# TRANSPORT PROPERTIES IN DRIVEN GRANULAR MIXTURES AT LOW-DENSITY: SOME APPLICATIONS

Vicente Garzó

Departamento de Física and Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, Badajoz, Spain

Nagi Khalil

IFISC (CSIC-UIB), Universitat de les Illes Balears, Palma de Mallorca, Spain

*Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto*

# OUTLINE

**1**. Driven granular mixtures at low-density. Boltzmann kinetic equation for ***smooth*** inelastic hard spheres

**2**. Homogeneous steady state (HSS)

**3**. Navier-Stokes hydrodynamics: transport coefficients

**4**. *Stability* anaysis of the HSS

**5.** 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

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

***Coefficient of restitution***

$$\boxed{0 < \alpha \leq 1}$$

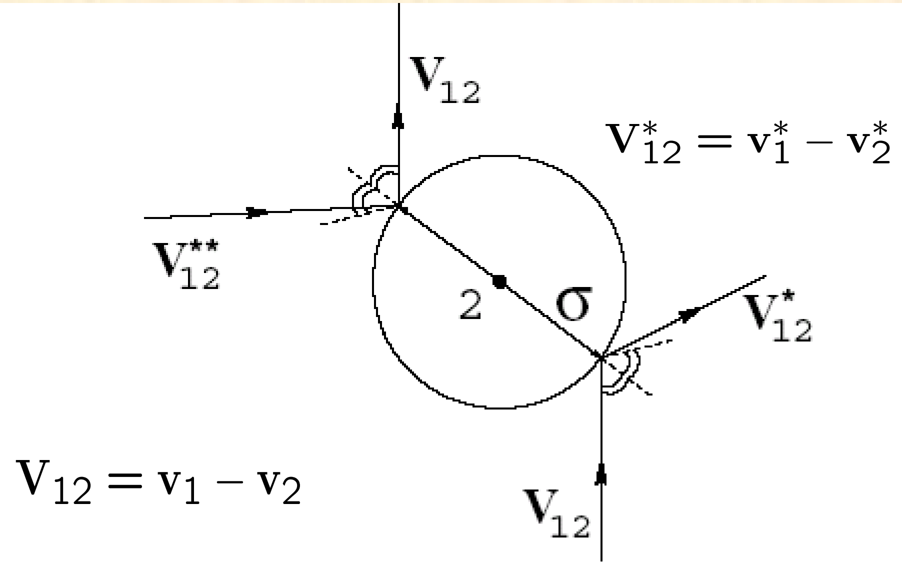



FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

Direct collision

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

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

*Momentum* conservation

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

*Collisional* energy change

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

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

In real experiments, external energy must be injected into the system to compensate for the energy lost by collisions. ***Nonequilibrium*** steady states. Most of the simulations are carried out under steady state conditions (external nonconservative forces)

The effect of the interstitial fluid (like air) surrounding the grains is usually neglected in most of the theoretical works

At a kinetic theory level, description of gas-solid flows is intricate:
(i) there are two different phases and (ii) set of two coupled Boltzmann equations for each one of the phases

Both previous effects can be modeled by the introduction of external forces (``*thermostats*'')

# Driven granular monocomponent granular gases

Inspired in Andrea Puglisi and coworkers. Interaction of a granular gas with a thermal bath at fixed temperature

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathcal{F} f = J[f, f]$$

Operator representing the effect of an external force on solid particles

Thermostat constituted by two different terms: (i) viscous drag force plus (ii) stochastic force

$$\mathbf{F} = \mathbf{F}^{\mathsf{drag}} + \mathbf{F}^{\mathsf{st}}$$

Viscous drag force proportional to the velocity of particles. This force attempts to model the friction of solid particles on the surrounding interstitial gas

$$\mathbf{F}^{\mathsf{drag}} = -m\gamma_{\mathsf{b}} \left(\mathbf{v} - \mathbf{U}_g\right)$$

*Friction* or drift coefficient

Flow velocity of the interstitial gas

***Stochastic force***: tries to simulate the kinetic energy gain due to eventual collisions with the more rapid molecular surrounding gas. It does this by adding a random velocity to each particle between successive collisions.

[Williams and MacKintosh, PRE **54**, R9 (1996)]

Gaussian white noise. It is represented by a Fokker-Planck operator in the BE

$$\boxed{\mathcal{F}^{\mathrm{st}} f \to -\frac{1}{2}\xi_{\mathrm{b}}^2 \frac{\partial^2 f}{\partial v^2}}$$

van Noije and Ernst, GM **1**, 57 (1998)

*Strength* of the correlation

## Boltzmann equation for *driven* granular gases

$$\partial_t f + \mathbf{v}\cdot\nabla f - \gamma_\mathrm{b}\Delta\mathbf{U}\cdot\frac{\partial f}{\partial\mathbf{v}} - \gamma_\mathrm{b}\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{V}f - \frac{1}{2}\xi_\mathrm{b}^2\frac{\partial^2 f}{\partial v^2} = J[f,f]$$

$$\Delta\mathbf{U} = \mathbf{U} - \mathbf{U}_g \qquad \mathbf{V} = \mathbf{v} - \mathbf{U}$$

Similar kinetic equation to a model for gas-solid ***suspensions***
(VG et al. J. Fluid Mech. **712**, 129 (2012))

## Boltzmann equation for *driven* granular mixtures

There is some flexibility in the choice of the external forces for mixtures since either one takes both forces to be the same for each species or they can be chosen to be functions of mass of each species

To cover both possibilities $\mathcal{F}_i f_i = \mathcal{F}_i^{\mathrm{drag}} f_i + \mathcal{F}_i^{\mathrm{st}} f_i$

$$\mathcal{F}_i^{\mathrm{drag}} f_i = -\frac{\gamma_{\mathrm{b}}}{m_i^{\beta}} \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{v} - \mathbf{U}_g) f_i$$

$$\mathcal{F}_i^{\mathrm{st}} f_i = -\frac{1}{2} \frac{\xi_{\mathrm{b}}^2}{m_i^{\lambda}} \frac{\partial^2}{\partial v^2} f_i$$

Particular choices: 1. Stochastic thermostat $(\gamma_b = 0, \quad \lambda = 0)$

$$\mathcal{F}_i f_i = -\frac{1}{2}\xi_b^2 \frac{\partial^2}{\partial v^2} f_i$$

(Henrique *et al.* PRE **63**, 011304 (2000);
Barrat and Trizac, GM **4**, 57 (2002),
Dahl *et al.* PRE **66**, 041301 (2002))

2. Fokker-Planck model $(\beta = 1, \quad \lambda = 2, \quad \mathbf{U} = \mathbf{U}_g)$

$$\mathcal{F}_i f_i = -\frac{\gamma_b}{m_i}\frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{v} - \mathbf{U}) f_i - \frac{1}{2}\frac{\xi_b^2}{m_i^2}\frac{\partial^2}{\partial v^2} f_i$$

(Hayakawa, PRE **68**, 031304 (2003)
Sarracino *et al.* JSTAT P04013 (2010))

$$\boxed{\partial_t f_i + \mathbf{v}\cdot\nabla f_i - \frac{\gamma_\mathrm{b}}{m_i^\beta}\Delta\mathbf{U}\cdot\frac{\partial f_i}{\partial\mathbf{v}} - \frac{\gamma_\mathrm{b}}{m_i^\beta}\frac{\partial}{\partial\mathbf{v}}\cdot\mathbf{V} f_i - \frac{1}{2}\frac{\xi_\mathrm{b}^2}{m_i^\lambda}\frac{\partial^2 f_i}{\partial v^2} = \sum_{j=1}^{2} J_{ij}\left[f_i, f_j\right]}$$

Results derived from this Boltzmann equation could be applicable to bidisperse granular ***suspensions*** at low-density

# MACROSCOPIC BALANCE EQUATIONS

***Hydrodynamic*** fields

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

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

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

Collision operators conserve the particle number of each species and the total momentum but the total energy is not conserved.

$$\int \mathrm{d}\mathbf{v} J_{ij}=0$$

$$\sum_{i,j}\int \mathrm{d}\mathbf{v}\left\{m_i\mathbf{v},\frac{m_i}{2}V^2\right\}J_{ij}=\{\mathbf{0},-dnT\zeta\}$$

Cooling rate

# Balance equation for the partial densities

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

# Balance equation for the flow velocity

$$\boxed{\rho D_t \mathbf{U} + \nabla \cdot \mathsf{P} = -\gamma_{\mathsf{b}} \left( \Delta \mathbf{U} \sum_i \frac{m_i n_i}{m_i^{\beta}} + \sum_i \frac{\mathbf{j}_i}{m_i^{\beta}} \right)}$$

