Γ-convergence approach for Large Deviations Problems In Interacting Diffusion systems

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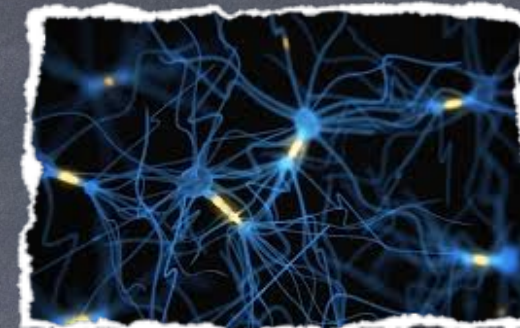
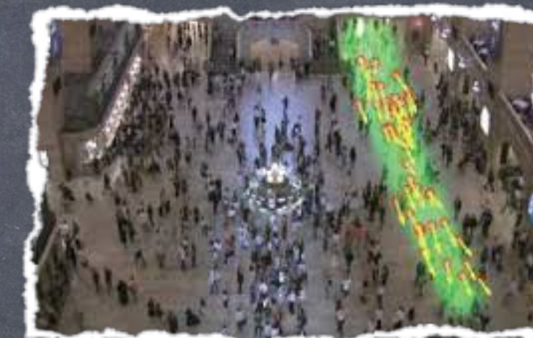
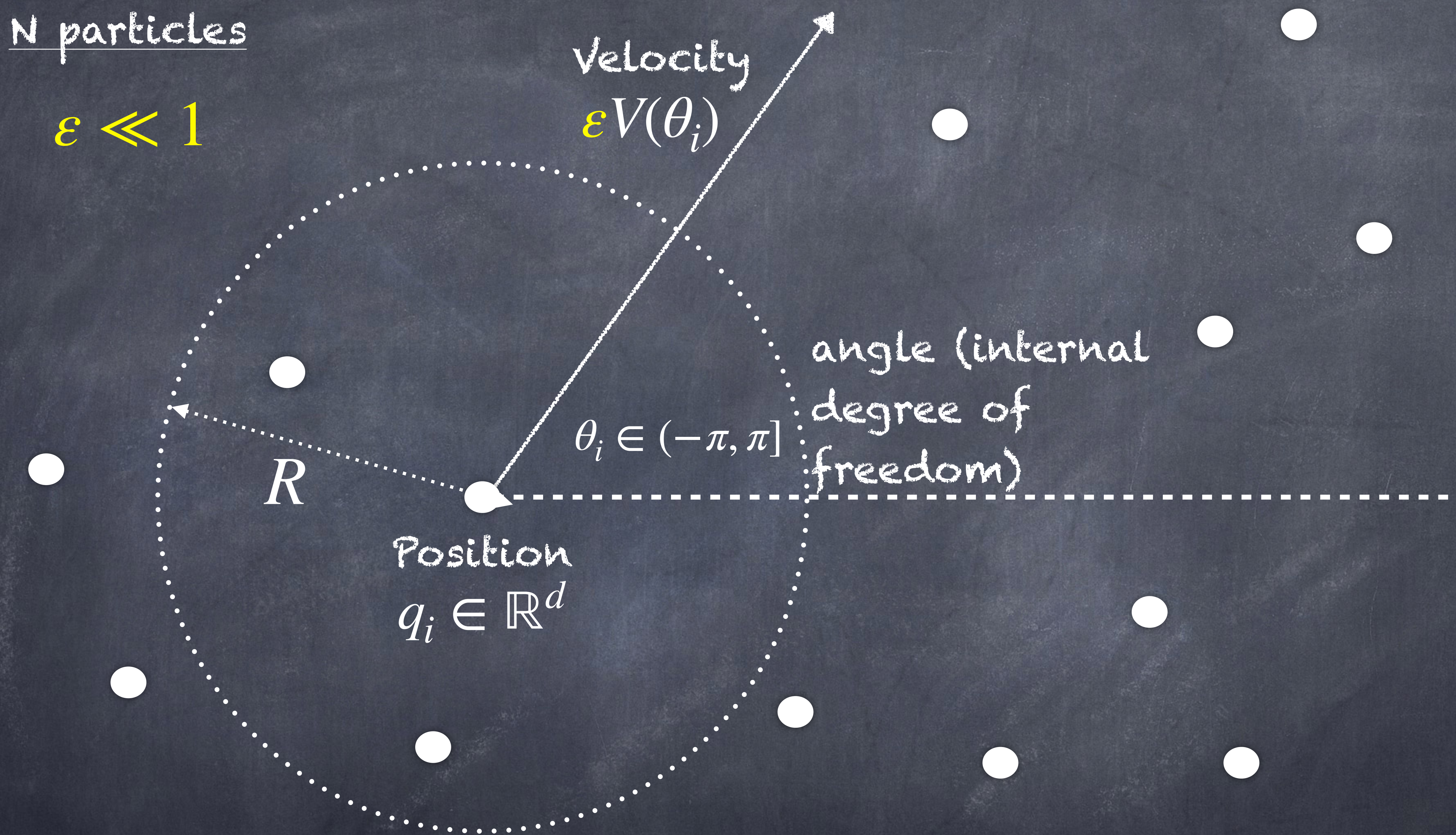



