Energy production rates in fluid mixtures of inelastic rough hard spheres

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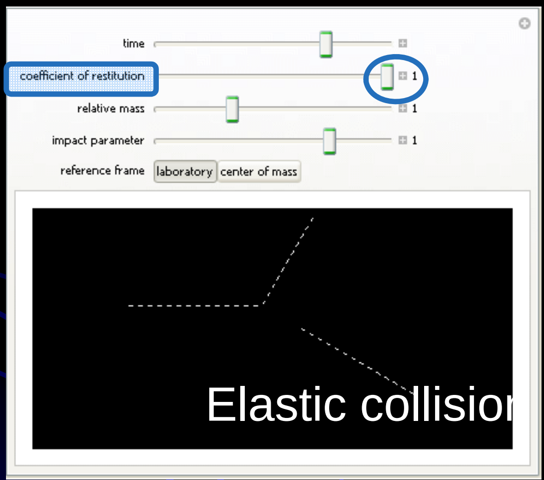
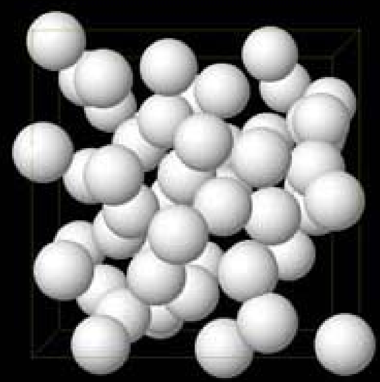
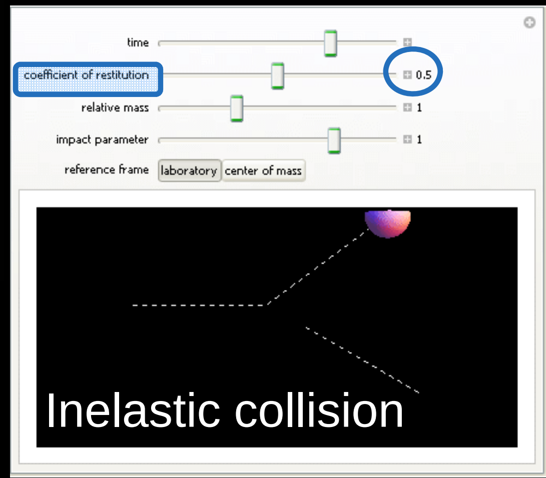
Minimal model of a granular gas: A gas of *identical smooth inelastic* hard spheres



Elastic collision



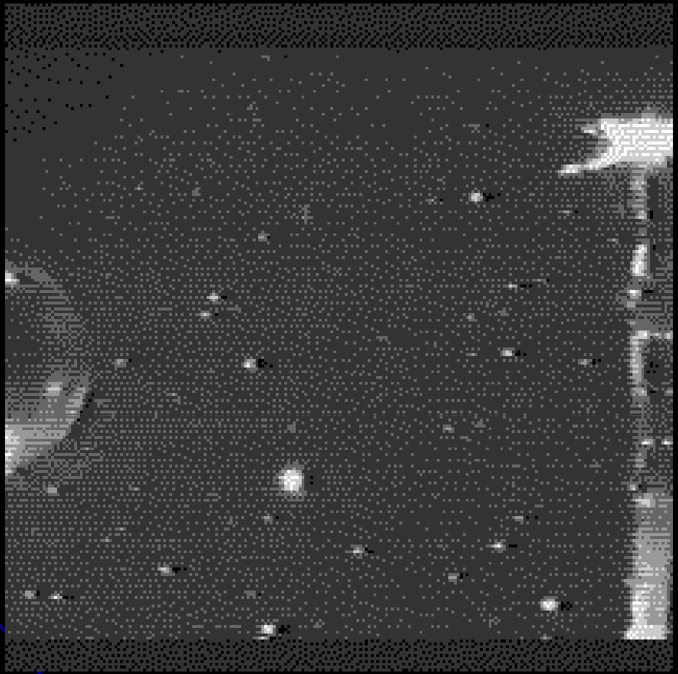


Inelastic collision

http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

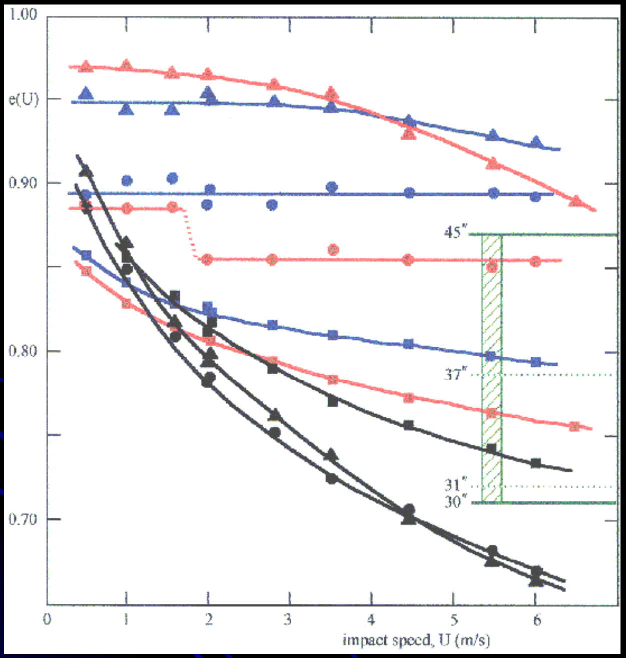
This minimal model ignores …

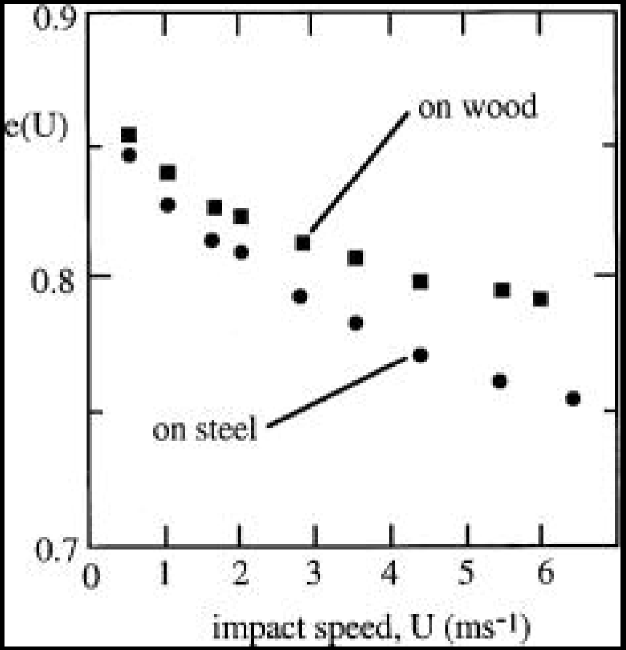
Interstitial fluid



Caltech Granular Flows Group (http://www.its.caltech.edu/~granflow/)