# Balance equation for the granular temperature

$$\boxed{(D_t + \zeta)\, T + \frac{2}{dn} (\mathsf{P} : \nabla \mathbf{U} + \nabla \cdot \mathbf{q}) - \frac{T}{n} \sum_i \frac{\nabla \cdot \mathbf{j}_i}{m_i} = -\frac{2\gamma_{\mathsf{b}}}{dn} \sum_i \frac{\Delta \mathbf{U} \cdot \mathbf{j}_i}{m_i^{\beta}} - 2\gamma_{\mathsf{b}} \sum_i \frac{n_i T_i}{m_i^{\beta}} + \frac{\xi_{\mathsf{b}}^2}{n} \sum_i \frac{n_i m_i}{m_i^{\lambda}}}$$

$$D_t \equiv \partial_t + \mathbf{v} \cdot \nabla$$

Mass flux of species $i$

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

Pressure tensor

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

Heat flux

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

# HOMOGENEOUS STEADY STATES (HSS)

Most simple situation: the partial densities and temperature are spatially *uniform* and with a selection of frame of reference

$$\mathbf{U} = \mathbf{U}_g = \mathbf{0}$$

*Partial* temperatures: associated with the kinetic energy of species *i*

$$T_i = \frac{m_i}{dn_i} \int \mathrm{d}\mathbf{v}\; v^2 f_i(\mathbf{v})$$

$$\boxed{\partial_t f_i - \frac{\gamma_\mathsf{b}}{m_i^\beta}\frac{\partial}{\partial \mathbf{v}}\cdot \mathbf{v} f_i - \frac{1}{2}\frac{\xi_\mathsf{b}^2}{m_i^\lambda}\frac{\partial^2 f_i}{\partial v^2} = \sum_{j=1}^{2} J_{ij}\left[f_i, f_j\right]}$$

Extension to dense gases (Enskog equation) is quite simple $J_{ij} \to \chi_{ij} J_{ij}$

After a transient regime, the system achieves a *steady* state. The (asymptotic) steady partial temperatures obey the coupled equations

$$\boxed{\frac{2T_i}{m_i^\beta}\gamma_\mathsf{b} + \zeta_i T_i = \frac{\xi_\mathsf{b}^2}{m_i^{\lambda-1}}}$$

Partial cooling rates $\zeta_i = -\frac{m_i}{d n_i T_i}\sum_{j=1}^{2}\int d\mathbf{v}\, v^2 J_{ij}[f_i, f_j]$

## Elastic collisions

When both partial distribution functions are Maxwellian distributions at the *same* temperature, then partial cooling rates vanish and

$$T_i^{\mathrm{el}} = \frac{\xi_{\mathrm{b}}^2}{2\gamma_{\mathrm{b}} m_i^{\lambda-\beta-1}}$$

Energy equipartition is fulfilled for equal masses or when $\lambda - \beta = 1$

Equivalent to ``Fluctuation-dissipation'' relation

``Bath temperature´´ $T_i^{\mathrm{el}} = T_{\mathrm{b}} = \frac{\xi_{\mathrm{b}}^2}{2\gamma_{\mathrm{b}}(2\overline{m})^{\lambda-\beta-1}}, \quad \overline{m} = \frac{m_1 m_2}{m_1 + m_2}$

Dimensional analysis requires that the distribution functions have the *scaled* forms

$$\boxed{f_i(\mathbf{v},\gamma_\mathsf{b},\xi_\mathsf{b}^2) = n_i v_\mathsf{th}^{-d}\varphi_i\left(x_1,\mathbf{c},\xi^*,\gamma^*\right)}$$

$$v_\mathsf{th} = \sqrt{2T/\overline{m}}, \quad \mathbf{c} = \mathbf{v}/v_\mathsf{th}$$

$$\xi^* = \frac{\xi_\mathsf{b}^2}{n\sigma_{12}^{d-1}\overline{m}^{\lambda-1}T v_\mathsf{th}}, \quad \gamma^* = \frac{\gamma_\mathsf{b}}{n\sigma_{12}^{d-1}\overline{m}^{\beta}v_\mathsf{th}} = \omega^*\xi^{*1/3}$$

Scaled distributions verify the BE

$$\boxed{\frac{1}{2}\zeta_i^*\frac{\partial}{\partial\mathbf{c}}\cdot\mathbf{c}\varphi_i - \frac{1}{2}\frac{\xi^*}{M_i^{\lambda-1}\chi_i}\frac{\partial}{\partial\mathbf{c}}\cdot\mathbf{c}\varphi_i - \frac{1}{4}\frac{\xi^*}{M_i^\lambda}\frac{\partial^2}{\partial c^2}\varphi_i = \sum_{j=1}^2 J_{ij}^*[\varphi_i,\varphi_j]}$$

$$\zeta_i^* = \zeta_i/n\sigma_{12}^{d-1}v_\mathsf{th}, \quad M_i = m_i/\overline{m}, \quad \chi_i = T_i/T$$

Once the scaled distributions are obtained , the partial cooling rates can be determined and hence the partial temperatures

$$T^* \left[1-(M_i/2)^{\lambda-1-\beta}T_i^*\right]\xi^* = M_i^{\lambda-1}\zeta_i^* T_i^*$$

$$T_i^* = T_i/T_\mathrm{b}, \quad T^* = T/T_\mathrm{b} = x_1 T_1^* + x_2 T_2^*$$

Well-possed mathematical problem: partial temperatures are given in terms of the model parameters, concentration, and the mechanical parameters of the mixture

Unfortunately, the scaled distributions are not ***exactly*** known for inelastic collisions

A good estimate for the scaled distributions is to consider the low order truncation in a Laguerre (Sonine) polynomial expansion

$$\varphi_i(\mathbf{c}) \to \varphi_{i,\mathrm{M}}(\mathbf{c}) \left\{ 1 + \frac{\lambda_i}{4} \left[ \theta_i^2 c^4 - (d+2)\theta_i c^2 + \frac{d(d+2)}{4} \right] \right\}$$

$$\varphi_{i,\mathrm{M}}(\mathbf{c}) = \pi^{-d/2} \theta_i^{d/2}\, e^{-\theta_i c^2}, \qquad \theta_i = m_i T / (\overline{m} T_i)$$

Deviations of the scaled distributions from their Maxwellians forms (kurtosis or cumulants)

$$\boxed{\lambda_i = 2 \left[ \frac{4}{d(d+2)} \theta_i \int \mathrm{d}\mathbf{c}\; c^4 \varphi(\mathbf{c}) - 1 \right]}$$

As usual, only ***linear*** contributions in cumulants are retained

Comparison against MD simulations for dense systems (hard spheres)
(Khalil and VG, J. Chem. Phys. **140**, 164901 (2014))

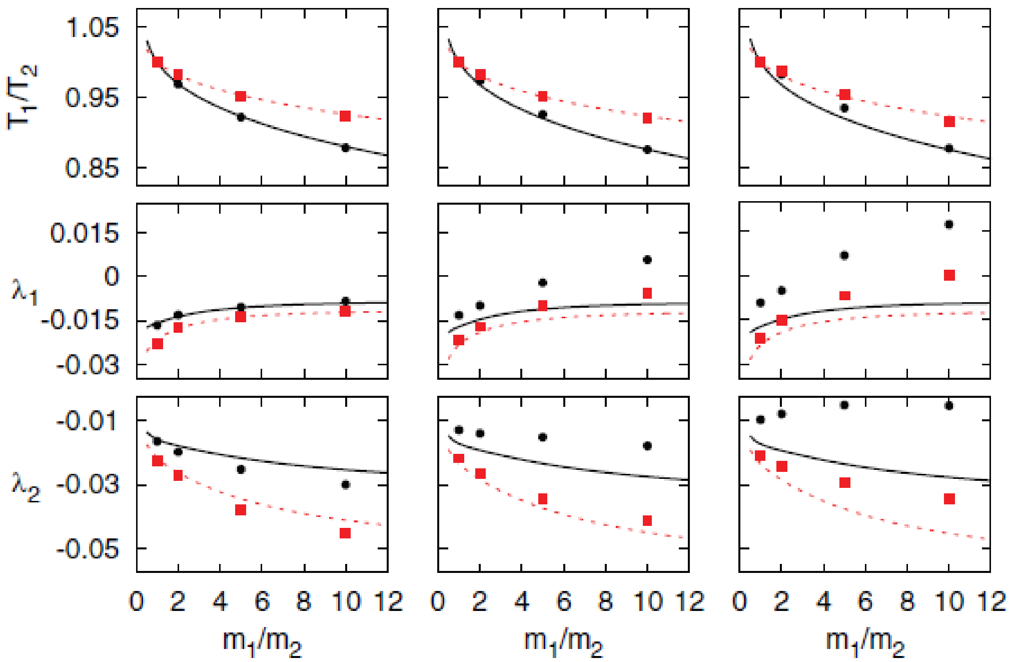



FIG. 3. Case I: Plot of the temperature ratio $T_1/T_2$ and the cumulants $\lambda_1$ and $\lambda_2$ as a function of the mass ratio $m_1/m_2$ for $\sigma_1/\sigma_2 = \phi_1/\phi_2 = 1$, and two different values of the (common) coefficient of restitution $\alpha$: $\alpha = 0.8$ (solid lines and circles) and $\alpha = 0.9$ (dashed lines and squares). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The first, second, and third columns correspond to $\phi = 0.00785$, $\phi = 0.1$, and $\phi = 0.2$, respectively.