Goal: Introduce a Large Deviations approach to study the link between fluctuating kinetics and fluctuating hydrodynamics (e.g. in active matter models)


N particles
$\varepsilon \ll 1$
Velocity
$\varepsilon V(\theta_i)$
R
$\theta_i \in (-\pi, \pi]$
angle (internal degree of freedom)
Position
$q_i \in \mathbb{R}^d$

Example ('Ising model' of active matter)

$$
\boxed{
\begin{aligned}
dq_i &= \varepsilon\,(\cos(\theta_i), \sin(\theta_i))\,dt,\\
d\theta_i &= -\sin(\theta_i)dt - \frac{1}{\mathcal{N}_i}\sum_{j\in\mathcal{V}_i}\cos(\theta_i-\theta_j)dt + \sqrt{2}\,d\eta_i(t)
\end{aligned}
}
$$

Independent Brownian motions

$$\mathcal{V}_i := \{j \in \{1,\ldots,N\}\ ;\ |q_i - q_j| \le R\},\quad \mathcal{N}_i = \sharp\mathcal{V}_i$$

Slow-fast extended systems of interacting diffusions

$$\varepsilon \ll 1, \quad N \gg 1$$

$$dq_i = \varepsilon\, V(\theta_i)dt,$$

$$d\theta_i = -\,[\Gamma \partial_\theta \mathbb{U}](\theta_i)dt - \frac{1}{\mathcal{N}_i}\sum_{j\in\mathcal{V}_i}\Gamma(\theta_i)F(\theta_i,\theta_j)dt + \sqrt{2\Gamma(\theta_i)}\, d\eta_i(t)$$

Independent Brownian motions

$\mathbb{U}(\theta) := U(\theta) - \log\Gamma(\theta)$: Effective potential

$\Gamma(\theta)$: diffusion coefficient

$F(\theta,\theta') = \nabla_\theta W(\theta,\theta')$: binary interaction with radius R

The dependence in the potentials on Γ is here to assure that if $R=\infty$ then the angles (autonomous) dynamics is reversible w.r.t. the Gibbs measure. Our results could bypass this assumption if the model does not present phase transitions.

Kinetic Limit: $$\lim_{R\to 0}\lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N}\delta_{(q_i(t),\theta_i(t))}(dq,d\theta) = f^{\varepsilon}(q,\theta,t)\,dq d\theta$$

$$\partial_t f^{\varepsilon} := \mathcal{D}_{f^{\varepsilon}}(f^{\varepsilon}) - \varepsilon\mathcal{T}(f^{\varepsilon})$$

Dissipative term

Transport term

$$\mathcal{D}_f(g) := \partial_\theta\left(\Gamma\left[\partial_\theta U + \frac{F(f)}{\Pi(f)}\right]g + \Gamma\,\partial_\theta g\right),$$

$$\mathcal{T}(g) := V(\theta)\cdot\nabla g\,.$$

spatial density:

$$\rho(q) := \Pi(f)(q) := \int_{-\pi}^{\pi} f(q,\theta')d\theta'$$

effective force:

$$F(f)(q,\theta) := \int_{-\pi}^{\pi} d\theta'\,F(\theta,\theta')\,f(q,\theta')\,d\theta',$$

Local equilibria $\mathscr{D}_f(f) = 0$

We assume all local equilibria (equilibria of the fast dynamics) are in the form

$$f_{\mathrm{le}}(q,\theta) = \rho(q) G(\theta)$$

with

$$\left[\partial_\theta U + F(G)\right] G + \partial_\theta G = 0 \qquad \int_{-\pi}^{\pi} G(\theta) = 1$$

