Navier-Stokes velocity distribution of a granular gas in the heat flux problem

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From gases to glasses in granular matter: Thermodynamic and hydrodynamic aspects
June 27-30 2005, Lyon, France

Model

- Smooth inelastic hard spheres (mass m, diameter σ, coefficient of normal restitution α)
- Post-collision velocities:

$$\mathbf{v}' = \mathbf{v} - \frac{1+\alpha}{2}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$

Relative velocity

$$\mathbf{v}_1' = \mathbf{v}_1 + \frac{1+\alpha}{2}(\mathbf{g}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$

Boltzmann equation

- Dilute granular gas
- Absence of velocity correlations before collision

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

Inelastic collisions

dimensionality

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

Collisional balance

$$\int \mathrm{d}\mathbf{v} \begin{Bmatrix} 1 \\ \mathbf{v} \\ V^2 \end{Bmatrix} J[f,f] = \begin{Bmatrix} 0 \\ \mathbf{0} \\ -\frac{d}{m}\zeta m T \end{Bmatrix}$$

Cooling rate

- Conservation of mass
- Conservation of momentum
- Dissipation of energy

"Normal" or hydrodynamic solutions

- All space and time dependence is determined by the hydrodynamic fields:

$$f(\mathbf{r}, \mathbf{v}, t) = f[\mathbf{v}|n, \mathbf{u}, T]$$

- It applies to both steady and unsteady states (after a few mean free times and a few mean free paths away from boundaries).
- It is not restricted to weak hydrodynamic gradients.

Weak hydrodynamic gradients → Chapman-Enskog expansion

(at fixed α: uncoupling between α and ∇)

$\epsilon \sim \nabla$: uniformity parameter

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \cdots$$

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

$$\partial_t^{(0)} T = -\zeta_0 T \Rightarrow \partial_t^{(0)} = -\zeta_0 T \partial_T$$

Zeroth-order: (local) Homogeneous Cooling State (HCS)

$$\frac{1}{2}\zeta_0 \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} f_0) = J[f_0, f_0]$$

$$f_0(\mathbf{V}) = n\pi^{-d/2} v_T^{-d} f_0^*(c)$$ scaling

$$\mathbf{c} \equiv \mathbf{V}/v_T, \quad v_T \equiv \sqrt{2T/m}$$

Thermal speed

Kurtosis and high-energy tail of the HCS

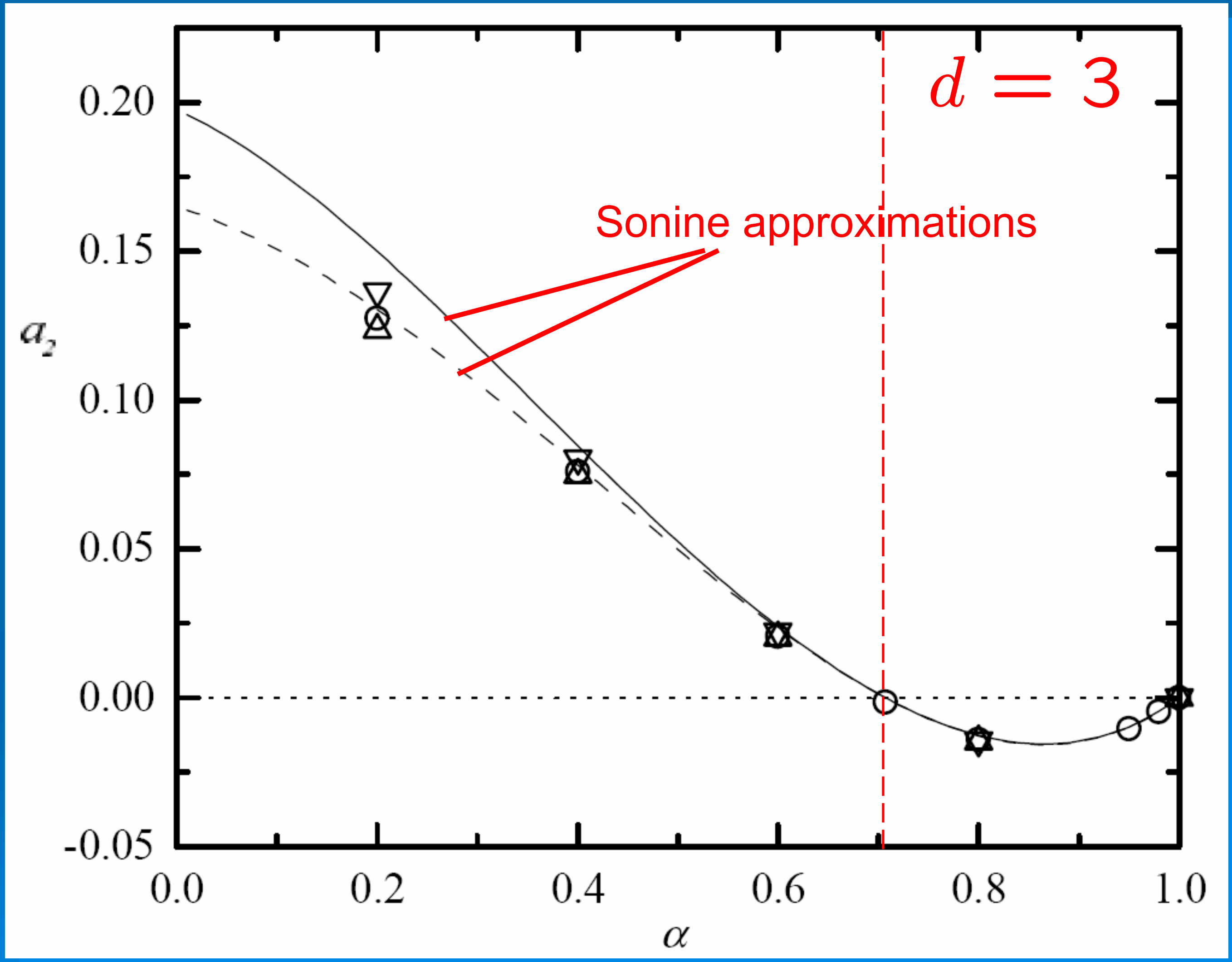
$$f_0^*(c) \neq f_M^*(c) = \pi^{-d/2} e^{-c^2}$$ Maxwellian

$$f_0^*(c) = f_M^*(c) \left[1 + \sum_{k=2}^{\infty} a_k L_k^{\left(\frac{d-2}{2}\right)}(c^2) \right]$$

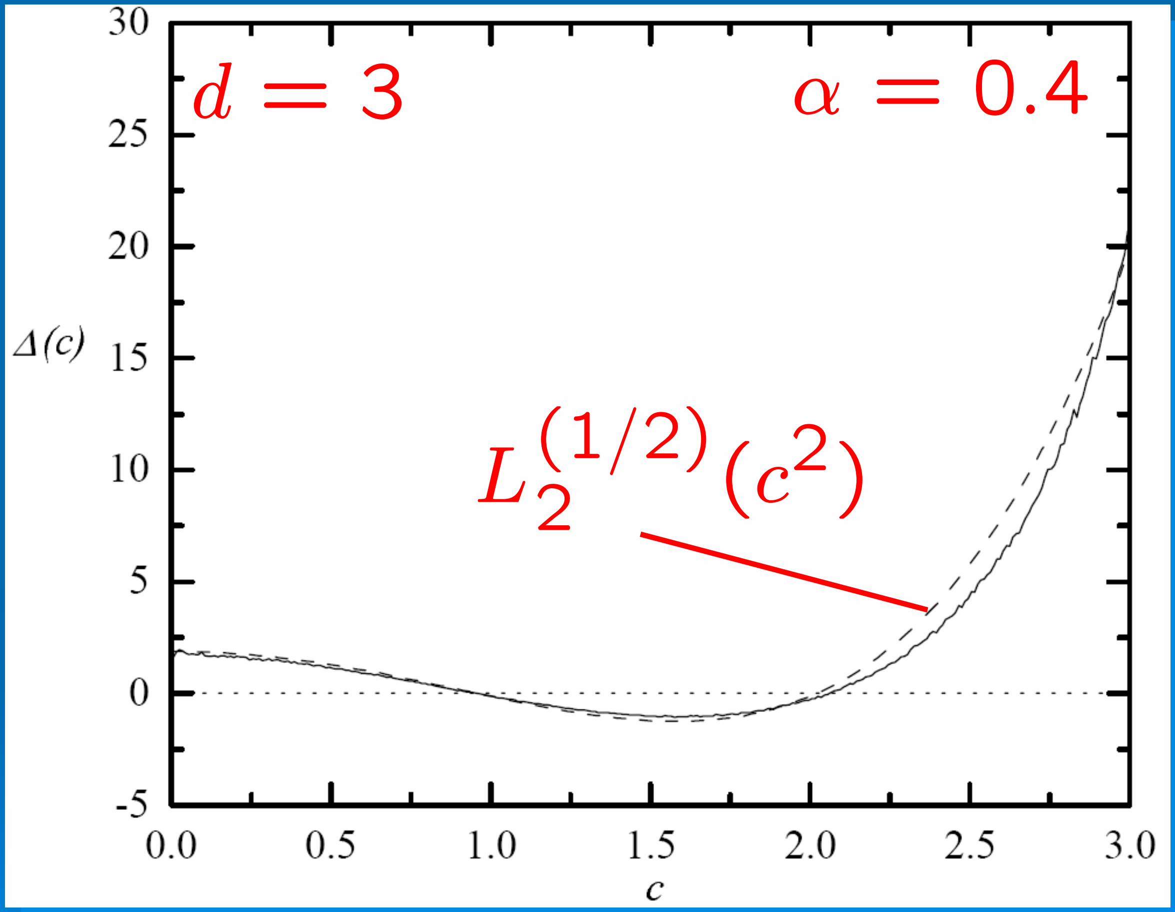
$a_2 = \dfrac{4}{d(d+2)} \langle c^4 \rangle - 1$: fourth cumulant

$f_0^*(c) \to e^{-Ac}$: high-energy overpopulation

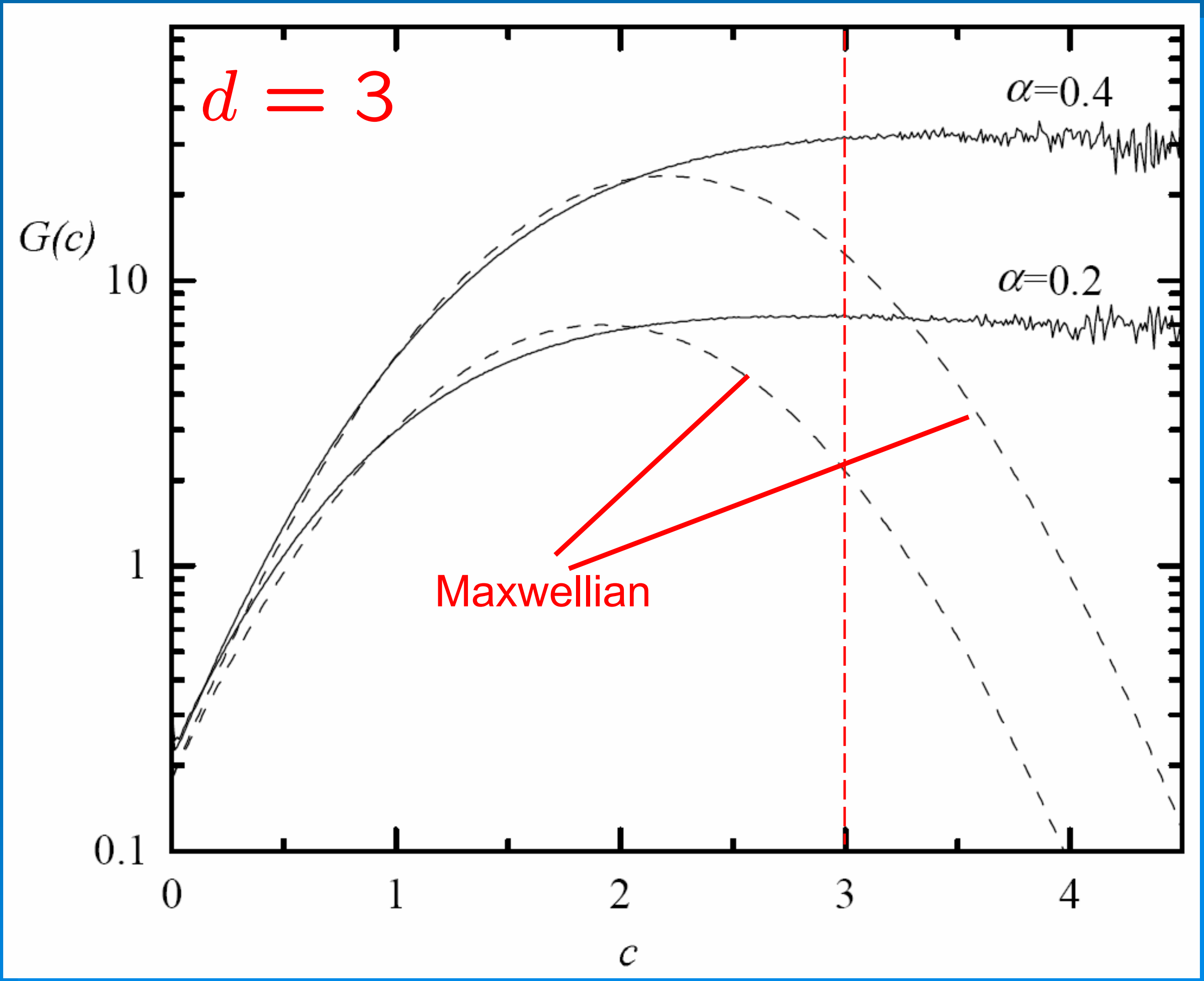
J.M. Montanero & A.S., Gran. Matt. **2**, 53 (2000)