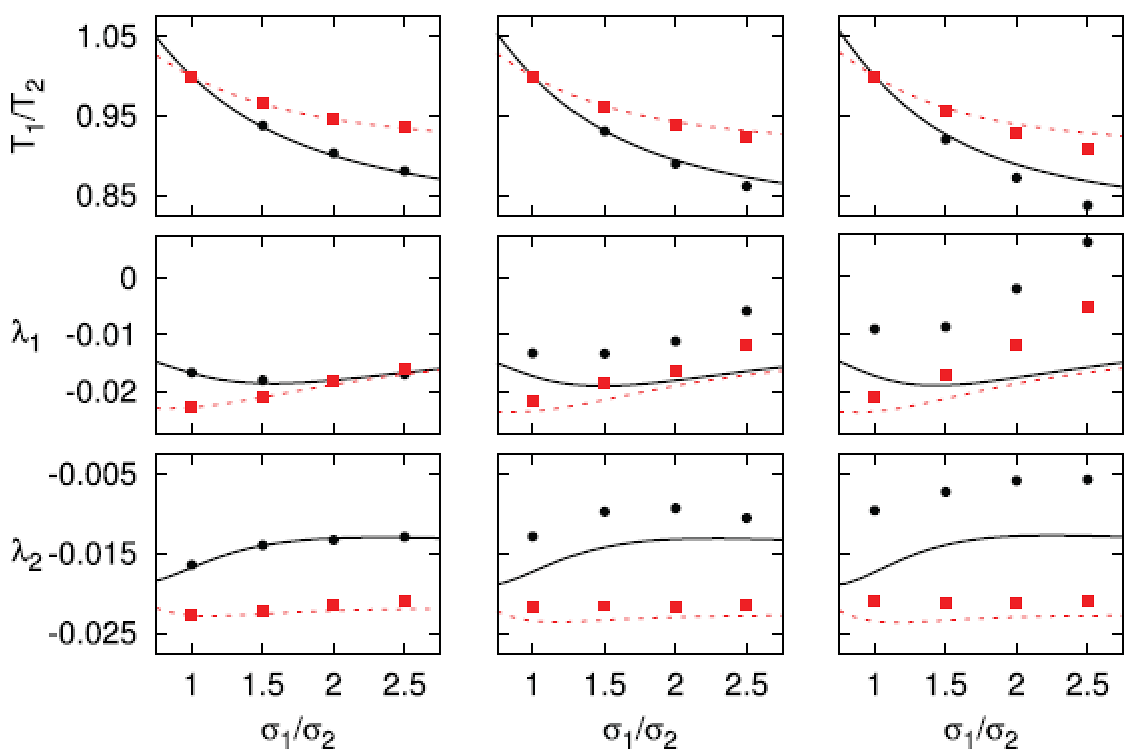



FIG. 4. Case II: Plot of the temperature ratio $T_1/T_2$ and the cumulants $\lambda_1$ and $\lambda_2$ as a function of the size ratio $\sigma_1/\sigma_2$ for $m_1/m_2 = \phi_1/\phi_2 = 1$, and two different values of the (common) coefficient of restitution $\alpha$: $\alpha = 0.8$ (solid lines and circles) and $\alpha = 0.9$ (dashed lines and squares). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The first, second, and third columns correspond to $\phi = 0.00785$, $\phi = 0.1$, and $\phi = 0.2$, respectively.

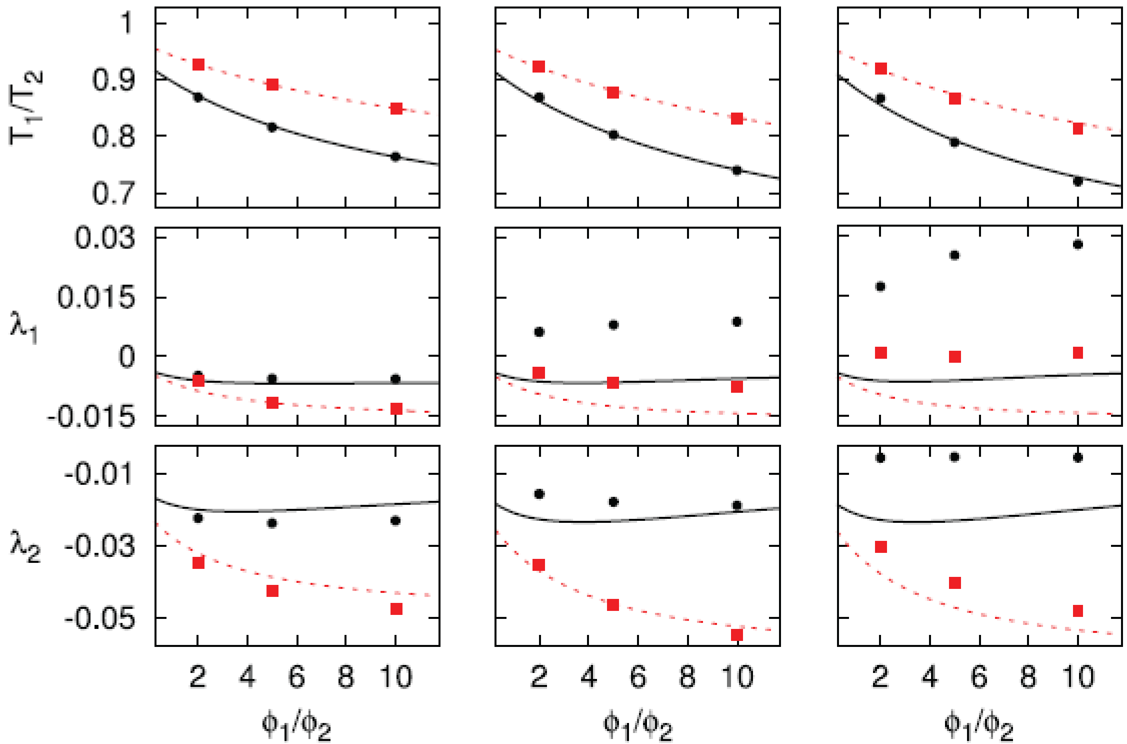



FIG. 5. Case III: Plot of the temperature ratio $T_1/T_2$ and the cumulants $\lambda_1$ and $\lambda_2$ as a function of the composition $\phi_1/\phi_2$ for $m_1/m_2=\sigma_1/\sigma_2=1$, and two different values of the (common) coefficient of restitution $\alpha$: $\alpha=0.8$ (solid lines and circles) and $\alpha=0.9$ (dashed lines and squares). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The first, second, and third columns correspond to $\phi=0.00785$, $\phi=0.1$, and $\phi=0.2$, respectively.

$$m_1/m_2=8, \sigma_1/\sigma_2=8$$

$$\frac{\phi_1}{\phi_2}=\frac{x_1\sigma_1^3}{x_2\sigma_2^3}$$

# CHAPMAN-ENSKOG SOLUTION

The HSS is perturbed by *small* spatial gradients. Nonzero contributions to the mass, momentum, and heat fluxes. Boltzmann equation can be solved by means of the Chapman-Enskog method

***Normal*** or hydrodynamic solution. For times longer than the mean free time

$$f_i(\mathbf{r},\mathbf{v},t)=f_i\left[\mathbf{v}|x_1(\mathbf{r},t),p(\mathbf{r},t),T(\mathbf{r},t),\mathbf{U}(\mathbf{r},t)\right]$$

This functional dependence can be made local in space and time through an expansion in powers of spatial gradients

$$f_i = f_i^{(0)} + \epsilon\, f_i^{(1)} + \epsilon^2 f_i^{(2)} + \cdots$$

Implicit gradient of a hydrodynamic field

Some considerations:

(i) Driven parameters of the model do not induce any flux (zeroth-order in gradients)

(ii) Difference of the mean velocities is assumed to be at least of first order in gradients. In the absence of gradients $\mathbf{U} = \mathbf{U}_g$

