BOLTZMANN KINETIC THEORY FOR INELASTIC MAXWELL MIXTURES

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OUTLINE

0. SOME GENERALITIES

1. INELASTIC MAXWELL MODELS (IMM) FOR MIXTURES

2. HOMOGENEOUS COOLING STATE (HCS)

3. CHAPMAN-ENSKOG SOLUTION

4. TRANSPORT COEFFICIENTS

5. ONSAGER'S RECIPROCAL RELATIONS

6. CONCLUSIONS

Granular materials are ubiquitous in nature and industry. Some examples: storage of cereals in silo's, transport of coal and of pills, landslides and formation of dunes, planetary rings,....

Collection of a large number of discrete macroscopic solid (grains) particles. Interstices between the particles are filled with fluid (air or water).

Dry granular materials: interparticle forces dominate over the fluid-particle interactions (single-phase systems).

Grains are of macroscopic size: ***inelastic*** interactions. Lost of kinetic energy in each collision.

Laboratory experiments and industrial processes: total number of grains is much smaller than Avogrado's number. However, their number is large enough to justify a statistical description.

Rapid flow regime: grains move like atoms or molecules in classical fluids. Grains move ballistically and collide with other grains. I'm interested here in this regime (fluidized system).

Main difference between ordinary and granular fluids: character of the interactions. Notion of Gibbsian equilibrium does not apply to granular fluids (inherent nonequilibrium behavior).

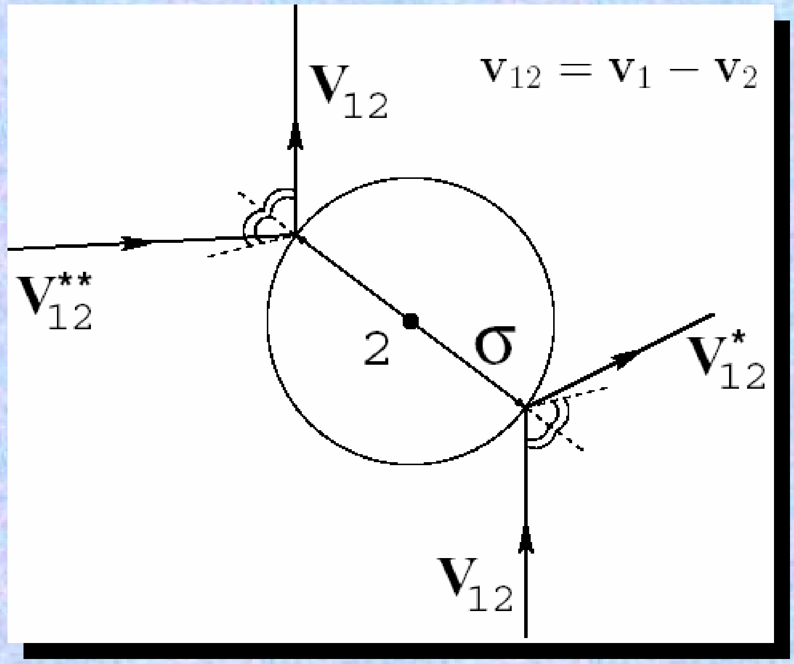
Kinetic theory is still applicable since it does not make any assumption on the conservative or dissipative nature of the interactions.

We want to understand only the effects of collisional dissipation by isolating it from other important properties of granular media in an idealized model. This allows us to identify which qualitative features can be attributed primarily to dissipation.

Granular fluids: Dense fluid with very short range and strongly repulsive interactions.

↓ Idealized model

Smooth hard spheres with inelastic collisions (IHS)



Interactions modelled as ***instantaneous*** collisions

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

Normal (constant) restitution coefficient

$$0 < \alpha \leq 1$$

Direct collision: $\{\mathbf{v}_1, \mathbf{v}_2\} \rightarrow \{\mathbf{v}_1^*, \mathbf{v}_2^*\}$

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

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

Inverse (restituting) collision: $\{\mathbf{v}_1^{**}, \mathbf{v}_2^{**}\} \rightarrow \{\mathbf{v}_1, \mathbf{v}_2\}$

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

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

In a collision, total momentum is conserved but ***not*** the total energy

$$\Delta E = -\frac{1}{4}m(1-\alpha^2)(\mathbf{v}_{12} \cdot \widehat{\boldsymbol{\sigma}})^2$$

Properties of IHS are quite different from those found for elastic had spheres

BOLTZMANN kinetic theory (low-density gas):

Velocity distribution function $f(\mathbf{r}, \mathbf{v}; t)$

Crucial assumptions: Binary collisions+velocities of particles before collisions are uncorrelated (***molecular chaos***)

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

$$J[\mathbf{v}_1|f, f] = \sigma^{d-1} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) \left[\alpha^{-2} f(\mathbf{v}_1^{**}) f(\mathbf{v}_2^{**}) - f(\mathbf{v}_1) f(\mathbf{v}_2)\right]$$

Boltzmann collision operator

Some ***success*** of kinetic theory description for granular fluids

PHYSICAL REVIEW E VOLUME 59, NUMBER 5 MAY 1999

Dense fluid transport for inelastic hard spheres

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Measurements of Grain Motion in a Dense, Three-Dimensional Granular Fluid