$$\Delta(c) \equiv \frac{1}{a_2}\left[\frac{f_0^*(c)}{f_M^*(c)} - 1\right]$$

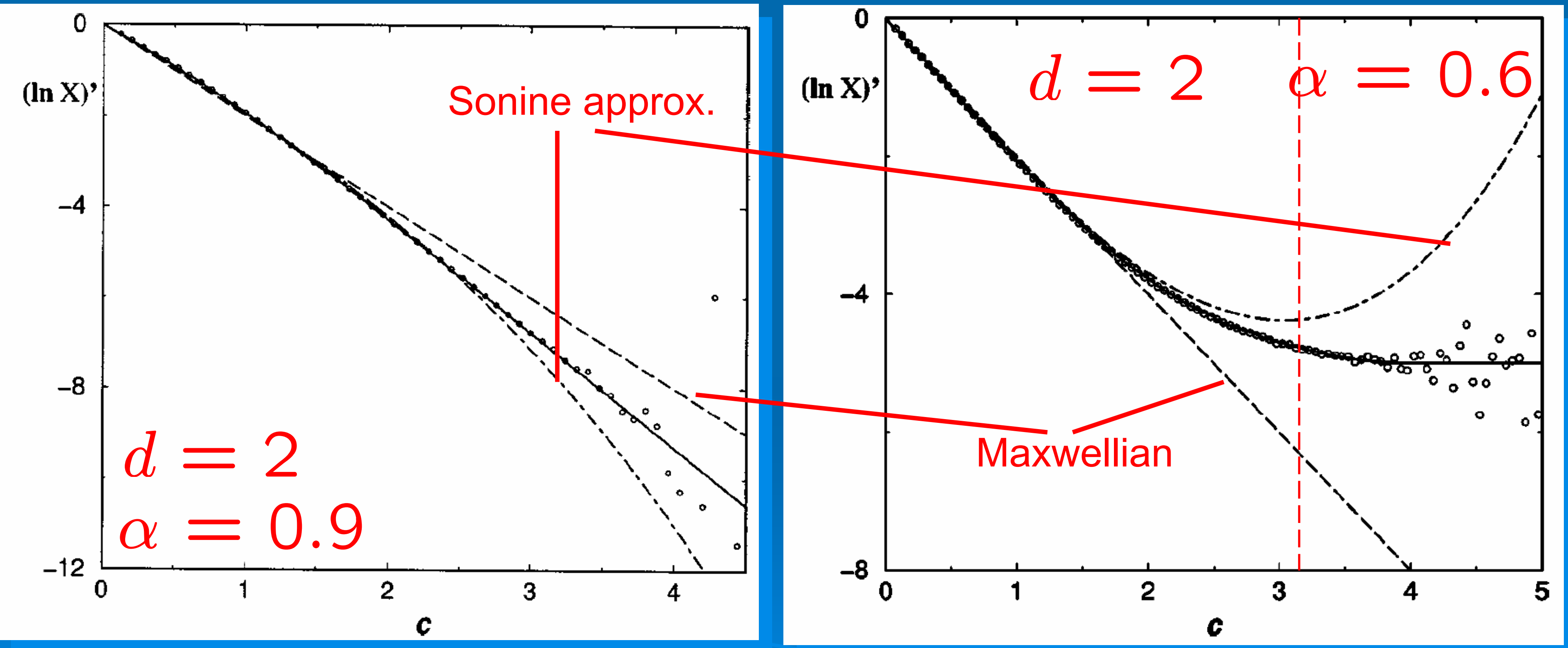


$$G(c) \equiv e^{Ac} f_0^*(c)$$



J.J. Brey & M.J. Ruiz-Montero, Phys. Rev. E **70**, 051301 (2004)

$$(\ln X)' \rightarrow \partial \ln f_0^*(c)/\partial c$$



First-order: Navier-Stokes (NS) velocity distribution

$$f_1 = \mathbf{X}\cdot\nabla \ln T + \mathbf{Y}\cdot\nabla \ln n + \mathsf{Z} : \nabla \mathbf{u}$$

$$\tilde{\mathcal{L}}\mathbf{X}(\mathbf{V}) = \mathbf{A}(\mathbf{V})$$

Inhomogeneous term

$$\tilde{\mathcal{L}} \equiv \frac{\zeta_0}{2}\frac{\partial}{\partial \mathbf{V}}\cdot\mathbf{V} - \frac{\zeta_0}{2} + \mathcal{L}$$

Linearized collision operator (around HCS)

$$\mathbf{A}(\mathbf{V}) \equiv \frac{1}{2}\left(\mathbf{V}\frac{\partial}{\partial \mathbf{V}}\cdot\mathbf{V} - v_T^2\frac{\partial}{\partial \mathbf{V}}\right) f_0(\mathbf{V})$$

First-order: Navier-Stokes (NS) velocity distribution

$$f_1 = \mathbf{X} \cdot \nabla \ln T + \mathbf{Y} \cdot \nabla \ln n + \mathsf{Z} : \nabla \mathbf{u}$$

$$\tilde{\mathcal{L}}' \mathbf{X}'(\mathbf{V}) = \mathbf{A}'(\mathbf{V}), \qquad \mathbf{X}' \equiv \mathbf{X} - \frac{1}{2}\mathbf{Y}$$

Combined function

$$\tilde{\mathcal{L}}' \equiv \frac{\zeta_0}{2} \frac{\partial}{\partial \mathbf{V}} \cdot \mathbf{V} + \mathcal{L}$$

$$\mathbf{A}'(\mathbf{V}) \equiv \frac{1}{2}\left(\frac{\partial}{\partial \mathbf{V}} \cdot \mathbf{V}\mathbf{V} - \frac{1}{2} v_T^2 \frac{\partial}{\partial \mathbf{V}}\right) f_0(\mathbf{V})$$

Structure of X(V) and X'(V)

Mean free path

$$\mathbf{X}(\mathbf{V}) = \lambda f_M(V)\Phi(c)\mathbf{c}$$

$$\Phi(c) = \sum_{k=1}^{\infty} b_k L_k^{(d/2)}(c^2):$$ Sonine expansion

$$b_k \propto \int \mathrm{d}\mathbf{c}\, L_k^{(d/2)}(c^2)\mathbf{c}\cdot\mathbf{X}(\mathbf{V})$$

$$\propto \underbrace{\langle L_k^{(d/2)}(c^2)c_x\rangle}_{\text{Full average}} \propto \underbrace{\langle L_k^{(1/2)}(c_x^2)c_x\rangle}_{\text{One-dimensional average}}$$

Transport coefficients

Thermal conductivity

- Heat flux: $\mathbf{q} = -\kappa \nabla T - \mu \nabla n$

Diffusion thermo-effect

$$\kappa = -\frac{m}{2Td} \int \mathrm{d}\mathbf{V}\, V^2 \mathbf{V} \cdot \mathbf{X}(\mathbf{V})$$

$$\mu = -\frac{m}{2nd} \int \mathrm{d}\mathbf{V}\, V^2 \mathbf{V} \cdot \mathbf{Y}(\mathbf{V})$$

$$\kappa \propto b_1, \qquad \kappa' \equiv \kappa - \frac{n}{2T}\mu \propto b_1'$$

Combined thermal conductivity

Green-Kubo expressions

$$\widetilde{\mathcal{L}}\mathbf{X} = \mathbf{A} \Rightarrow \mathbf{X}(\mathbf{V}) = \int_0^\infty \mathrm{d}s\, e^{-\widetilde{\mathcal{L}}s}\mathbf{A}(\mathbf{V})$$

$$\kappa = -\frac{m}{2Td}\int_0^\infty \mathrm{d}s \int \mathrm{d}\mathbf{V}\, V^2\mathbf{V}\cdot e^{-\widetilde{\mathcal{L}}s}\mathbf{A}(\mathbf{V})$$

First Sonine approximation

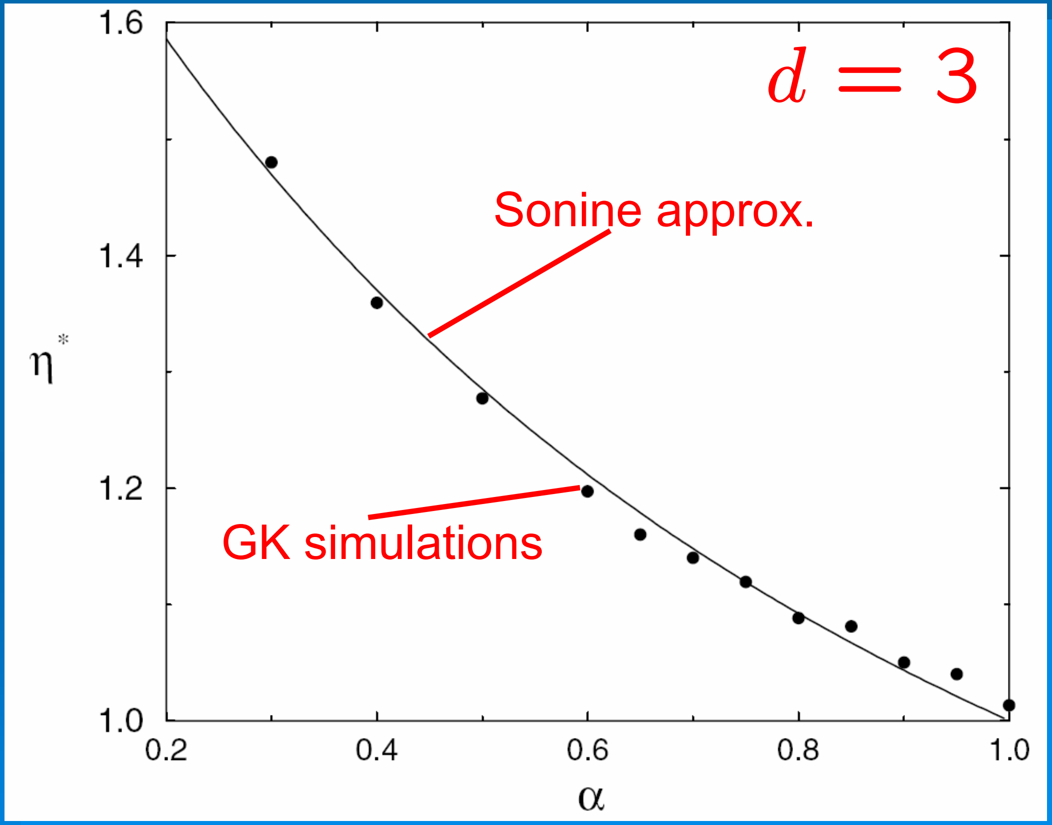
$$\widetilde{\mathcal{L}}\mathbf{X} = \mathbf{A}, \qquad \mathbf{X}(\mathbf{V}) = \lambda f_M(V)\Phi(c)\mathbf{c}$$

Ansatz: $\Phi(c) \to b_1 L_1^{(d/2)}(c^2)$

$$\kappa \propto \frac{\int \mathrm{d}\mathbf{c}\, c^2 \mathbf{c} \cdot \mathbf{A}(\mathbf{V})}{\int \mathrm{d}\mathbf{c}\, c^2 \mathbf{c} \cdot \widetilde{\mathcal{L}} f_M(V) L_1^{(d/2)}(c^2)\mathbf{c}}$$

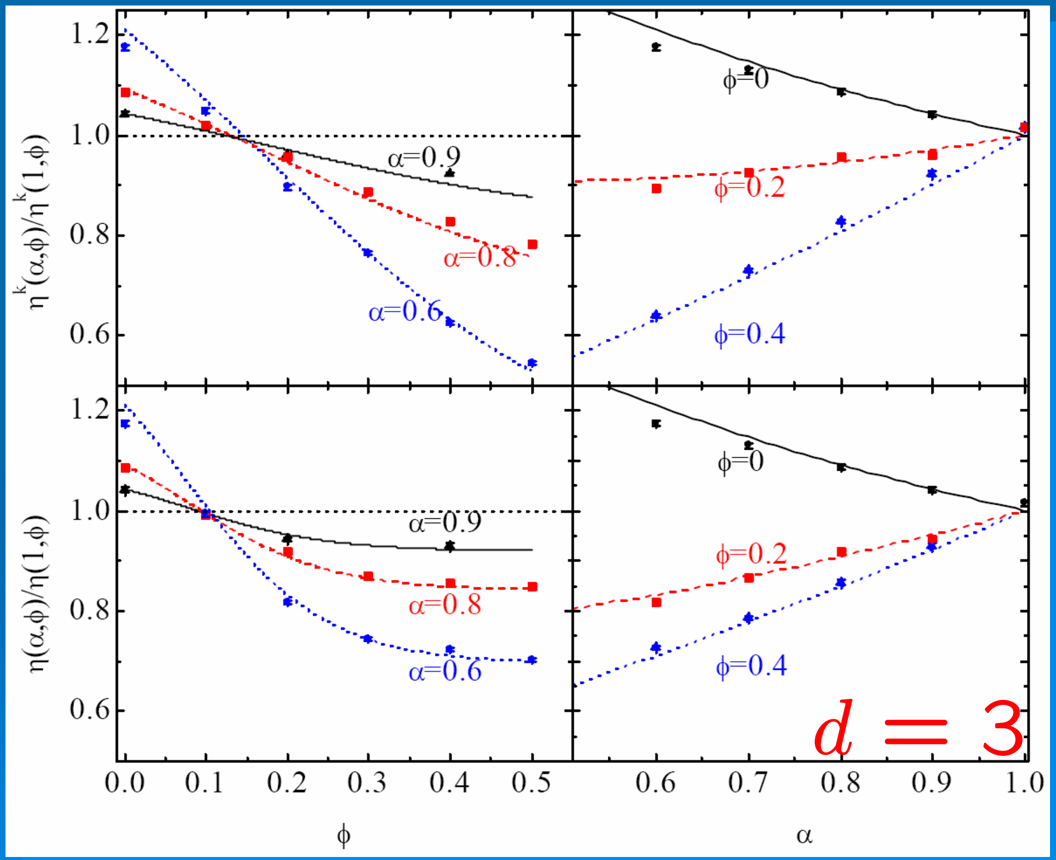
How good is the Sonine approximation for the shear viscosity?