Assumption
G is unique

Valid for
small
interactions

Notation: $\langle h \rangle_G = \int h(\theta)\, G(\theta)\, d\theta$

Hydrodynamic limits via a Chapman-Enskog expansion

$$\tilde{f}^{\varepsilon}(q,\theta,t) = f^{\varepsilon}(q,\theta,t\varepsilon^{-1})$$

Density in a long (Euler) time scale

$$\tilde{\rho}_0^{\varepsilon}(q,t) = \int_{-\pi}^{\pi} \tilde{f}^{\varepsilon}(q,\theta,t)d\theta$$

Spatial density

Hydrodynamic limit:

$$\partial_t \tilde{\rho}_0^{\varepsilon} + \langle V \rangle_G \cdot \nabla \tilde{\rho}_0^{\varepsilon} - \varepsilon \nabla \cdot \mathbf{D} \nabla \tilde{\rho}_0^{\varepsilon} = O(\varepsilon^2)$$

Finite size fluctuations: fluctuating kinetic equation

$$\partial_t \tilde{f}^\varepsilon + \mathcal{T}(\tilde{f}^\varepsilon) = \varepsilon^{-1}\mathcal{D}_{\tilde{f}^\varepsilon}(\tilde{f}^\varepsilon) + (\varepsilon N)^{-1/2}\mathcal{N}\left(\sqrt{\Gamma \tilde{f}^\varepsilon}\right)$$

Center transport term by changing frame and look in a longer (diffusive) time scale

$$\bar{f}^\varepsilon(q,\theta,t) := \tilde{f}^\varepsilon(q + t\varepsilon^{-1}\langle V\rangle_G, \theta, t\varepsilon^{-1}) \,.$$

$$\mathcal{N}(g) := \sqrt{2}\,\partial_\theta(\eta\, g)$$

$$\eta := \eta(q,\theta,t)$$

White noise

$$\varepsilon\partial_t \bar{f}^\varepsilon + \mathcal{T}_0(\bar{f}^\varepsilon) = \varepsilon^{-1}\mathcal{D}_{\bar{f}^\varepsilon}(\bar{f}^\varepsilon) + N^{-1/2}\mathcal{N}\left(\sqrt{\Gamma \bar{f}^\varepsilon}\right)$$

Centered transport term:

$$\mathcal{T}_0(g) := \overline{V}\cdot\nabla g, \quad \overline{V}(\theta) = V(\theta) - \langle V\rangle_G$$

Fluctuating hydrodynamic limits via a Chapman-Enskog expansion

$$\tilde{f}^{\varepsilon}(q,\theta,t) = f^{\varepsilon}(q,\theta,t\varepsilon^{-1})$$

Density in long (Euler) time scale

$$\tilde{\rho}_0^{\varepsilon}(q,t) = \int_{-\pi}^{\pi} \tilde{f}^{\varepsilon}(q,\theta,t)d\theta$$

Spatial density

Semi-explicit matrices

Fluctuating hydrodynamic limit:

$$\partial_t \tilde{\rho}_0^{\varepsilon} + \langle V \rangle_G \cdot \nabla \tilde{\rho}_0^{\varepsilon} - \varepsilon \nabla \cdot \mathbf{D} \, \nabla \, \tilde{\rho}_0^{\varepsilon} + \sqrt{\frac{2\varepsilon}{N}} \nabla \cdot \left(\sqrt{\tilde{\rho}_0^{\varepsilon}} \sigma \, \zeta \right) \; = \; o(1)$$

$\zeta := \zeta(q,t)$ is a space-time white noise

A LD interpretation of these formal derivations

- The correct interpretation of the (ill defined) fluctuating equation is a large deviations principle for the corresponding density.
- The convergence of the fluctuating kinetic equation to the fluctuating hydrodynamic equation is established at the level of large deviations functionals.
- The right notion of convergence of LD functionals is the Gamma-convergence.