Non-constant coefficient of restitution

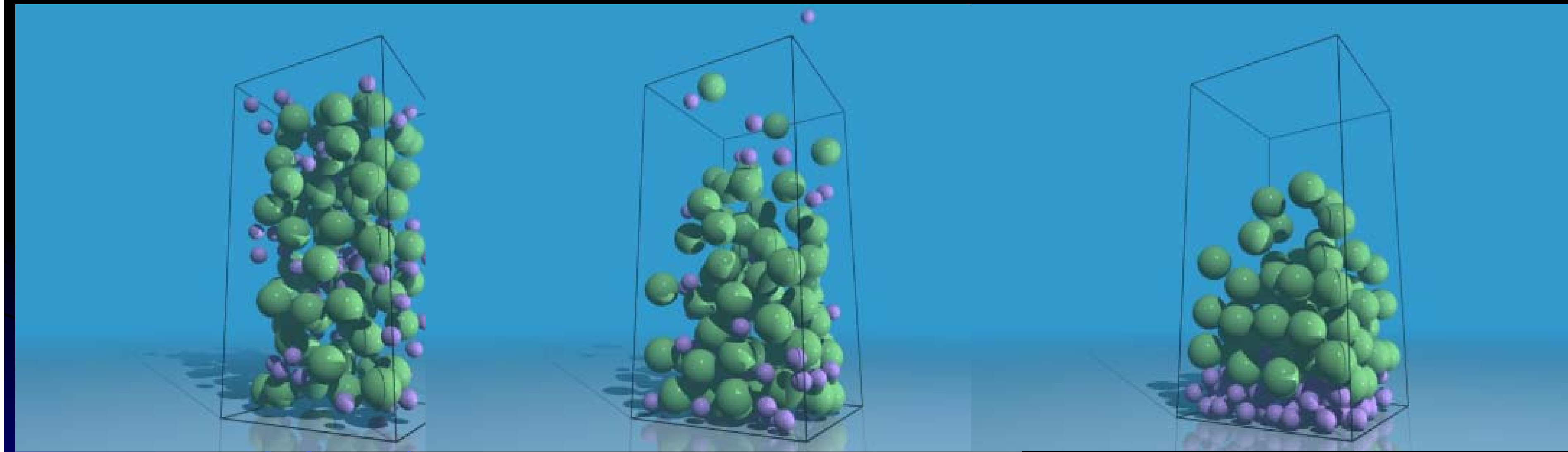




www.oxfordcroquet.com/tech/

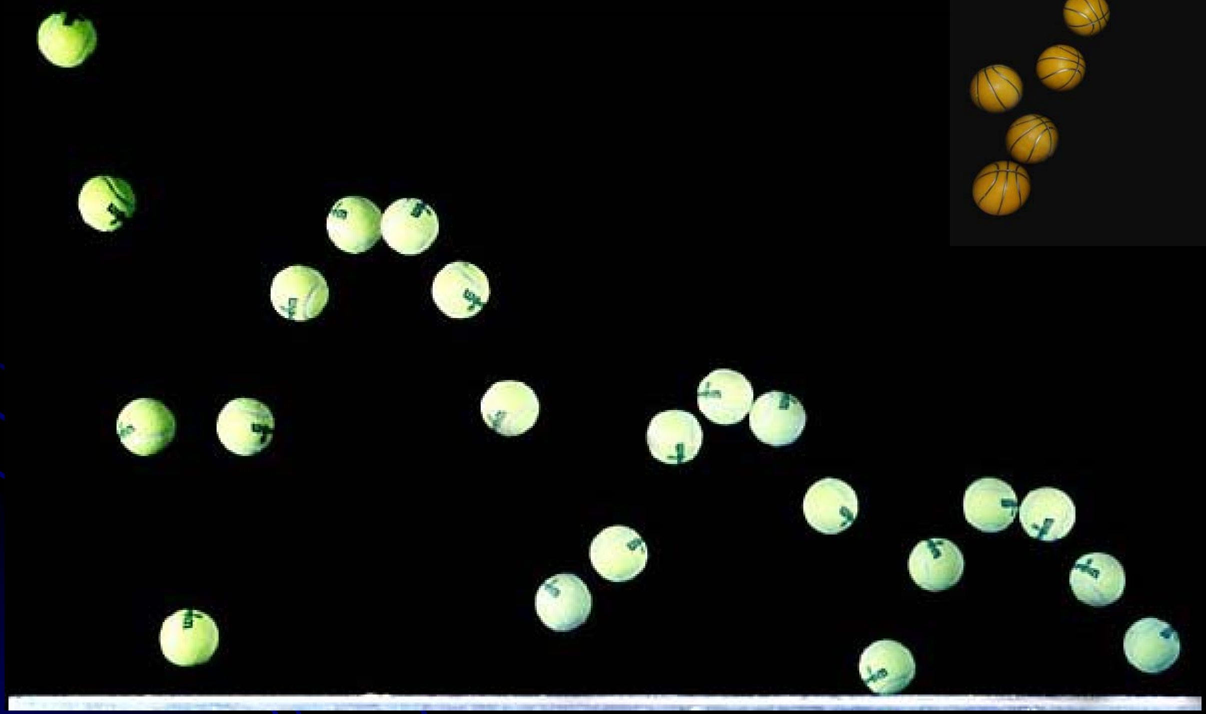
Non-spherical shape

Polydispersity



http://www.cmt.york.ac.uk/~ajm143/nuts.html

Roughness



Model of a granular gas:
A *mixture* of *inelastic rough* hard spheres

This model unveils an inherent breakdown of energy equipartition in granular fluids, even in homogeneous and isotropic states

Several circles
(Kandinsky, 1926)

Galatea of the Spheres
(Dalí, 1952)

Our aim

To derive manageable expressions for the (partial) *energy* production rates associated with each degree of freedom and each *binary collision*

Scheme of the derivation (arXiv:0910.5614)

Collision rules

↓ 1st BBGKY equation

1. Formally exact expressions

↓ $f_{ij}^{(2)} \to \bar{f}_{ij}^{(2)} \equiv \langle f_{ij}^{(2)} \rangle_\Omega$

2. Two-body averages

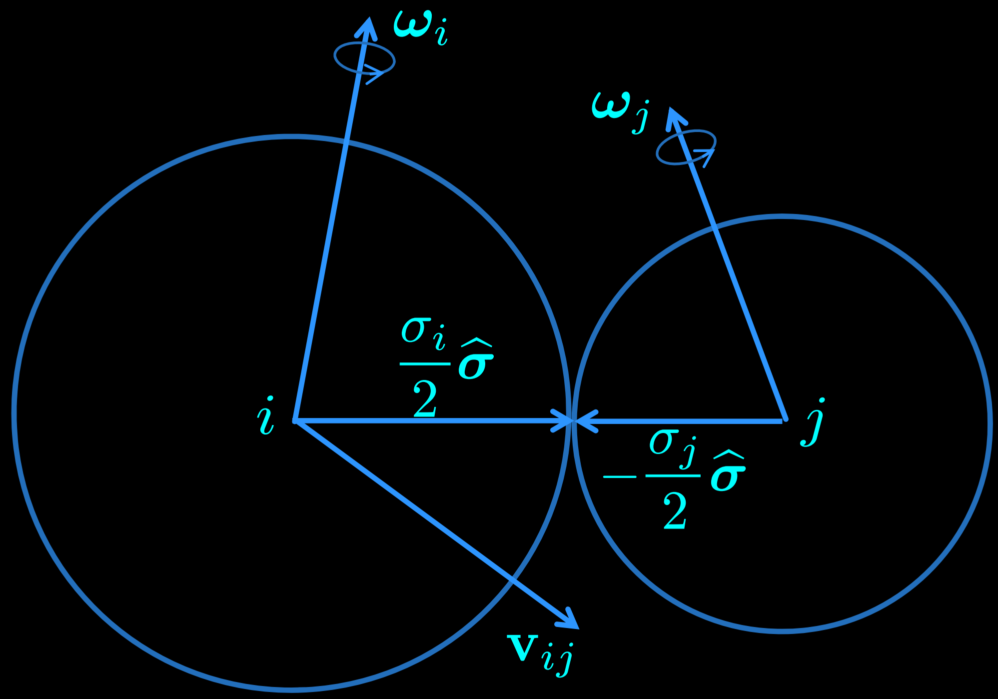
↓ Information-theory estimate of $\bar{f}_{ij}^{(2)}$

3. Final results

Material parameters:

- Masses m_i
- Diameters σ_i
- Moments of inertia I_i
- Coefficients of normal restitution α_{ij}
- Coefficients of tangential restitution β_{ij}
- $\alpha_{ij} = 1$ for perfectly elastic particles
- $\beta_{ij} = -1$ for perfectly smooth particles
- $\beta_{ij} = +1$ for perfectly rough particles

Collision rules



Notation: $\widetilde{\alpha}_{ij} \equiv m_{ij}\left(1+\alpha_{ij}\right), \quad \widetilde{\beta}_{ij} \equiv \frac{m_{ij}\kappa_{ij}}{1+\kappa_{ij}}\left(1+\beta_{ij}\right)$

$$m_{ij} \equiv \frac{m_i m_j}{m_i + m_j}, \quad \kappa_{ij} \equiv \kappa_i \kappa_j \frac{m_i + m_j}{\kappa_i m_i + \kappa_j m_j}, \quad \kappa_i \equiv \frac{I_i}{m_i(\sigma_i/2)^2}$$

Energy collisional loss

$$E_{ij} = \frac{1}{2}m_i v_i^2 + \frac{1}{2}m_j v_j^2 + \frac{1}{2}I_i\omega_i^2 + \frac{1}{2}I_j\omega_j^2$$

$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha_{ij}^2)\times\cdots \\ &\quad -(1-\beta_{ij}^2)\times\cdots \end{aligned}$$

Energy is conserved *only* if the spheres are

- elastic (α_{ij}=1) and
- either
  - perfectly smooth (β_{ij}=-1) or
  - perfectly rough (β_{ij}=+1)

Partial (granular) temperatures

Translational temperatures: $T_i^{\mathrm{tr}} = \dfrac{m_i}{3} \langle (\mathbf{v}_i - \mathbf{u})^2 \rangle$

Rotational temperatures: $T_i^{\mathrm{rot}} = \dfrac{I_i}{3} \langle \omega_i^2 \rangle = \dfrac{m_i \kappa_i}{12} \sigma_i^2 \langle \omega_i^2 \rangle$

Total temperature: $T = \sum_i \dfrac{n_i}{2n} \left(T_i^{\mathrm{tr}} + T_i^{\mathrm{rot}} \right)$

Collisional rates of change for temperatures

Energy production rates:

$$\xi_i^{\rm tr} = -\frac{1}{T_i^{\rm tr}}\left(\frac{\partial T_i^{\rm tr}}{\partial t}\right)_{\rm coll}, \quad \xi_i^{\rm tr} = \sum_j \xi_{ij}^{\rm tr}$$

Binary collisions

$$\xi_i^{\rm rot} = -\frac{1}{T_i^{\rm rot}}\left(\frac{\partial T_i^{\rm rot}}{\partial t}\right)_{\rm coll}, \quad \xi_i^{\rm rot} = \sum_j \xi_{ij}^{\rm rot}$$

Net *cooling* rate:

$$\zeta = -\frac{1}{T}\left(\frac{\partial T}{\partial t}\right)_{\rm coll}, \quad \zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\rm tr}T_i^{\rm tr} + \xi_i^{\rm rot}T_i^{\rm rot}\right)$$