J.J. Brey *et al*., J. Phys: Condens. Matt. **17**, S2489 (2005)



How good is the Sonine approximation for the shear viscosity?

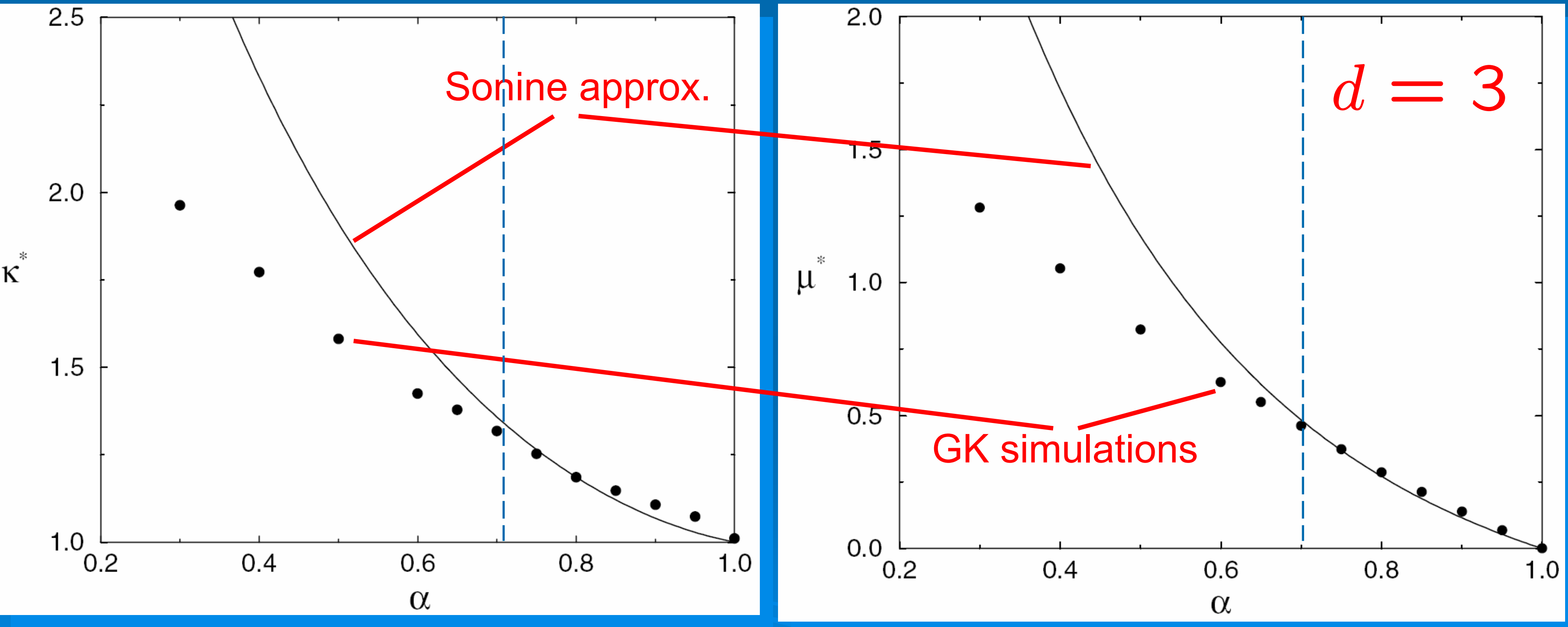
J.M. Montanero *et al.*, Proceedings of RGD 24 (AIP, 2005)



Lines: Sonine approximation
Symbols: Simulations on a *heated* simple shear flow

How good is the Sonine approximation for the heat transport coefficients?

J.J. Brey *et al.*, J. Phys: Condens. Matt. **17**, S2489 (2005)



The first Sonine approximation is not appropriate for the NS distribution functions $\mathbf{X}(\mathbf{V})$ and $\mathbf{X}'(\mathbf{V})$ at high inelasticity ($\alpha \lesssim 0.7$)

$$\mathbf{X}(\mathbf{V}) = \lambda f_M(V)\Phi(c)\mathbf{c}$$

$$\Phi(c) = \sum_{k=1}^{\infty} b_k L_k^{(d/2)}(c^2)$$

$\Phi(c) - b_1 L_1^{(d/2)}(c^2)$: not negligible

$b_2, b_3, \ldots$: not negligible

Our aim:

- Devise a simulation method to obtain $\mathbf{X}(\mathbf{V})$.
- Measure b_1, b_2, and b_3.
- Check consistency with the results for κ obtained from the GK relations.
- Compare $\Phi(c)$ with $\Phi_N(c) \equiv \sum_{k=1}^{N} b_k L_k^{(d/2)}(c^2)$

for N=1,2,3.

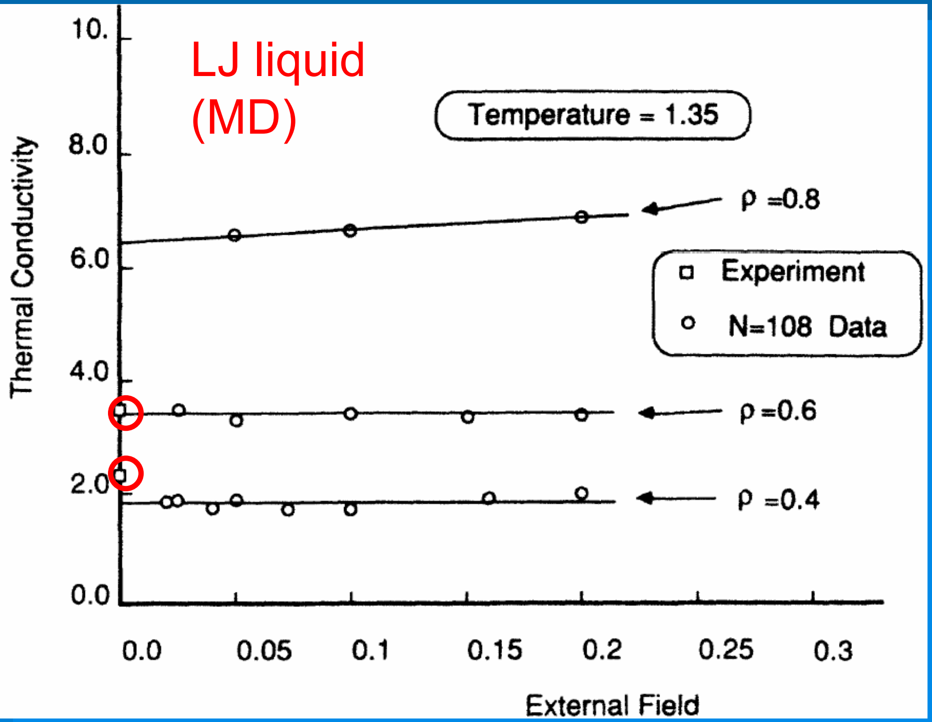
Truncated Sonine expansion

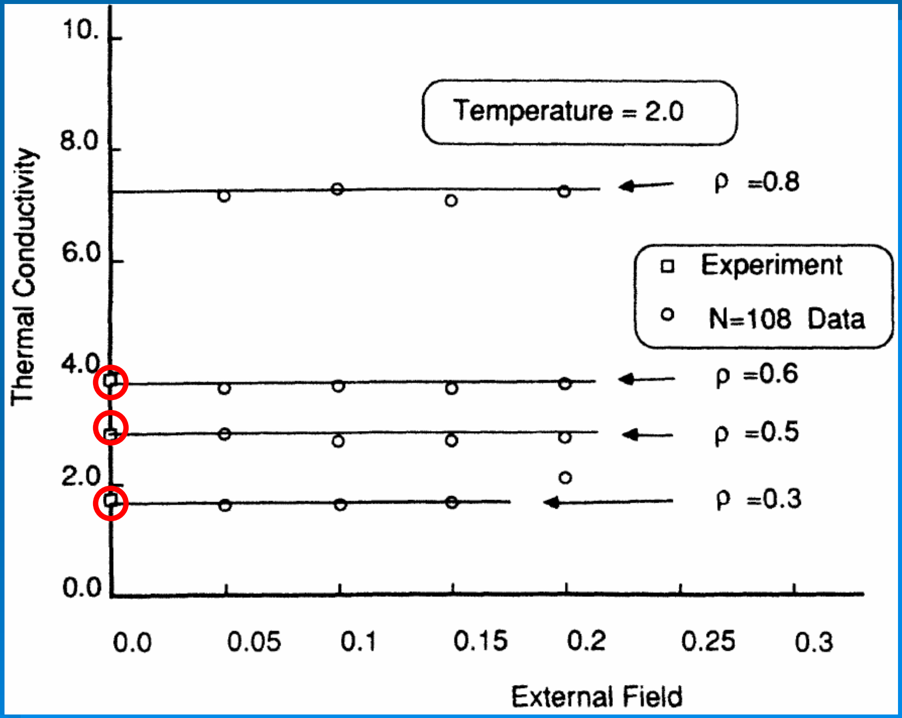
Main features of the method

- Spatially uniform system.
- Steady state.
- Application of a non-conservative, anisotropic external force of strength measured by a parameter ε.
- This parameter mimics the effect of a thermal gradient: $\varepsilon \sim \lambda \nabla \ln T \Rightarrow \mathbf{q} = -\kappa (T/\lambda) \varepsilon$.
- In the limit $\varepsilon \rightarrow 0$ one must have $f(\mathbf{V}) \simeq f_0(\mathbf{V}) + f_1(\mathbf{V})$.