# ZEROTH-ORDER DISTRIBUTION FUNCTION

$$\partial_t^{(0)} f_i^{(0)} - \frac{\gamma_\mathrm{b}}{m_i^\beta}\frac{\partial}{\partial \mathbf{v}}\cdot \mathbf{V} f_i^{(0)} - \frac{1}{2}\frac{\xi_\mathrm{b}^2}{m_i^\lambda}\frac{\partial^2}{\partial v^2} f_i^{(0)} = \sum_{j=1}^{2} J_{ij}[f_i^{(0)}, f_j^{(0)}]$$

Balance equations at zeroth-order

$$\partial_t^{(0)} x_1 = 0, \quad \partial_t^{(0)} \mathbf{U} = \mathbf{0}, \quad T^{-1}\partial_t^{(0)} T = p^{-1}\partial_t^{(0)} p = -\Lambda^{(0)}$$

$$\boxed{\Lambda^{(0)} \equiv 2\gamma_\mathrm{b} \sum_{i=1}^{2} \frac{x_i \chi_i}{m_i^\beta} - \frac{\xi_\mathrm{b}^2}{p}\sum_{i=1}^{2}\frac{\rho_i}{m_i^\lambda} + \zeta^{(0)}}$$

Steady-state condition: $\Lambda^{(0)} = 0$

Steady-state condition establishes a mapping between the partial densities, the pressure, and the temperature

Subtle and original point: Since the hydrodynamic fields are specified separately in the ***local*** reference state, then the collisional cooling cannot be in general compensated for by the energy injected in the system by the driving force

The presence of the external thermostat introduces the possibility of a local energy unbalance

$$\boxed{\partial_t^{(0)} T \neq 0, \qquad \partial_t^{(0)} p \neq 0}$$

## *Local* zeroth-order distribution

$$f_i^{(0)}(\mathbf{r},\mathbf{v},t) = x_i(\mathbf{r},t)\frac{p(\mathbf{r},t)}{T(\mathbf{r},t)}v_{\text{th}}(\mathbf{r},t)^{-d}\varphi_i\left(x_1,\mathbf{c},\gamma^*,\xi^*\right)$$

The dependence of the zeroth-order distribution on temperature and pressure is explicit and also through the (reduced) velocity and driven parameters

$$\partial_t^{(0)} f_i^{(0)} = -\Lambda^{(0)}\left(T\partial_T + p\partial_p\right) f_i^{(0)}$$

$$\left(T\partial_T + p\partial_p\right) f_i^{(0)} = -\frac{1}{2}\frac{\partial}{\partial \mathbf{v}}\cdot\left(\mathbf{V} f_i^{(0)}\right) - \frac{3}{2}\xi^*\frac{\partial f_i^{(0)}}{\partial \xi^*}$$

We are interested in obtaining the transport coefficents in the steady-state. These coefficients depend on the derivatives of temperature ratio on concentration, and driven parameters

# NAVIER-STOKES TRANSPORT COEFFICIENTS

The first-order distribution function is

$$f_i^{(1)} = \mathcal{A}_i \cdot \nabla x_1 + \mathcal{B}_i \cdot \nabla p + \mathcal{C}_i \cdot \nabla T + \mathcal{D}_{i,k\ell} \frac{1}{2} \left( \nabla_k U_\ell + \nabla_\ell U_k - \frac{2}{d} \delta_{k\ell} \nabla \cdot \mathbf{U} \right) + \mathcal{E}_i \nabla \cdot \mathbf{U} + \mathcal{G}_i \cdot \Delta \mathbf{U}$$

The ***unknowns*** verify a set of coupled linear integral equations. They can be solved approximately by considering the leading terms in a Sonine polynomial expansion

Constitutive equations for the mass, momentum, and heat fluxes. Linear deviations from the steady state. Transport coefficients evaluated when the steady state conditions applies. Significant simplification

Mass flux

$$\mathbf{j}_1^{(1)} = -\left(\frac{m_1 m_2 n}{\rho}\right) D \nabla x_1 - \frac{\rho}{p} D_p \nabla p - \frac{\rho}{T} D_T \nabla T - D_U \Delta \mathbf{U}$$

Pressure tensor

$$P_{k\ell}^{(1)} = -\eta \left(\partial_k U_\ell + \partial_\ell U_k - \frac{2}{d}\delta_{k\ell} \nabla \cdot \mathbf{U}\right)$$

Heat flux

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

(N. Khalil, VG PRE **88**, 052201 (2013))

## *Nine* transport coefficients

$$\begin{pmatrix} D \\ D_p \\ D_T \\ D_U \\ D'' \\ L \\ \kappa \\ \kappa_U \\ \eta \end{pmatrix} = \begin{pmatrix} \text{diffusion coefficient} \\ \text{pressure diffusion coefficient} \\ \text{thermal diffusion coefficient} \\ \text{velocity diffusion coefficient} \\ \text{Dufour coefficient} \\ \text{pressure energy coefficient} \\ \text{thermal conductivity} \\ \text{velocity conductivity} \\ \text{shear viscosity} \end{pmatrix}$$

These coefficients are determined at the steady state

$$\Lambda^{(0)} = 0$$

Transport coefficients associated with the mass flux

$$D = -\frac{\rho}{d m_2 n} \int \mathrm{d}\mathbf{v}\, \mathbf{V} \cdot \mathcal{A}_1$$

$$D_p = -\frac{m_1 p}{d \rho} \int \mathrm{d}\mathbf{v}\, \mathbf{V} \cdot \mathcal{B}_1$$

$$D_T = -\frac{m_1 T}{d \rho} \int \mathrm{d}\mathbf{v}\, \mathbf{V} \cdot \mathcal{C}_1$$

$$D_U = -\frac{m_1}{d} \int \mathrm{d}\mathbf{v}\, \mathbf{V} \cdot \mathcal{G}_1$$

Shear viscosity coefficient $$\eta = -\frac{1}{(d-1)(d+2)} \sum_{i=1}^{2} \int d\mathbf{v}\, m_i V_k V_\ell \mathcal{D}_{i,k\ell}$$

Transport coefficients associated with the heat flux

$$D'' = -\frac{1}{dT^2} \sum_{i=1}^{2} \int d\mathbf{v}\, \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{A}_i$$

$$L = -\frac{1}{d} \sum_{i=1}^{2} \int d\mathbf{v}\, \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{B}_i$$

$$\kappa = -\frac{1}{d} \sum_{i=1}^{2} \int d\mathbf{v}\, \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{C}_i$$

$$\kappa_U = -\frac{1}{d} \sum_{i=1}^{2} \int d\mathbf{v}\, \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{G}_i$$

As an example, let us consider the diffusion (coupled) transport coefficients

$$\mathcal{A}_1(\mathbf{V}) \to -f_{1,M}\mathbf{V}\frac{m_1 m_2 n}{\rho n_1 T_1}D, \quad \mathcal{A}_2(\mathbf{V}) \to f_{2,M}\mathbf{V}\frac{m_1 m_2 n}{\rho n_2 T_2}D$$

$$\mathcal{B}_1(\mathbf{V}) \to -f_{1,M}\mathbf{V}\frac{\rho}{p n_1 T_1}D_p, \quad \mathcal{B}_2(\mathbf{V}) \to f_{2,M}\mathbf{V}\frac{\rho}{p n_2 T_2}D_p$$

$$\mathcal{C}_1(\mathbf{V}) \to -f_{1,M}\mathbf{V}\frac{\rho}{T n_1 T_1}D_T, \quad \mathcal{C}_2(\mathbf{V}) \to f_{2,M}\mathbf{V}\frac{\rho}{T n_2 T_2}D_T$$

$$f_{i,M}(\mathbf{V}) = n_i\left(\frac{m_i}{2\pi T_i}\right)^{d/2}\exp\left(-\frac{m_i V^2}{2T_i}\right)$$

## Simple limit case (tracer limit)

Relevant transport coefficient: tracer diffusion coefficient

$$D = \frac{\rho T}{m_1 m_2 n \sigma_{12}^{d-1} v_{\text{th}}} D^*$$

$$\boxed{D^* = \frac{\chi_1}{\nu_D + \mu_{21}^{\beta} \omega^* \xi^{*1/3}}}$$

$$\mu_{ij} = \frac{m_i}{m_i + m_j}$$

$$\nu_D = \frac{2\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)} (1+\alpha_{12}) \mu_{21} \sqrt{\mu_{12} + \mu_{21}\chi_1}$$

