SEGREGATION BY THERMAL DIFFUSION OF AN INTRUDER IN A GRANULAR DENSE GAS

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OUTLINE

1. *Segregation* problem: thermal (Soret) diffusion

2. *Hydrodynamic* description

3. Revised (*inelastic*) Enskog kinetic theory

4. *Phase-diagrams* for BNE/RBNE transition

5. Summary and conclusions

Segregation and **mixing** of dissimilar grains is one of the most interesting problems in vibrated granular mixtures

Extensive **observational** evidence but much less is known from a more *fundamental* point of view

Several mechanisms have been proposed:
Archimedean buoyancy, void filling, convection, frictional properties,…..
thermal (Soret) diffusion

Large shaking amplitude

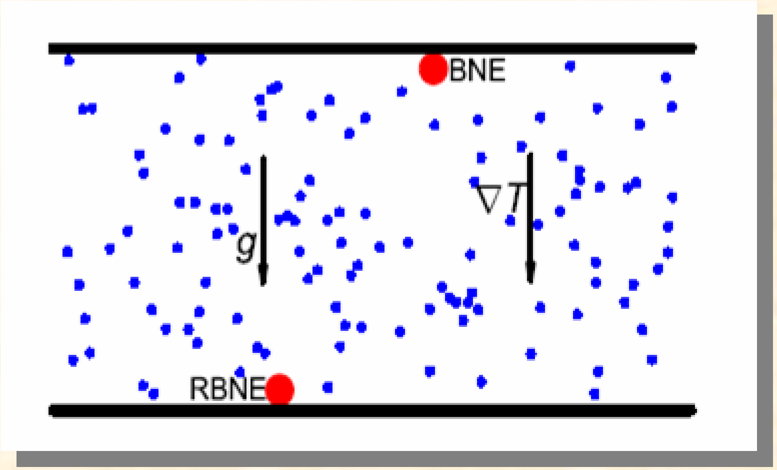
↓

Sample resembles a ***granular gas***

Kinetic theory tools provide a good framework to describe granular systems under rapid flow conditions

The **revised Enskog** equation can be a reliable and accurate theory to study segregation for granular mixtures at *moderate* densities (*molecular chaos* assumption can be still a good approximation)

Objective: Segregation problem driven by the presence of a thermal gradient and the gravitational field in a *moderately* dense ganular fluid



Model system: dense *granular* fluid+**intruder**

(binary mixture in the **tracer** limit)

Early theoretical attempts:

Dense gases: *Homogeneous* temperature

- *Elastic* systems: Jenkins and Yoon PRL 2002
- *Quasielastic* particles: Trujillo, Alam & Herrmann EPL 2003

Dilute gases: *Inhomogeneous* temperature

- *Weak* dissipation: Serero et al. JFM 2006
- *Arbitrary* degree of dissipation:

Brey et al. PRL 2005; Garzó EPL 2006

Our theory
(i) goes beyond weak dissipation limit, (ii) combined effect of gravity and thermal gradient, (iii) applies for moderate densities

It covers some of the aspects *not* previously accounted for in previous theories, but it also assumes a **Navier-Stokes** description (first order in spatial gradients)

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:

$$\frac{\partial p}{\partial z} = \frac{\partial p}{\partial T}\partial_z T + \frac{\partial p}{\partial n}\partial_z n = -\rho g$$

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

$$j_z = -\frac{m_0^2}{\rho} D_0 \partial_z n_0 - \frac{m_0 m}{\rho} D \partial_z n - \frac{\rho}{T} D^T \partial_z T$$

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

Density gradients in terms of gravity and thermal gradient

$$\Lambda = \frac{\beta D^{T*} - (p^* + g^*)(D_0^* + D^*)}{\beta D_0^*}$$

$$p^* = p/nT, g^* = \rho g/n\partial_z T < 0$$

$$\beta = p^* + \phi\partial_\phi p^*, \phi = [\pi^{d/2}/2^{d-1}d\Gamma(d/2)]n\sigma^d$$