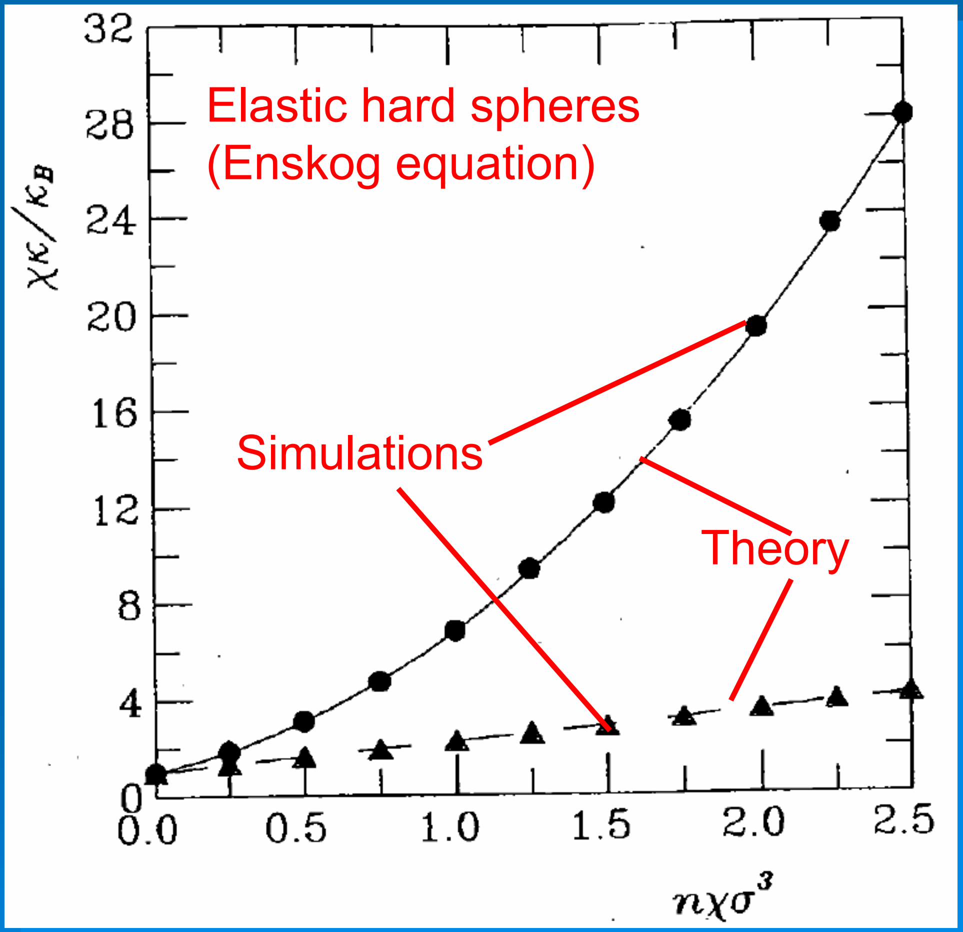
This method was already proposed by Evans (1982) and Gillan & Dixon (1983) in the case of normal fluids

D.J. Evans, Phys. Rev. A **34**, 1449 (1986)





J.M. Montanero, A.S., Proceedings of RGD 20 (Peking U.P., 1997)



First step: Express $\mathbf{A}(\mathbf{V})$ and $\mathbf{A}'(\mathbf{V})$ as divergences in velocity space

$$
\begin{aligned}
\mathbf{A}(\mathbf{V}) &\equiv \frac{1}{2}\left(\mathbf{V}\frac{\partial}{\partial \mathbf{V}}\cdot\mathbf{V} - v_T^2\frac{\partial}{\partial \mathbf{V}}\right) f_0(\mathbf{V}) \\
&= -\frac{\partial}{\partial \mathbf{V}}\cdot \mathsf{F}(\mathbf{V}) f_0(\mathbf{V})
\end{aligned}
$$

Non-conservative external force

$$
F_{ij}(\mathbf{V}) \equiv -\frac{1}{2}\left(\frac{V^2}{d-1} - v_T^2\right)\delta_{ij} - \frac{d-2}{2(d-1)} V_i V_j
$$

First step: Express $\mathbf{A}(\mathbf{V})$ and $\mathbf{A}'(\mathbf{V})$ as divergences in velocity space

$$\mathbf{A}'(\mathbf{V}) \equiv \frac{1}{2}\left(\frac{\partial}{\partial \mathbf{V}} \cdot \mathbf{V}\mathbf{V} - \frac{1}{2} v_T^2 \frac{\partial}{\partial \mathbf{V}}\right) f_0(\mathbf{V})$$

$$= -\frac{\partial}{\partial \mathbf{V}} \cdot \mathsf{F}'(\mathbf{V}) f_0(\mathbf{V})$$

$$F'_{ij}(\mathbf{V}) \equiv \frac{1}{4} v_T^2 \delta_{ij} - \frac{1}{2} V_i V_j$$

Second step: Formulate the Boltzmann equation

Total external force

$$\partial_t f + \frac{\partial}{\partial \mathbf{V}} \cdot \left(\frac{\zeta}{2}\mathbf{V} + \lambda^{-1}\mathsf{F} \cdot \boldsymbol{\epsilon} \right) f \quad = \quad J[f,f] + \frac{\zeta}{2}(f - f_0)$$

Clonation/annihilation term

$$\boldsymbol{\epsilon} \to \mathbf{0} \Rightarrow f \to f_0 + f_1, \qquad f_1 = \lambda^{-1}\mathbf{X} \cdot \boldsymbol{\epsilon}$$

Second step: Formulate the Boltzmann equation

Total external force

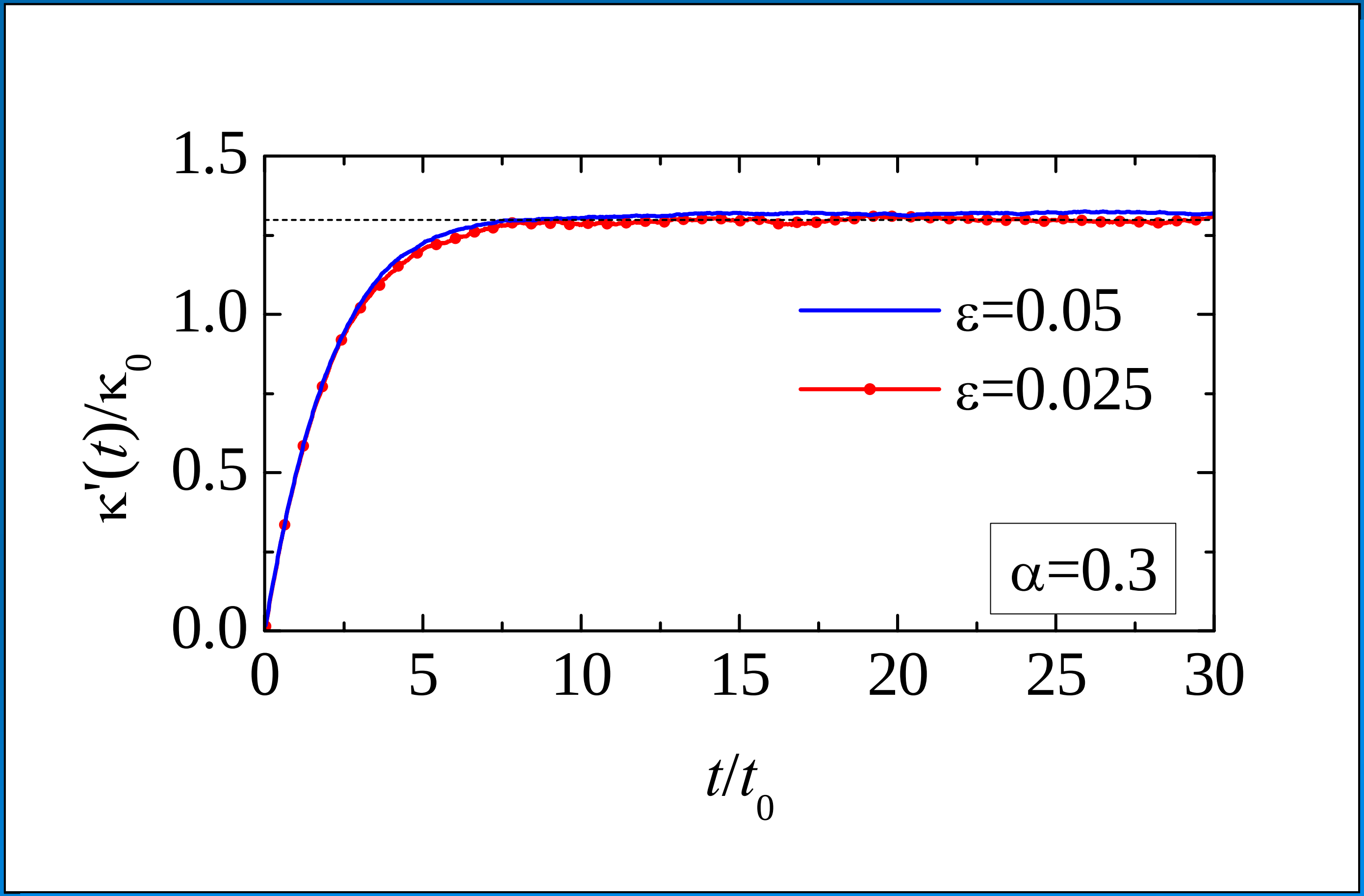
$$\partial_t f + \frac{\partial}{\partial \mathbf{V}} \cdot \left(\frac{\zeta}{2}\mathbf{V} + \lambda^{-1}\mathsf{F}' \cdot \boldsymbol{\epsilon} \right) f = J[f,f]$$

$$\boldsymbol{\epsilon} \to \mathbf{0} \Rightarrow f \to f_0 + f_1 \qquad f_1 = \lambda^{-1}\mathbf{X}' \cdot \boldsymbol{\epsilon}$$

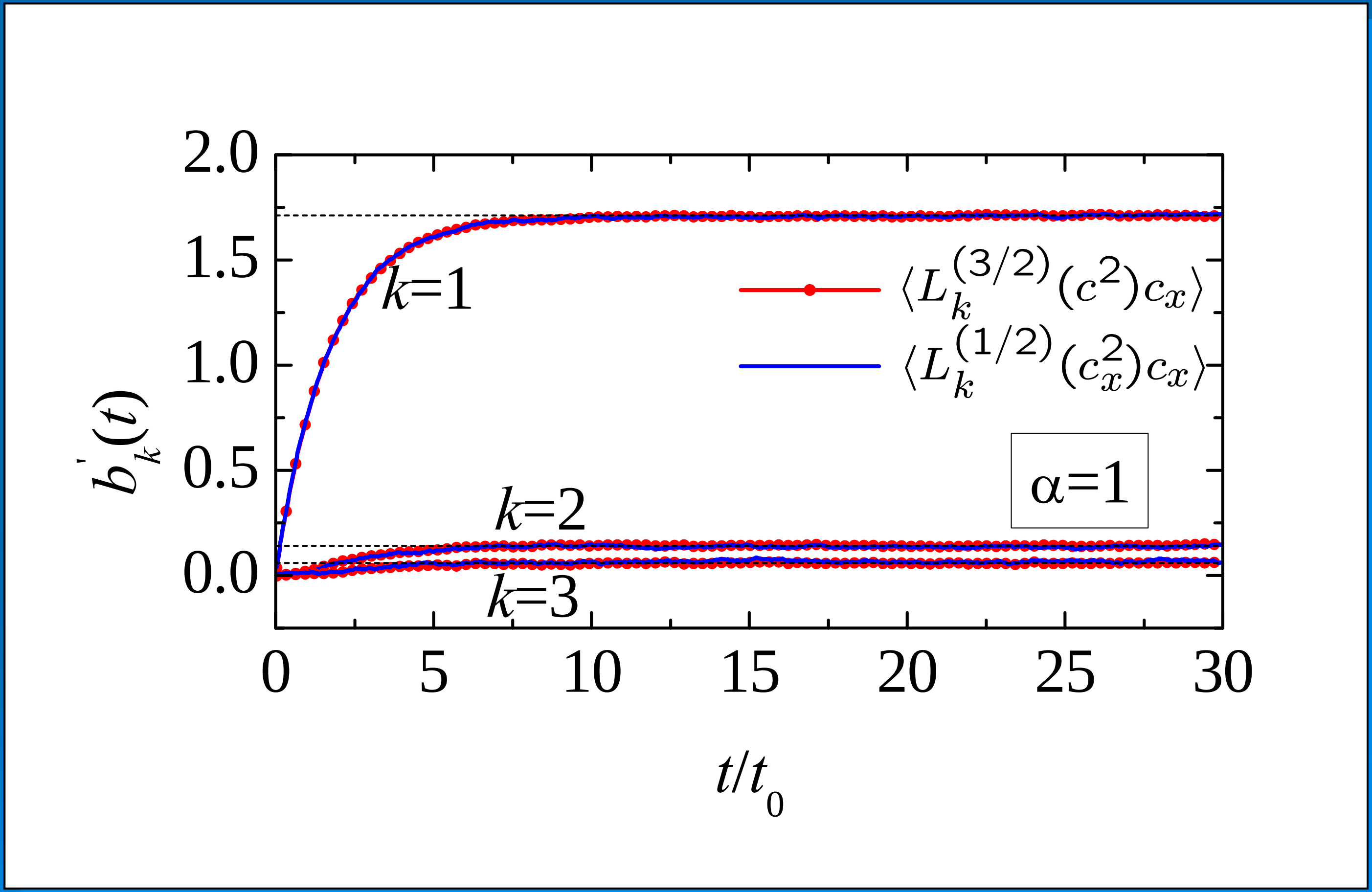
Simulation details

- Direct Simulation Monte Carlo (DSMC) method to solve the Boltzmann equation.
- We consider d=3 and restrict ourselves to the case of $\mathbf{X}'(\mathbf{V})$ and $\kappa' = \kappa$-$(n/2T)\mu$.
- Range of inelasticities: $0.3 \leq \alpha \leq 1$.
- Strength parameter: $\boldsymbol{\varepsilon} = \varepsilon\,\mathbf{x}$, $\varepsilon = 0.025$.
- 2×10^5 simulated particles.
- 200 independent replicas.
- Time step: $0.03t_0$, $t_0=\lambda/\mathrm{v}_T$.