Dawson-Gärtner theory:

$$\mathbb{P}\left(\bar{f}_N^\varepsilon(q,\theta,t) \approx g(q,\theta,t) \text{ on } [0,T]\right) \sim \exp(-N\mathscr{I}_T^\varepsilon(g))$$

with the rate functional

$$\mathscr{I}_T^\varepsilon(f) = \frac{1}{4}\int_0^T \int_{\mathbb{R}^d} \left\| A_f^\varepsilon(f) \right\|_{-1,\Gamma f}^2 dq\ dt$$

where

$$A_f^\varepsilon(f) = \varepsilon\partial_t f + \mathscr{T}_0(f) - \varepsilon^{-1}\mathscr{D}_f(f)$$

and

$$\|g\|_{-1,h}^2 = \inf_\varphi \left\{ \int \frac{\varphi^2}{h}\, dq\, d\theta\ ,\ \partial_\theta\varphi = g \right\}$$

$$= 2\sup_\varphi \left\{ \int g\varphi\, dq\, d\theta - \frac{1}{2}\int (\partial_\theta\varphi)^2 h\, dq\, d\theta \right\}$$

formally:

$$\|g\|_{-1,h}^2 = \text{"} \int h^{-1}(\partial_\theta^{-1} g)^2 dq d\theta \text{"}$$

This form is well understood in view of the fluctuating kinetic equation

$$A_{\bar{f}^\varepsilon}(\bar{f}^\varepsilon) = N^{-1/2}\mathcal{N}\left(\sqrt{\Gamma\bar{f}^\varepsilon}\right)$$

$$\mathcal{N}(g) := \sqrt{2}\,\partial_\theta(\eta\, g)$$
$$\eta := \eta(q,\theta,t)$$

White noise

since formally

$$\mathbb{P}(\eta(q,\theta,t) = g) \sim exp(-\int g^2\, dqd\theta dt)$$

The fluctuating hydrodynamic equation can be interpreted similarly as a large deviations principle for the empirical spatial density.

Theorem (Barré, B., Chetrite, Chopra, Mariani)

The large deviations functional $\mathscr{I}^{\varepsilon}_T$ converges to

(for the Gamma-convergence)

$$\mathscr{I}_T(f) = \begin{cases} \frac{1}{4}\int_0^T \left\| \partial_t \rho - \nabla \cdot \mathbf{D}\nabla\rho \right\|^2_{-1,\rho\sigma} dt \\ \qquad\qquad \text{if } f(q,\theta,t) = f_{\mathrm{le}}(q,\theta,t) = \rho(q,t)G(\theta), \\ +\infty \quad \text{otherwise,} \end{cases}$$

Gamma-convergence (motivating example)

$$F_\varepsilon(u) = \int_0^1 a\left(\frac{x}{\varepsilon}\right) |\, u'(x) \,|^2 \, dx$$

$a : \mathbb{R} \to (0, +\infty)$
1-periodic function

For any u, we have that

$$\lim_{\varepsilon \to 0} F_\varepsilon(u) = F_0(u)$$

with

$$F_0(u) = \bar{a} \int_0^1 |\, u'(x) \,|^2 \, dx$$

$$\bar{a} = \int_0^1 a(x)dx$$

We have that

$$\Gamma - \lim_{\varepsilon \to 0} F_\varepsilon(u) = F(u)$$

with

$$F(u) = \underline{a}^{-1} \int_0^1 |\, u'(x) \,|^2 \, dx$$

$$\underline{a} = \int_0^1 a^{-1}(x)dx$$

This is the correct answer!
The minimizer of F_ε converge to the minimizer of F, not of F_0.

Linearized operator

$$\mathscr{L}_f(g) := \lim_{\delta \to 0} \frac{\mathscr{D}_{f+\delta g}(f+\delta g) - \mathscr{D}_f(f)}{\delta}$$

Recall that G is the unique local equilibrium

$$\mathscr{L}_G(g) = \partial_\theta \left(\Gamma[\partial_\theta U + F(G) + \partial_\theta] g \right)$$
$$+ \partial_\theta \left(\Gamma G \left[F(g) - \left\langle \frac{g}{G} \right\rangle_G F(G) \right] \right)$$

Our main assumption is that (can be proved for weak interactions)

$$\mathrm{Ker}(\mathscr{L}_G^\dagger) = \mathrm{Span}(\mathbf{1}), \quad \mathrm{Ker}(\mathscr{L}_{\mathbf{G}}) = \mathrm{Span}(\mathbf{G})$$

$$\mathrm{Range}(\mathscr{L}_G^\dagger) = \left\{ u \; ; \; \langle u \rangle_G = 0 \right\}, \quad \mathrm{Range}(\mathscr{L}_G) = \left\{ u \; ; \; \langle \tfrac{u}{G} \rangle_G = 0 \right\}$$

Gamma-convergence

Definition

A sequence of functional $F^\nu : E \to \mathbb{R}$ defined on some topological space E $\Gamma-$converges to $F : E \to \mathbb{R}$ as $\nu \to 0$ if