Determine the dependence of thermal diffusion on

$$\{m_0/m, \sigma_0/\sigma, \alpha, \alpha_0, \phi, g^*\}$$

Enskog kinetic theory: transport coefficients and equation of state

V. Garzó, J. Dufty, C. Hrenya PRE **76,** 0313303; 031304 (2007)

Binary mixture in the *tracer limit* for the intruder

Tracer limit : $n_0/n \to 0$

Granular dense *fluid*

$$\left(\partial_t + \mathbf{v}\cdot\nabla + \mathbf{g}\cdot\frac{\partial}{\partial\mathbf{V}} - \frac{1}{2}\frac{T}{m}\zeta\frac{\partial^2}{\partial V^2}\right) f = J[f,f]$$

gravity

White-noise thermostat

$$\begin{aligned} J\,[f,f] \;&\equiv\; \sigma^{d-1}\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathrm{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathrm{g}) \\ &\times\left[\alpha^{-2}\chi\left(\mathbf{r}_1,\mathbf{r}_1-\boldsymbol{\sigma}\mid\{n(t)\}\right) f(\mathbf{r}_1,\mathbf{v}_1'';t)f(\mathbf{r}_1-\boldsymbol{\sigma},\mathbf{v}_2'';t)\right. \\ &\left.-\chi\left(\mathbf{r}_1,\mathbf{r}_1+\boldsymbol{\sigma}\mid\{n(t)\}\right) f(\mathbf{r}_1,\mathbf{v}_1;t)f(\mathbf{r}_1+\boldsymbol{\sigma},\mathbf{v}_2;t)\right] \end{aligned} \tag{1}$$

Scattering rules

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

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

Intruder

$$\left(\partial_t + \mathbf{v}\cdot\nabla + \mathbf{g}\cdot\frac{\partial}{\partial \mathbf{V}} - \frac{1}{2}\frac{T_0}{m_0}\zeta_0\frac{\partial^2}{\partial V^2}\right) f_0 = J_0[f_0, f]$$

$$\begin{aligned} J_0\left[f_0, f\right] \equiv\ & \overline{\sigma}^{d-1}\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}) \\ & \times\left[\alpha_0^{-2}\chi_0\left(\mathbf{r}_1, \mathbf{r}_1 - \overline{\boldsymbol{\sigma}} \mid \{n(t)\}\right) f(\mathbf{r}_1, \mathbf{v}_1''; t) f(\mathbf{r}_1 - \overline{\boldsymbol{\sigma}}, \mathbf{v}_2''; t)\right. \\ & \left. -\chi\left(\mathbf{r}_1, \mathbf{r}_1 + \overline{\boldsymbol{\sigma}} \mid \{n(t)\}\right) f(\mathbf{r}_1, \mathbf{v}_1; t) f(\mathbf{r}_1 + \overline{\boldsymbol{\sigma}}, \mathbf{v}_2; t)\right] \end{aligned} \qquad (1)$$

$$\overline{\sigma} = (\sigma_0 + \sigma)/2$$

Scattering rules

$$\mathbf{v}_1'' = \mathbf{v}_1 - \frac{m}{m+m_0}\left(1+\alpha_0^{-1}\right)(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})\hat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2'' = \mathbf{v}_2 + \frac{m_0}{m+m_0}\left(1+\alpha_0^{-1}\right)(\hat{\boldsymbol{\sigma}}\cdot\mathbf{g})\hat{\boldsymbol{\sigma}}$$

Mass balance for intruders

$$D_t n_0 + n_0 \nabla\cdot\mathbf{u} + \frac{\nabla\cdot\mathbf{j}}{m_0} = 0$$

$$\mathbf{j} = m_0 \int d\mathbf{v}\, \mathbf{V}\, f_0(\mathbf{v})$$

Mass flux

Steady state without convection (**u**=**0**) → **j**=**0**

Chapman-Enskog expansion: *Normal* or hydrodynamic solution to the set of coupled Enskog equations

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

$$f(\mathbf{r},\mathbf{v};t) = f(\mathbf{v}|\{n(\mathbf{r},t)\},\mathbf{U}(\mathbf{r},t),T(\mathbf{r},t)\})$$

$$f_0(\mathbf{r},\mathbf{v};t) = f_0(\mathbf{v}|\{n_0(\mathbf{r},t)\},\mathbf{U}(\mathbf{r},t),T(\mathbf{r},t)\})$$

This representation can also apply for situations where spatial gradients are ***not*** small. For ***small*** spatial gradients,

$$f = f^{(0)} + f^{(1)} + \cdots$$

$$f_0 = f_0^{(0)} + f_0^{(1)} + \cdots$$

First order: *Navier-Stokes* description. Explicit forms for the mass transport coefficients

LOCAL HOMOGENEOUS STATE FOR INTRUDERS

The reference state $f_0^{(0)}$ is not the local equilibrium distribution. Its explicit form is not known

$$-\frac{\zeta_0^{(0)}T_0}{2m_0}\frac{\partial^2}{\partial V^2}f_0^{(0)} = J_0^{(0)}[f_0^{(0)}, f^{(0)}]$$