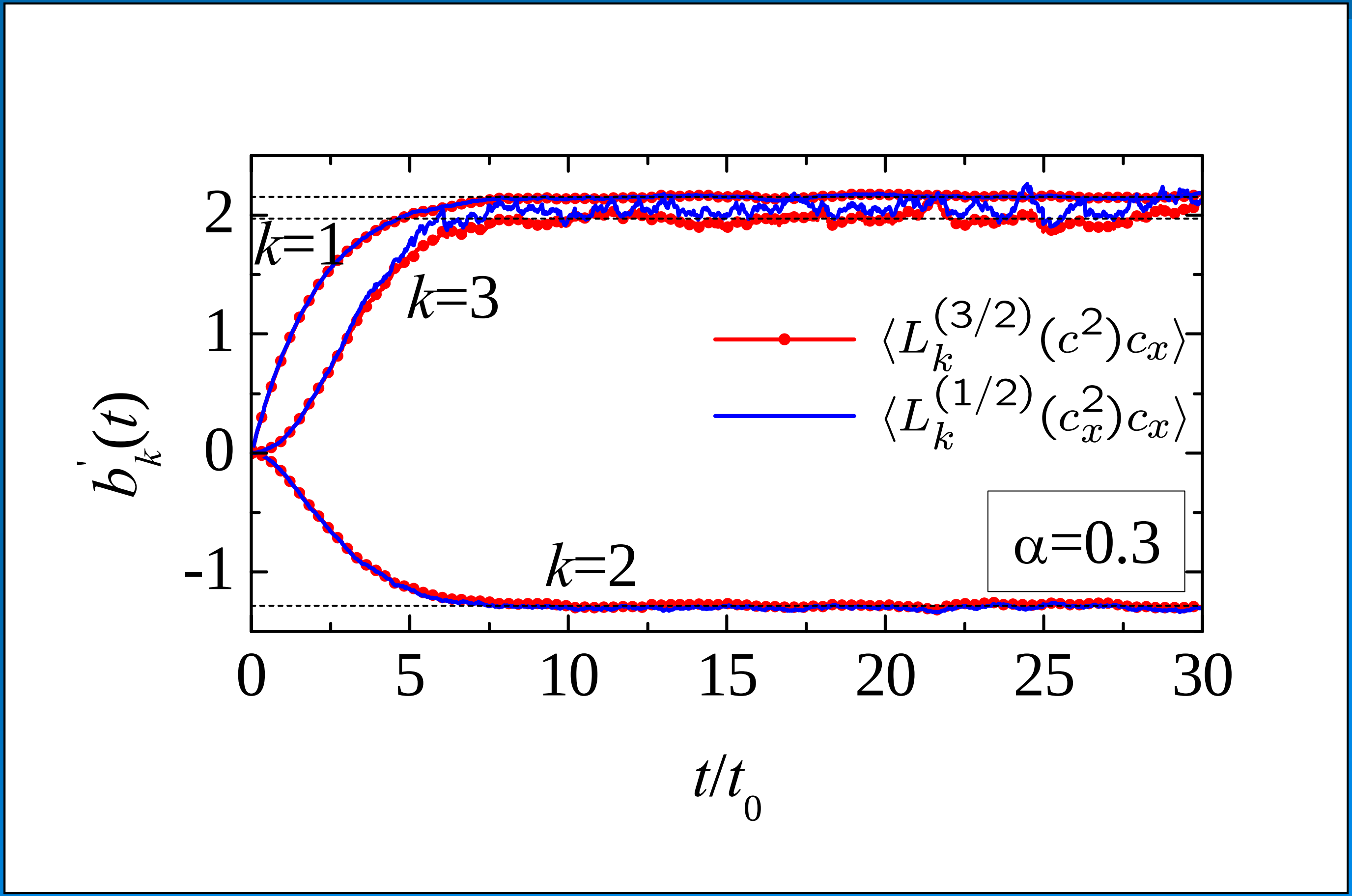
Toward the steady state



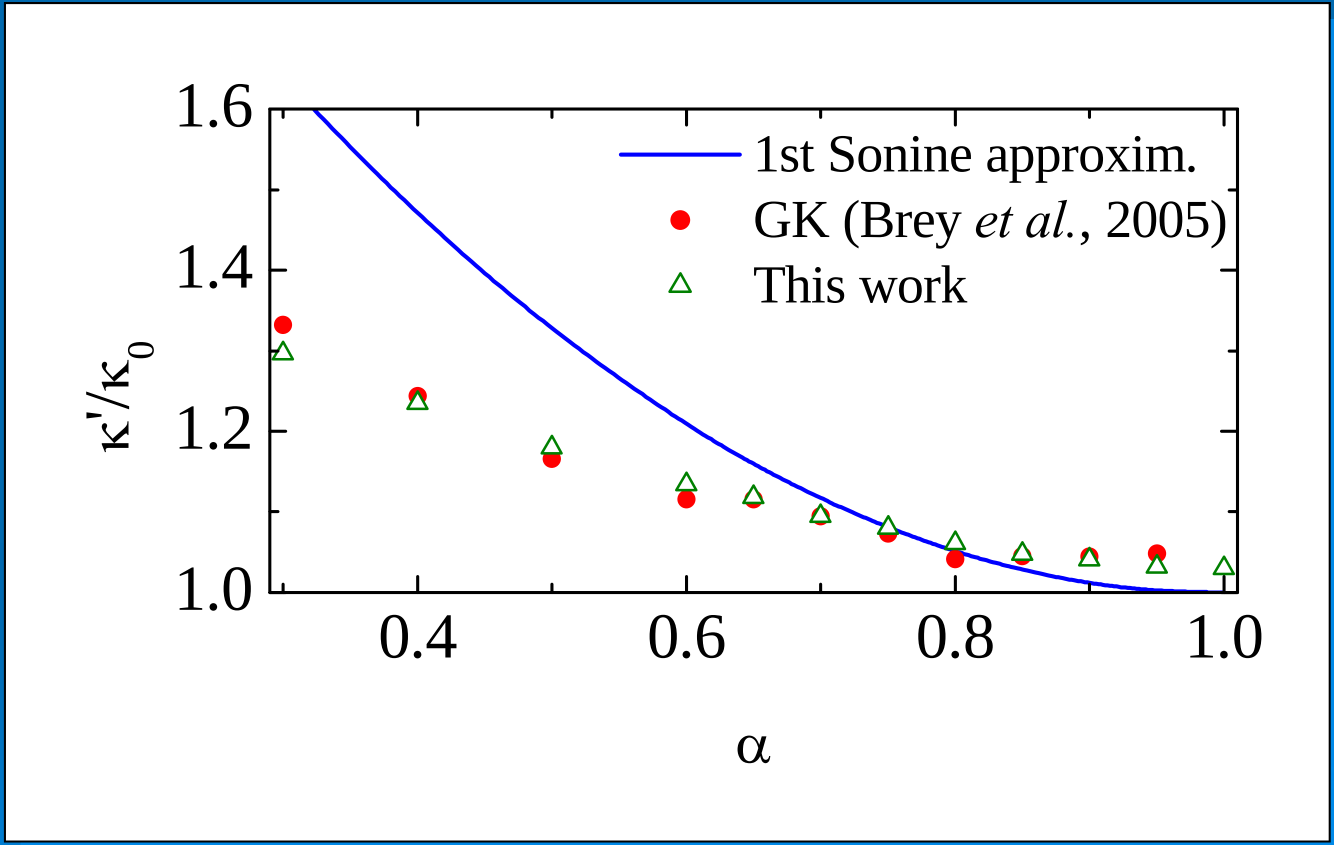
Toward the steady state



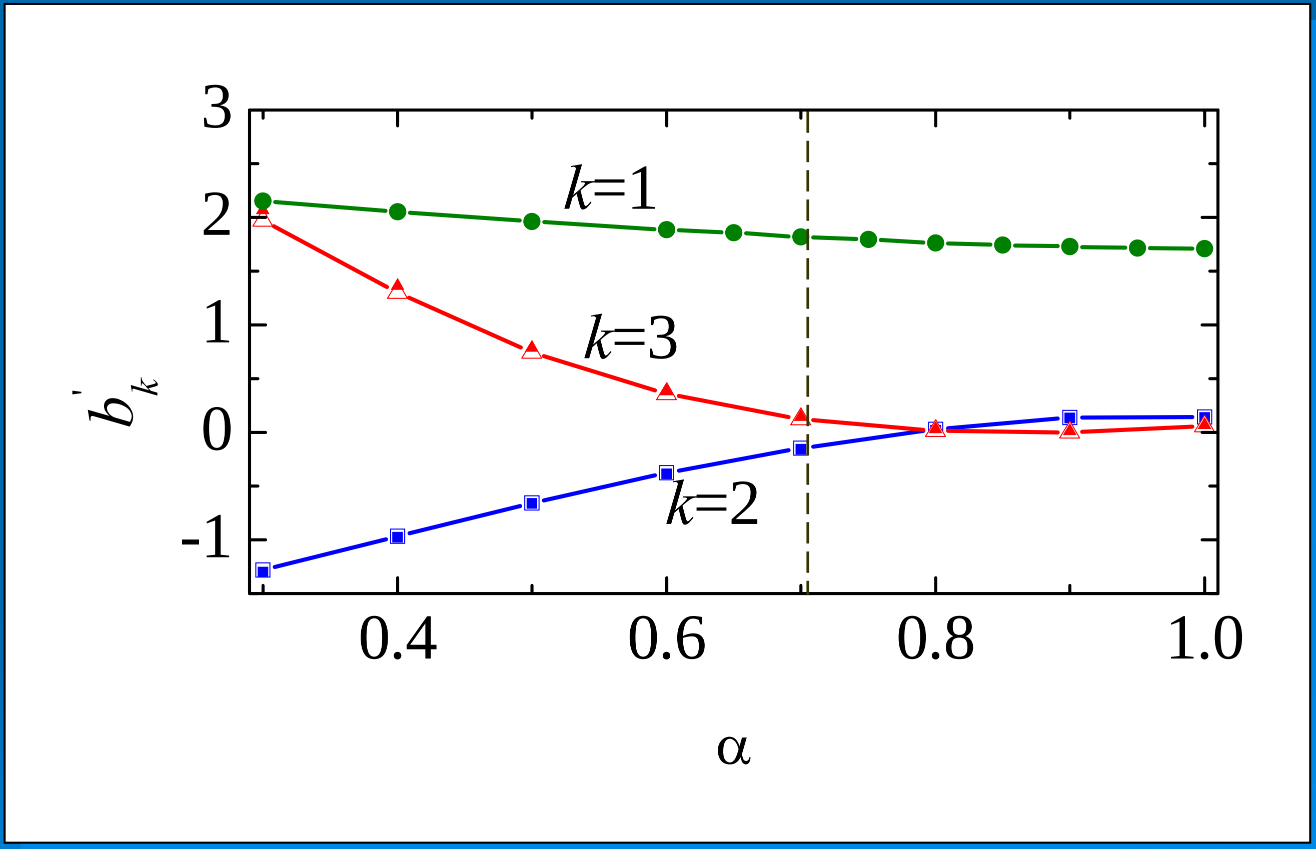
Toward the steady state



(Combined) Thermal conductivity



Sonine coefficients



(Marginal) NS distribution function

$$g(V_x) = \int_{-\infty}^{\infty} \mathrm{d}V_y \int_{-\infty}^{\infty} \mathrm{d}V_z f(\mathbf{V})$$

$$g(V_x) = \underbrace{g_0(V_x)}_{\text{Even function}} + \underbrace{g_1(V_x)}_{\text{Odd function}}$$