1. 1st BBGKY equation. Formally exact results

$$\xi_{ij}^{\rm tr} = -\frac{m_i\sigma_{ij}^2}{3n_i T_i^{\rm tr}}\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \int d\mathbf{v}_j \int d\boldsymbol{\omega}_j \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}}) \times f_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{r}_i+\sigma_{ij}\widehat{\boldsymbol{\sigma}},\mathbf{v}_j,\boldsymbol{\omega}_j)\left[(\mathbf{v}_i'-\mathbf{u})^2-(\mathbf{v}_i-\mathbf{u})^2\right]$$

$$\xi_{ij}^{\rm rot} = -\frac{I_i\sigma_{ij}^2}{3n_i T_i^{\rm rot}}\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \int d\mathbf{v}_j \int d\boldsymbol{\omega}_j \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}}) \times f_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{r}_i+\sigma_{ij}\widehat{\boldsymbol{\sigma}},\mathbf{v}_j,\boldsymbol{\omega}_j)\left(\omega_i'^2-\omega_i^2\right)$$

Collision rules

Pre-collisional two-body correlation function (at contact)

2. Approximation
(weak inhomogeneities and/or low density)

$$f_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{r}_i+\sigma_{ij}\widehat{\boldsymbol{\sigma}},\mathbf{v}_j,\boldsymbol{\omega}_j)\to\bar{f}_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{v}_j,\boldsymbol{\omega}_j)$$

$$\bar{f}_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{v}_j,\boldsymbol{\omega}_j)\equiv\frac{\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})f_{ij}^{(2)}(\mathbf{r}_i,\mathbf{v}_i,\boldsymbol{\omega}_i;\mathbf{r}_i+\sigma_{ij}\widehat{\boldsymbol{\sigma}},\mathbf{v}_j,\boldsymbol{\omega}_j)}{\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})(\mathbf{v}_{ij}\cdot\widehat{\boldsymbol{\sigma}})}$$

$$\xi_{ij}^{\mathrm{tr}},\xi_{ij}^{\mathrm{rot}}=\mathrm{L.C.}\begin{cases}\langle v_{ij}\mathbf{v}_i\cdot\mathbf{v}_{ij}\rangle\\\langle(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\cdot(\mathbf{v}_i\times\mathbf{v}_j)\rangle\\\langle v_{ij}\,(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)^2\rangle\\\dots\end{cases}$$

Two-body averages
(at contact)

3. Information-theory estimates

Pair correlation function (at contact)

$$\bar{f}_{ij}^{(2)}(\mathbf{v}_i, \boldsymbol{\omega}_i; \mathbf{v}_j, \boldsymbol{\omega}_j) \to \boxed{\chi_{ij}} \left(\frac{m_i m_j}{4\pi^2 T_i^{\text{tr}} T_j^{\text{tr}}} \right)^{3/2} e^{-m_i \frac{(\mathbf{v}_i - \mathbf{u})^2}{2T_i^{\text{tr}}} - m_j \frac{(\mathbf{v}_j - \mathbf{u})^2}{2T_j^{\text{tr}}}} \times f_i^{\text{rot}}(\boldsymbol{\omega}_i) f_j^{\text{rot}}(\boldsymbol{\omega}_j)$$

Final results.
Energy production rates

$$\xi_{ij}^{\text{tr}} = \frac{\nu_{ij}}{m_i T_i^{\text{tr}}}\left[2\left(\widetilde{\alpha}_{ij}+\widetilde{\beta}_{ij}\right)T_i^{\text{tr}} - \left(\widetilde{\alpha}_{ij}^2+\widetilde{\beta}_{ij}^2\right)\left(\frac{T_i^{\text{tr}}}{m_i}+\frac{T_j^{\text{tr}}}{m_j}\right) - \widetilde{\beta}_{ij}^2\left(\frac{T_i^{\text{rot}}}{m_i\kappa_i}+\frac{T_j^{\text{rot}}}{m_j\kappa_j}\right)\right]$$

$$\xi_{ij}^{\text{rot}} = \frac{\nu_{ij}}{m_i\kappa_i T_i^{\text{rot}}}\widetilde{\beta}_{ij}\left[2T_i^{\text{rot}} - \widetilde{\beta}_{ij}\left(\frac{T_i^{\text{tr}}}{m_i}+\frac{T_j^{\text{tr}}}{m_j}+\frac{T_i^{\text{rot}}}{m_i\kappa_i}+\frac{T_j^{\text{rot}}}{m_j\kappa_j}\right)\right]$$

$$\nu_{ij} \equiv \frac{4\sqrt{2\pi}}{3}\chi_{ij} n_j \sigma_{ij}^2\sqrt{\frac{T_i^{\text{tr}}}{m_i}+\frac{T_j^{\text{tr}}}{m_j}}$$ Effective collision frequencies

Final results.
Net cooling rate

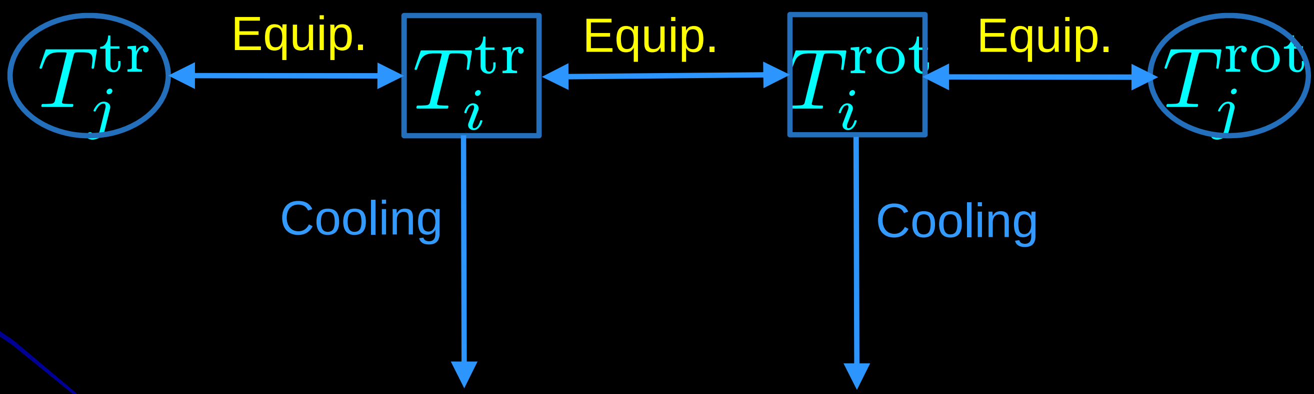
$$\zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\rm tr} T_i^{\rm tr} + \xi_i^{\rm rot} T_i^{\rm rot}\right)$$

$$\zeta = \sum_{ij} \frac{n_i \nu_{ij}}{4nT} \frac{m_i m_j}{m_i + m_j} \left[(1-\alpha_{ij}^2) \left(\frac{T_i^{\rm tr}}{m_i} + \frac{T_j^{\rm tr}}{m_j} \right) + \frac{\kappa_{ij}}{1+\kappa_{ij}} (1-\beta_{ij}^2) \left(\frac{T_i^{\rm tr}}{m_i} + \frac{T_j^{\rm tr}}{m_j} + \frac{T_i^{\rm rot}}{m_i \kappa_i} + \frac{T_j^{\rm rot}}{m_j \kappa_j} \right) \right]$$

Decomposition

Energy production rates = Equipartition rates + Cooling rates

Net cooling rate = Σ Cooling rates



Simple application: Homogeneous Cooling State (HCS)

The HCS is

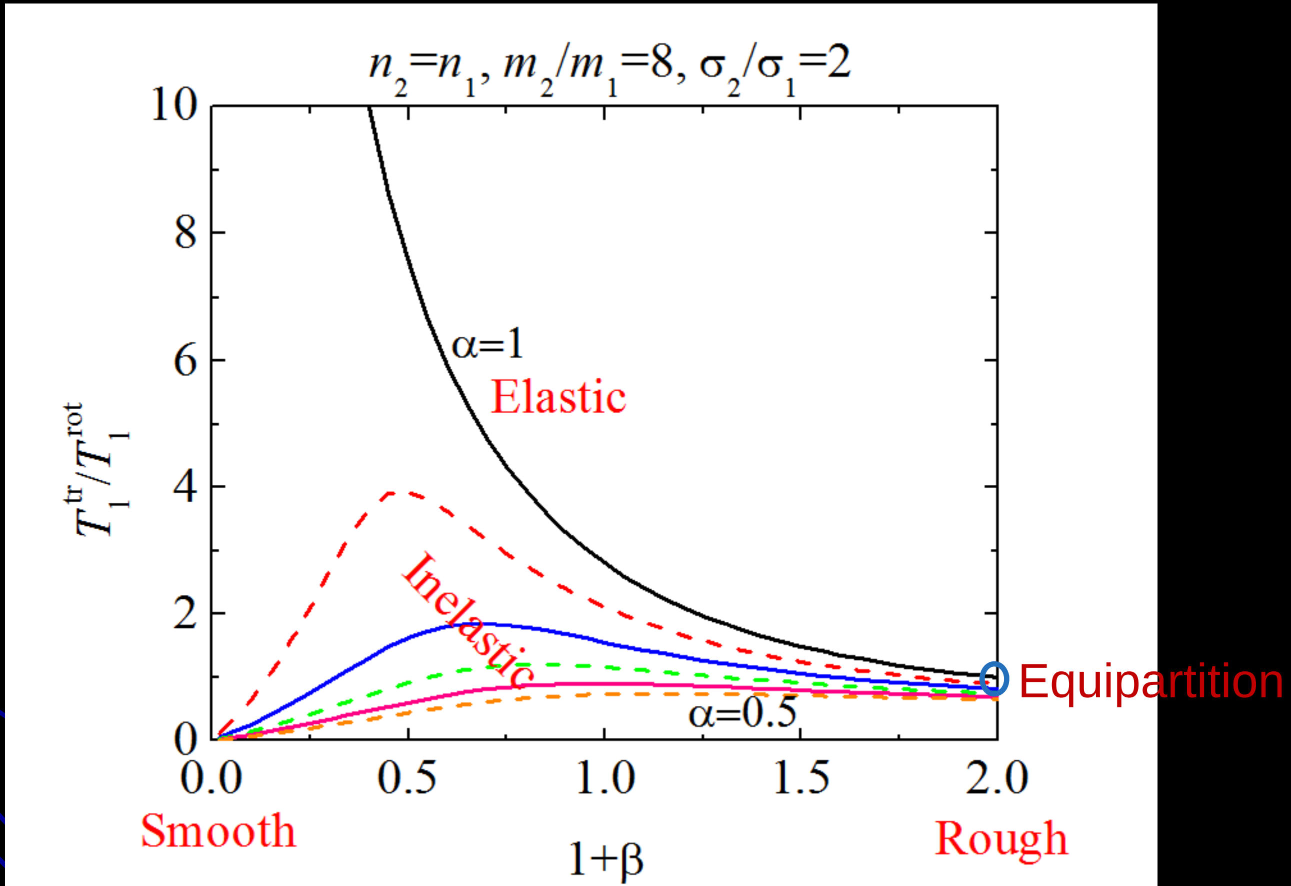
- Spatially homogeneous
- Isotropic
- Undriven
- Freely cooling