Scaled form: $$f_0^{(0)}(V) = n_0 v_o^{-d}(T)\Phi_0(V/v_o)$$

Sonine polynomial expansion

Thermal speed: $$v_0 = \sqrt{2T/m}$$

Condition to determine T_0/T: covariance of the stochastic acceleration is taken to be the same for both species (fluid particles and intruder)

$$\frac{T_0 \zeta_0^{(0)}}{m_0} = \frac{T \zeta^{(0)}}{m}$$

Barrat&Trizac, Gran. Matt. **4**, 57 (2002)

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

$$d n_0 T_0 = \int d\mathbf{v} m_0 V^2 f_0^{(0)}$$

Differs from the **HCS** condition (*undriven* case)

$$\zeta_0^{(0)} = \zeta^{(0)}$$

Garzó&Dufty PRE **60**, 5706 (1999)

Simplest approximation: *Maxwellians* at different temperatures T and T_0

$$\zeta^* \to \frac{\Omega_d}{\sqrt{2\pi} d} \chi (1 - \alpha^2)$$

$$\zeta_0^* \to \frac{\Omega_d}{d\sqrt{\pi}} \left(\frac{1+\omega}{2} \right)^{d-1} \chi_0 \frac{1+\alpha_0}{1+M} \sqrt{\frac{1+\theta}{\theta}} \left[2 - \frac{1+\theta}{1+M}(1+\alpha_0) \right]$$

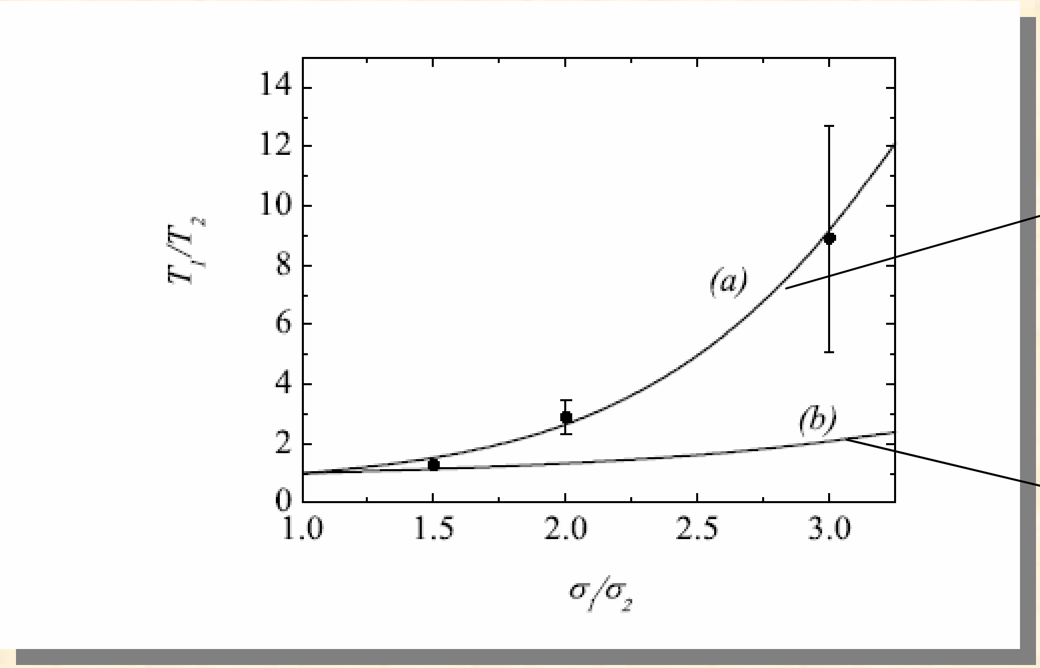
$$M = \frac{m_0}{m}, \omega = \frac{\sigma_0}{\sigma}, \theta = \frac{m_0 T}{m T_0}$$

$$\zeta^* = \zeta / \nu$$

$$\zeta_0^* = \zeta_0^{(0)} / \nu$$

Comparison with **experimental/simulation** results of Schroter, Ulrich, Kreft, Swift&Swinney (PRE **74**, 011307 (2006))

