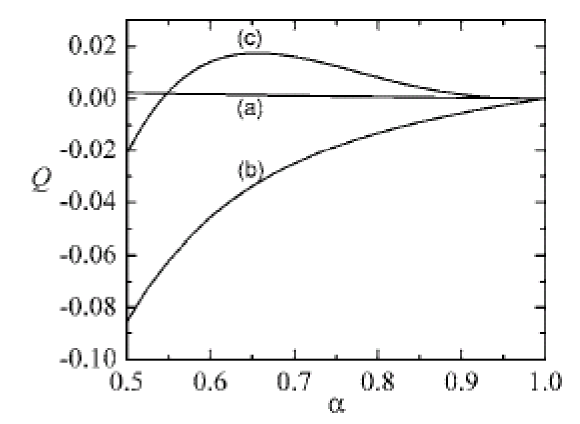
(Onsager's theorem)

NO *time* reversal *invariance* for granular fluids:
Onsager's relations are not expected to apply

Quantitative extent of violation: $L_{12} = L_{21}, L_{1q} \neq L_{q1}, C_p \neq C'_p \neq 0$

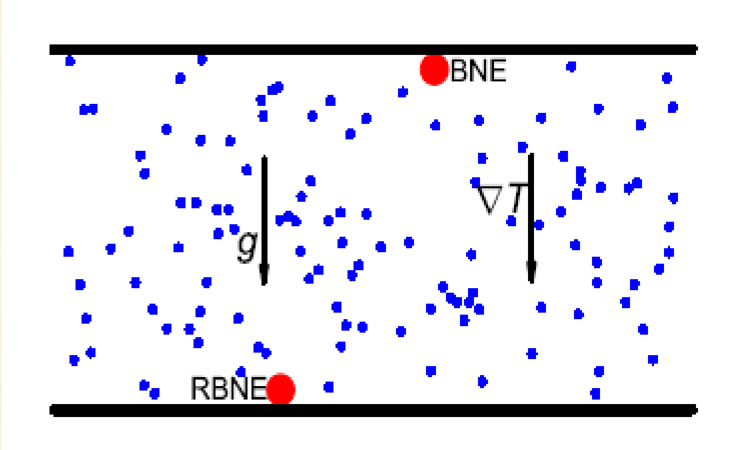






VG&Montanero&Dufty, Phys. Fluids **18**, 083395 (2006)

Segregation of an intruder in a granular gas



Segregation driven by *gravity* and *thermal gradients*: thermal (Soret) diffusion

Mechanical parameters of the system

$$\{m, m_0, \sigma, \sigma_0, \alpha, \alpha_0\}$$

Collisional dissipation

We assume that $\sigma_0 > \sigma$

Experimental conditions: *inhomogeneous* steady state without convection (*zero* mass flux) and gradients along the z direction

$$-\Lambda \partial_z \ln T = \partial_z \ln(n_0/n)$$

$\Lambda > 0 \longrightarrow$ Intruder rises with respect fluid (**BNE**)

$\Lambda < 0 \longrightarrow$ Intruder falls with respect fluid (**RBNE**)

Hydrodynamic description to evaluate thermal diffusion Λ

a) *Momentum* balance equation:

$$\frac{\partial p}{\partial z} = -\rho g$$

$$p = nT$$

b) *Constitutive* equation for the mass flux of intruder:

$$j_z = -\frac{m_0}{\rho} D \partial_z x_0 - \frac{\rho}{p} D_p \partial_z p - \frac{\rho}{T} D_T \partial_z T$$

Non-convecting steady state $\longrightarrow j_z = 0$

Mole fraction gradient in terms of gravity and thermal gradient

$$\Lambda = \frac{\rho}{x_0 m_0} \frac{D_T - D_p g^*}{D}$$

$$g^* = \frac{m g}{\partial_z T} < 0$$

Order parameter for the transition BNE/RBNE

$$\theta = \frac{mT_0}{m_0 T}$$

Brey, Ruiz-Montero& Moreno PRL **95**, 098001 (2005); VG EPL **75**, 521 (2006)

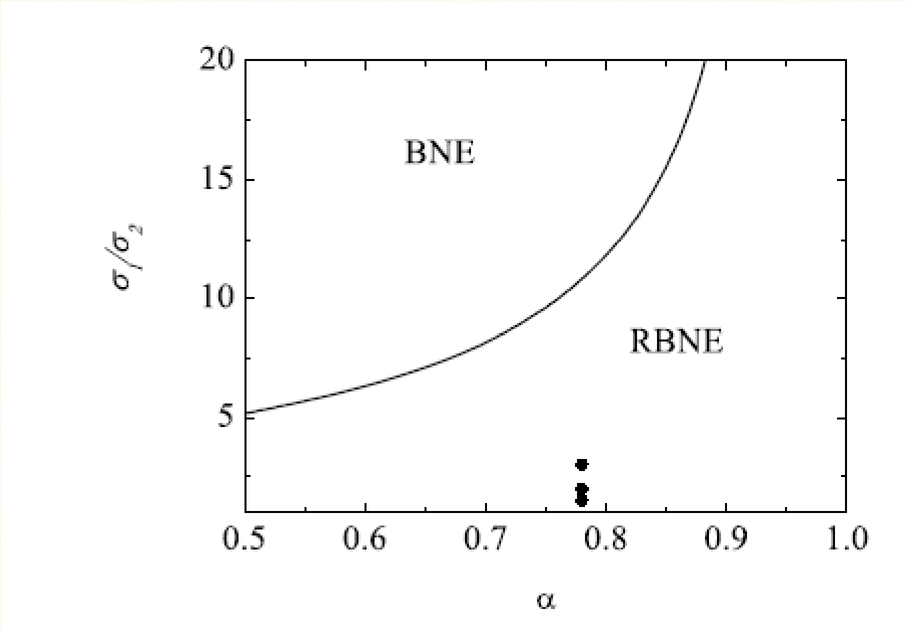
If $\theta>1$ ($\theta<1$), then BNE (RBNE)