$$\frac{\partial T}{\partial t} = -\zeta T$$

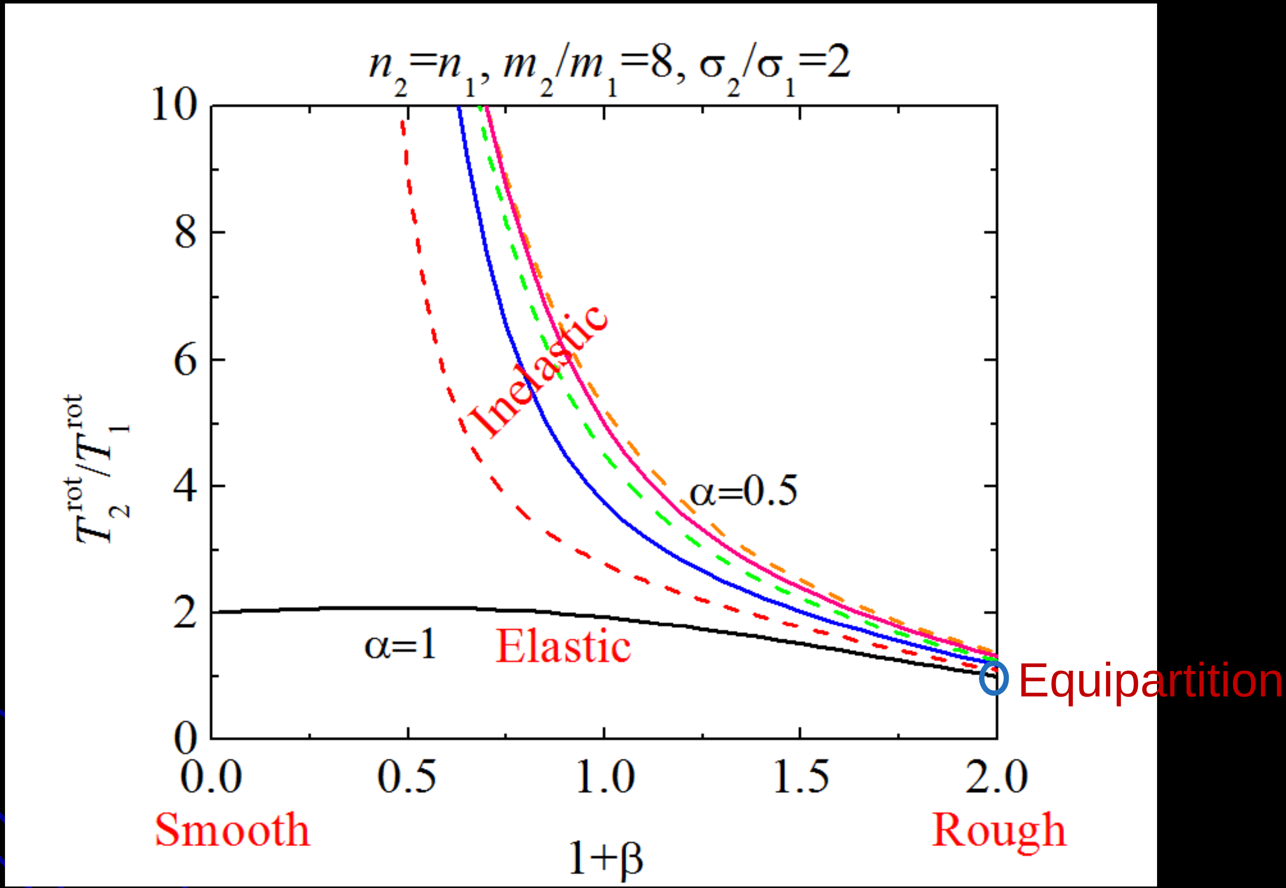
$$\frac{\partial}{\partial t}\frac{T_i^{\rm tr}}{T} = -\left(\xi_i^{\rm tr} - \zeta\right)\frac{T_i^{\rm tr}}{T}, \quad \frac{\partial}{\partial t}\frac{T_i^{\rm rot}}{T} = -\left(\xi_i^{\rm rot} - \zeta\right)\frac{T_i^{\rm rot}}{T}$$

$$t \to \infty \Rightarrow \xi_1^{\rm tr} = \xi_2^{\rm tr} = \cdots = \xi_1^{\rm rot} = \xi_2^{\rm rot} = \cdots$$

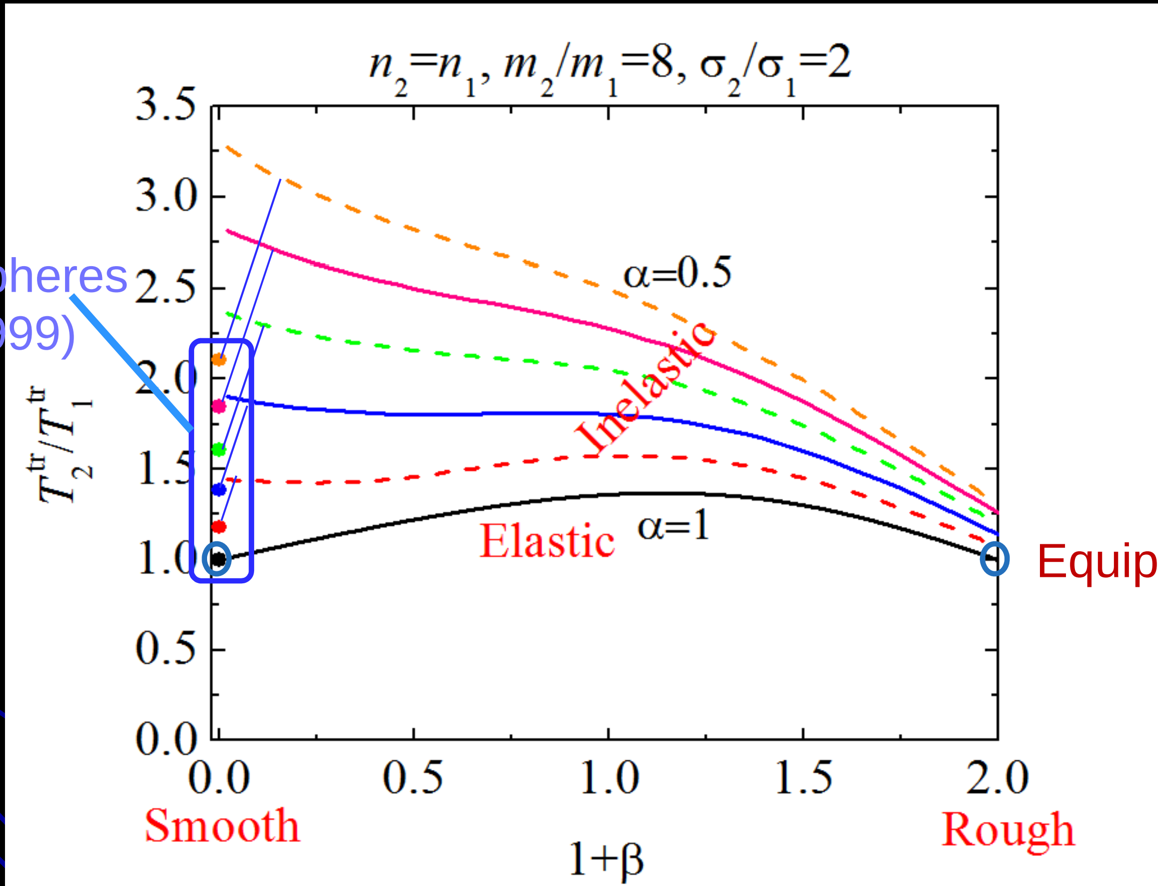
Translational/Rotational



Rotational/Rotational



Translational/Translational



"Pure" smooth spheres (Garzó&Dufty, 1999)