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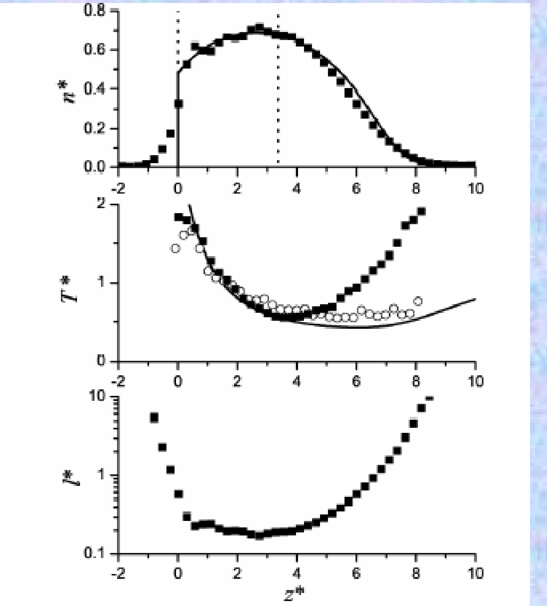
In summary, we have used NMR methods to measure three-dimensional grain motion and density and granular temperature profiles for a vibrofluidized granular system composed of irregularly shaped mustard seeds. The dense lower region of the sample is well described by a hydrodynamic theory for inelastic hard spheres. Thus, the continuum theory appears accurate in spite of the small number of grains in the sample and the steep granular temperature gradient. In the upper region of the sample the mean free path becomes long, and the horizontal and vertical grain velocities become decoupled in a manner that is not described by the theory.



Real granular system is characterized by some degrees of polydispersity in mass and size (granular mixtures)

Difficulties of getting microscopic expressions for transport coefficients increase for multicomponent systems

Transport coefficients $\longrightarrow$ Linear integral equations (Sonine polynomial approximation)

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Hydrodynamics for a granular binary mixture at low density

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Alternative: **Inelastic Maxwell models** (IMM)

Its collision rate is velocity independent but their collision rules are the same as for IHS

Potential interaction ??

Perhaps, the cost of sacrificing physical realism can be in part compensated by getting **exact** results

Many results for homogeneous states, but much less is known for ***inhomogeneous*** situations (**transport coefficients**)

BOLTZMANN EQUATION FOR INELASTIC MAXWELL MIXTURES

Binary mixture: $\{m_1, m_2, \sigma_1, \sigma_2, \alpha_{11}, \alpha_{22}, \alpha_{12}\}$

Velocity distribution function of species *r* $f_r(\mathbf{r}, \mathbf{v}_1, t)$

$$(\partial_t + \mathbf{v} \cdot \nabla) f_r(\mathbf{r}, \mathbf{v}; t) = \sum_s J_{rs} [\mathbf{v} | f_r(t), f_s(t)]$$

$$J_{rs} [\mathbf{v}_1 | f_r, f_s] = \frac{\omega_{rs}(\mathbf{r}, t; \alpha_{rs})}{n_s(\mathbf{r}, t)\Omega_d} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}} \left[\alpha_{rs}^{-1} f_r(\mathbf{r}, \mathbf{v}_1', t) f_s(\mathbf{r}, \mathbf{v}_2', t) - f_r(\mathbf{r}, \mathbf{v}_1, t) f_s(\mathbf{r}, \mathbf{v}_2, t)\right]$$

Free parameters chosen to optimize agreement with IHS

Coefficient of restitution for collisions of type r-s $\alpha_{rs} \leq 1$

$$\mathbf{v}_1' = \mathbf{v}_1 - \mu_{sr}\left(1+\alpha_{rs}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}, \quad \mathbf{v}_2' = \mathbf{v}_2 + \mu_{rs}\left(1+\alpha_{rs}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mu_{rs} = m_r/(m_r+m_s)$$

Energy lost in each collision →

$$\Delta E = -\frac{1}{2}\frac{m_r m_s}{m_r+m_s}(1-\alpha_{rs}^2)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})^2$$

Hydrodynamic fields:

$$n_r = \int d\mathbf{v}\, f_r(\mathbf{v}),$$

$$\rho\mathbf{u} = \sum_r \rho_r\mathbf{u}_r = \sum_r \int d\mathbf{v} m_r \mathbf{v} f_r(\mathbf{v}),$$

$$nT = p = \sum_r n_r T_r = \sum_r \frac{m_r}{d}\int d\mathbf{v} V^2 f_r(\mathbf{v})$$

$$\mathbf{V} = \mathbf{v} - \mathbf{u}$$

Collisional invariants

$$\int d\mathbf{v} J_{rs}[\mathbf{v}|f_r, f_s] = 0,$$

$$\sum_{r,s} \int d\mathbf{v} m_r \mathbf{v} J_{rs}[\mathbf{v}|f_r, f_s] = 0,$$

$$\sum_{r,s} \int d\mathbf{v} \frac{1}{2} m_r V^2 J_{rs}[\mathbf{v}|f_r, f_s] = -\frac{d}{2} n T \zeta$$

Cooling rate

$\zeta \longrightarrow$ Fractional energy changes per unit time

Total energy is ***not*** conserved

Macroscopic balance equations

$$D_t n_r + n_r \nabla \cdot \mathbf{u} + \frac{\nabla \cdot \mathbf{j}_r}{m_r} = 0 \ ,$$

$$D_t \mathbf{u} + \rho^{-1} \nabla \cdot \mathsf{P} = 0 \ ,$$

$$D_t T - \frac{T}{n} \sum_r \frac{\nabla \cdot \mathbf{j}_r}{m_r} + \frac{2}{dn} \left(\nabla \cdot \mathbf{q} + \mathsf{P} : \nabla \mathbf{u} \right) = -\zeta T$$

$$\mathbf{j}_r = m_r \int d\mathbf{v}\, \mathbf{V}\, f_r(\mathbf{v})$$

$$\mathsf{P} = \sum_r \int d\mathbf{v}\, m_r \mathbf{V}\mathbf{V}\, f_r(\mathbf{v})$$

$$\mathbf{q} = \sum_r \int d\mathbf{v}\, \frac{1}{2} m_r V^2 \mathbf{V}\, f_r(\mathbf{v})$$