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



Thermostat case

Dilute gas

Undriven case

V. Garzó, EPL **75**, 521 (2006)

First order solution

$$\mathbf{j}^{(1)} = -\frac{m_0^2}{\rho} D_0 \nabla n_0 - \frac{m m_0}{\rho} D \nabla n - \frac{\rho}{T} D^T \nabla T$$

$$D^T = -\frac{m_0}{\rho d} \int d\mathbf{v} \mathbf{V} \cdot \mathcal{A}_0 (\mathbf{V})$$

$$D_0 = -\frac{\rho}{m_0 n_0 d} \int d\mathbf{v} \mathbf{V} \cdot \mathcal{B}_0 (\mathbf{V})$$

$$D = -\frac{1}{d} \int d\mathbf{v} \mathbf{V} \cdot \mathcal{C}_0 (\mathbf{V})$$

Transport coefficients given in terms of solutions of ***linear integral equations***. Approximate method: Sonine polynomial expansion

$$\mathcal{A}_0(\mathbf{V}) \to -f_{0,M}(\mathbf{V})\frac{\rho}{n_0 T_0}\mathbf{V} D^T$$

$$\mathcal{B}_0(\mathbf{V}) \to -f_{0,M}(\mathbf{V})\frac{m_0^2}{\rho T_0}\mathbf{V} D_0$$

$$\mathcal{C}_0(\mathbf{V}) \to -f_{0,M}(\mathbf{V})\frac{m_0}{n_0 T_0}\mathbf{V} D$$

$$f_{0,M}(\mathbf{V}) = n_0 \left(\frac{m_0}{2\pi T_0}\right)^{d/2} \exp\left(-\frac{m_0 V^2}{2T_0}\right)$$

Navier-Stokes transport coefficients

$$D_0^* = \frac{\gamma}{\nu_D},$$

$$D^{T*} = -\frac{M}{\nu_D}\left(p^* - \frac{\gamma}{M}\right) + \frac{(1+\omega)^d}{2\nu_D}\frac{M}{1+M}\chi_0 \phi (1+\alpha_0),$$

$$D^* = -\frac{M}{\nu_D}\beta + \frac{1}{2\nu_D}\frac{\gamma + M}{1+M}\frac{\phi}{T}\left(\frac{\partial \mu_0}{\partial \phi}\right)_{T,n_0}(1+\alpha_0)$$

μ_0 : chemical potential of intruder

$\gamma = T_0/T, \beta = p^* + \phi \partial_\phi p^*, M = m_0/m, \omega = \sigma_0/\sigma$

Equation of state

$$p^* = p/nT = 1 + 2^{d-2}\chi\phi(1+\alpha)$$

Pair correlation function

Segregation criterion for BNE/RBNE $\longrightarrow$ $\Lambda = 0$

$$g^*(\gamma - M\beta) - \gamma\phi\frac{\partial p^*}{\partial \phi} + \frac{(1+\omega)^d}{2}\frac{M}{1+M}\chi_0\phi(1+\alpha_0)\left[(p^*+g^*)(1+\frac{\gamma}{M})\Delta - \beta\right] = 0$$

Garzó, PRE **78**, 020301 (R) (2008)

$$\gamma = T_0/T, M = m_0/m, \omega = \sigma_0/\sigma, \Delta = ((1+\omega)^{-d}/T\chi_0)(\partial_\phi \mu_0)_{T,n_0}$$

Special cases:

a) $m_0 = m, \sigma_0 = \sigma, \alpha = \alpha_0 \longrightarrow$ No segregation

b) Dilute gas (ϕ=0) $(p^* = 1, \beta = 1)$

$$\frac{T_0}{T} = \frac{m_0}{m}$$

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

Due to the lack of energy equipartition, criterion is rather complicated since it involves all the parameter space *c)* Gravity dominates over thermal gradient $\quad (|g^*| \to \infty)$

$$\frac{1+\frac{(1+\omega)^d}{2}\chi_0\phi(1+\alpha_0)\frac{\gamma+M}{1+M}\frac{\Delta}{\gamma}}{1+2^{d-2}\chi\phi(1+\alpha)\left[1+\phi\partial_\phi \ln(\phi\chi)\right]}\frac{mT_0}{m_0T}-1=0$$

Different from
$$\frac{1+\frac{(1+\omega)^d}{2}\chi_0\phi}{1+2^{d-1}\chi\phi}\frac{mT_0}{m_0T}-1=0$$

Jenkins and Yoon, PRL **88**, 194301 (2002);
Trujillo, Alam and Herrmann, EPL **64**, 190 (2003)