$$g_1(V_x) = \frac{1}{2}\left[g(V_x) - g(-V_x)\right]$$

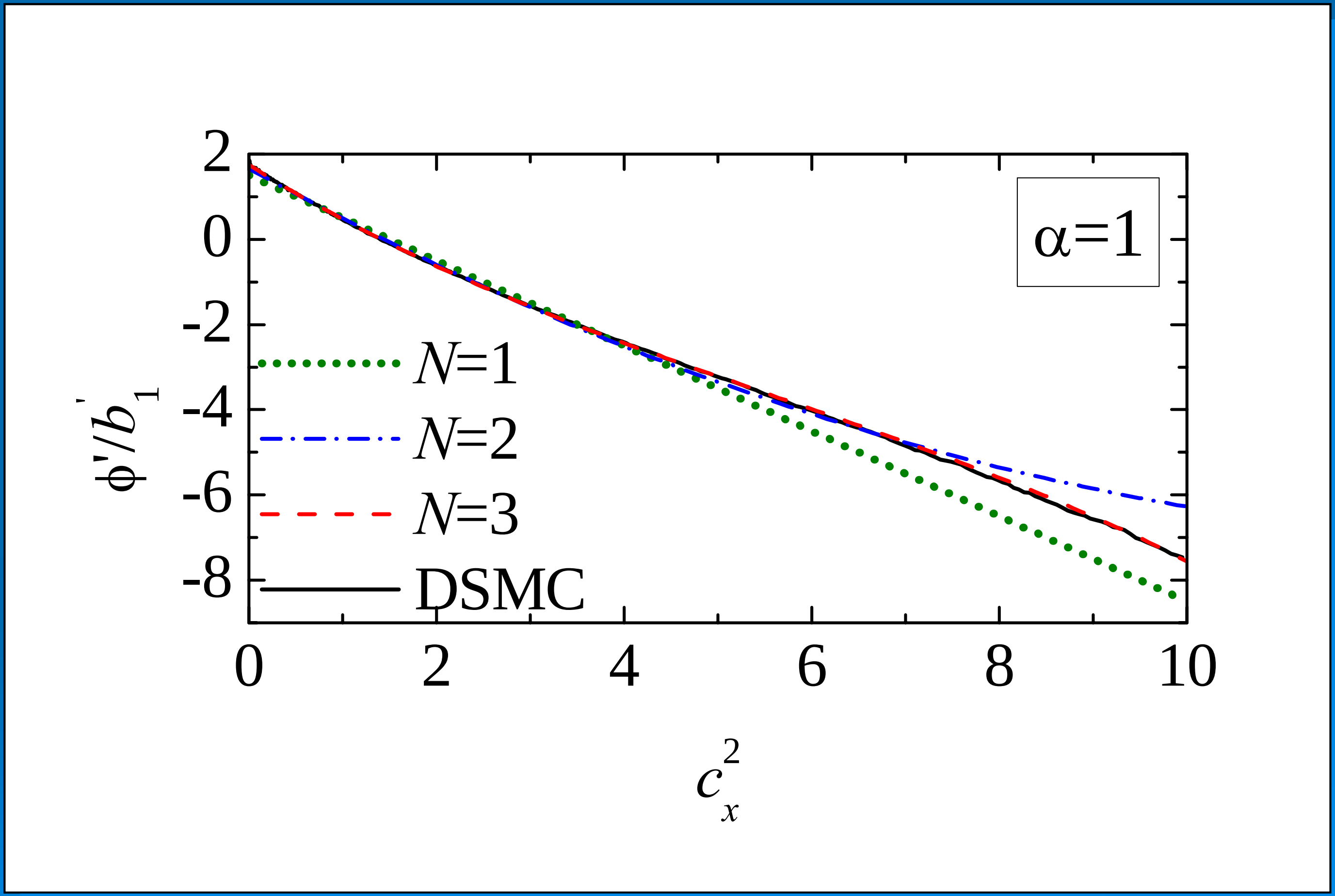
Structure of $g_1(V_x)$

$$g_1(V_x) = g_M(V_x)\phi'(c_x)c_x\epsilon$$

$$\phi'(c_x) = \sum_{k=1}^{\infty} b'_k L_k^{(1/2)}(c_x^2)$$

$$\phi'_N(c_x) \equiv \sum_{k=1}^{N} b'_k L_k^{(1/2)}(c_x^2)$$

Comparison between $\phi'(c_x)$ and $\phi_N'(c_x)$



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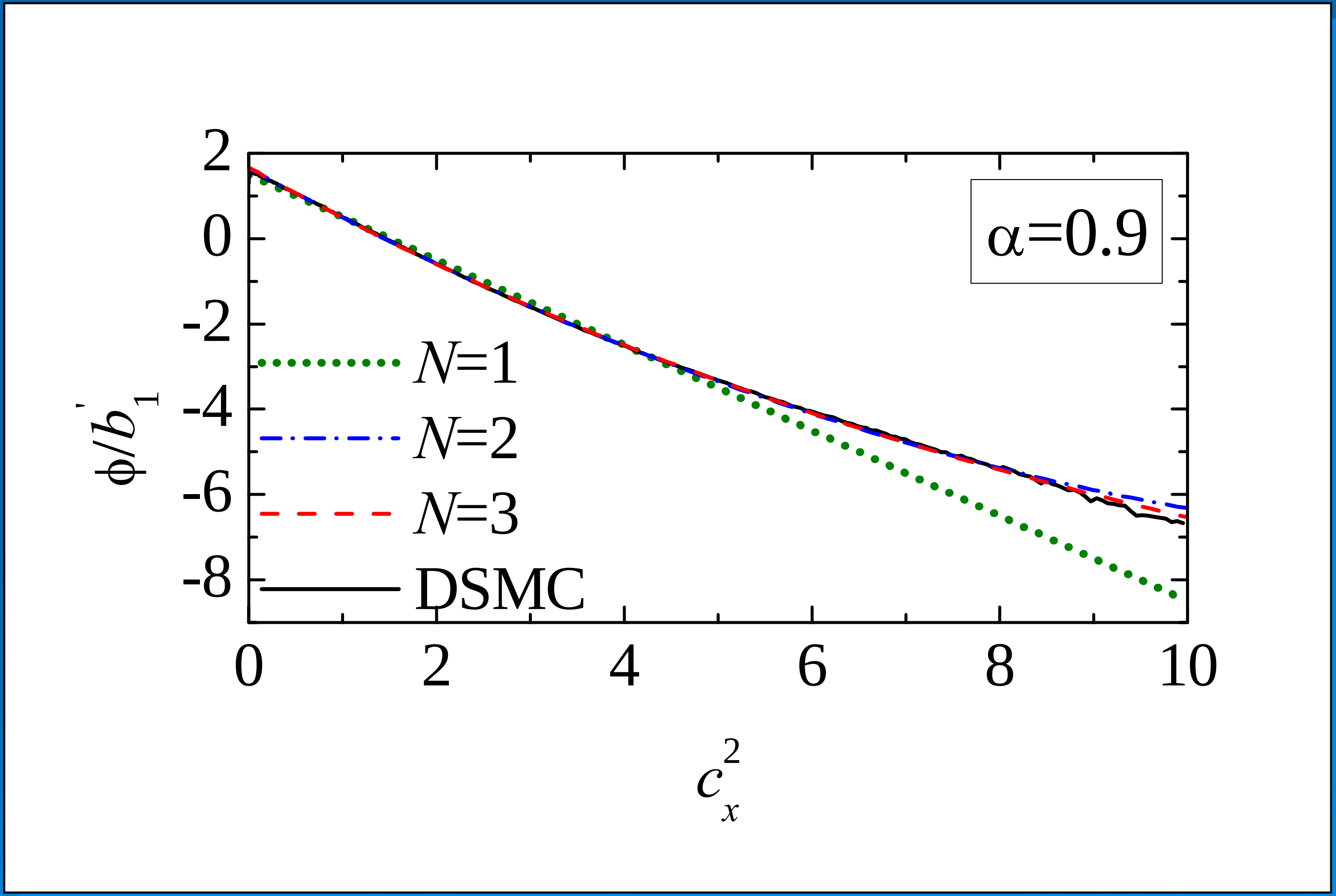

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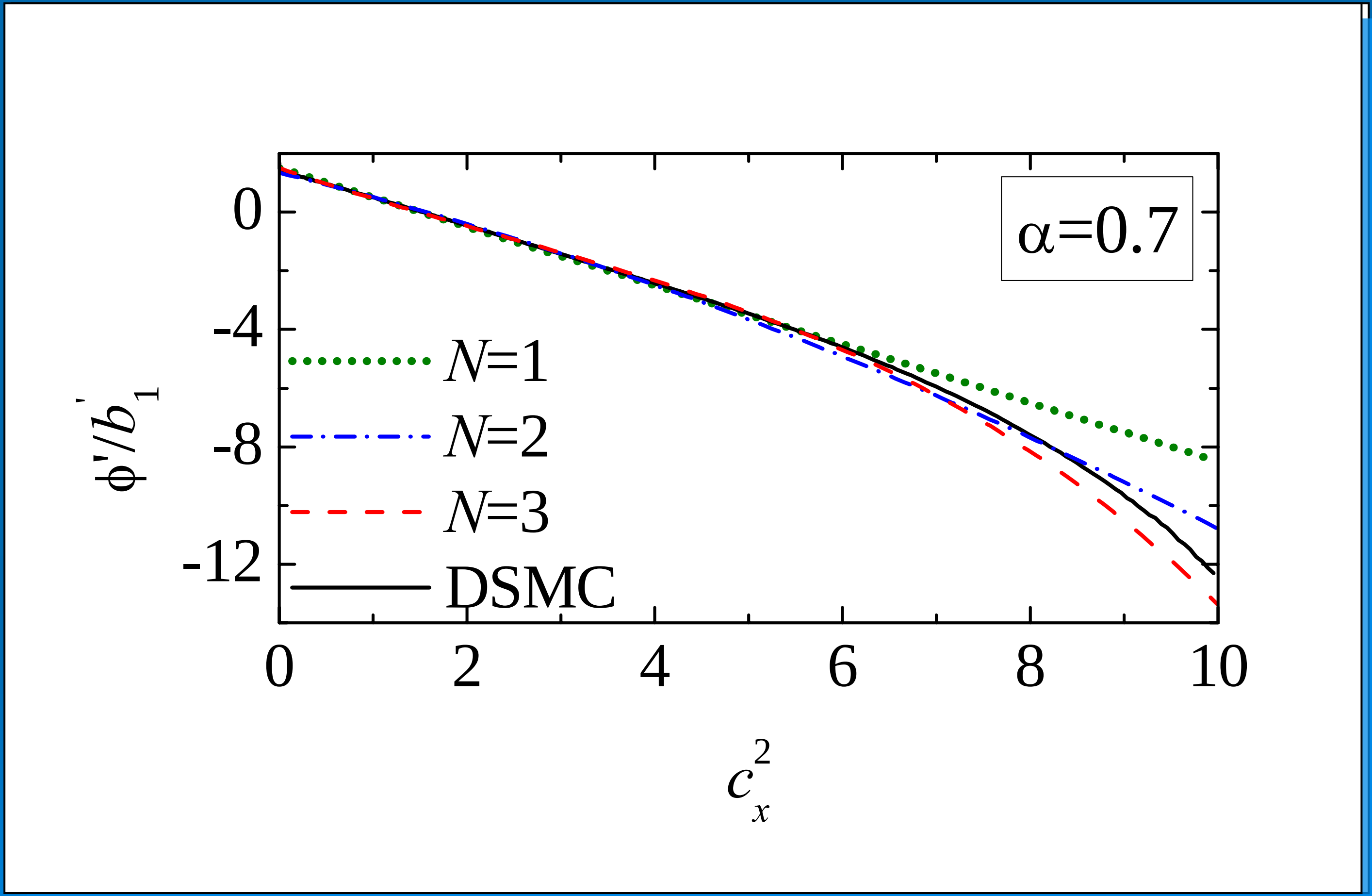
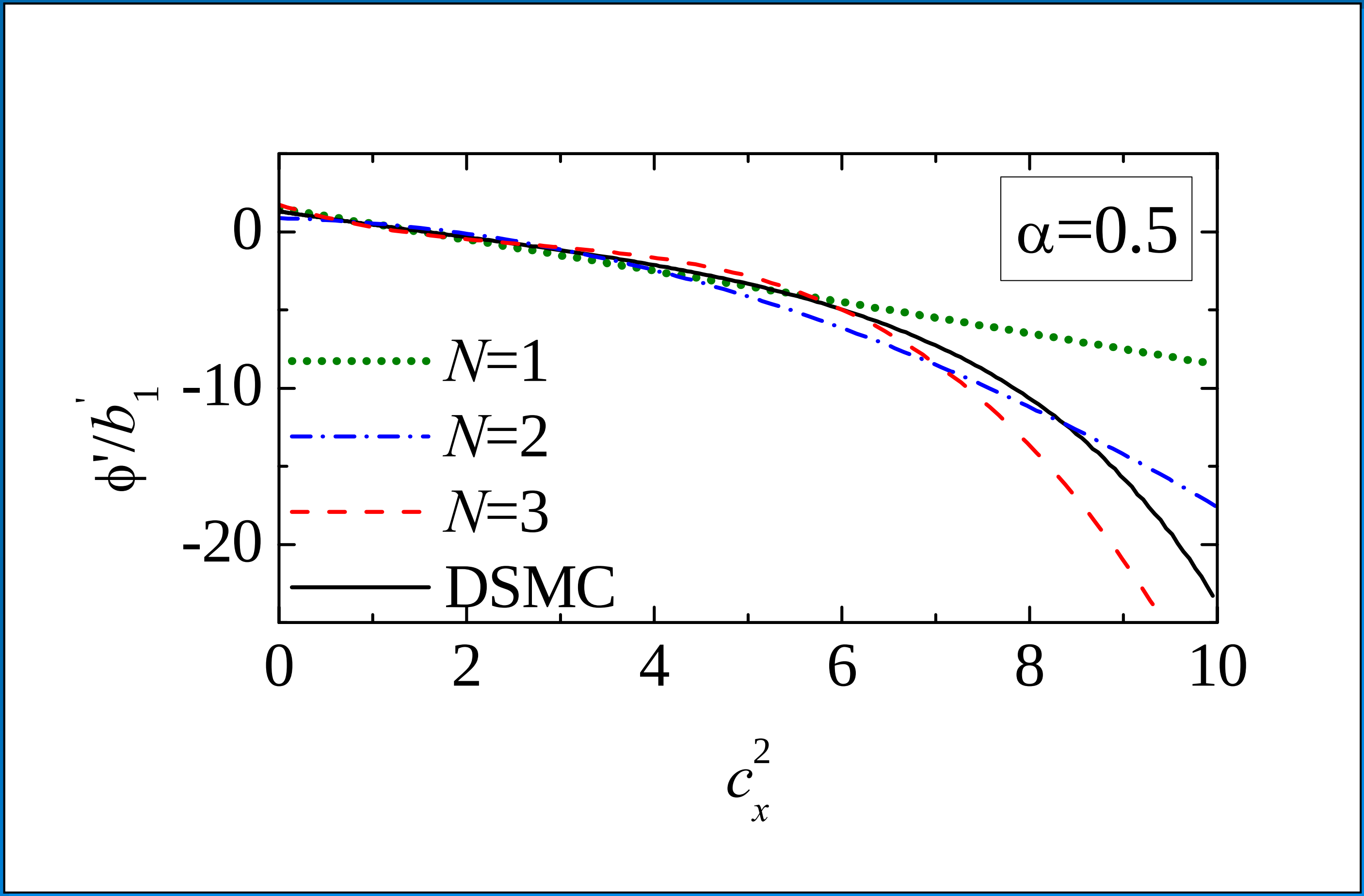
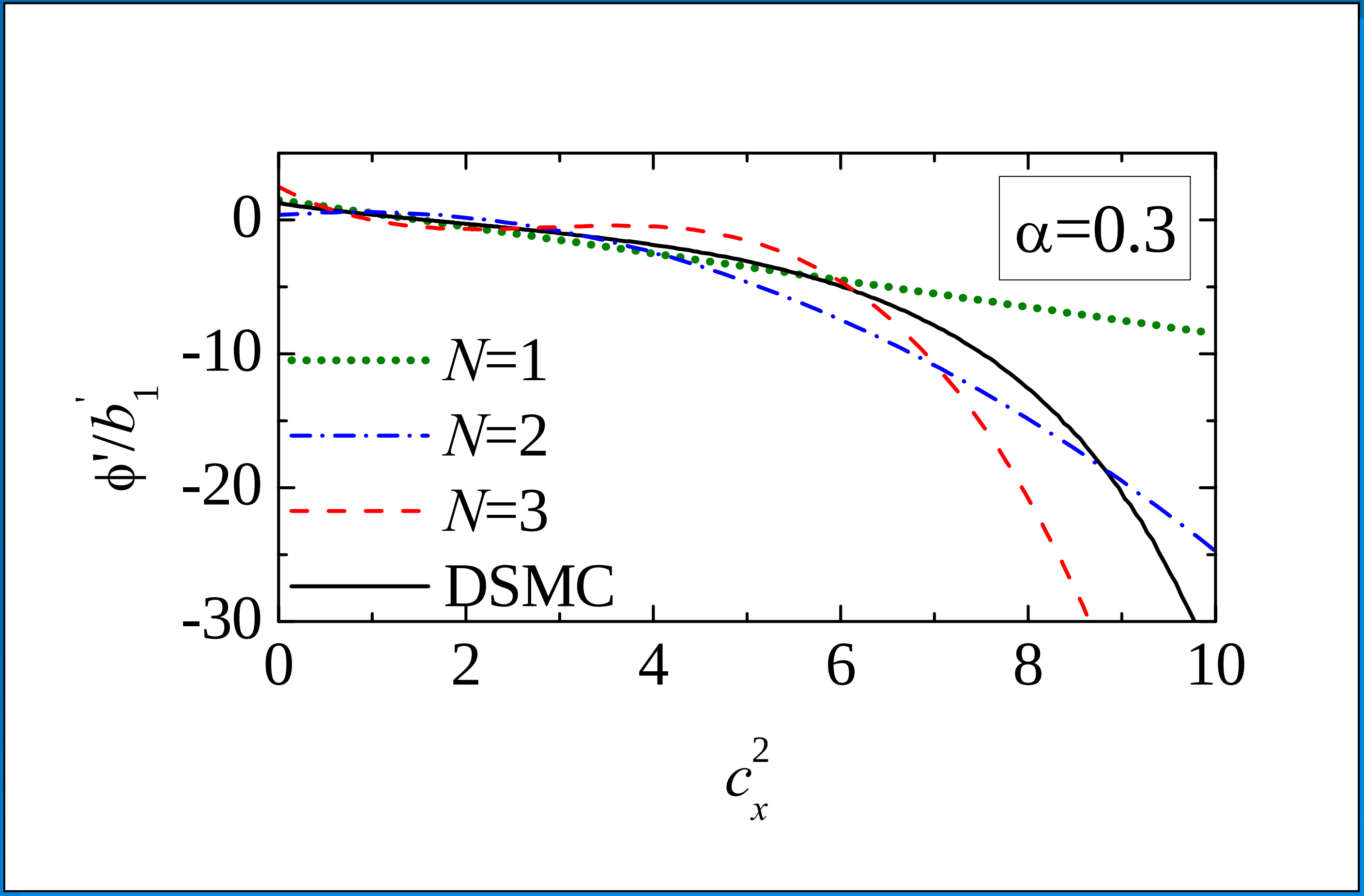


