Thermal fluctuations in a kinetic model for multicomponent fluids

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Outline

Kinetic model — Introducing kinetic theory for isothermal binary mixtures
- Binary Boltzmann equation
- Non-ideal effects
- Thermal fluctuations

Technicalities — Sketching how to apply fluctuation-dissipation theorem
- Equilibrium correlations
- Noise correlations

Numerics — Checking theoretics with numerical simulations
- Homogeneous ideal mixture
- Homogeneous interacting mixture
- Non-homogeneous interacting mixture

Conclusions — Summarizing results
Kinetic model
The probability of finding a blue, resp. green, particle at \( t \) in a phase space volume \( d\omega = dr dv \) around \((r, v)\) is \( f^b(t, r, v) d\omega \), resp. \( f^g(t, r, v) d\omega \).

\[
\rho^b = \int f^b dv \\
j^b = \int vf^b dv
\]

**Equilibrium distribution**

\[
f^b_{\text{eq}}(r, v) = \rho^b(r) \left( \frac{m}{2\pi k_B T} \right)^{D/2} e^{-\frac{m}{2k_B T} |v|^2} \\
f^b \rightarrow f^b_{\text{eq}} \implies \nabla \rho^b = 0
\]
The body-force acceleration $a^b = a[\rho^g]$ exerted by a blue particle is assumed to depend on the green mass distribution.

The non-ideal binary Boltzmann equation is:

$$\partial_t f^b + v \cdot \nabla f^b = \text{Coll}(f^b, f^g) - a^b \cdot \nabla v f^b$$

The equilibrium distribution is:

$$f^{b\text{eq}}(r, v) = \rho^b(r) \left( \frac{m}{2\pi k_B T} \right)^{D/2} e^{-\frac{m}{2k_B T} |v|^2}$$

$$f^b \rightarrow f^{b\text{eq}} \implies \nabla \rho^b = \frac{m}{k_B T} \rho^b a[\rho^g]$$
Fluctuating non-ideal binary Boltzmann equation

\[ \partial_t f^b + v \cdot \nabla f^b = \text{Coll}(f^b, f^g) - a^b \cdot \nabla v f^b + \xi^b \]

Averages over all possible trajectories \( \langle \cdot \rangle \) are equivalent to canonical ensemble averages.

\[ \rho^b = \int f^b dv \]
\[ j^b = \int v f^b dv \]
\[ \xi^b_\rho = \int \xi^b dv \]
\[ \xi^b_j = \int v \xi^b dv \]

Equilibrium distribution

\[ f^b_{eq}(r, v) = \rho^b(r) \left( \frac{m}{2\pi k_B T} \right)^{D/2} e^{-\frac{m}{2k_B T} |v|^2} \]
\[ \langle f^b \rangle \rightarrow f^b_{eq} \implies \nabla \rho^b = \frac{m}{k_B T} \rho^b a[\rho^g] \]

Langevin equation - FDT

\[ \frac{dV}{dt} = -\lambda V + \xi \]
\[ \langle V^2 \rangle \rightarrow E \implies \langle \xi^2 \rangle = 2\lambda E \]
Multicomponent Boltzmann equation

\[ \partial_t f_s^s + v \cdot \nabla f_s^s = (\text{Coll} f_s) - a^s \cdot \nabla v f_s^s + \xi_s^s \]

The Boltzmann distributions are labeled by the species index \( s = b, g, \ldots \) and are collected in \( f = (f_s^s)_{s=b,g,\ldots} \).

\[ \rho_s = \int f_s^s dv \]
\[ j_s = \int v f_s^s dv \]
\[ \xi_{\rho} = \int \xi_s dv \]
\[ \xi_j = \int v \xi_s dv \]

Equilibrium distribution

\[ f_{eq}^s(r,v) = \rho_s^s(r) \left( \frac{m}{2\pi k_B T} \right)^{D/2} e^{-\frac{m}{2k_B T} |v|^2} \]

\[ \langle f_s^s \rangle \rightarrow f_{eq}^s \quad \Rightarrow \quad \nabla \rho_s^s = \frac{m}{k_B T} \rho_s^s a[\rho] \]

Langevin equation - FDT

\[ \frac{dV_i}{dt} = -(L V)_i + \xi_i \]
\[ \langle V_i V_j^* \rangle \rightarrow E_{ij} \quad \Rightarrow \quad \langle \xi_i \xi_j^* \rangle = (LE + EL)_{ij} \]
Multicomponent Boltzmann equation

\[ \partial_t f^s + v \cdot \nabla f^s = (\text{Coll} f)^s - a^s \cdot \nabla v f^s + \xi^s \]

The Boltzmann distributions are labeled by the species index \( s = b, g, \ldots \) and are collected in \( f = (f^s)_{s=b,g,...} \).

\[ \rho^s = \int f^s dv \]
\[ j^s = \int v f^s dv \]

Equilibrium distribution

\[ f_{eq}^s(r, v) = \rho^s(r) \left( \frac{m}{2\pi k_B T} \right)^{D/2} e^{-\frac{m}{2k_B T}|v|^2} \]
\[ \langle f^s \rangle \rightarrow f_{eq}^s \implies \nabla \rho^s = \frac{m}{k_B T} \rho^s a[\rho] \]