Both criteria agree under some approximations

Phase diagrams for *three-dimensional* systems

$$\chi = \frac{1 - \frac{1}{2}\phi}{(1-\phi)^3}$$

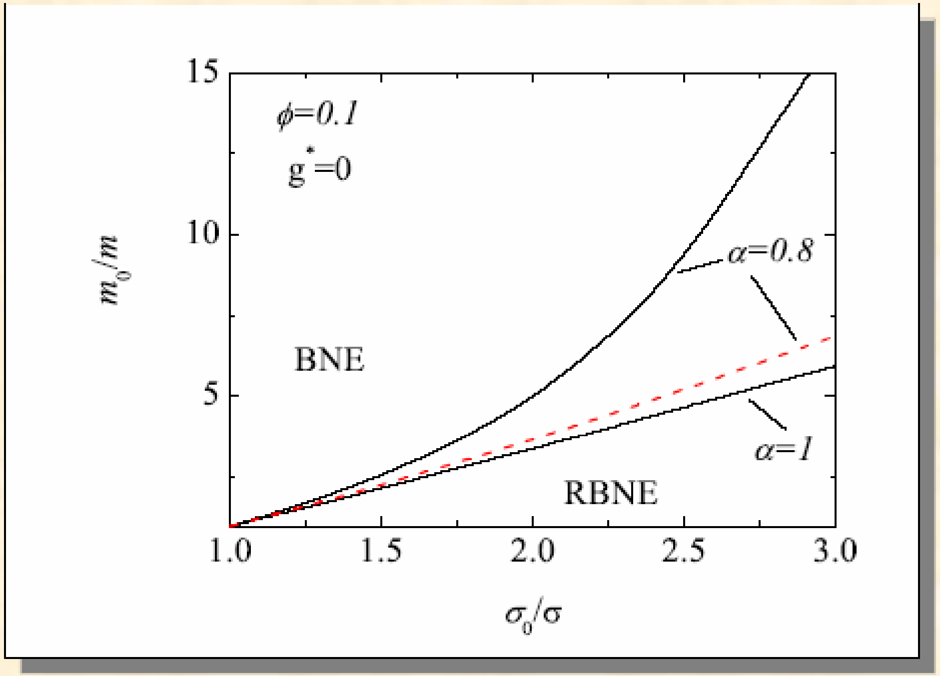
$$\chi_0 = \frac{1}{1-\phi} + 3\frac{\omega}{1+\omega}\frac{\phi}{(1-\phi)^2} + 2\frac{\omega^2}{(1+\omega)^2}\frac{\phi^2}{(1-\phi)^3}$$

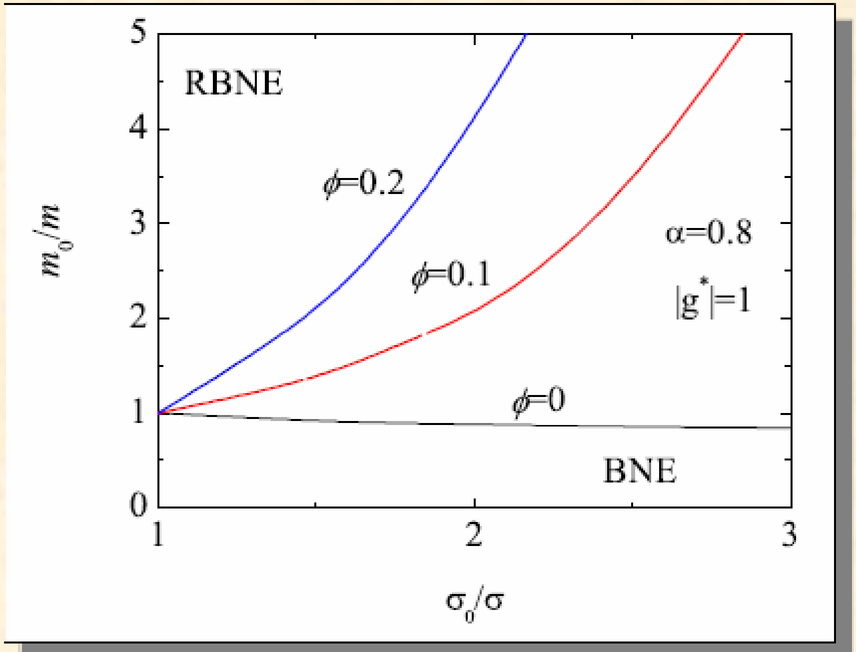
$$\begin{aligned}\frac{\mu_0}{T} = \; & \ln n_0 - \ln(1-\phi) + (1+4\chi\phi)\omega^3\phi + 3\omega(1+\omega)\frac{\phi}{(1-\phi)} + \frac{9}{2}\omega^2\frac{\phi^2}{(1-\phi)^2} \\ & +3\omega^2\left[\ln(1-\phi) + \frac{\phi}{(1-\phi)} - \frac{\phi^2}{2(1-\phi)^2}\right] - \omega^3\left[2\ln(1-\phi) + \frac{\phi(2-\phi)}{(1-\phi)}\right] + c\end{aligned} \quad (1)$$