Equipartition

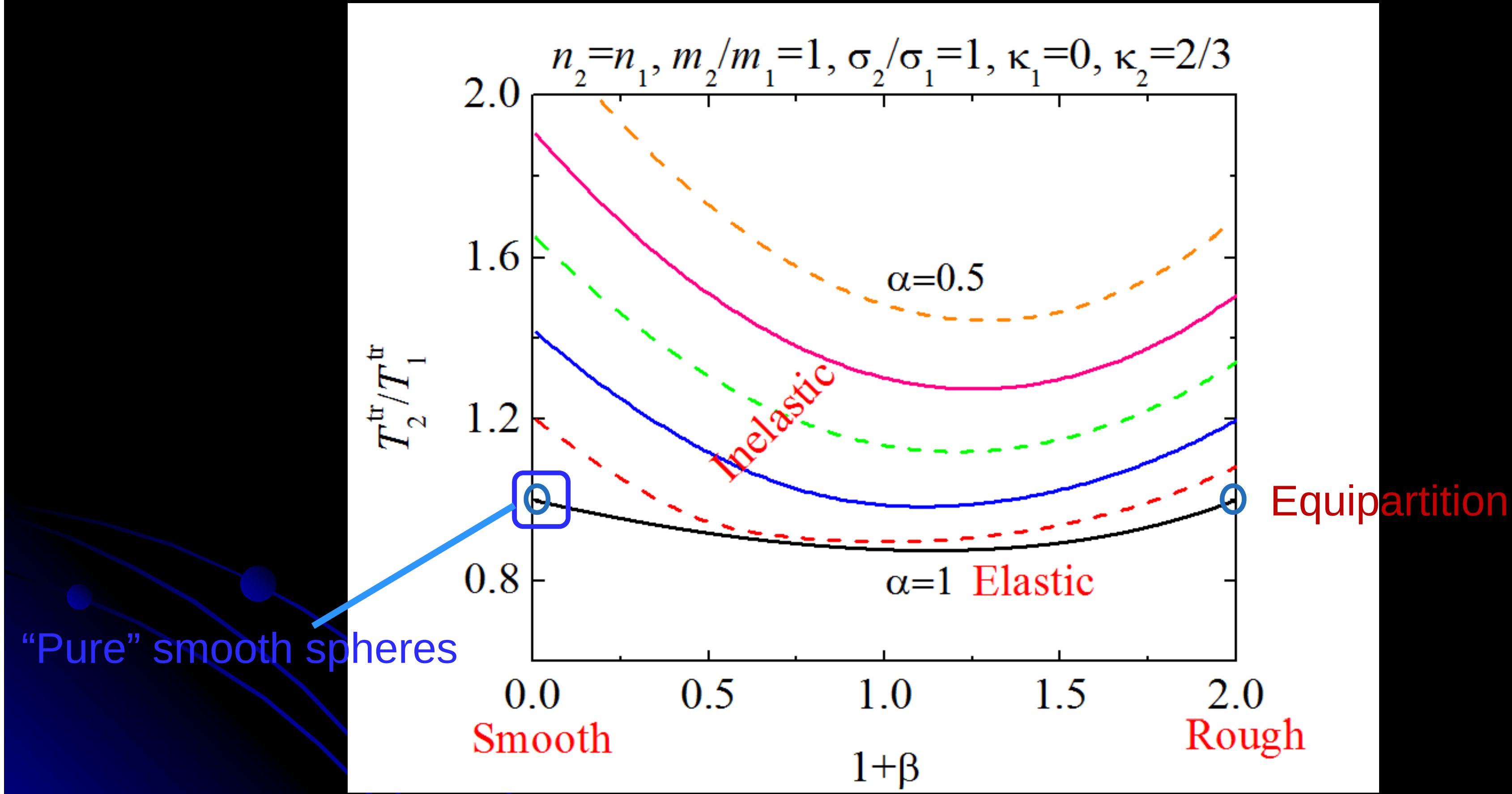
"Ghost" effect: A tiny amount of roughness has dramatic effects on the temperature ratio (enhancement of non-equipartition)

Conclusions and outlook

- Collisional energy production rates obtained for mixtures of inelastic rough hard spheres.
- Interesting non-equipartition phenomena in the HCS (“ghost” effect).
- Simulations planned to test the theoretical predictions.
- Proposal of a simple model kinetic equation for the single-component case.
- Solution of the above model in the uniform shear flow. Simulations planned.
- Derivation of the Navier-Stokes constitutive equations.

Thanks for your attention!

Translational/Translational



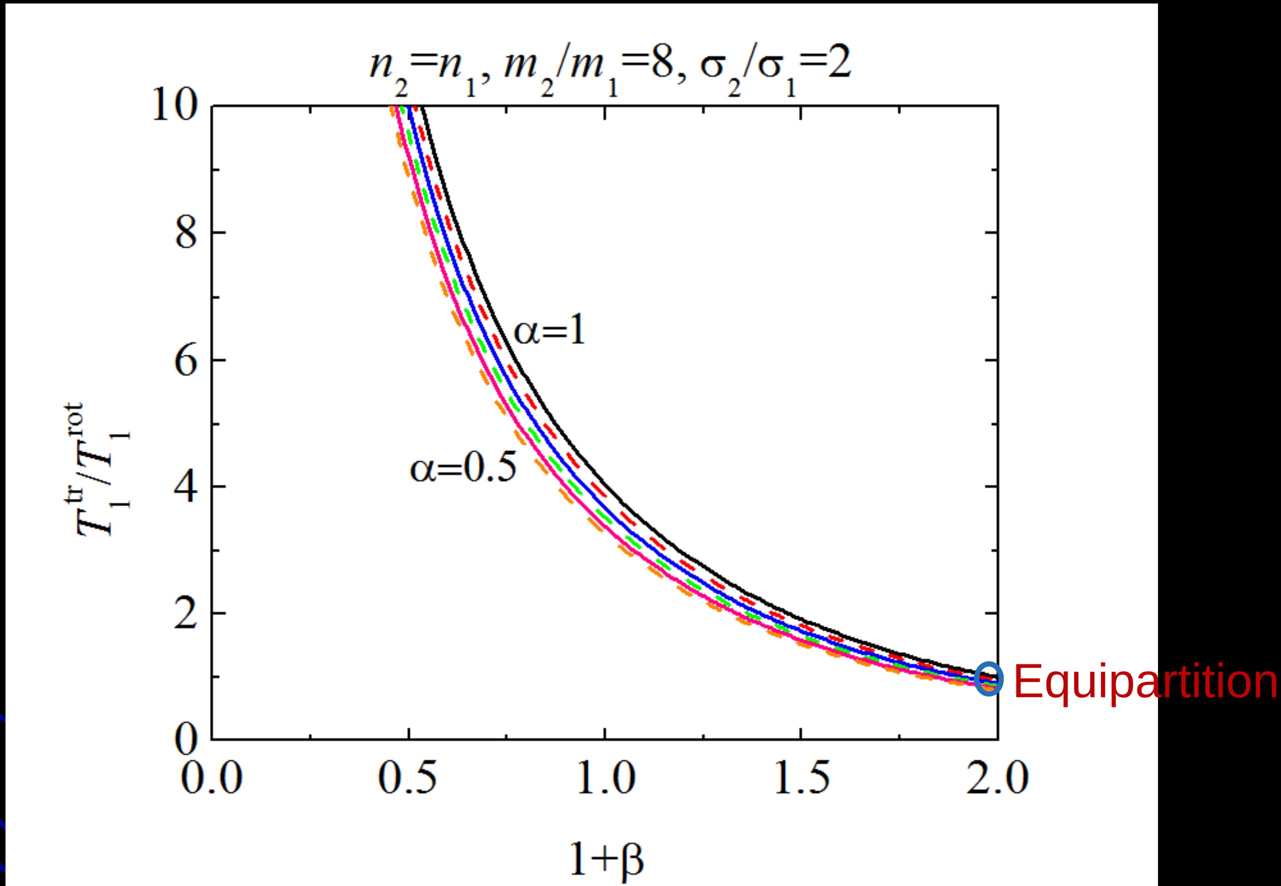
"Ghost" effect: A tiny amount of roughness has dramatic effects on the temperature ratio