Due to the lack of energy equipartition, criterion is rather complicated since it involves all the parameter space

If $T_0=T$, segregation is predicted for particles that differ only in mass !!

Comparison with experiments of Schroter et al.
(PRE **74**, 011307 (2006))

$$m_1/m_2 = x_2/x_1 = (\sigma_1/\sigma_2)^3, \alpha = 0.78$$



VG, EPL **75**, 521 (2006);
VG, EPJ E **29**, 261 (2009)

Consistent with experiments and simulations

MIXTURES OF INELASTIC ROUGH HARD SPHERES

Influence of ***roughness*** on the properties of the system. Rotational degrees of freedom are also affected by the collisional dissipation. Very complex problem

Some previous results for monodisperse gases: Golshtein&Shapiro, JFM (1993); Huthmann&Zippelius, PRE (1997); Huthmann et al. PRE (1999); Zippelius, Physica A (2006)…..

No equipartition of energy : $T_{\mathsf{tr}} \neq T_{\mathsf{rot}}$

To the best of my knowledge, no results for multicomponent systems….

Objective: Analyze the ***homogeneous*** state (HCS)

$$(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}'_{ij}) = -\alpha_{ij}(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{ij}), \quad 0 < \alpha_{ij} \leq 1$$

$$(\widehat{\boldsymbol{\sigma}} \times \mathbf{g}'_{ij}) = -\beta_{ij}(\widehat{\boldsymbol{\sigma}} \times \mathbf{g}_{ij}), \quad -1 \leq \beta_{ij} \leq 1$$

Coefficent of tangential restitution

$\beta_{ij} = -1, \alpha_{ij} < 1 \longrightarrow$ Smooth spheres

Boltzmann collision operator

$$J_{ij}[f_i,f_j] = \sigma_{ij}^{d-1} \int d\mathbf{v}_2 \int d\mathbf{w}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12}) \left[\alpha_{ij}^{-2}\beta_{ij}^{-2} f_i' f_j' - f_i f_j\right]$$

Collisional transfer of momentum and energy in terms of averages involving f_i and f_j

Simplifications:

- Isotropic distributions
- NO correlation between rotational and translational degrees of freedom

$$f_i(v_i, w_i) = f_i^{\mathrm{tr}}(v_i) f_i^{\mathrm{rot}}(w_i)$$

•Maxwell distributions

$$f_i^{\mathrm{tr}}(v_i) = n_i \left(\frac{m_i}{2\pi T_i^{\mathrm{tr}}}\right)^{3/2} \exp\left(-\frac{m_i v_i^2}{2T_i^{\mathrm{tr}}}\right)$$

Partial temperatures :

$$T_i^{\mathrm{tr}} = \frac{m_i}{3}\langle v_i^2\rangle$$

$$T_i^{\mathrm{rot}} = \frac{I_i}{3}\langle w_i^2\rangle$$

Partial cooling rates :

$$\zeta_{ij}^{\text{tr}} \equiv -\frac{\widetilde{J}_{ij}[v_i^2]}{n_i \langle v_i^2 \rangle}$$

$$\zeta_{ij}^{\text{rot}} \equiv -\frac{\widetilde{J}_{ij}[w_i^2]}{n_i \langle w_i^2 \rangle}$$

Parameter space: $\left\{ m_i, n_i, \sigma_i, I_i, \alpha_{ij}, \beta_{ij} \right\}$