- for any $x \in E$ and any sequence $x^\nu \to x$,

  $$\lim_{\mu \to 0} \inf_{\nu \leq \mu} F^\nu(x^\nu) \geq F(x)$$

- for any $x \in E$ there is a sequence $x^\nu \to x$,

  $$\lim_{\mu \to 0} \sup_{\nu \leq \mu} F^\nu(x^\nu) \leq F(x)$$

$\Gamma - \liminf$

Consider any sequence $f^\varepsilon = f + \varepsilon f_1 + \varepsilon^2 f_2 + O(\varepsilon^3)$

We have to prove

$$\boxed{\liminf_{\varepsilon\to 0} \ \mathscr{I}^\varepsilon_T(f^\varepsilon) \ \geq \ \mathscr{I}_T(f)}$$

with

$$\mathscr{I}_T(f) = \begin{cases} \frac{1}{4}\int_0^T \left\| \partial_t \rho - \nabla \cdot \mathbf{D} \nabla \rho \right\|^2_{-1,\rho\sigma} dt \\ \qquad \text{if } f(q,\theta,t) = f_{\mathrm{le}}(q,\theta,t) = \rho(q,t)G(\theta), \\ +\infty \quad \text{otherwise,} \end{cases}$$

Sup-formula for the H_{-1}-norm gives

$$\mathscr{I}^\varepsilon_T(f^\varepsilon) = \frac{1}{4}\int_0^T \int_{\mathbb{R}^d} \left\| A^\varepsilon_{f^\varepsilon}(f^\varepsilon) \right\|^2_{-1,\Gamma f^\varepsilon} dq \ dt$$

$$\geq \frac{1}{4}\int_0^T dt \left\{ 2\langle \varphi, A^\varepsilon_{f^\varepsilon}(f^\varepsilon)\rangle - \langle [\partial_\theta \varphi]^2, \Gamma f^\varepsilon \rangle \right\}$$

Choose the best test function φ

$$A^\varepsilon_f(f) = \varepsilon \partial_t f + \mathscr{T}_0(f) - \varepsilon^{-1} \mathscr{D}_f(f)$$

We see that f shall be a local equilibrium $f(q,\theta,t) = \rho(q,t)G(\theta)$ Otherwise Infinite

We choose the test function in the form

$$\varphi^{\varepsilon}(q,\theta,t) = \varepsilon^{-1}\varphi_{-1}(q,\theta,t) + \varphi_0(q,\theta,t)$$

Then we have

$$\mathcal{J}_T^{\varepsilon}(f^{\varepsilon}) \geq \frac{1}{2}\int_0^T dt \left\{\varepsilon^{-2}X_t + \varepsilon^{-1}Y_t + Z_t\right\} \ + \ O(\varepsilon)$$

This sign implies φ_{-1} shall not depend on θ

with

$$X = -\frac{1}{2}\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_{\mathrm{le}}\rangle \leq 0$$

$$Y = \Big\langle \varphi_{-1}, \mathcal{T}_0(f_{\mathrm{le}}) - \mathcal{L}_G(f_1)\Big\rangle - \frac{1}{2}\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_1\rangle - \langle(\partial_\theta\varphi_{-1})(\partial_\theta\varphi_0), \Gamma f_{\mathrm{le}}\rangle$$

$$Z = \Big\langle \varphi_0, \mathcal{T}_0(f_{\mathrm{le}}) - \mathcal{L}_G(f_1)\Big\rangle + \Big\langle \varphi_{-1}\,,\ \big[\partial_t f_{\mathrm{le}} + \mathcal{T}_0(f_1) - \partial_\theta \mathcal{Q}(f_{\mathrm{le}}, f_1, f_2)\big]\Big\rangle$$
$$-\frac{1}{2}\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_2\rangle - \langle(\partial_\theta\varphi_{-1})(\partial_\theta\varphi_0), \Gamma f_1\rangle - \frac{1}{2}\langle(\partial_\theta\varphi_0)^2, \Gamma f_{\mathrm{le}}\rangle$$

We choose the test function in the form

$$\varphi^{\varepsilon}(q,\theta,t) = \varepsilon^{-1}\varphi_{-1}(\theta,t) + \varphi_0(q,\theta,t)$$