↓

$$\left(\frac{\partial\mu_0}{\partial\phi}\right)_{T,n_0}$$

Three-dimensional system (d=3), $\alpha=\alpha_0$

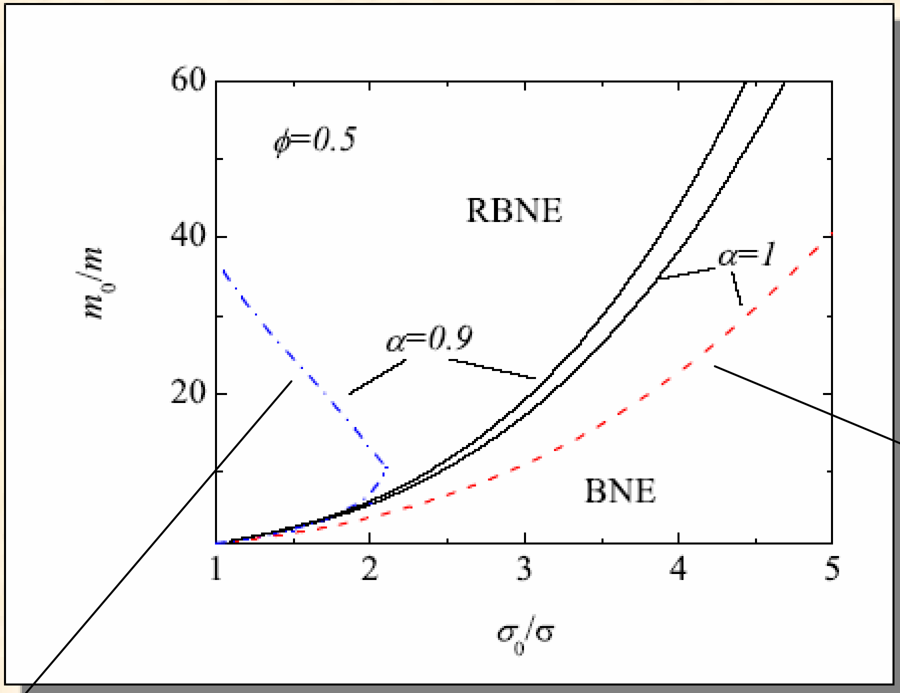




Galvin, Dahl & Henya, JFM **528**, 207 2005

Similar trends observed in the experiments of Breu *et al*. PRL **90**, 014302 (2003)

$$|g^*| = \infty$$



Jenkins&Yoon, PRL (2002)

Trujillo, Alam& Herrmann EPL (2003)

Positive aspects

- Realistic theory based on the inelastic Enskog kinetic theory to study segregation of an intruder in a moderately granular dense gas.
- New aspects covered by theory: finite density, combined effect of thermal gradients and gravity and not limited to weak dissipation
- Consistent with MD and experiments

Limitations

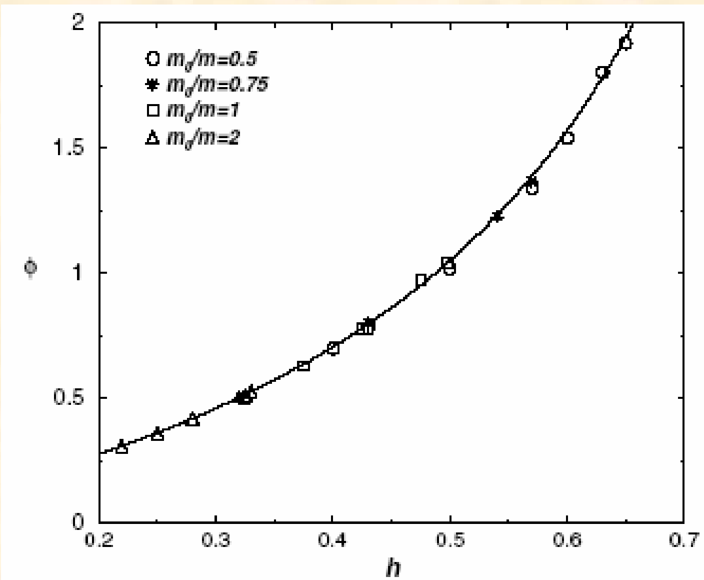
- Tracer limit. Extension to finite composition
- *Vibrating* wall effect
- Transport *linear* theory. Kinetic models