Maxwell potential: nice mathematical properties of the Boltzmann collision operator

Velocity moment of order *k* of the Boltzmann collision operator

only involves moments of order less than or equal to *k*

Elastic fluids: Nonlinear transport properties

Inelastic fluids: ***Exact*** results

Balance equations become a closed set once the fluxes and the cooling rate are obtained in terms of the hydrodynamic fields and their gradients

Chapman-Enskog solution $\longrightarrow$ Hydrodynamic regime

Normal solution

$$f_r(\mathbf{r},\mathbf{v},t) = f_r[\mathbf{v}|x_1(t),p(t),T(t),\mathbf{u}(t)]$$

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

$$\epsilon \sim \mathcal{O}(\nabla) : \frac{\text{mean free time}}{\text{hydrodynamic length}}$$

$$\partial_t = \partial_t^{(0)} + \epsilon \partial_t^{(1)} + \cdots.$$

T(t) $\longrightarrow$ Reference state is **not** the local equilibrium distribution

Some **controversy** about the possibility of going from kinetic theory to hydrodynamics by using the C-E expansion

Time scale for T is set by the cooling rate instead of gradients. In this new time scale, T is much faster than the usual hydrodynamic scale. Some hydrodynamic excitations decay much slower than temperature

For large inelasticity, perhaps there were no time scale separation between the hydrodynamic and kinetic contributions to the time evolution of the system: no aging to hydrodynamics (no normal solution)

We assume the validity of a hydrodynamic description and compare the predictions based on this assumption with numerical solutions (DSMC method)

Local homogeneous cooling state (HCS)

$$\partial_t f_r^{(0)}(V;t) = \sum_s J_{rs}[f_r^{(0)}, f_s^{(0)}]$$

Normal solution $\longrightarrow$

$$f_r^{(0)}(\mathbf{V},t) = n_r v_0^{-d}(t)\Phi_r(V/v_0(t))$$

$$v_0(t) = \sqrt{2T(t)(m_1+m_2)/m_1 m_2}$$

$$\partial_t T = -\zeta^{(0)} T, \quad \partial_t T_r = -\zeta_r^{(0)} T_r \longrightarrow \partial_t \ln T_1(t)/T_2(t) = \zeta_2^{(0)} - \zeta_1^{(0)}$$

$$T(t) = \frac{T(0)}{\left[1+\frac{1}{2}\zeta(0)t\right]^2}$$

Haff's law

Since $f_r^{(0)}$ depends on time only through *T(t)*

↓ HCS condition

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

We adjust free parameters of the model to get the same cooling rates as for IHS

$$\omega_{rs} = 4x_s \left(\frac{\sigma_{rs}}{\sigma_{12}}\right)^{d-1} \left(\frac{\theta_r + \theta_s}{\theta_r \theta_s}\right)^{1/2} \nu_0$$

$$\nu_0 = \frac{\Omega_d}{4\sqrt{\pi}} n \sigma_{12}^{d-1} v_0$$

The fact that both partial temperatures could be different does not mean that there are additional degrees of freedom

$$T_1(t) = \frac{\gamma}{1+x_1(\gamma-1)} T(t), \quad T_2(t) = \frac{1}{1+x_1(\gamma-1)} T(t)$$

Temperature ratio

Deviation of the distribution functions from their Maxwellian forms

$$c_r = 2\left[\frac{4}{d(d+2)}\theta_r^2 \langle v^{*4}\rangle_r - 1\right],$$

$$\langle v^{*4}\rangle_r = \int d\mathbf{v}^* v^{*4} \Phi_r(v^*),$$

After a transient regime, one expects that the system reaches a hydrodynamic regime (HCS) with stationary values independent of the initial conditions