Then we have

$$\mathcal{I}_T^{\varepsilon}(f^{\varepsilon}) \geq \frac{1}{2}\int_0^T dt\,\left\{\varepsilon^{-2}X_t + \varepsilon^{-1}Y_t + Z_t\right\} \;+\; O(\varepsilon)$$

since φ_{-1} doesn't depend on θ one can check it vanishes

with

$$X = \cancel{-\frac{1}{2}\left\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_{\mathrm{le}}\right\rangle} \leq 0$$

$$Y = \Big\langle \varphi_{-1}, \cancel{\mathcal{T}_0(f_{\mathrm{le}}) - \mathcal{L}_G(f_1)} \Big\rangle - \cancel{\frac{1}{2}\left\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_1\right\rangle} - \cancel{\left\langle(\partial_\theta\varphi_{-1})(\partial_\theta\varphi_0), \Gamma f_{\mathrm{le}}\right\rangle}$$

$$Z = \Big\langle \varphi_0, \mathcal{T}_0(f_{\mathrm{le}}) - \mathcal{L}_G(f_1) \Big\rangle + \Big\langle \varphi_{-1}\,,\ \big[\partial_t f_{\mathrm{le}} + \mathcal{T}_0(f_1) - \cancel{\partial_\theta \mathcal{Q}(f_{\mathrm{le}}, f_1, f_2)}\big] \Big\rangle$$

$$-\cancel{\frac{1}{2}\left\langle(\partial_\theta\varphi_{-1})^2, \Gamma f_2\right\rangle} - \cancel{\left\langle(\partial_\theta\varphi_{-1})(\partial_\theta\varphi_0), \Gamma f_1\right\rangle} - \frac{1}{2}\left\langle(\partial_\theta\varphi_0)^2, \Gamma f_{\mathrm{le}}\right\rangle$$

$$Z = \left\langle \varphi_0, \mathcal{T}_0(f_{\rm le}) - \mathcal{L}_G(f_1) \right\rangle + \left\langle \varphi_{-1}\,,\, \left[\partial_t f_{\rm le} + \mathcal{T}_0(f_1)\right] \right\rangle \;-\; \frac{1}{2}\langle(\partial_\theta\varphi_0)^2, \Gamma f_{\rm le}\rangle$$

Choose then φ_0, φ_{-1} such that

$$\mathcal{L}_G^\dagger\varphi_0 - \mathcal{T}_0^\dagger\varphi_{-1} = 0 = \mathcal{L}_G^\dagger\varphi_0 + \mathcal{T}_0\varphi_{-1}$$

The terms with f_1 disappear

Observe then that

$$\mathcal{T}_0(\varphi_{-1})(q,\theta,t) = \overline{V}(\theta)\cdot\nabla\varphi_{-1}(q,t)$$

and choose $\quad \varphi_0(q,\theta,t) = \psi(\theta)\cdot\nabla\varphi_{-1}(q,t), \quad (\mathcal{L}_G^\dagger\psi)(\theta) = -\,\bar{V}(\theta)$

$$\langle\varphi_0, \mathcal{T}_0(f_{\rm le})\rangle = -\int dq\; \varphi_{-1}(q,t)\;\nabla\cdot\mathbf{D}\,\nabla\rho(q,t)$$

$$\langle\varphi_{-1}\,, \partial_t f_{\rm le}\rangle = \int dq\; \varphi_{-1}(q,t)\;\partial_t\rho(q,t)$$

$$\langle(\partial_\theta\varphi_0)^2, \Gamma f_{\rm le}\rangle = \int dq\; \rho(q,t)\;\nabla\varphi_{-1}(q,t)\;\cdot\;\sigma\nabla\varphi_{-1}(q,t)$$

We got

$$\mathcal{J}_T^{\varepsilon}(f^{\varepsilon}) \geq \frac{1}{4}\int_0^T dt \left\{ 2\int dq\, \varphi_{-1}(q,t)\, \Big[\partial_t \rho(q,t)\, dq - \nabla \cdot \mathbf{D}\, \nabla \rho(q,t)\Big] - \int dq\, \rho(q,t)\, \nabla \varphi_{-1}(q,t) \;\cdot\; \sigma \nabla \varphi_{-1}(q,t) \right\} \;+\; O(\varepsilon)\,.$$

We can optimize over φ_{-1} to get the result (the sup of the rhs becomes the H_{-1} norm we were looking for).

Summary:

- We introduced a LD approach to connect fluctuating kinetics to fluctuating hydrodynamics
- This approach is based on clean mathematical statements, even if a totally rigorous proof is still missing (work for some variations of the model)

- <u>Open problem 1:</u> extend this approach in the presence of phase transitions.
- <u>Open problem 2:</u> extend this approach when the velocity depends V also on the position $V(q,\theta)$.