Simple application: White-noise heating (steady state)

$$T_1^{\rm tr}\xi_1^{\rm tr} = T_2^{\rm tr}\xi_2^{\rm tr} = \cdots$$

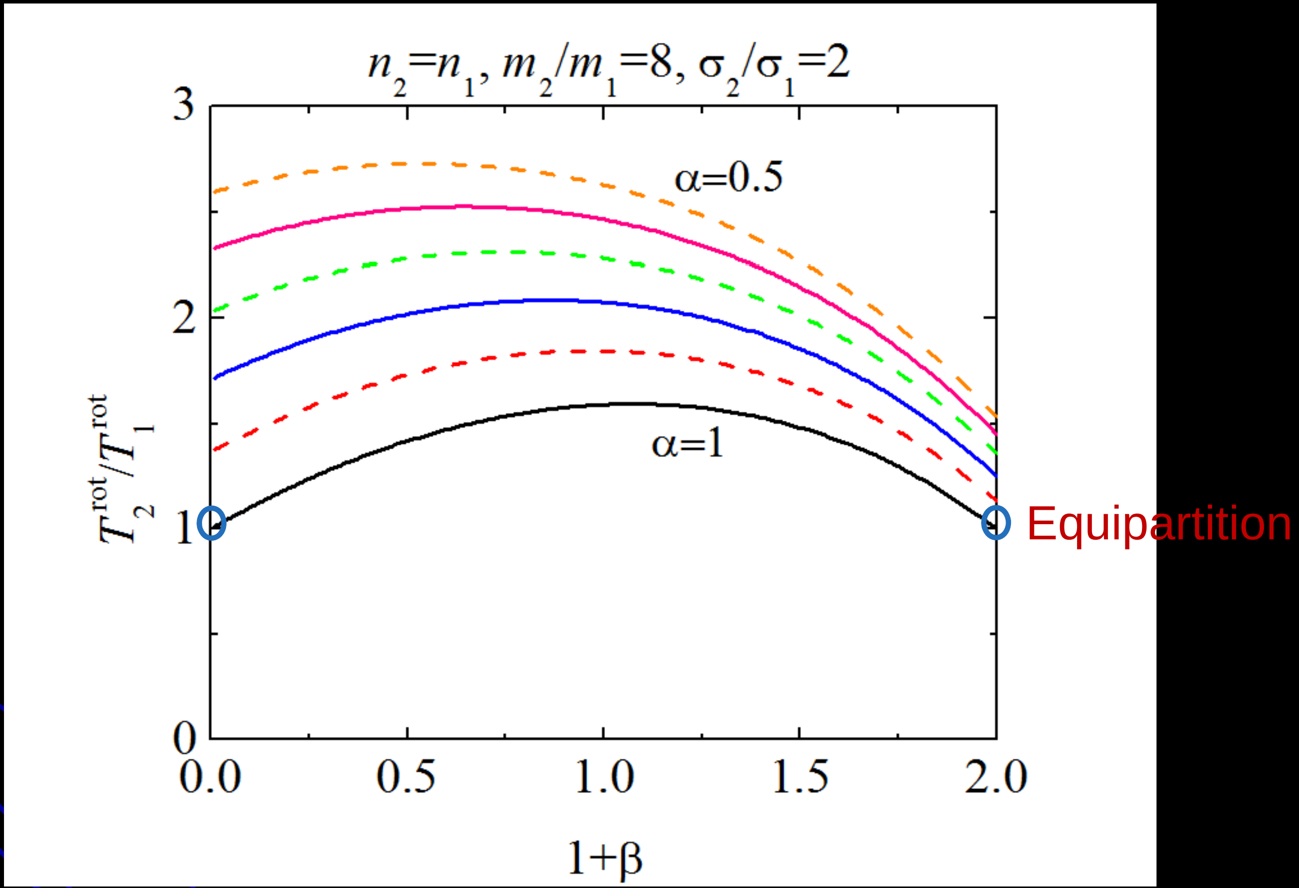
$$\xi_1^{\rm rot} = \xi_2^{\rm rot} = \cdots = 0$$

Translational/Rotational



Weak influence of inelasticity

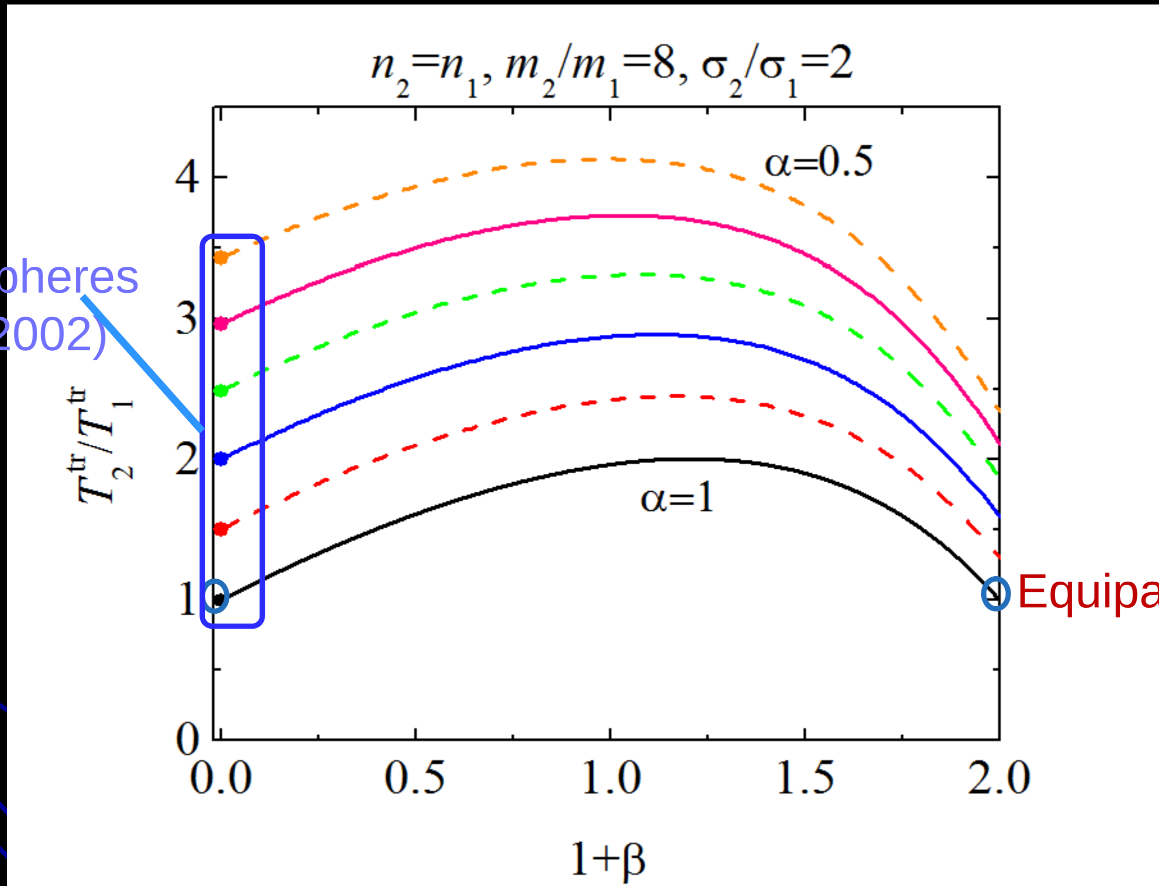
Rotational/Rotational



Same qualitative behavior for different inelasticities

Translational/Translational

"Pure" smooth spheres (Barrat&Trizac, 2002)



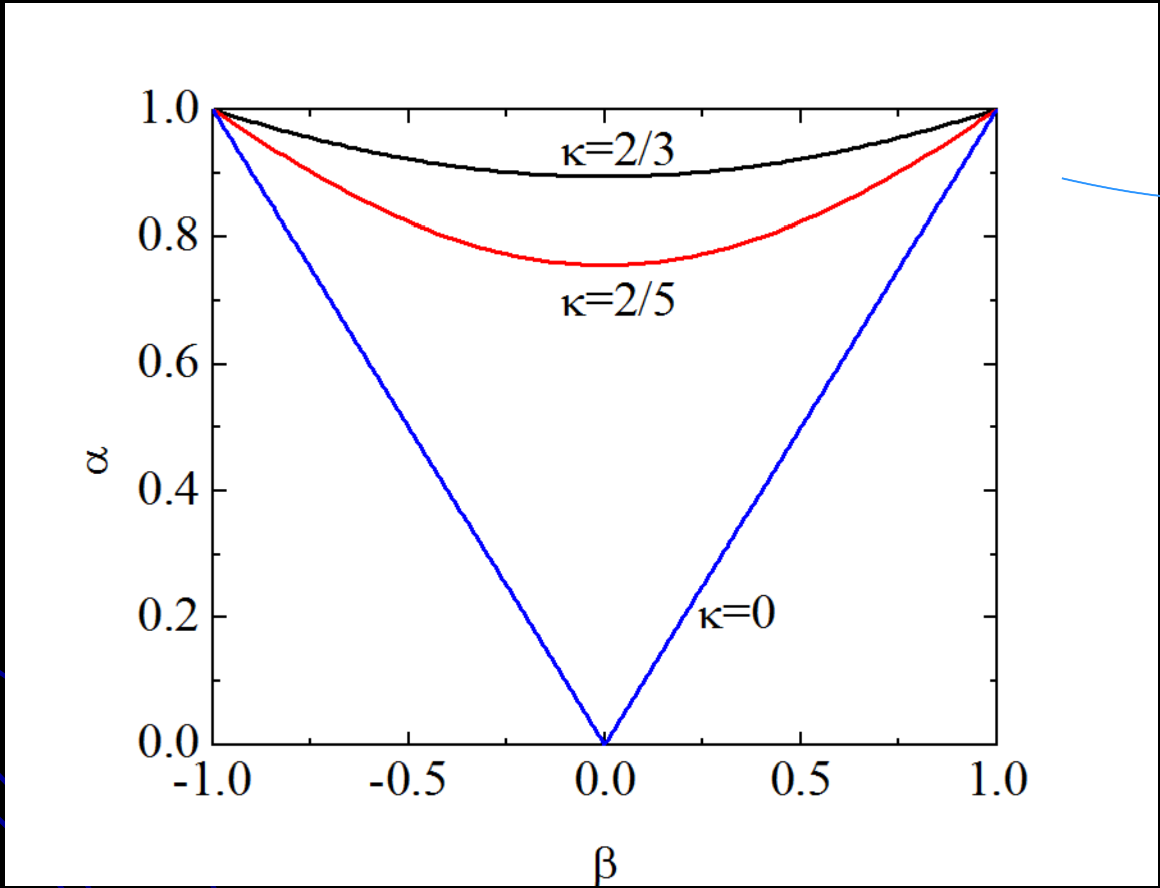
Equipartition

No "ghost" effect! (steady state)