Brownian limit $(m_1/m_2 \to \infty)$ (Sarracino et al. JSTAT P04013 (2010))

$$\overline{D} = \frac{T_2 D^*}{m_1 n \sigma_{12}^{d-1} v_{\rm th}}$$

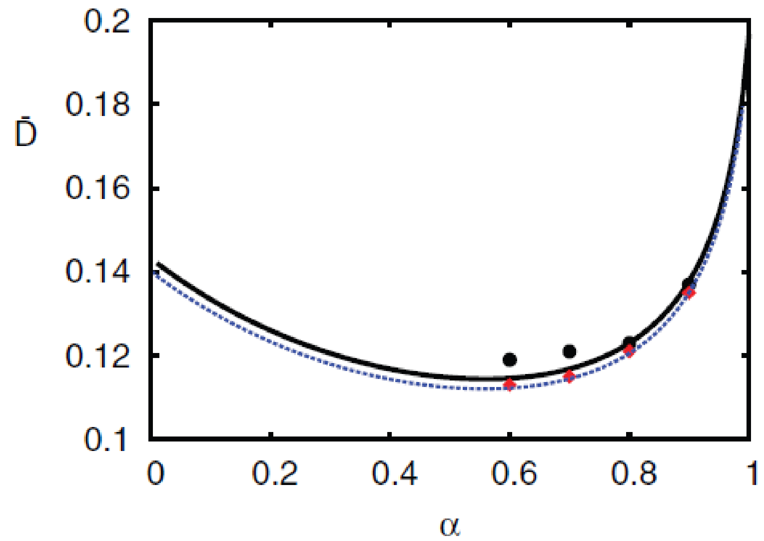
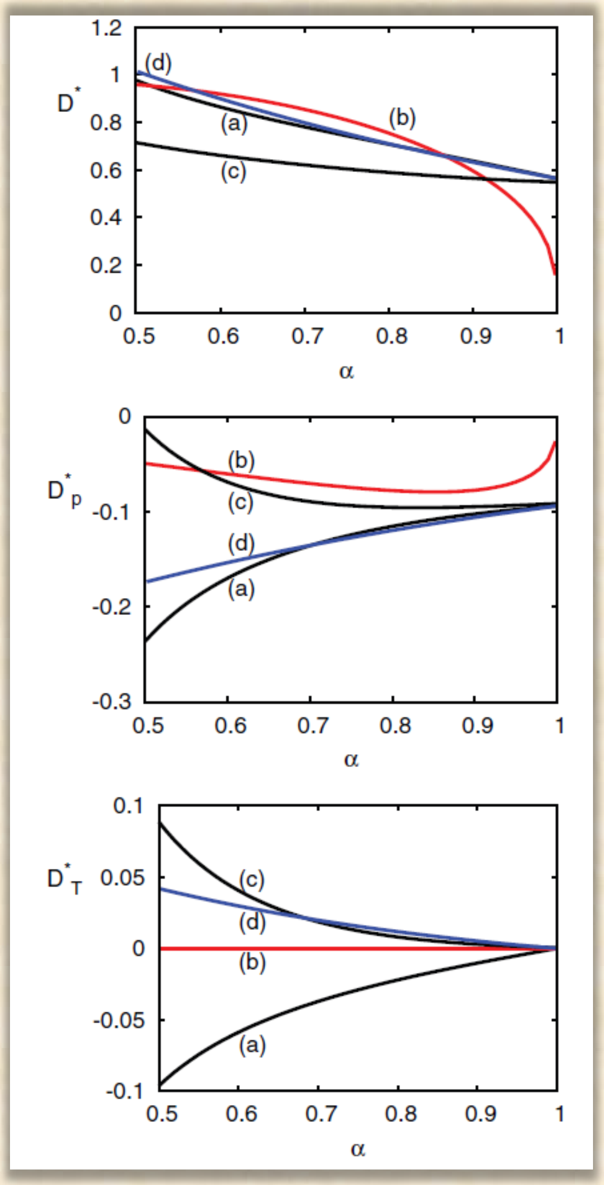



FIG. 3. (Color online) Plot of the self-diffusion coefficient $\overline{D}$ as a function of the (common) coefficient of restitution $\alpha \equiv \alpha_{22} = \alpha_{12}$ for a two-dimensional system ($d = 2$). The parameters of the system are $m_1 = 100m_2$, $\sigma_1 = \sigma_2$, $\phi = 0.007\,85$, $\xi_b^2 = 0.2$, and $\gamma_b = 0.1$. Symbols are the simulation results obtained in Ref. [30] by means of the DSMC method (red diamonds) and MD simulations (black circles). The solid line is the theoretical result obtained from Eq. (92) for $m_1 = 100m_2$, while the dashed line corresponds to the theoretical result obtained from Eq. (95) in the Brownian limit $(m_1/m_2 \to \infty)$.