Study of HCS

Homogenous cooling state

$$f_i(v_i, t) = f_i(v_i, T(t))$$

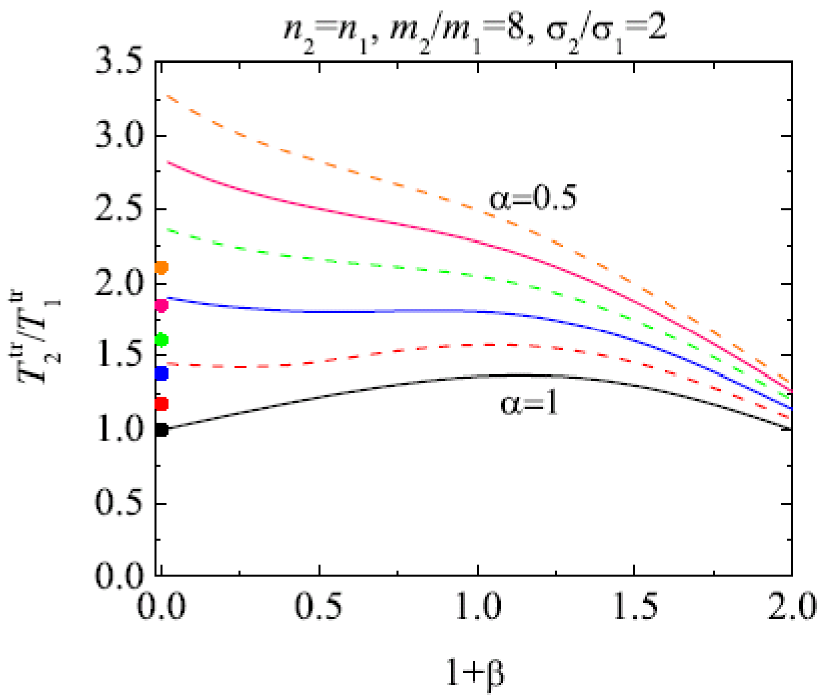
$$\partial_t T_i^{\mathrm{tr}} = -\sum_j \zeta_{ij}^{\mathrm{tr}} T_i^{\mathrm{tr}}$$

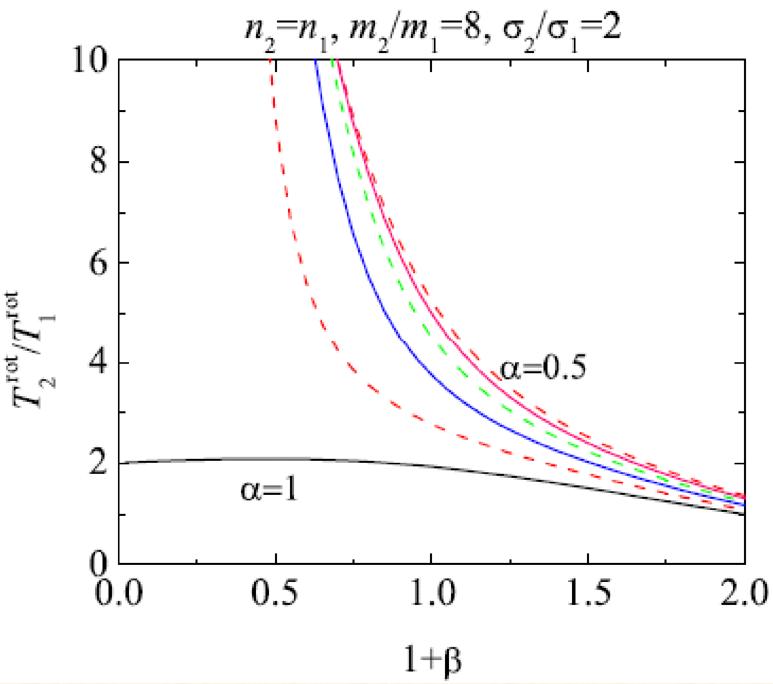
$$\partial_t T_i^{\mathrm{rot}} = -\sum_j \zeta_{ij}^{\mathrm{rot}} T_i^{\mathrm{rot}}$$

Normal solution ⟶ Temperature ratios are constant

$$\sum_j \zeta_{ij}^{\mathrm{tr}} = \sum_j \zeta_{ij}^{\mathrm{rot}}$$

Particular case: binary mixture ⟶ $T_1^{\mathrm{tr}}/T_2^{\mathrm{tr}}, T_1^{\mathrm{rot}}/T_2^{\mathrm{rot}}, T^{\mathrm{tr}}/T^{\mathrm{rot}}$





$\beta = -1$ → Smooth spheres

$\alpha = 1$ → Elastic collisions

CONCLUSIONS

✓Hydrodynamic description (derived from kinetic theory) appears to be a powerful tool for analysis and predictions of rapid flow gas dynamics of granular mixtures.

✓New and interesting result: partial temperatures (which measure the mean kinetic energy of each species) are different (breakdown of energy equipartition theorem). Not surprising feature since granular matter is inherently in non-equilibrium.

✓Energy nonequipartition has important and new quantitiative effects on macroscopic properties (transport coefficients, Einstein and Onsager relations, segregation criterion,…) of the system

PERSPECTIVES

Extension to inelastic **rough** spheres

Influence of **interstitial** fluid on grains (suspensions)

Granular hydrodynamics for **far from equilibrium** steady states

UEx (Spain)

- José María Montanero
- Francisco Vega Reyes
- Andrés Santos

External collaborations

- James W. Dufty (University of Florida, USA)
- Christine Hrenya, Steven Dahl (University of Colorado, USA)
- Gilberto Kremer (Un. Federal Paraná, Brazil)

Ministerio de Educación y Ciencia (Spain) Grant no. FIS2007-60977
Junta de Extremadura Grant No. GRU09038

European Union
European Regional Development Fund

IWNET 2009, August 24-28, Cuernavaca, Mexico

Thanks for your attention and….

HASTA LA PRÓXIMA, CUATES