Time evolution for the temperature ratio

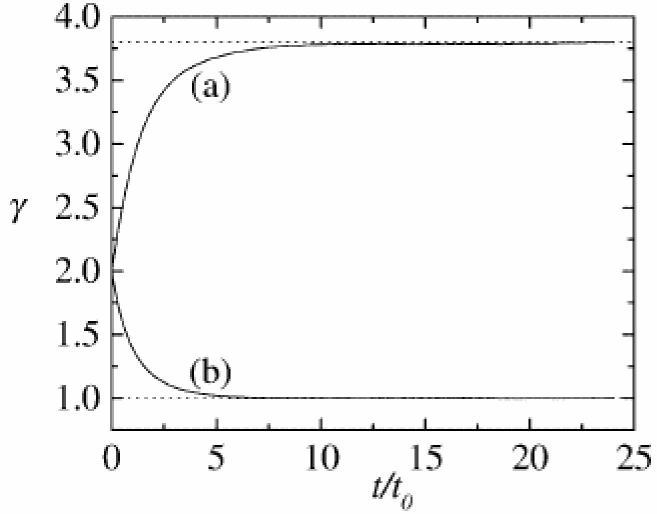
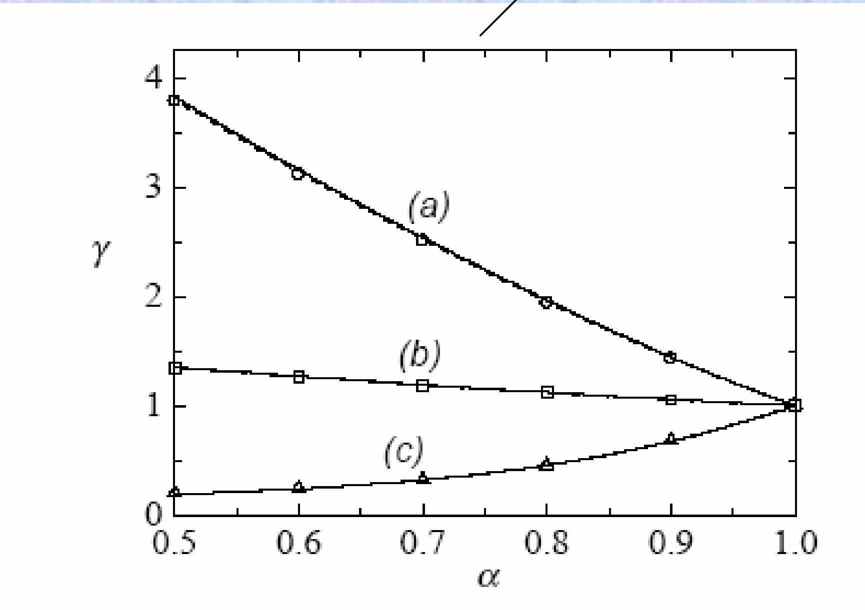
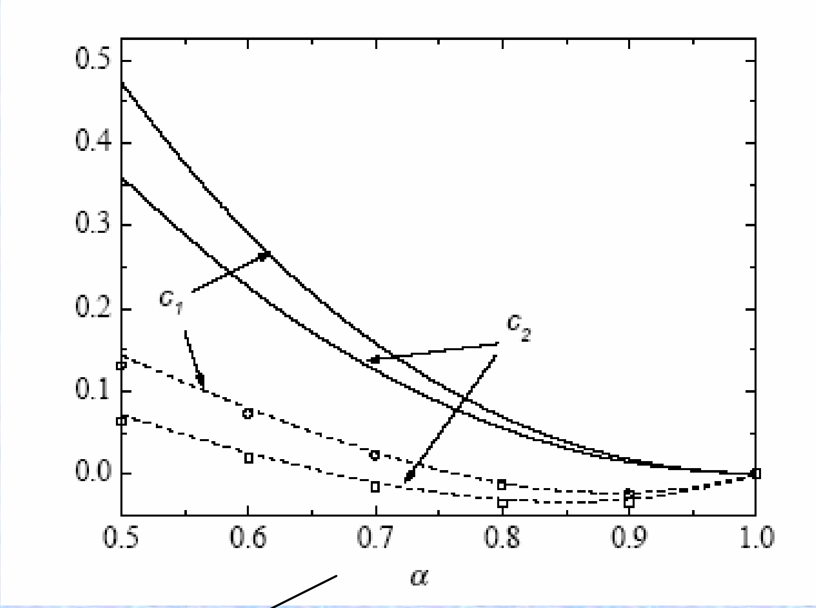


Fig. 1. Time evolution of $\gamma(t) = T_1(t)/T_2(t)$ for $n^* = 0$, $\delta = 2$, $w = 1$, $\mu = 10$, and $\alpha = 0.5$ (a) and $\alpha = 1$ (b). The dotted lines refer to the theoretical predictions. Time is measured in units of $t_0 \equiv \lambda_{11}/v_{01}(0)$

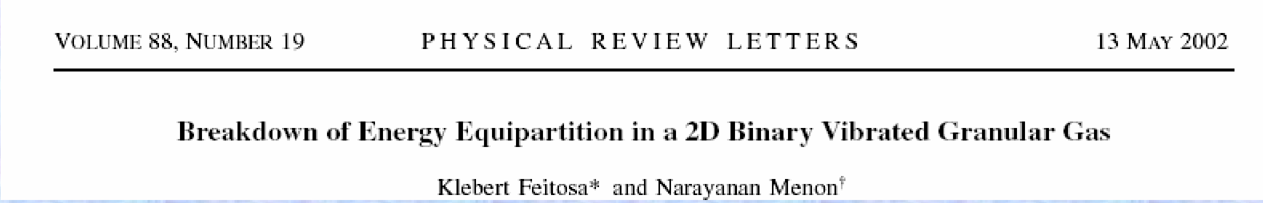
Montanero and Garzó, Gran. Matt. 2002

Breakdown of energy equipartition





Fourth-cumulant (Non-Gaussianity)



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Breakdown of Energy Equipartition in a 2D Binary Vibrated Granular Gas

Klebert Feitosa* and Narayanan Menon†

First-order solution (Navier-Stokes hydrodynamic equations)

$$\left(\partial_t^{(0)} + \mathcal{L}_r\right) f_r^{(1)} + \mathcal{M}_r f_s^{(1)} = \mathbf{A}_r \cdot \nabla x_1 + \mathbf{B}_r \cdot \nabla p + \mathbf{C}_r \cdot \nabla T + D_{r,ij} \nabla_i u_j$$