Comparison between $\phi'(c_x)$ and $\phi_N'(c_x)$

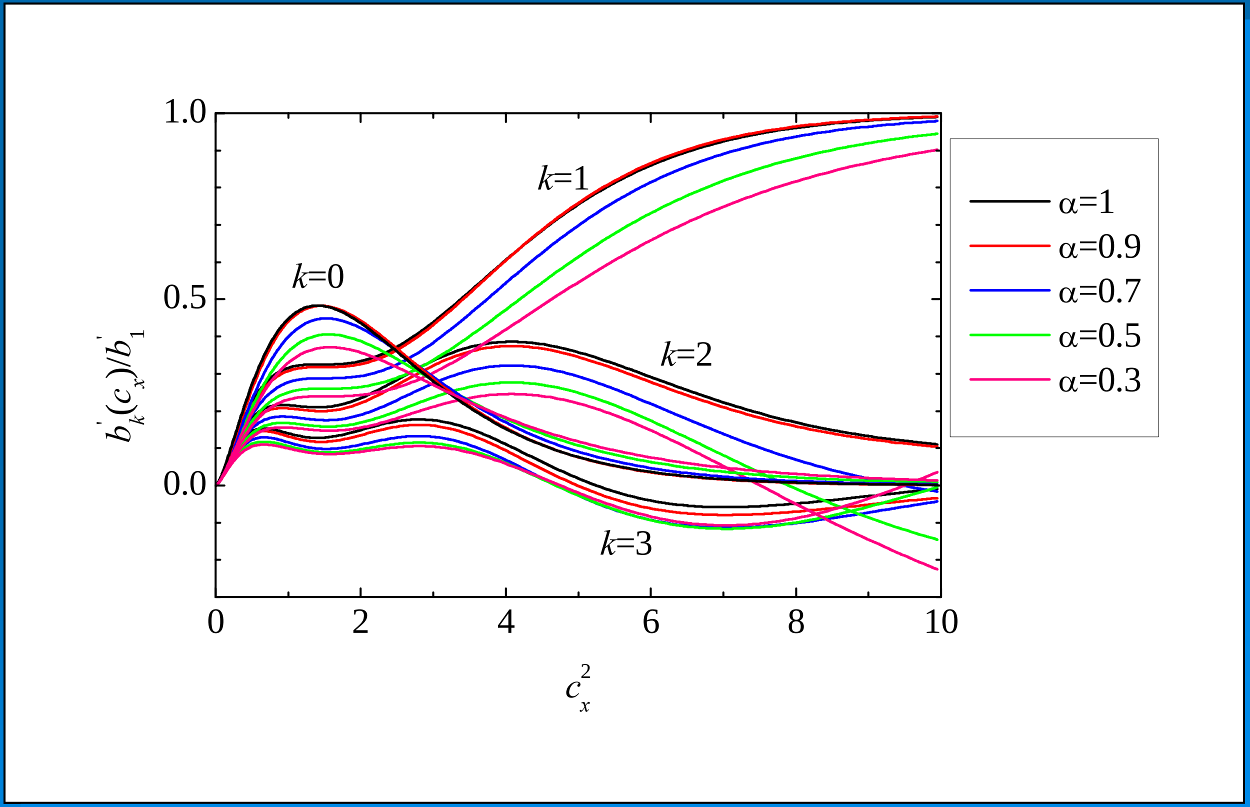


Comparison between $\phi'(c_x)$ and $\phi_N'(c_x)$



Which velocity range is relevant for b_1'?

$$b'_k(c_k) \propto \int_0^{c_x} \mathrm{d}u_x \, L_k^{(1/2)}(u_x^2) u_x^2 e^{-u_x^2} \phi'(u_x)$$