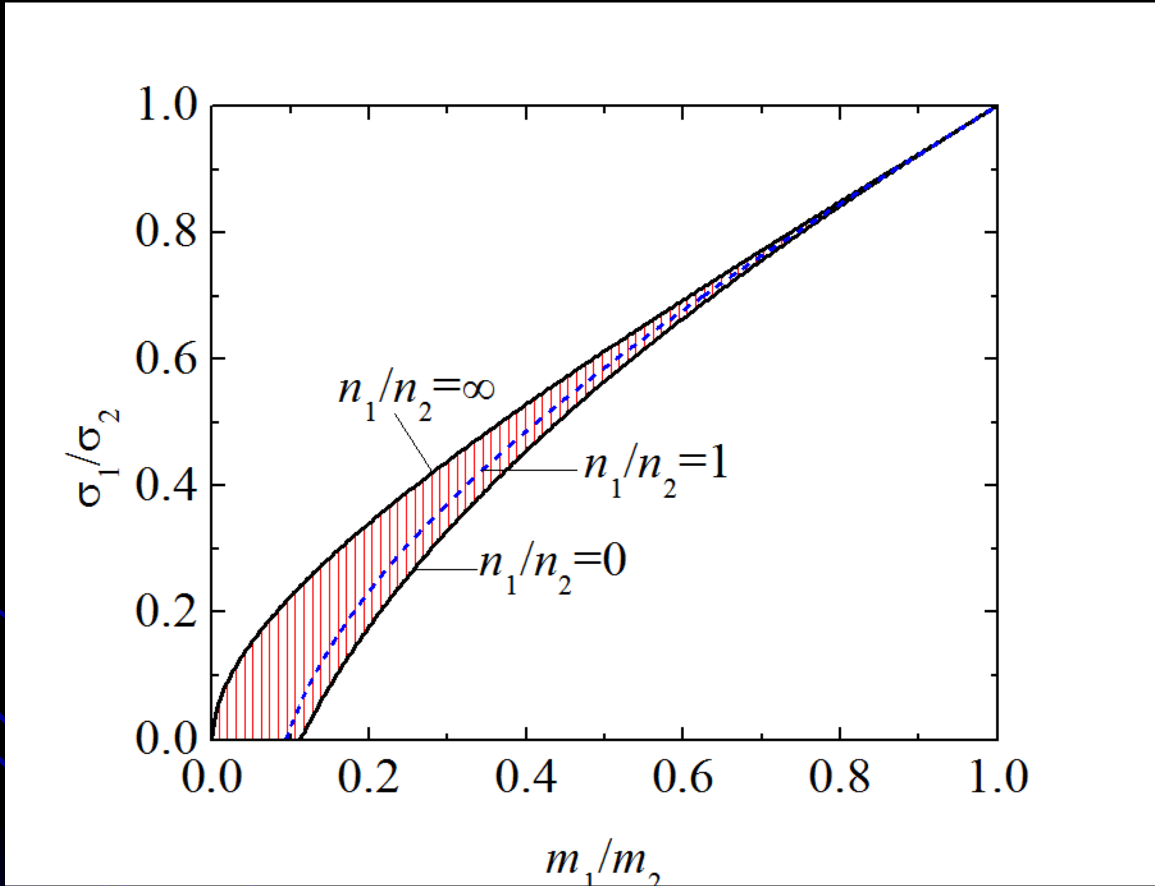
Locus of equipartition: Under which conditions does equipartition hold?

- Coefficients of normal restitution $\alpha_{11} = \alpha_{12} = \alpha_{22} = \alpha$
- Coefficients of tangential restitution $\beta_{11} = \beta_{12} = \beta_{22} = \beta$
- Inertia-moment parameters $\kappa_1 = \kappa_2 = \kappa$
- Size ratio $\sigma_1/\sigma_2 = \text{free}$
- Mass ratio $m_1/m_2 = \text{free}$
- Mole fraction $n_1/(n_1 + n_2) = \text{free}$

First condition: $\begin{cases} 1-\alpha^2 = \frac{1-\kappa}{1+\kappa}(1-\beta^2) \\ \beta = \pm 1 \end{cases}$ HCS White noise



Second condition: $$\frac{n_1}{n_2} = \frac{\sigma_{12}^2\sqrt{\frac{m_2}{m_1}} - \sigma_2^2\sqrt{\frac{m_1+m_2}{2m_2}}}{\sigma_{12}^2\sqrt{\frac{m_1}{m_2}} - \sigma_1^2\sqrt{\frac{m_1+m_2}{2m_1}}}$$



Simple kinetic model for *monodisperse* inelastic rough hard spheres

Three key ingredients we want to keep:

1. $(\partial_t T^{\text{tr}})_{\text{coll}} = -\xi^{\text{tr}} T^{\text{tr}}$

2. $(\partial_t T^{\text{rot}})_{\text{coll}} = -\xi^{\text{rot}} T^{\text{rot}}$

3. $$\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j] = \frac{1+\alpha_{ij}+\beta_{ij}\kappa_{ij}/(1+\kappa_{ij})}{2} \times \int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j] \Big|_{\substack{\alpha_{ij}=1 \\ \beta_{ij}=-1}}$$

Elastic smooth spheres

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

$$\begin{aligned} J[f,f] \;\to\; & -\lambda\nu_0\,(f-f_0) \\ & +\frac{\xi^{\rm tr}}{2}\frac{\partial}{\partial\mathbf{v}}\cdot[(\mathbf{v}-\mathbf{u})f]+\frac{\xi^{\rm rot}}{2}\frac{\partial}{\partial\boldsymbol{\omega}}\cdot(\boldsymbol{\omega}f)\end{aligned}$$

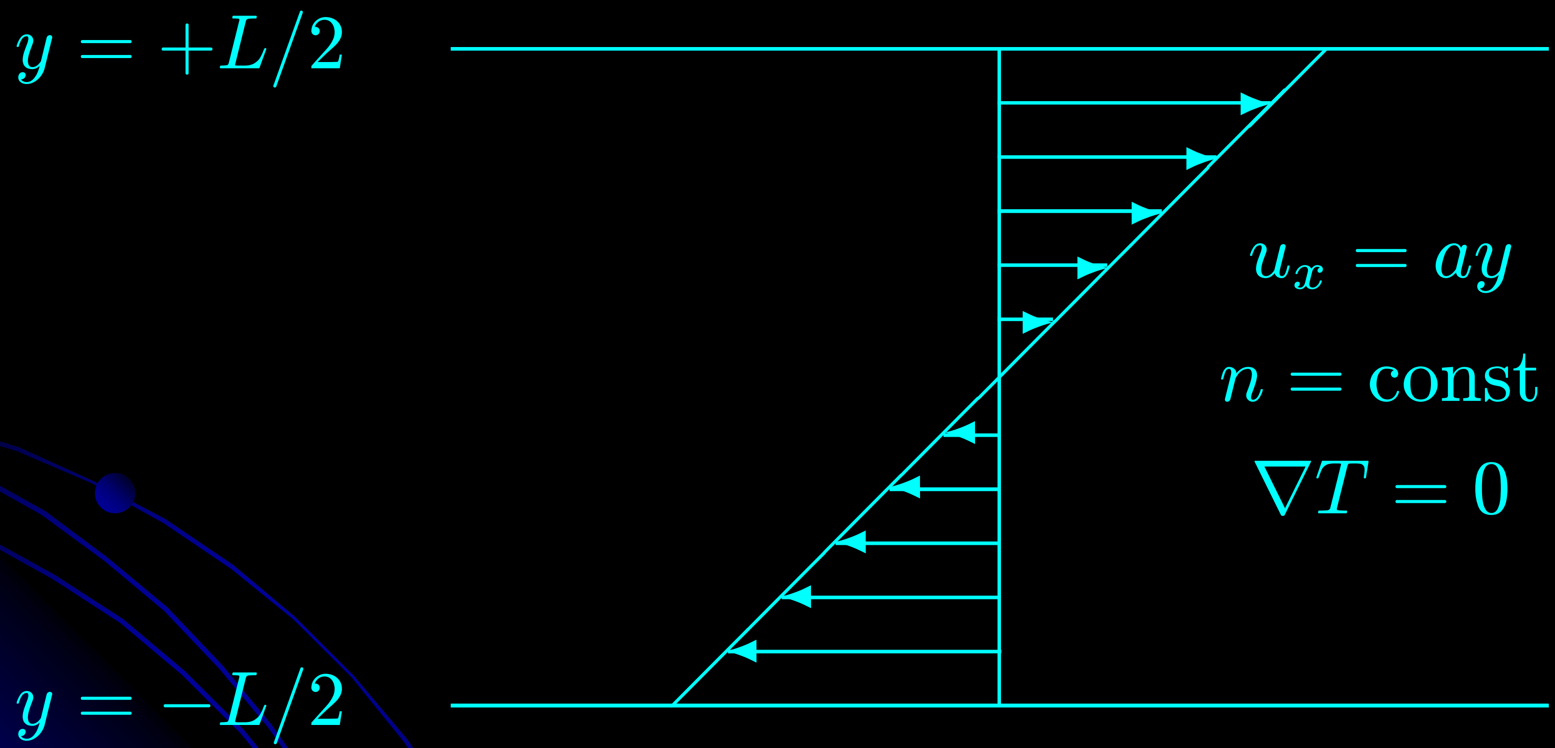
$$\lambda\equiv\frac{1+\alpha}{2}+\frac{\kappa}{1+\kappa}\frac{1+\beta}{2},\quad \nu_0=\frac{16\sqrt{\pi}}{5}n\sigma^2\sqrt{T^{\rm tr}/m}$$

$$f_0=n\left(\frac{mI}{4\pi^2T^{\rm tr}T^{\rm rot}}\right)^{3/2}\exp\left[-\frac{m(\mathbf{v}-\mathbf{u})^2}{2T^{\rm tr}}-\frac{I\omega^2}{2T^{\rm rot}}\right]$$