Linearized Boltzmann collision operators

$$\mathcal{L}_r f_r^{(1)} = -\left(J_{rr}[f_r^{(0)}, f_r^{(1)}] + J_{rr}[f_r^{(1)}, f_r^{(0)}] + J_{rs}[f_r^{(1)}, f_s^{(0)}]\right),$$

$$\mathcal{M}_r f_s^{(1)} = -J_{rs}[f_r^{(0)}, f_s^{(1)}].$$

Normal solution:

$$\partial_t^{(0)} x_r = 0, \quad \partial_t^{(0)} \mathbf{u} = \mathbf{0}, \quad T^{-1} \partial_t^{(0)} T = p^{-1} \partial_t^{(0)} p = -\zeta^{(0)}$$

$$\mathbf{A}_r(\mathbf{V}) = -\left(\frac{\partial}{\partial x_1} f_r^{(0)}\right)_{p,T} \mathbf{V},$$

$$\mathbf{B}_r(\mathbf{V}) = -\frac{1}{p}\left[f_r^{(0)}\mathbf{V} + \frac{p}{\rho}\left(\frac{\partial}{\partial \mathbf{V}} f_r^{(0)}\right)\right],$$

$$\mathbf{C}_r(\mathbf{V}) = \frac{1}{T}\left[f_r^{(0)} + \frac{1}{2}\frac{\partial}{\partial \mathbf{V}} \cdot \left(\mathbf{V} f_r^{(0)}\right)\right]\mathbf{V},$$

$$D_{r,ij}(\mathbf{V}) = \frac{\partial}{\partial V_j}\left(V_i f_r^{(0)}\right) - \frac{1}{d}\delta_{ij}\frac{\partial}{\partial \mathbf{V}} \cdot \left(\mathbf{V} f_r^{(0)}\right).$$

Orthogonality conditions:

$$\int d\mathbf{v}\left[f_r^{(1)}(\mathbf{v}) - f_r^{(0)}(\mathbf{v})\right] = 0,$$

$$\sum_r \int d\mathbf{v} m_r \mathbf{v}\left[f_r^{(1)}(\mathbf{v}) - f_r^{(0)}(\mathbf{v})\right] = 0,$$

$$\sum_r \int d\mathbf{v}\frac{m_r}{2}v^2\left[f_r^{(1)}(\mathbf{v}) - f_r^{(0)}(\mathbf{v})\right] = 0.$$

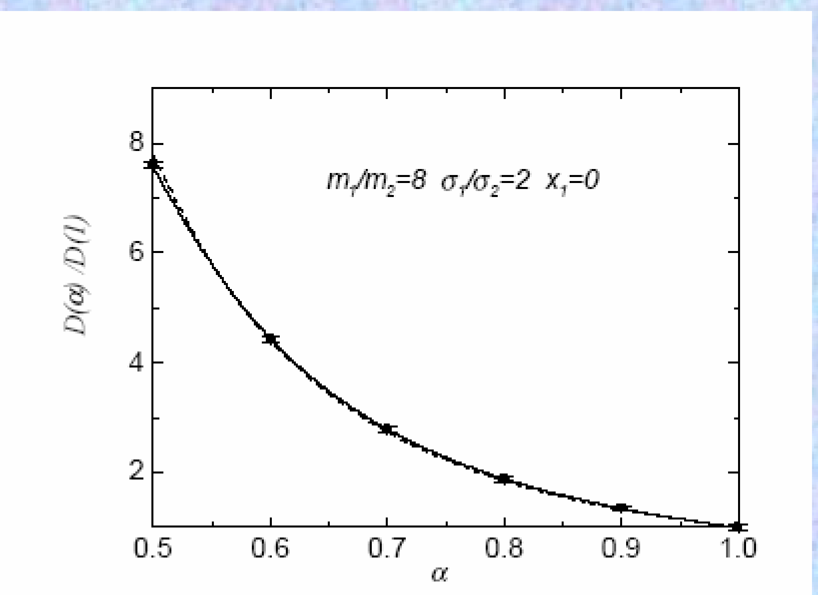
Navier-Stokes transport coefficients

$$\mathbf{j}_1 = -\frac{m_1 m_2 n}{\rho} D \nabla x_1 - \frac{\rho}{p} D_p \nabla p - \frac{\rho}{T} D' \nabla T, \quad \mathbf{j}_2 = -\mathbf{j}_1$$

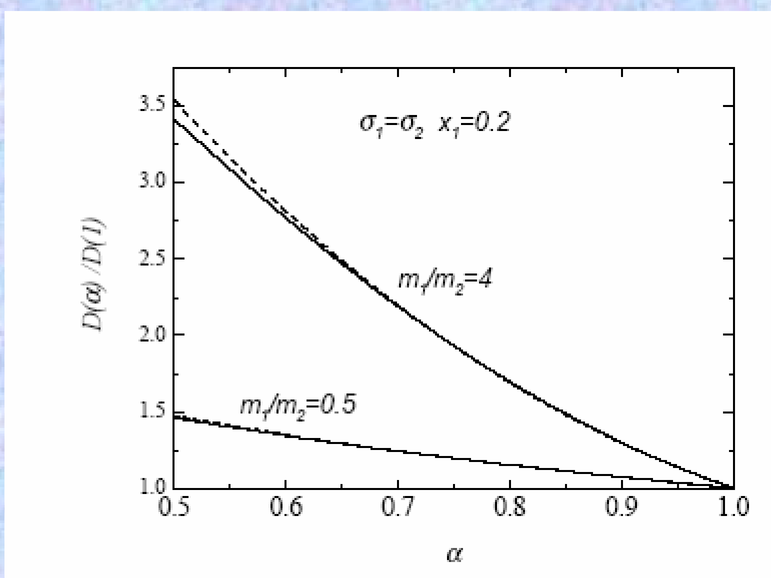
$$\mathbf{q} = -T^2 D'' \nabla x_1 - L \nabla p - \lambda \nabla T,$$

$$P_{ij} = p\delta_{ij} - \eta \left(\nabla_j u_i + \nabla_i u_j - \frac{2}{d} \delta_{ij} \nabla \cdot \mathbf{u} \right)$$