Hard disks

$$\boxed{x_1 = \frac{1}{2}, \sigma_1/\sigma_2 = 1, m_1/m_2 = 2}$$

(a) Global stochastic thermostat

$$(\gamma_b = \lambda = 0)$$

(b) Local stochastic thermostat

$$(\gamma_b = \lambda = 0)$$

(c) Stochastic bath with friction

$$(\xi_b^2 = 0.2, \gamma_b = 0.1, \lambda = 2, \beta = 1)$$

(d) Undriven system

$$(\xi_b^2 = \gamma_b = 0)$$

$$\boxed{x_1 = \frac{1}{2}, \sigma_1/\sigma_2 = 1}$$

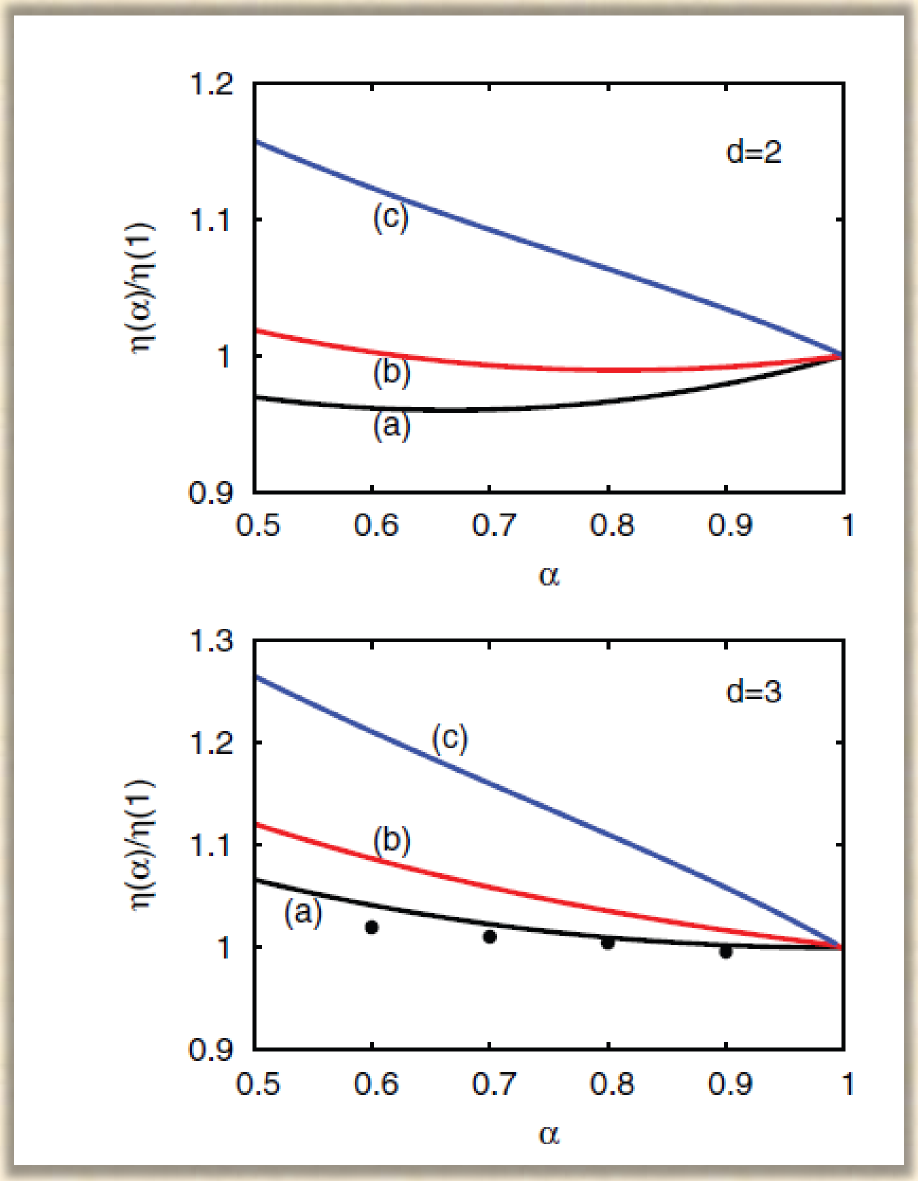
$$(a) m_1/m_2 = 1,$$

$$(b) m_1/m_2 = 2,$$

$$(c) m_1/m_2 = 4$$

Stochastic thermostat

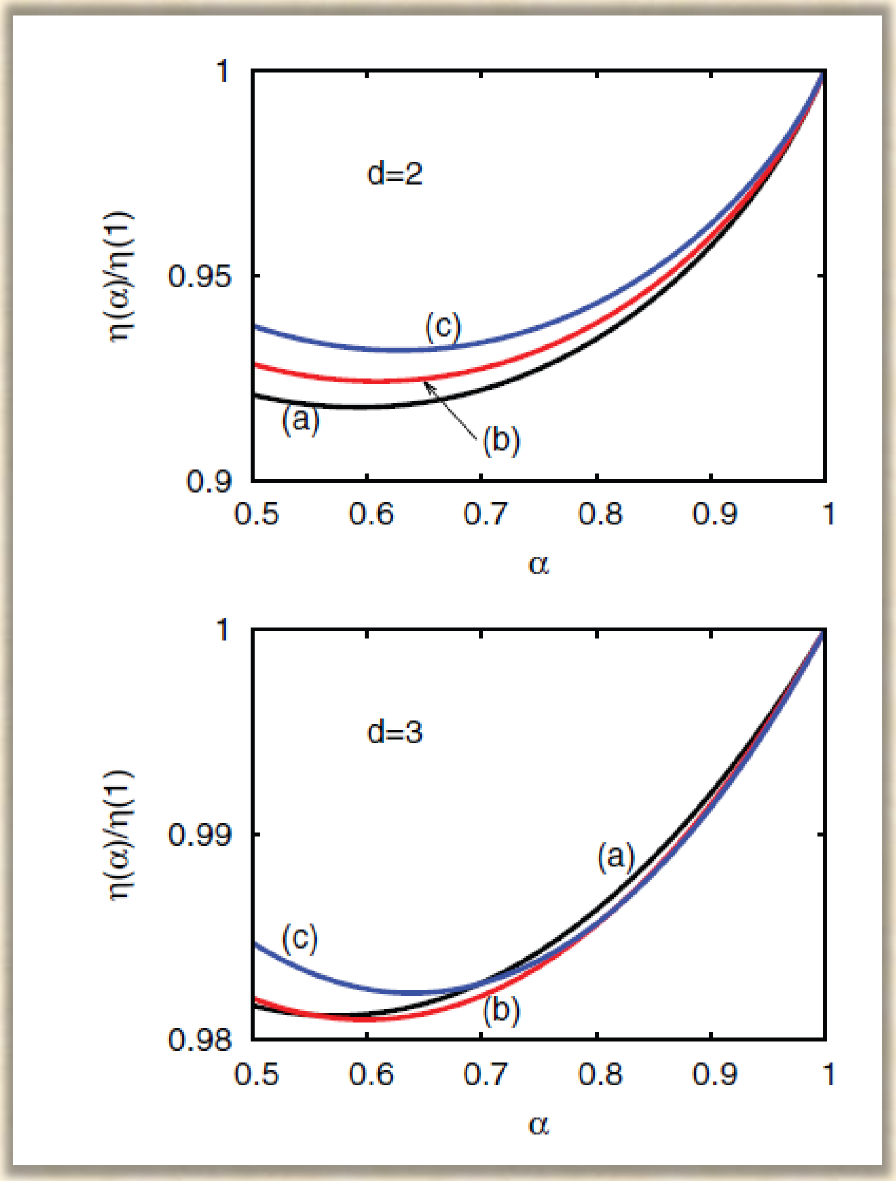
$$(\gamma_b = \lambda = 0)$$



Stochastic bath with friction

$$(\xi_b^2 = 0.2, \gamma_b = 0.1, \lambda = 2, \beta = 1)$$

Small relative deviations form their elastic values



## Heat flux conjugate to temperature gradient (Onsager's reciprocal relation)

$$\mathbf{J}_q \equiv \mathbf{q}^{(1)} - \frac{d+2}{2} T \sum_{i=1}^{2} \frac{\mathbf{j}_i^{(1)}}{m_i} = \frac{p\rho}{m_1 m_2 n^2} \kappa_T \mathbf{j}_1^{(1)} - \kappa' \nabla T - L_p \nabla p - \kappa'_U \Delta \mathbf{U}$$

$$\kappa_T = \frac{TD''}{D} - \frac{d+2}{2}\frac{n}{\rho}(m_2 - m_1)$$ → Thermal diffusion (Soret)

$$\kappa' = \kappa - \frac{\rho^2 T D'' D_T}{m_1 m_2 n D}$$ → Thermal conductivity

$$L_p = L - \frac{\rho^2 T D'' D_p}{m_1 m_2 n D}$$ → New coefficient; vanishes for elastic collisions

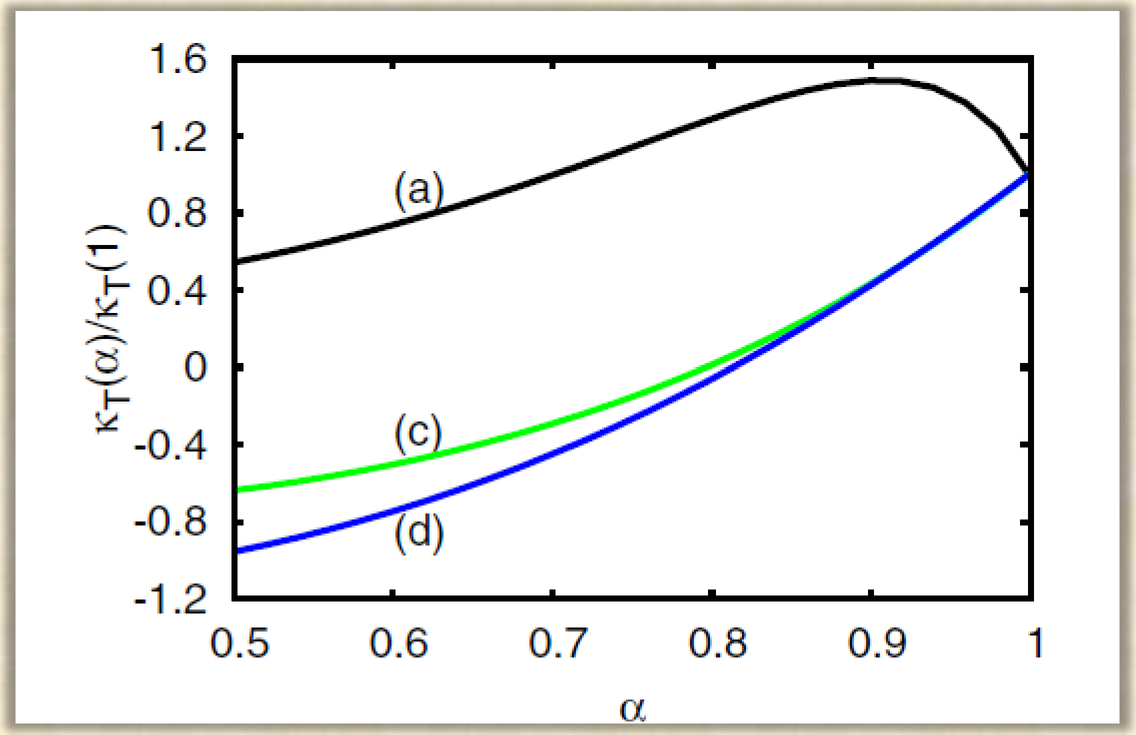
$$\kappa'_U = \kappa - \frac{\rho^2 T D'' D_U}{m_1 m_2 n D}$$

# Thermal diffusion factor

Stochastic bath with friction

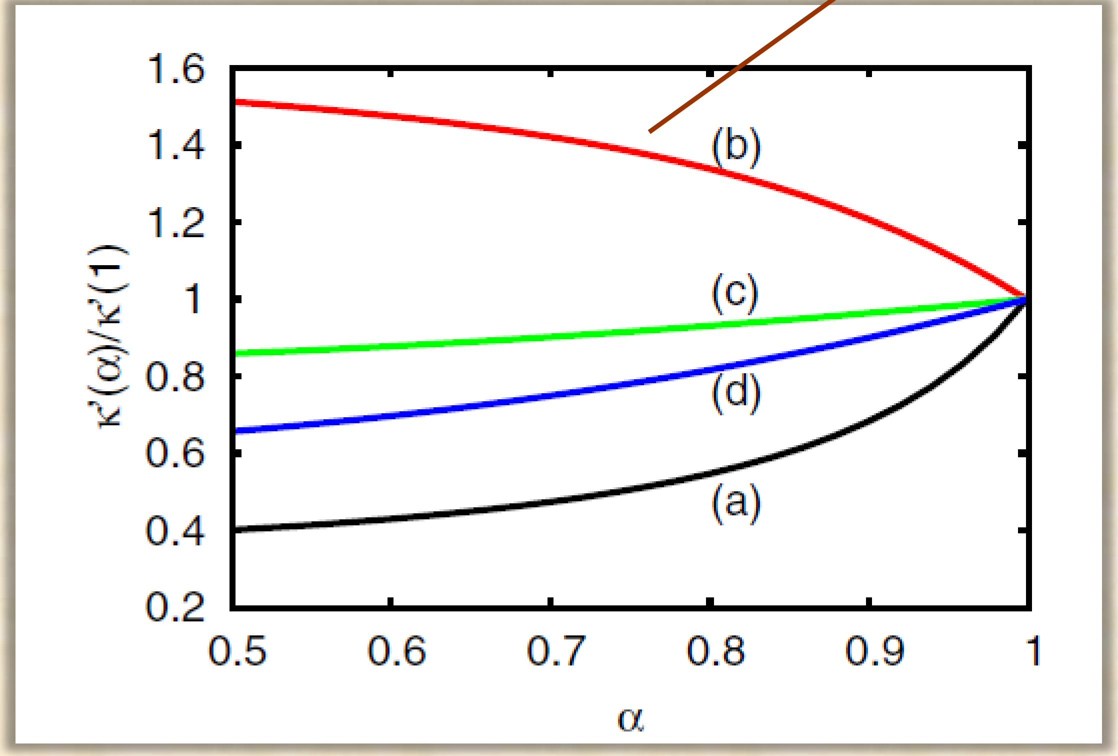
$$d = 3, x_1 = 0.2, \sigma_1/\sigma_2 = 1,$$