Work to be done……

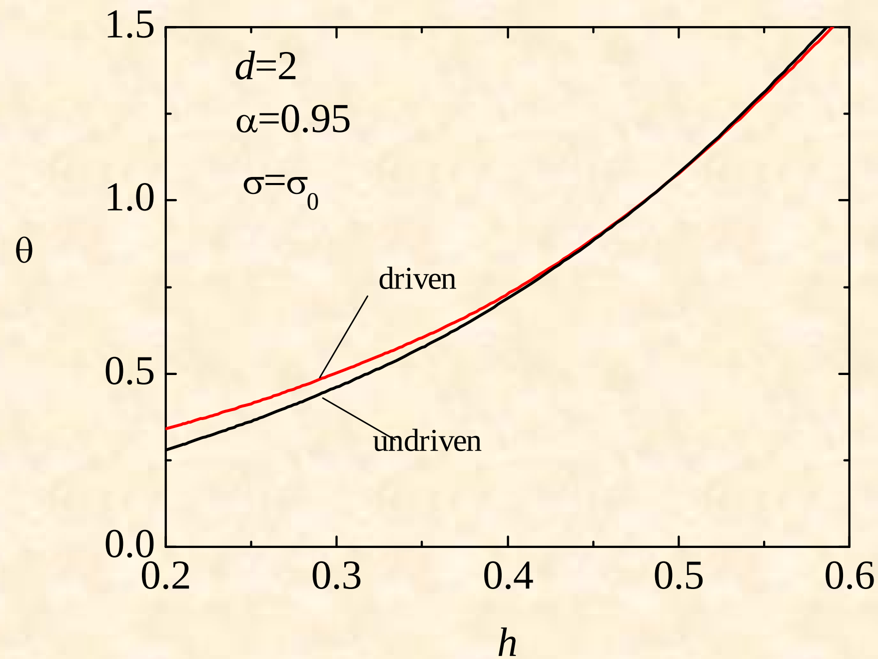
Many thanks for your attention !!

$$h = \frac{m}{m+m_0}\frac{1+\alpha_0}{2}, \theta = \frac{mT_0}{m_0 T}$$

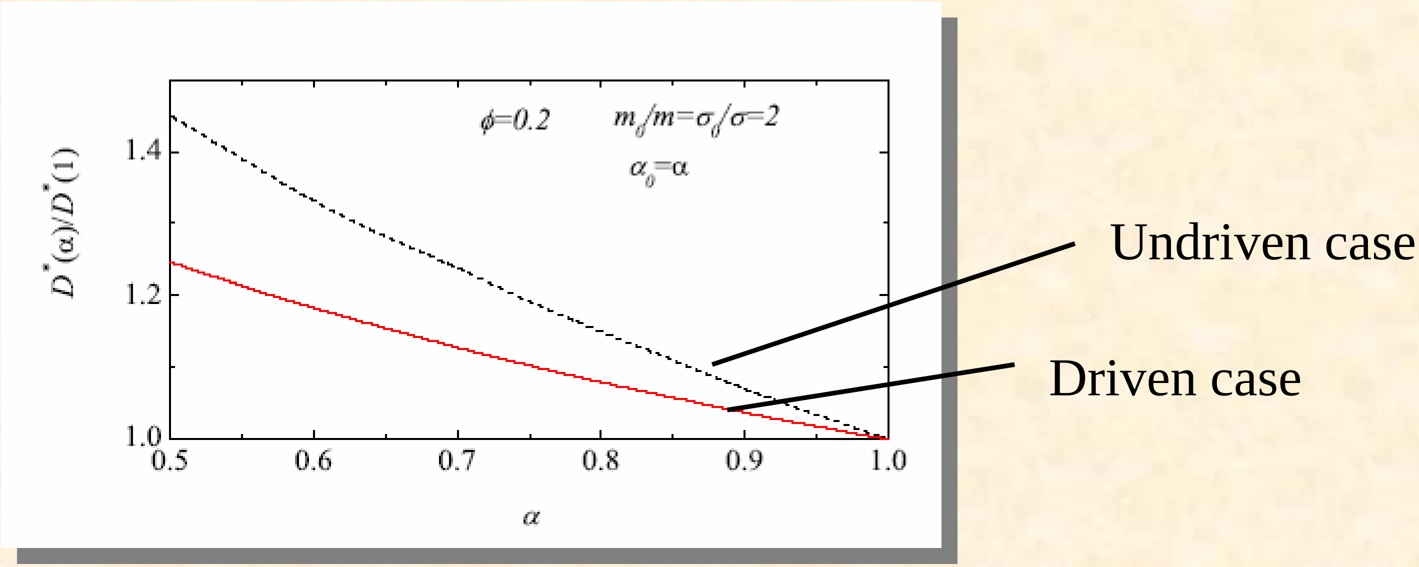
$$\frac{T_0\zeta_0^{(0)}}{m_0} = \frac{T\zeta^{(0)}}{m}$$
$$\zeta_0^{(0)} = \zeta^{(0)}$$