An even simpler version ...

$$\left\{\begin{array}{rcl} \partial_t f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)+\mathbf{v}\cdot\nabla f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t) & = & -\lambda\nu_0\left[f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)-f_0^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)\right] \\ & & +\frac{\xi^{\mathrm{tr}}}{2}\frac{\partial}{\partial\mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u})f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)\right] \\ \partial_t T^{\mathrm{rot}}+\nabla\cdot\left(\mathbf{u}\,T^{\mathrm{rot}}\right)=-\xi^{\mathrm{rot}}T^{\mathrm{rot}} & & \end{array}\right.$$

Application to simple shear flow



$$u_x = ay$$

$$n = \mathrm{const}$$

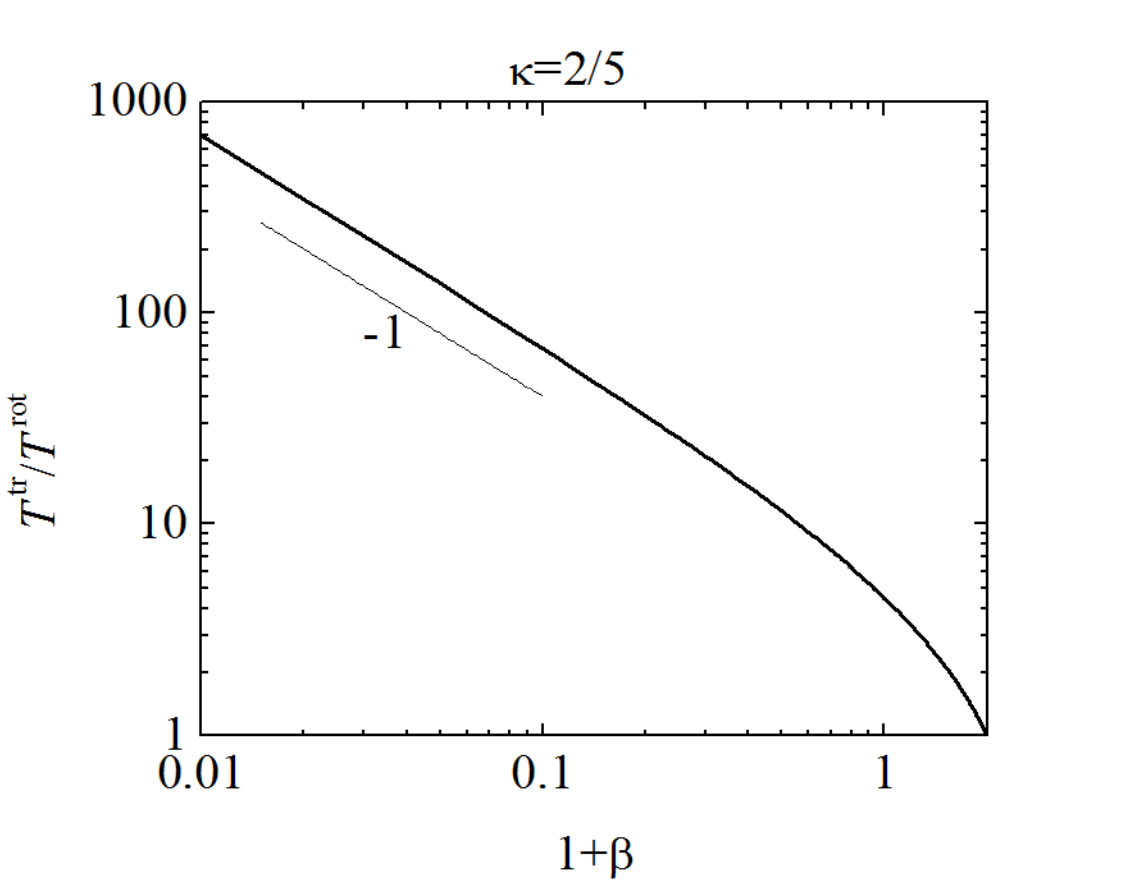
$$\nabla T = 0$$

Application to simple shear flow

Translational/Rotational temperature ratio

$$\xi^{\mathrm{rot}} = 0 \Rightarrow \boxed{\frac{T^{\mathrm{rot}}}{T^{\mathrm{tr}}} = \frac{\kappa(1+\beta)}{2\kappa+1-\beta}}$$

Independent of α



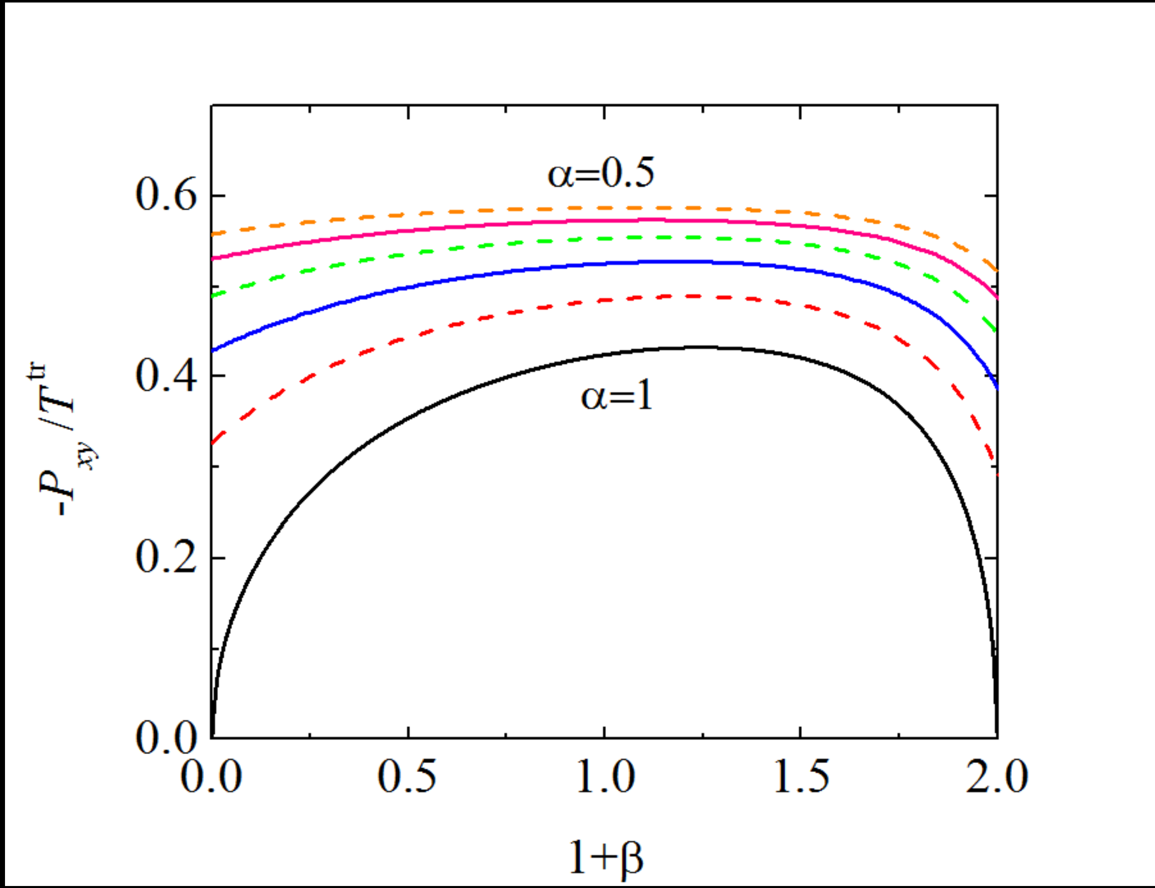
Application to simple shear flow

Shear stress

$$\frac{P_{xy}}{nT^{\text{tr}}} = -\frac{\sqrt{3\widehat{\xi}^{\text{tr}}/2}}{1+\widehat{\xi}^{\text{tr}}}$$

$$\widehat{\xi}^{\text{tr}} = \frac{5}{6}\frac{1-\alpha^2+2\kappa(1-\beta^2)/(2\kappa+1-\beta)}{1+\alpha+\kappa(1+\beta)/(1+\kappa)}$$

Scaled thermal rate



Application to simple shear flow

Anisotropic translational temperatures

$$\frac{T_x^{\rm tr}}{T^{\rm tr}} = \frac{1+3\widehat{\xi}^{\rm tr}}{1+\widehat{\xi}^{\rm tr}}$$

$$\frac{T_y^{\rm tr}}{T^{\rm tr}} = \frac{T_z^{\rm tr}}{T^{\rm tr}} = \frac{1}{1+\widehat{\xi}^{\rm tr}}$$