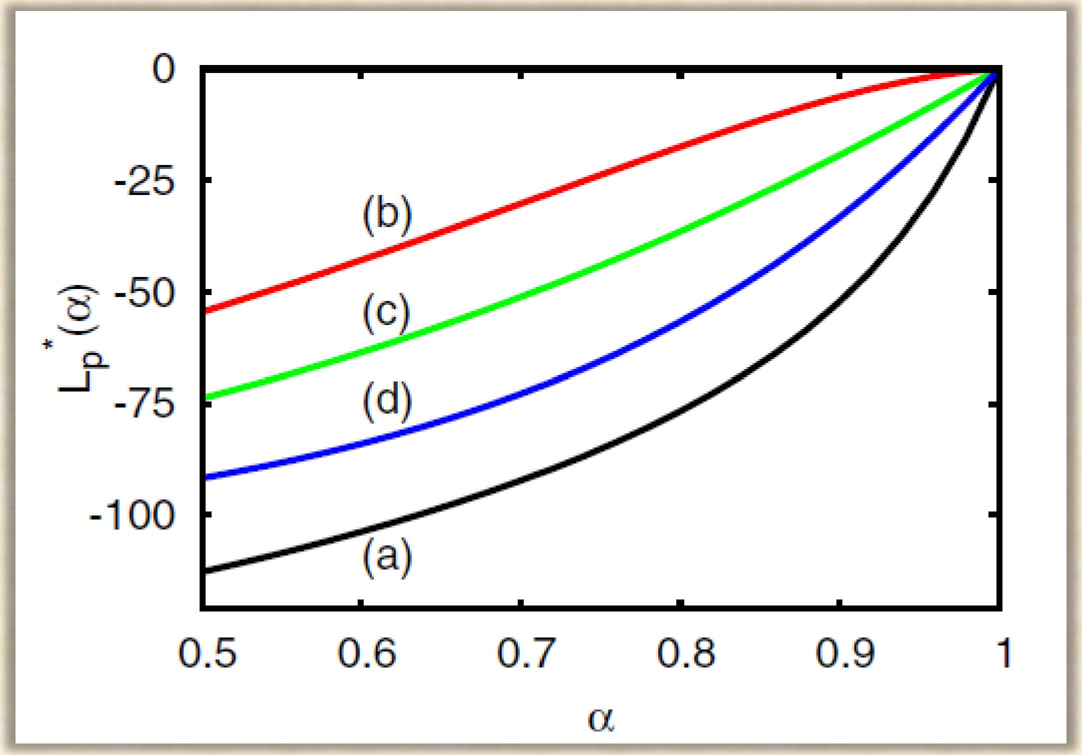
$$(a) m_1/m_2 = 0.5, (c) m_1/m_2 = 2, (d) m_1/m_2 = 4$$



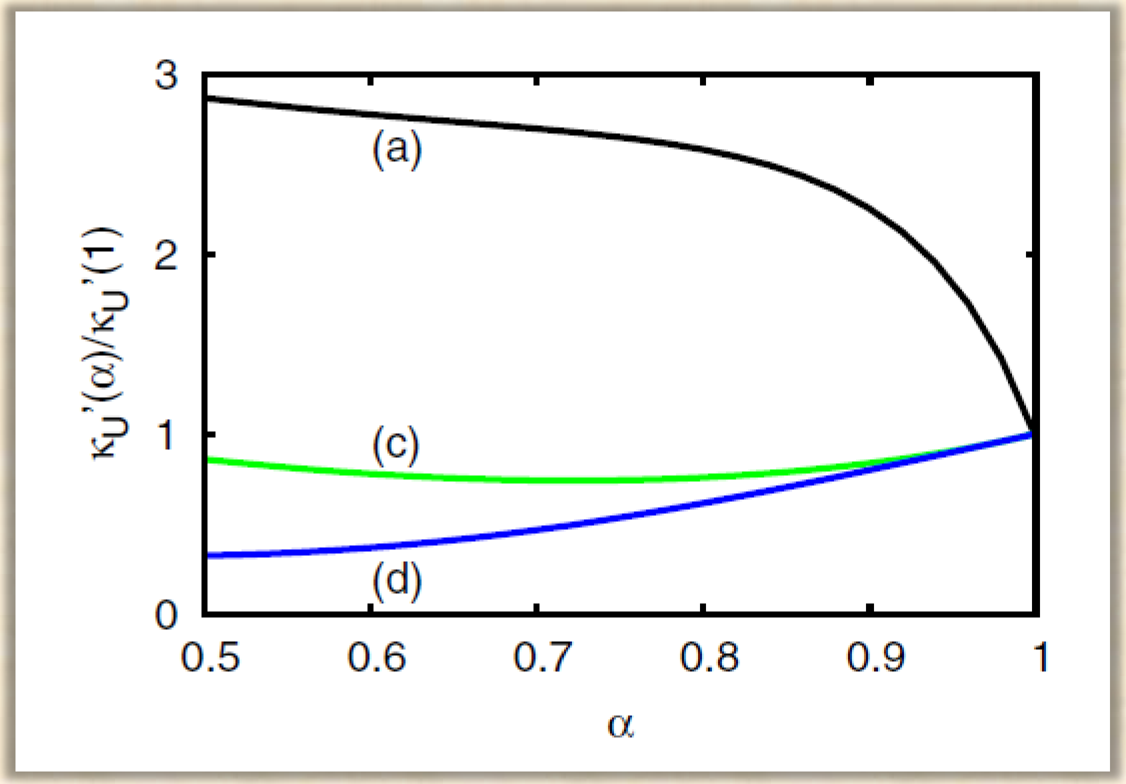
## Thermal conductivity coefficient

$m_1/m_2 = 1$






$$L_p^* = -\frac{2}{(d+2)\sqrt{\pi}}\frac{m_1+m_2}{p\sigma^{d-1}v_{\rm th}}L_p$$


3
2
1
0
0.5
0.6
0.7
0.8
0.9
1
(a)
(c)
(d)
κU'(α)/κU'(1)
α

# LINEAR STABILITY ANALYSIS OF THE HSS

We want to investigate the stability of the HSS with respect to long enough wavelength perturbations.

Stability analysis of the nonlinear hydrodynamic equations with respect to HSS for small initial excitations

**HSS solution** $\nabla x_{1s} = \nabla p_s = \nabla T_s = 0, \mathbf{U}_s = \mathbf{U}_{gs} = \mathbf{0},$

$$\partial_t T = 0, \quad 2M_i^{-\beta}\chi_{is}\gamma_s^* + \zeta_{is}^*\chi_{is} = M_i^{1-\lambda}\xi_s^*, i = 1, 2$$

This basic solution is stable or unstable to linear perturbations?