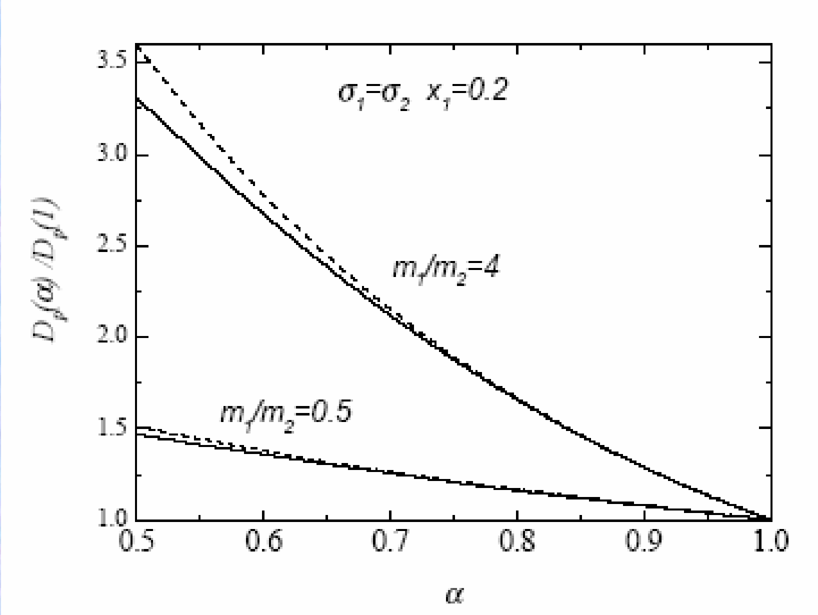
Seven transport coefficients in terms of dissipation and parameters of the mixture: **Exact** expressions



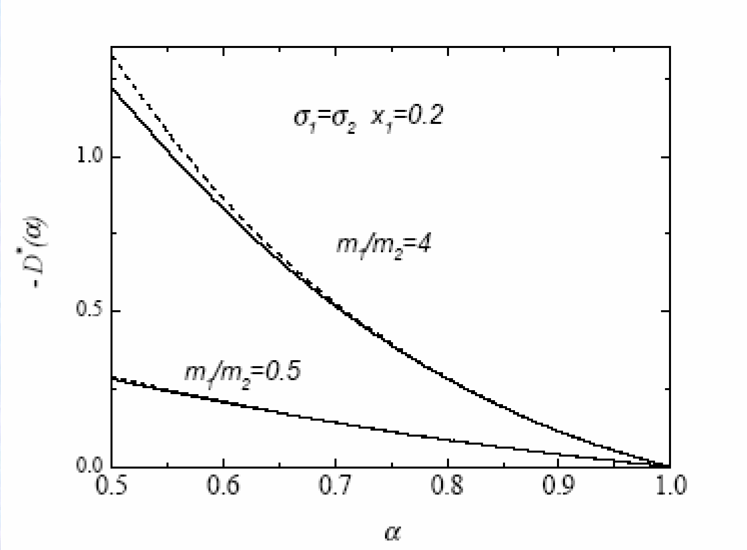
$m_1/m_2=8$ $\sigma_1/\sigma_2=2$ $x_1=0$
$D(\alpha)/D(1)$
α