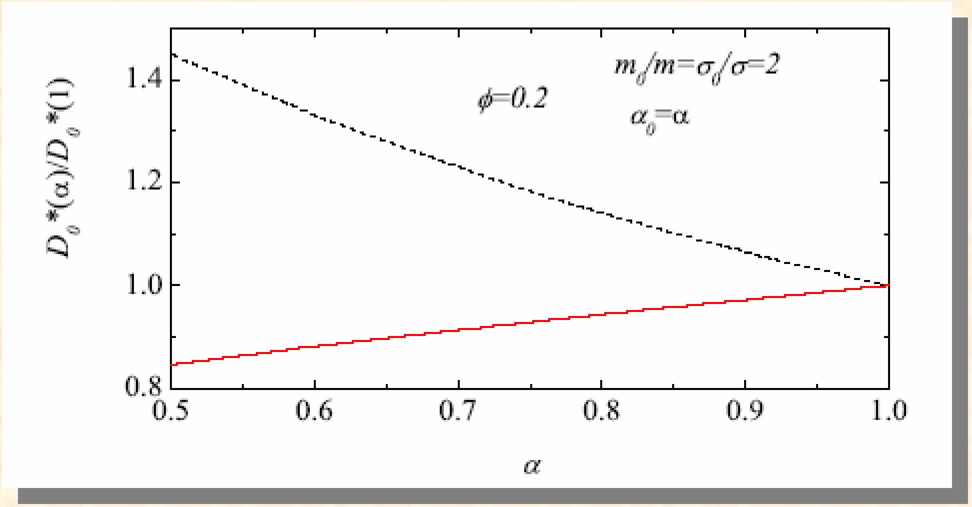
J. Brey, M.J.Ruiz-Montero, F. Moreno
PRL **95**, 098001 (2005)



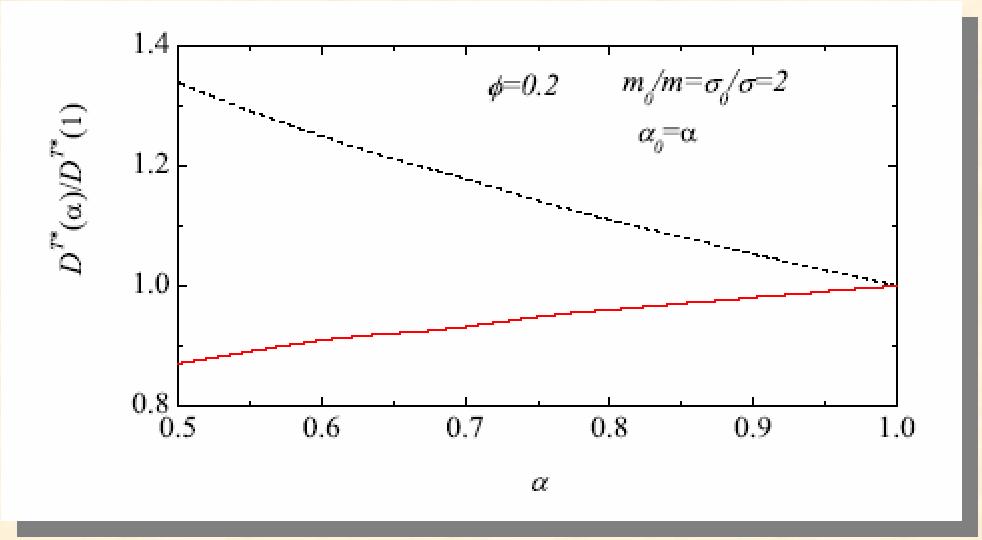
Tracer limit



φ=0.2
m0/m=σ0/σ=2
α0=α
D*(α)/D*(1)
α
Undriven case
Driven case



φ=0.2
m0/m=σ0/σ=2
α0=α
D0*(α)/D0*(1)
α



As expected, thermostat does not play a *neutral* role in the transport properties and/or energy nonequipartition

Garzó&Montanero, Physica A **313**, 336 2002);
Wang&Menon PRL **100**, 158001 (2008)