We linearize the Navier-Stokes equations with respect to the HSS solution. Deviations of the hydrodynamic fields from their values in HCS are *small*

$$\boxed{x_1(\mathbf{r},t) = x_{1s} + \delta x_1(\mathbf{r},t), p(\mathbf{r},t) = p_s + \delta p(\mathbf{r},t), \quad \mathbf{U}(\mathbf{r},t) = \delta\mathbf{U}(\mathbf{r},t), T(\mathbf{r},t) = T_s + \delta T(\mathbf{r},t)}$$

To compare with the results derived for ***undriven*** granular mixtures:

$$\boxed{d\tau = \nu_s dt, \qquad d\boldsymbol{\ell} = \frac{\nu_s}{v_{\text{th,s}}} d\mathbf{r}}$$

Set of Fourier transformed dimensionless variables:

$$\rho_{1,\mathbf{k}}(\tau) = \frac{\delta x_{1\mathbf{k}}(\tau)}{x_{1s}}, \qquad \Pi_{\mathbf{k}}(\tau) = \frac{\delta p_{\mathbf{k}}(\tau)}{p_s}$$

$$\mathbf{w}_{\mathbf{k}}(\tau) = \frac{\delta \mathbf{U}_{\mathbf{k}}(\tau)}{v_{\mathsf{th},s}}, \qquad \theta_{\mathbf{k}}(\tau) = \frac{\delta T_{\mathbf{k}}(\tau)}{T_s}$$

$$\delta y_{\mathbf{k}\beta}(\tau) = \int d\boldsymbol{\ell} e^{-i\mathbf{k}\cdot\boldsymbol{\ell}} \delta y_{\beta}(\boldsymbol{\ell}, \tau)$$

$$\delta y_{\mathbf{k}\beta} \equiv \left\{ \rho_{1,\mathbf{k}}, \Pi_{\mathbf{k}}, \mathbf{w}_{\mathbf{k}}, \theta_{\mathbf{k}} \right\}$$

Set of Fourier transformed dimensionless variables:

$$\rho_{1,\mathbf{k}}(\tau) = \frac{\delta x_{1\mathbf{k}}(\tau)}{x_{1H}}, \quad \rho_{\mathbf{k}}(\tau) = \frac{\delta n_{\mathbf{k}}(\tau)}{n_H}$$

$$\mathbf{w}_{\mathbf{k}}(\tau) = \frac{\delta \mathbf{U}_{\mathbf{k}}(\tau)}{v_H(\tau)}, \quad \theta_{\mathbf{k}}(\tau) = \frac{\delta T_{\mathbf{k}}(\tau)}{T_H(\tau)}$$

$$\delta y_{\mathbf{k}\beta}(\tau) = \int d\boldsymbol{\ell} e^{-i\mathbf{k}\cdot\boldsymbol{\ell}} \delta y_\beta(\boldsymbol{\ell}, \tau)$$

$$\delta y_{\mathbf{k}\beta} \equiv \left\{\rho_{1,\mathbf{k}}, \rho_{\mathbf{k}}, \mathbf{w}_{\mathbf{k}}, \theta_{\mathbf{k}}\right\}$$

As usual, transversal component of the velocity field is *decoupled* from the other modes. This identifies "d-1" shear (transversal) modes

$$\boxed{\frac{\partial \mathbf{w}_{\mathbf{k}\perp}}{\partial \tau} = \lambda_\perp \mathbf{w}_{\mathbf{k}\perp} \qquad \lambda_\perp = -\frac{\overline{m}p}{2\rho T}\eta^* k^2 + \gamma^* \left[\frac{\overline{m}p}{2\rho T}\delta m_\beta D_U^* - \frac{\rho_1 m_2^\beta + \rho_2 m_1^\beta}{\rho(m_1+m_2)^\beta}\right]}$$

$$\delta m_\beta \equiv \frac{m_2^\beta - m_1^\beta}{(m_1+m_2)^\beta}$$

$$\boxed{\mathbf{w}_{\mathbf{k}\perp}(\mathbf{k},\tau) = \mathbf{w}_{\mathbf{k}\perp}(0) e^{\lambda_\perp \tau}}$$

Transversal shear mode is linearly ***stable*** if $\lambda_\perp < 0$

For mechanically equivalent particles $D_U^* = 0 \rightarrow \lambda_\perp < 0$

For mixtures, it is easy to prove that

$$\boxed{\lambda_\perp \leq -\frac{\overline{m}p}{2\rho T}\eta^* k^2 - \gamma^* \frac{\rho \overline{m}^\beta}{\rho_1 m_1^\beta + \rho_2 m_2^\beta} < 0}$$

Transversal shear mode is always linearly stable

The remaining 4 longitudinal modes are *coupled* and are the eigenvalues of a 4X4 matrix

The eigenvalues are the solutions of a quartic equation. In general, they can be obtained by numerically solving this equaiton

Special simple case: mechanically equivalent particles of an inviscid fluid (k=0)

$$\lambda_{||} = \left(0, 0, -2\gamma^*(\mu_{12}^{\beta} + x_1 \delta m_{\beta}), \lambda_{\perp}\right) \leq 0$$

## General case

One of the longitudinal modes could be ***unstable*** for $k < k_{\parallel}^{c}$

The solutions to the hydrodynamic matrix leads to

$$k_{\parallel}^{c} = \left(0, 0, 0, 0, -\sqrt{-\frac{A}{B}}, \sqrt{-\frac{A}{B}}\right)$$

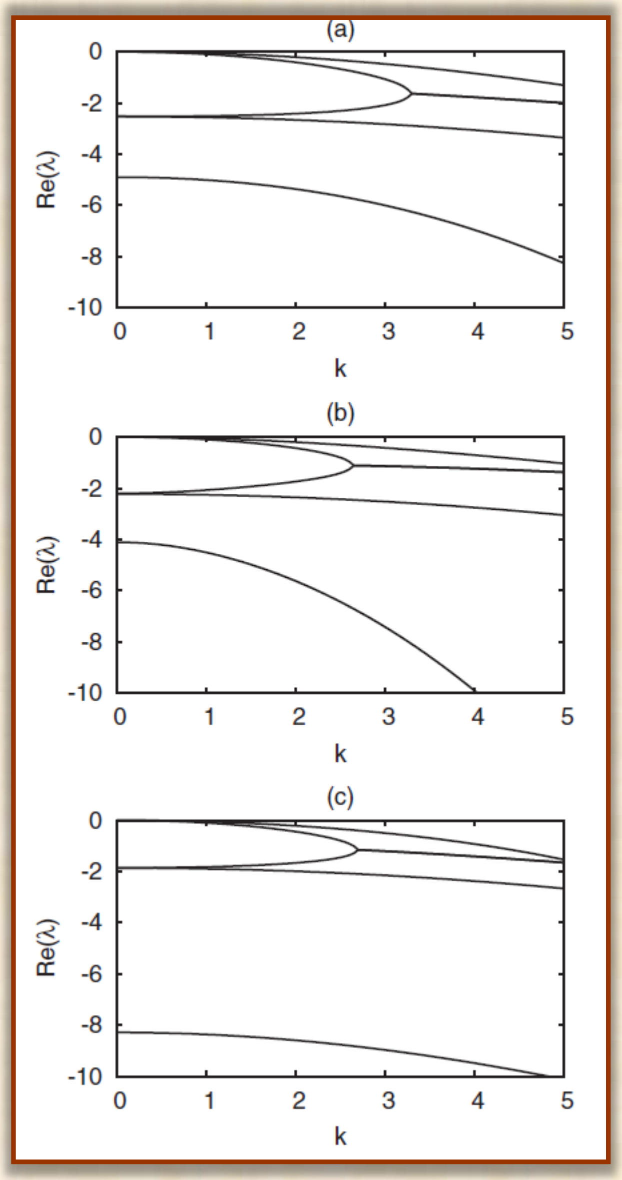
An analysis of the ratio A/B on the control parameters shows that this ratio is always positive. ***NO instabilites*** are found for the longitudinal modes in driven granular mixtures

Stochastic bath with friction

$$d = 3, x_1 = 0.2, \sigma_1/\sigma_2 = 1, \alpha = 0.9$$

$$(a) m_1/m_2 = 2, (c) m_1/m_2 = 3, (d) m_1/m_2 = 4$$

N. Khalil&VG, PRE **97**, 022902 (2018)



# CONCLUSIONS

✓Transport coefficients of a granular binary mixture driven by a stochastic bath with friction have been explicitly obtained from the Boltzmann kinetic equation. **9** relevant transport coefficients

✓***Stationary*** state has been considered for the sake of simplicity. However, the form of these coefficients depends not only on the properties of the steady state but also on the dynamics of the transport coefficients in the vicinity of the state state

✓***Homogeneous steady state (HSS)*****:** Temperature ratio and cumulants. Comparison between kinetic theory and MD shows excellent agreement for temperature ratio but significant discrepancies are found for cumulants at high densities

# CONCLUSIONS

✓Although the impact of inelasticity on transport is in general important, it is less significant than in the undriven case

✓Application: stability of the HSS. Stability analysis of the linearized Navier-Stokes hydrodynamic equations shows that the transversal (shear) y longitudinal modes are ***stable*** http://www.eweb.unex.es/eweb/fisteor/vicente/

Ministerio de Economía y Competitividad (Spain)
Grant no. FIS2016-76359-P, Junta de Extremadura Grant no. GR18079,
both partially financed by FEDER funds

JUNTA DE EXTREMADURA

Fondo Europeo de
Desarrollo Regional
“Una manera de hacer Europa”

Unión Europea