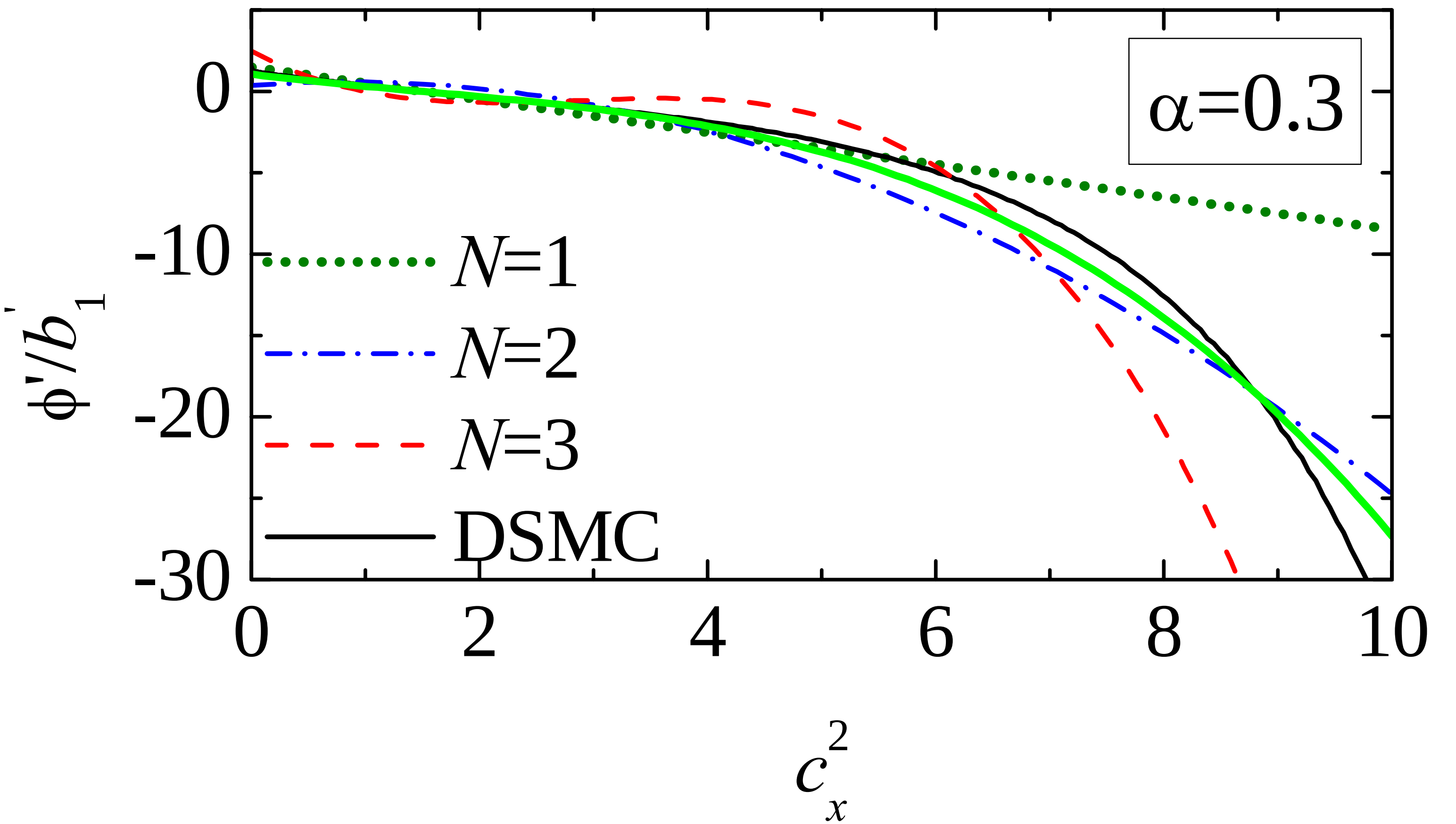


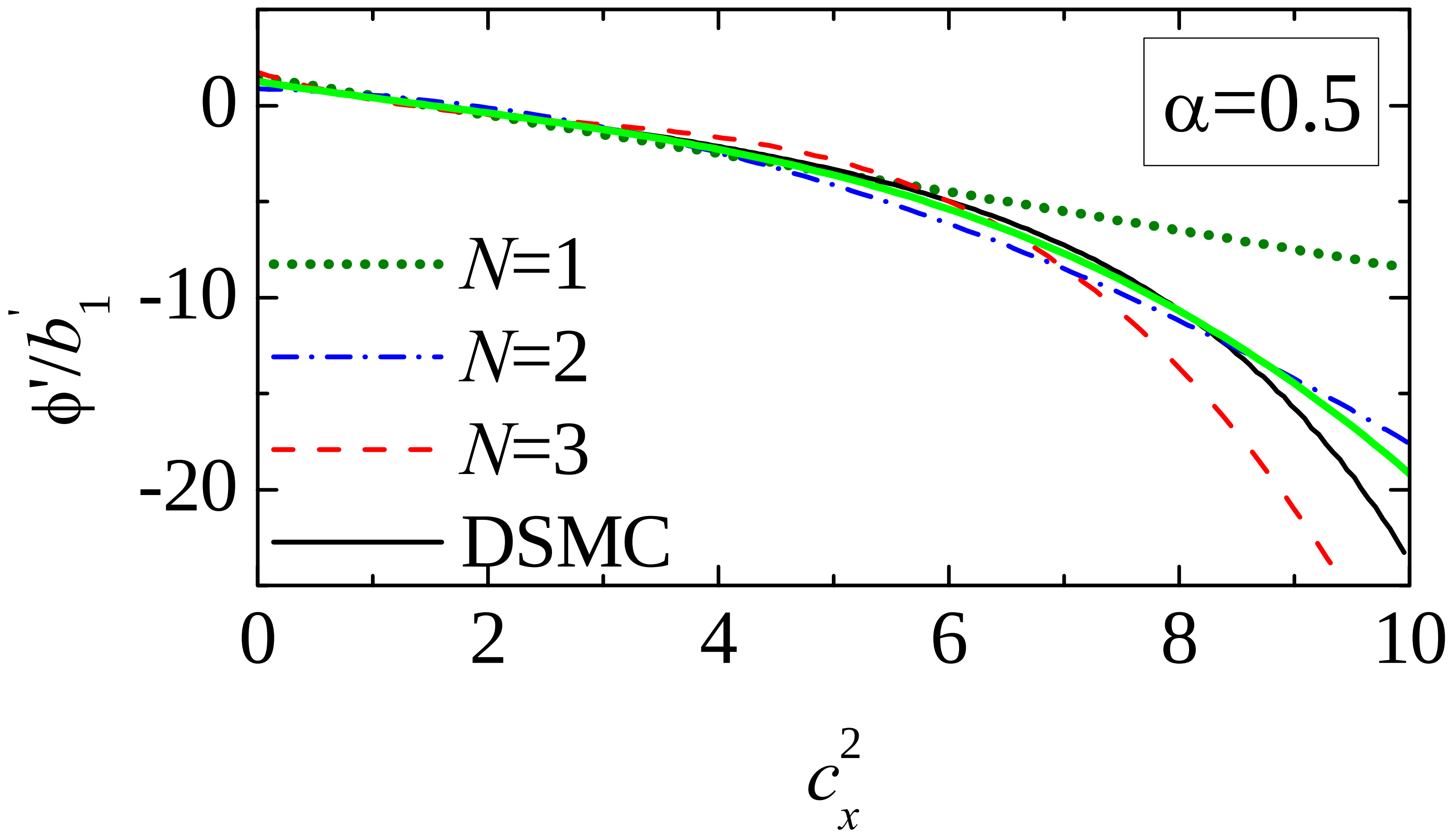
A *modified* (first) Sonine approximation

Old ansatz: $\Phi'(c) \propto \left(\frac{d+2}{2} - c^2\right)$

New ansatz: $\Phi'(c) \propto \frac{f_0^*(c)}{f_M^*(c)} \left[\frac{d+2}{2}(1+a_2) - c^2\right]$

$$\frac{f_0^*(c)}{f_M^*(c)} \approx 1 + a_2 L_2^{\left(\frac{d-2}{2}\right)}(c^2)$$


α=0.3
0
-10
-20
-30
0
2
4
6
8
10
φ'/b'1
N=1
N=2
N=3
DSMC
c²x


α=0.5
N=1
N=2
N=3
DSMC
0
-10
-20
0
2
4
6
8
10
φ'/b'_1
c_x^2

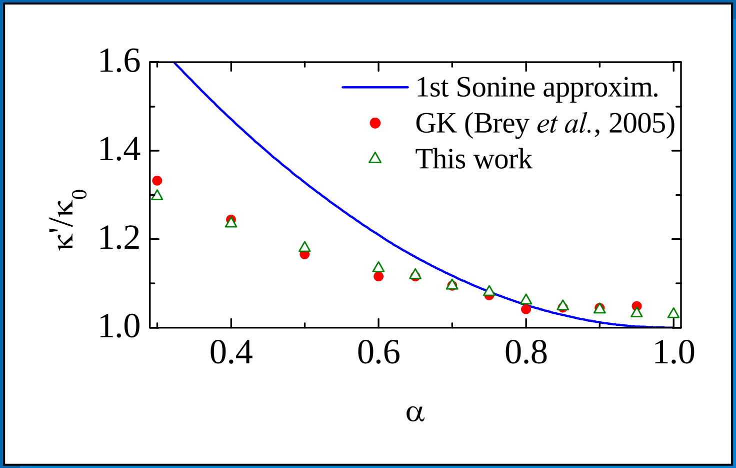
Conclusions (I)

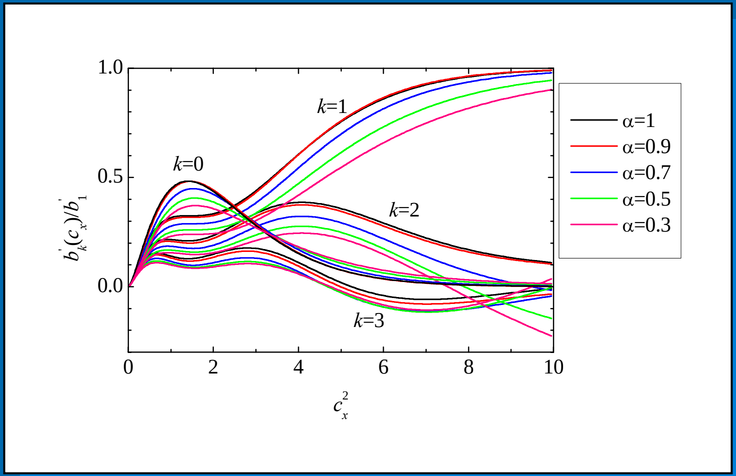
- The NS distribution function in the heat flux problem can be obtained by perturbing the HCS with an anisotropic, velocity-dependent external force (linear response).
- Simulations are easy: homogeneous steady state.
- The results for the thermal conductivity agree with those obtained from GK relations.

Conclusions (II)

- The conventional first Sonine approximation ceases to be reliable for $\alpha \lesssim 0.7$.
- The Sonine series expansion converges very slowly if $\alpha \lesssim 0.7$.
- A promising avenue consists of replacing the Maxwellian by the HCS as weight function in a modified first Sonine approximation.

THANKS!


1st Sonine approxim.
GK (Brey et al., 2005)
This work
κ'/κ0
α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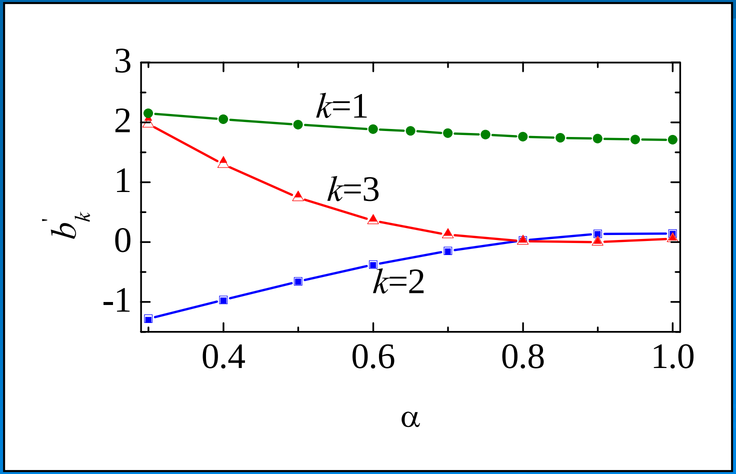
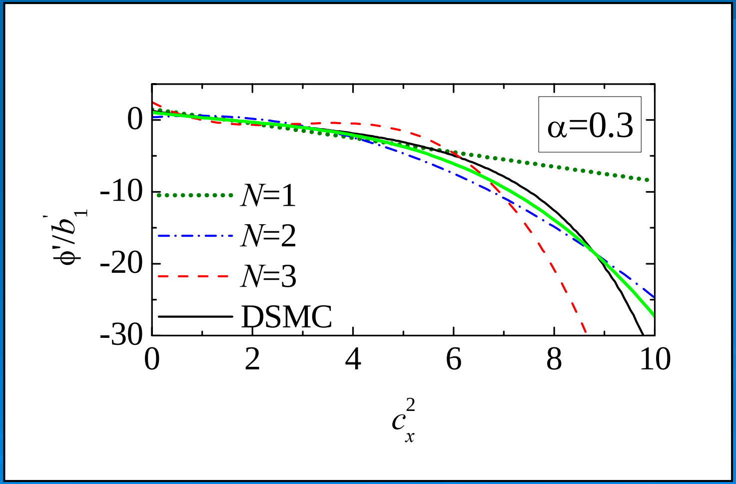
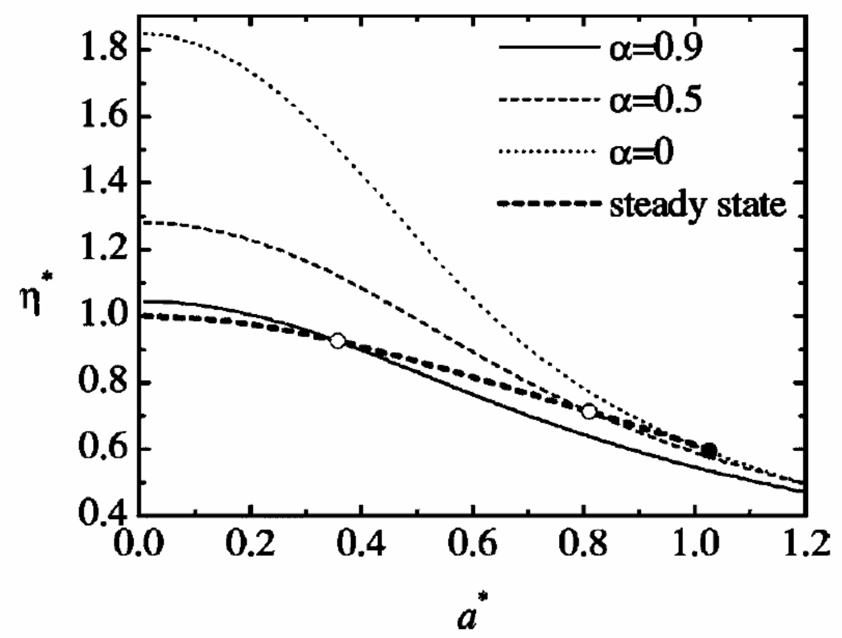
k=1
k=2
k=3
α=1
α=0.9
α=0.7
α=0.5
α=0.3


k=1
k=3
k=2
α

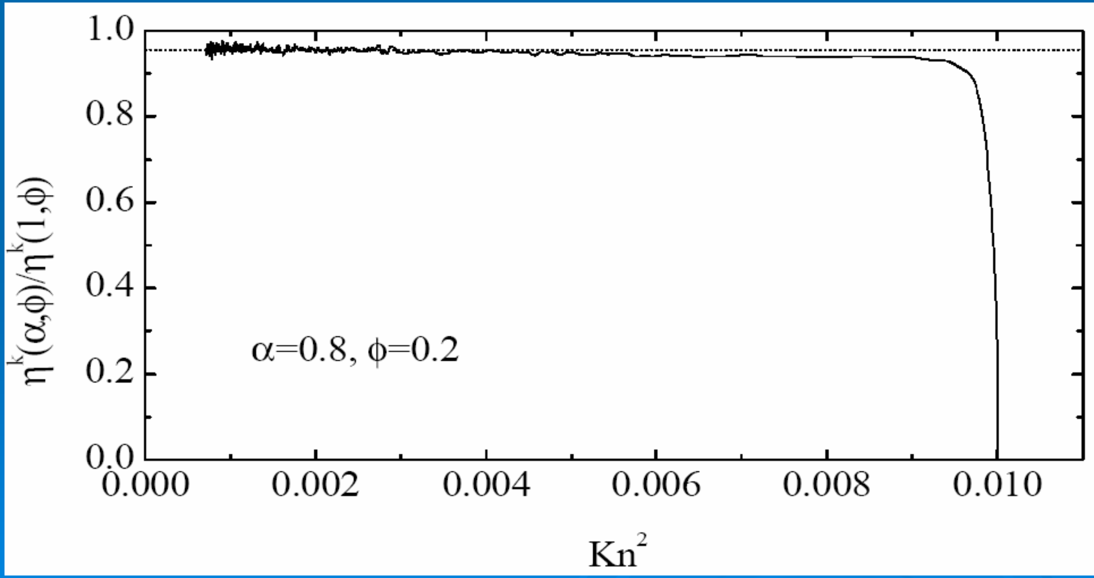

α=0.3
N=1
N=2
N=3
DSMC

A.S. *et al.*, Phys. Rev. E **69**, 061303 (2004)



Simple shear flow

M. Tij *et al.*, J. Stat. Phys. **103**, 1035 (2001)



Heated simple shear flow