Langevin equation - FDT

\[ \frac{dV_i}{dt} = -(LV)_i + \xi_i \]
\[ \langle V_i V_j^* \rangle \rightarrow E_{ij} \implies \langle \xi_i \xi_j^* \rangle = (LE + EL)_{ij} \]

Linearity:
Collisional operator and self-generated forcing are non-linear functional of \( f \)

\[ \implies \text{Small deviation from equilibrium} \]

ODE:
Non-ideal Boltzmann equation involves spatial and velocity gradient of \( f \)

\[ \implies \text{Kinetic modes, Fourier space} \]

Noise correlations

\[ \langle \xi^b \rho \xi^b \rangle = \langle \xi^b \rho \xi^g \rangle = 0 \]
\[ \langle \xi^b_j \xi^b_j \rangle = -\langle \xi^b_j \xi^g_j \rangle = 2\lambda k_B T \frac{\rho^b \rho^g}{\rho^b + \rho^g} 1 \]
Technicalities
Evolution equation for the distributions

\[ \partial_t f^s + \mathbf{v} \cdot \nabla f^s = (\text{Coll} f)^s - a^s \cdot \nabla_v f^s + \xi^s \]

\[ \rho^s = \int f^s \, dv \]
\[ j^s = \int v f^s \, dv \]
\[ \xi_\rho^s = \int \xi^s \, dv \]
\[ \xi_j^s = \int v \xi^s \, dv \]
Evolution equation for the velocity moments

\[ \partial_t f_a^s + \nabla \cdot (vf^s)_a = (\text{Coll}_a f_a)^s - a^s \cdot (\Phi f^s)_a + \xi_a^s \]

\[ \rho^s = \int f^s dv = f_0^s \]
\[ j^s = \int vf^s dv = f_1^s, \ldots, d \]
\[ \xi^s = \int \xi^s dv = \xi_0^s \]
\[ \xi_j^s = \int v\xi^s dv = \xi_1^s, \ldots, D \]

Hermite transformation

\[ f_a = \int H_a f dv \]
\[ H_0 = 1 \]
\[ H_1, \ldots, D = v \]

Linear evolution equation for the velocity moments

$$\partial_t \delta f_s^a + \nabla \cdot (v \delta f_s^a)_a = (\lambda_a \delta f_a^s) - a[\rho] \cdot (\Phi \delta f_s^a) - \delta a^s \cdot (\Phi f_{eq}^s)_a + \xi_s^a$$

\[\begin{align*}
\delta \rho^s &= \int \delta f^s dv = \delta f_0^s \\
\delta j^s &= \int v \delta f^s dv = \delta f_{1,\ldots,d}^s
\end{align*}\]

Hermite transformation

$$f_a = \int H_a f dv \quad H_0 = 1 \quad H_{1,\ldots,D} = v \quad \ldots$$

Small deviation from equilibrium

$$\delta f = f - f_{eq} \quad f_{eq} = \lim_{t \to \infty} \langle f \rangle$$
Kinetic model

Linear evolution equation for the Fourier-transformed velocity moments

$$
\partial_t \delta f^s_{a;k} + i k \cdot (v \delta f^s_k)_a = (\lambda_a \delta f_{a;k})^s - (a[\rho] * (\Phi \delta f^s)_a)_k - (\delta a^s * (\Phi f^s_{eq})_a)_k + \xi^s_{a;k}
$$

$$
\delta \rho^s_k = \int \delta f^s_k dv = \delta f^s_{0;k}
\delta j^s_k = \int v \delta f^s_k dv = \delta f^s_{1,\ldots,d;k}
\xi^s_\rho; k = \int \xi^s_k dv = \xi^s_{0;k}
\xi^s_j; k = \int v \xi^s_k dv = \xi^s_{1,\ldots,d;k}
$$

Hermite transformation

$$
f_a = \int H_a f dv \quad H_0 = 1 \quad H_{1,\ldots,D} = v \quad \ldots
$$

Small deviation from equilibrium

$$
\delta f = f - f_{eq} \quad f_{eq} = \lim_{t \to \infty} \langle f \rangle
$$

Fourier transformation

$$
f_k = \int e_k f dr \quad e_k = \frac{1}{(2\pi)^{D/2}} e^{-i k \cdot r}
$$

Linear evolution equation for the Fourier-transformed velocity moments

\[ \frac{\partial}{\partial t} \delta f_{a;\b}^{b} + i \mathbf{k} \cdot (v \delta f_{\b}^{b})_{a} = (\lambda_{a} \delta f_{a;\b})^{b} - (a[\rho] \ast (\Phi \delta f_{\b}^{b}))_{k} - (\delta a^{b} \ast (\Phi f_{eq}^{b}))_{k} + \xi_{a;\b}^{b} \]

\[ \delta \rho_{k}^{b} = \int \delta f_{\b}^{b} dv = \delta f_{0;\b}^{b} \]
\[ \delta j_{k}^{b} = \int v \delta f_{\b}^{b} dv = \delta f_{1,...,d;\b}^{b} \]
\[ \xi_{\rho}^{b} = \int \xi_{\b} dv = \xi_{0}^{b} \]
\[ \xi_{j}^{b} = \int v \xi_{\b} dv = \xi_{1,...,d}^{b} \]