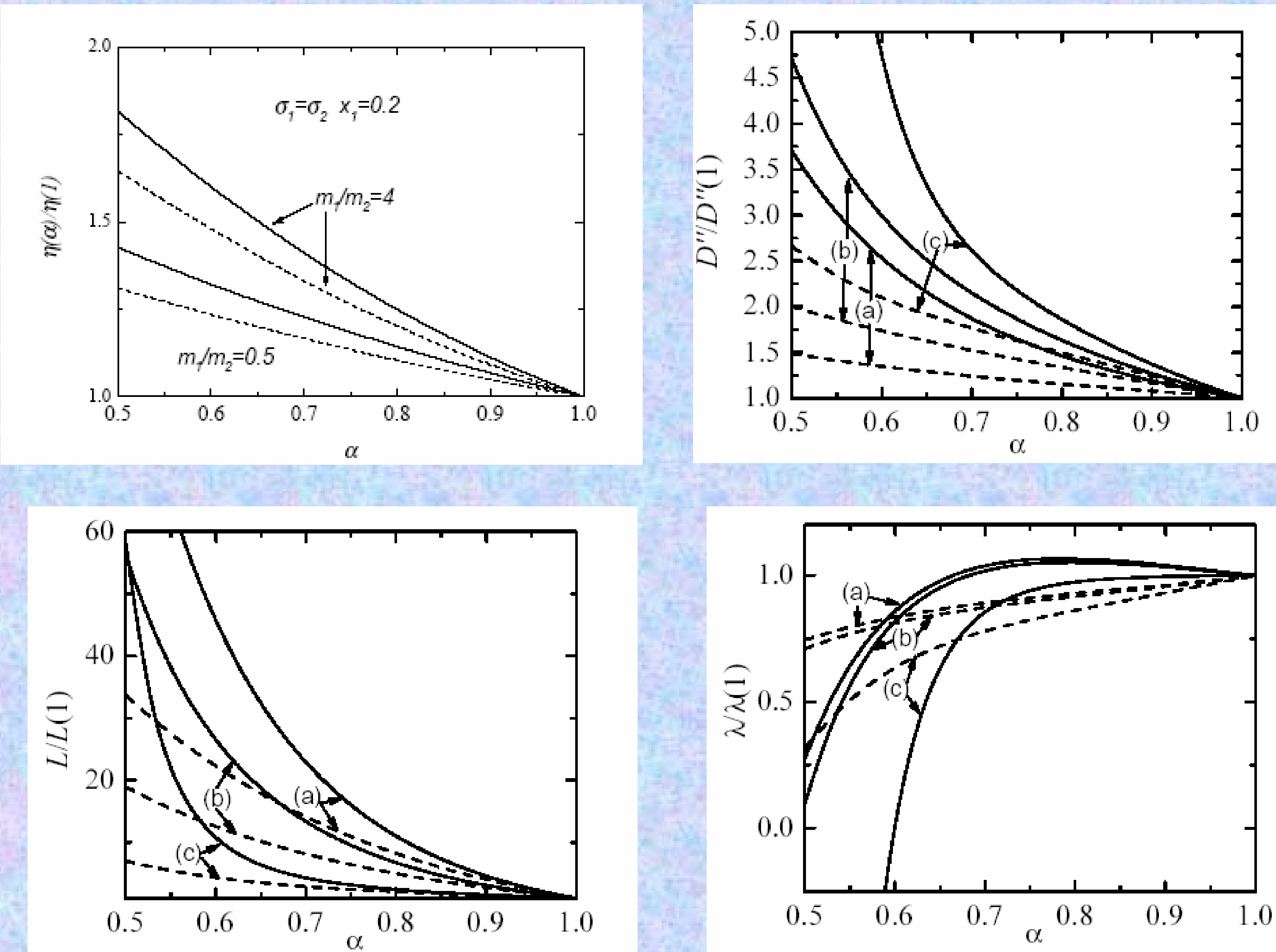
$\sigma_1=\sigma_2$ $x_1=0.2$
$m_1/m_2=4$
$m_1/m_2=0.5$
$D(\alpha)/D(1)$
α



$\sigma_1=\sigma_2$ $x_1=0.2$
$m_1/m_2=4$
$m_1/m_2=0.5$
$D_p(\alpha)/D_p(1)$
α



$\sigma_1=\sigma_2$ $x_1=0.2$
$m_1/m_2=4$
$m_1/m_2=0.5$
$-D^*(\alpha)$
α



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

$\sigma_1 = \sigma_2,\ x_1 = 0.2$

Onsager's constitutive equations for elastic mixtures:

$$\mathbf{j}_s = -\sum_{r=1}^{N} L_{sr} \left(\frac{\nabla \mu_r}{T}\right)_T - L_{sq}\frac{\nabla T}{T^2},$$

$$\mathbf{J}_q \equiv \mathbf{q} - \frac{d+2}{2} T \sum_{s=1}^{N} \frac{\mathbf{j}_s}{m_s}$$

$$= -L_{qq}\nabla T - \sum_{s=1}^{N} L_{qs} \left(\frac{\nabla \mu_s}{T}\right)_T .$$

$$\left(\frac{\nabla \mu_s}{T}\right)_T = \frac{1}{m_s}\nabla \ln(x_s p)$$

Onsager's reciprocal relations $\longrightarrow$ $L_{sr} = L_{rs}, \quad L_{sq} = L_{qs}$

Time reversal invariance

$$\mathbf{j}_1 = -\frac{m_1 m_2 \rho_1 \rho_2}{\rho^2} D \frac{(\nabla\mu_1)_T - (\nabla\mu_2)_T}{T} - C_p \nabla \ln p - \frac{\rho}{T} D' \nabla T,$$

$$\mathbf{J}_q = -\left(\frac{\rho_1\rho_2 T^2}{n\rho} D'' - \frac{d+2}{2} T \frac{m_2 - m_1}{\rho^2} \rho_1 \rho_2 D\right) \frac{(\nabla\mu_1)_T - (\nabla\mu_2)_T}{T}$$
$$-C_p' \nabla \ln p - \left(\lambda - \frac{d+2}{2} \frac{m_2 - m_1}{m_1 m_2} \rho D'\right) \nabla T,$$

Onsager´s phenomenological coefficients:

$$L_{11} = -L_{12} = \frac{m_1 m_2 \rho_1 \rho_2}{\rho^2} D, \quad L_{1q} = \rho T D',$$

$$L_{q1} = -L_{q2} = \frac{T^2 \rho_1 \rho_2}{n\rho} D'' - \frac{d+2}{2} \frac{T \rho_1 \rho_2}{\rho^2} (m_2 - m_1) D, \quad L_{qq} = \lambda - \frac{d+2}{2} \rho \frac{m_2 - m_1}{m_1 m_2} D'$$

Contributions **not** present in the elastic case: $C_p = C_p' = 0$

First Onsager´s relation $L_{12} = L_{21}$ holds since D is symmetric under the change