Equilibrium correlations

\[ \langle \delta \rho_{k}^{b} \delta \rho_{-k}^{g} \rangle = m \frac{\rho_{b}^{b}}{1 - \rho_{b}^{b} \rho_{g}^{g} \alpha_{k}^{2}} \]
\[ \langle \delta \rho_{k}^{b} \delta \rho_{-k}^{g} \rangle = -m \frac{\rho_{b}^{b} \rho_{g}^{g} \alpha_{k}^{2}}{1 - \rho_{b}^{b} \rho_{g}^{g} \alpha_{k}^{2}} \]
\[ \langle \delta j_{k} \delta j_{-k} \rangle = k_{B} T (\rho_{b}^{b} + \rho_{g}^{g}) \mathbf{1} \]
\[ (j = j_{b}^{b} + j_{g}^{g}) \]

... self-consistently derived in the theory!

Noise correlations

\[ \langle \xi_{\rho}^{b} \xi_{\rho}^{b} \rangle = \langle \xi_{\rho}^{b} \xi_{\rho}^{g} \rangle = 0 \]
\[ \langle \xi_{j}^{b} \xi_{j}^{b} \rangle = -\langle \xi_{j}^{b} \xi_{j}^{g} \rangle = 2 \lambda k_{B} T \frac{\rho_{b}^{b} \rho_{g}^{g}}{\rho_{b}^{b} + \rho_{g}^{g}} \mathbf{1} \]

... ↑ stochastic diffusion fluxes (sdf) ↑
Numerics
Lattice mutual interaction

\[ a^b(r) = -G \sum_{\ell} w_{\ell} c_{\ell} \rho^g(r + c_{\ell}) \quad \alpha_k = G(1 - \frac{1}{6}k^2) \]

\[ S_{\rho^b \rho^b}(k) = m \frac{\rho^b}{1 - \rho^b \rho^g \alpha_k^2} \]

\[ S_{\rho^b \rho^g}(k) = \frac{1}{2} \lambda k_B T \rho^b \rho^g \]

Noise correlations

\[ \langle \xi^b_{\rho} \xi^b_{\rho} \rangle = \langle \xi^b_{\rho} \xi^g_{\rho} \rangle = 0 \]

\[ \langle \xi^b_{j} \xi^b_{j} \rangle = -\langle \xi^b_{j} \xi^g_{j} \rangle = 2\lambda k_B T \frac{\rho^b \rho^g}{\rho^b + \rho^g} \]

Lattice mutual interaction

\[ a^b(r) = -G \sum_{\ell} w_{\ell} c_{\ell} \rho^g(r + c_{\ell}) \quad \alpha_k = G(1 - \frac{1}{6} k^2) \]

Noise correlations

\[ \langle \xi^b_{\rho} \xi^b_{\rho} \rangle = \langle \xi^b_{\rho} \xi^g_{\rho} \rangle = 0 \quad \langle \xi^b_{j} \xi^b_{j} \rangle = -\langle \xi^b_{j} \xi^g_{j} \rangle = 2\lambda k_B T \frac{\rho^b_{\rho} \rho^g_{\rho}}{\rho^b_{\rho} + \rho^g_{\rho}} 1 \]
Lattice mutual interaction

\[ a^b(r) = -G \sum_{\ell} w_{\ell} c_{\ell} \rho^g(r + c_{\ell}) \quad \alpha_k = G(1 - \frac{1}{6} k^2) \]

\[ P[h] \propto e^{-\frac{\gamma}{2k_B T} \int (\frac{dh}{dx})^2 dx} \]

\[ \langle |h_k|^2 \rangle = \frac{k_B T}{\gamma k^2} \]

Noise correlations

\[ \langle \xi^b_{\rho} \xi^b_{\rho} \rangle = \langle \xi^b_{\rho} \xi^g_{\rho} \rangle = 0 \quad \langle \xi^b_{j} \xi^b_{j} \rangle = -\langle \xi^b_{j} \xi^g_{j} \rangle = 2\lambda k_B T \frac{\rho^b_{\rho} \rho^g_{\rho}}{\rho^b_{\rho} + \rho^g_{\rho}} 1 \]
Conclusions

Kinetic model — A non-ideal kinetic model for mixture has been successfully extended to incorporate the effects of thermal fluctuations.

Technicalities — Application of fluctuation-dissipation theorem to derive the expression of both equilibrium and noise correlations directly at the kinetic level has allowed to go beyond hydrodynamics, by controlling thermalization of all the kinetic modes (velocity moments).

Numerics — Agreement between numerical simulations and theoretical expectations is very good for all wavevectors investigated in both homogeneous and non-homogeneous (phase separation) cases.

Conclusions — Conclusion, thanks for your attention!