$1 \leftrightarrow 2$

Second Onsager´s relation $L_{1q} = L_{q1}$ along with $C_p = C'_p = 0$

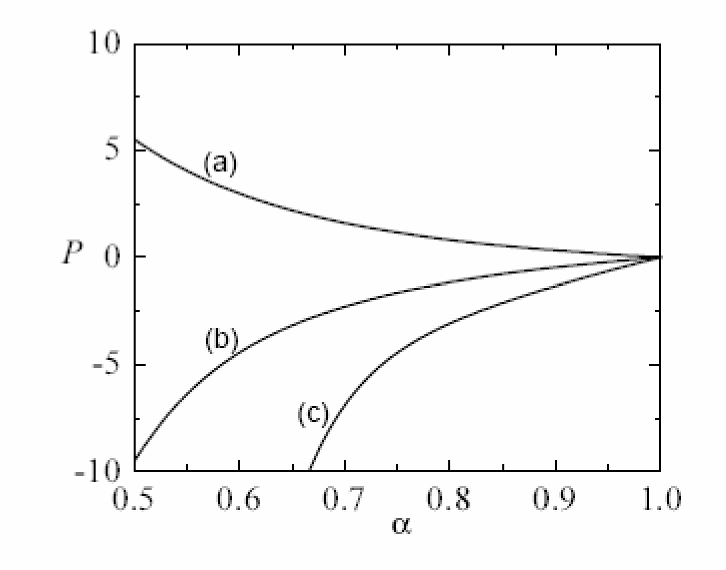
implies that

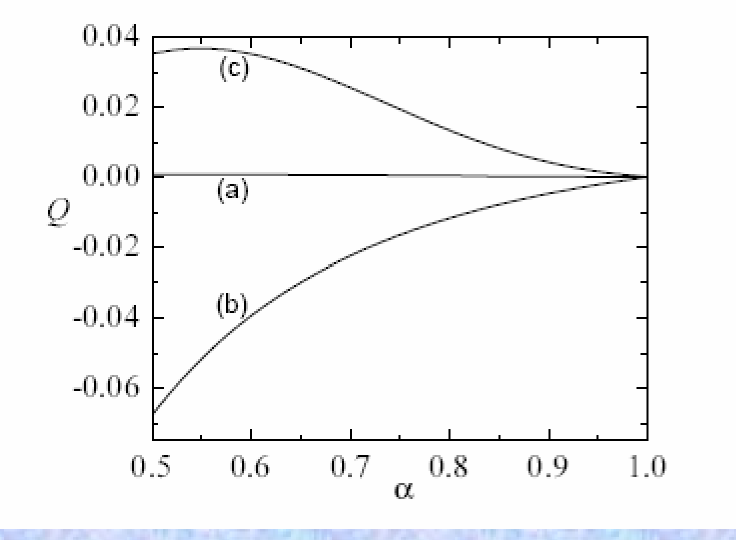
$$P(\alpha_{rs}) \equiv D''^* - \frac{d+2}{2}\frac{1-\mu^2}{\mu}D^* - \frac{1+\mu}{\mu}\frac{x_2+\mu x_1}{x_1 x_2}D'^* = 0,$$

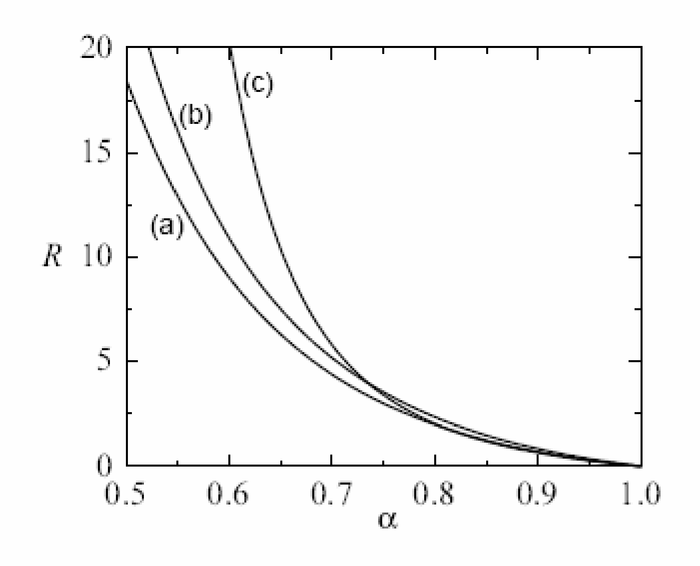
$$Q(\alpha_{rs}) \equiv D_p^* - x_1 x_2 \frac{1-\mu}{x_2+\mu x_1}D^* = 0,$$

$$R(\alpha_{rs}) \equiv L^* - \frac{d+2}{2}\frac{1-\mu^2}{\mu}Q - x_1 x_2 \frac{1-\mu}{x_2+\mu x_1}D''^* = 0.$$

In the elastic case, $P=Q=R=0$







$\sigma_1 = \sigma_2,\ x_1 = 0.2$

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

CONCLUSIONS

1. Hydrodynamic equations for a binary mixture of inelastic Maxwell molecules have been derived from the Boltzmann kinetic theory
2. Seven relevant transport coefficients given **exactly** in terms of the coefficients of restitution and parameters of the mixture.
3. Comparison with inelastic hard spheres shows reasonably good qualitative agreement, especially for the mass flux.
4. As expected, Onsager's relations do not apply for inelastic collisions.

(www.unex.es/fisteor/vicente)

Thanks for your attention