Mean field kinetic particles and the Vlasov-Fokker-Planck equation

Pierre Monmarché

CERMICS, École des Ponts ParisTech

groupe de travail de Probabilités du MAP5

Kinetic particle

- $X(t) \in \mathbb{R}^d$ position at time t
- $Y(t) \in \mathbb{R}^d$ velocity at time t
- $U : \mathbb{R}^d \to \mathbb{R}$ external potential
- $B(t)$ Brownian motion d-dimensional

Newton's law of motion :

$$\left\{ \begin{array}{rcl} \mathrm{d}X & = & Y\mathrm{d}t \\ \mathrm{d}Y & = & -\nabla U(X)\mathrm{d}t - Y\mathrm{d}t + \sqrt{2}\mathrm{d}B \end{array} \right.$$

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The law $m_t = \mathcal{L}(X_t, Y_t)$ is a (weak) solution of

$$\partial_t m_t + y \cdot \nabla_x m_t = \nabla_y \cdot \left(\nabla_y m_t + \left(\nabla U(x) + y \right) m_t \right),$$

the Langevin (or kinetic Fokker-Planck) equation.

Law of large numbers

- $Z_i = (X_i, Y_i)$ i.i.d. particles, $i \in [\![1, N]\!]$
- empirical measure

$$\pi_t^N = \frac{1}{N} \sum_{j=1}^{N} \delta_{Z_j}$$

Morally,

$$\pi_t^N \underset{N \to \infty}{\longrightarrow} m_t.$$

Mean field interaction

- $W : \mathbb{R}^d \to \mathbb{R}$ an even interaction potential

For $i \in [\![1, N]\!]$,

$$\begin{aligned} \mathrm{d}X_i &= Y_i \mathrm{d}t \\ \mathrm{d}Y_i &= -\nabla U(X_i)\mathrm{d}t - \frac{1}{N}\sum_{j=1}^{N} \nabla W(X_i - X_j)\mathrm{d}t - Y_i \mathrm{d}t + \sqrt{2}\mathrm{d}B_i \end{aligned}$$

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Assuming $\pi_t^N \underset{N\to\infty}{\longrightarrow} m_t$,

$$\partial_t m_t + y \cdot \nabla_x m_t = \nabla_y \cdot \left(\nabla_y m_t + \left(\nabla U + \nabla W * m_t + y\right) m_t\right)$$

with $\nabla W * m_t(x) = \int \nabla W(x-u) m_t(u,v)\mathrm{d}u\mathrm{d}v$ (Vlasov-Fokker-Planck).

Non-linear process

For $i \in [\![1, N]\!]$,

$$\begin{cases} \mathrm{d}\widetilde{X}_i &= \widetilde{Y}_i \mathrm{d}t \\ \mathrm{d}\widetilde{Y}_i &= -\nabla U\left(\widetilde{X}_i\right)\mathrm{d}t - \left(\nabla W * m_t\right)\left(\widetilde{X}_i\right) - \widetilde{Y}_i \mathrm{d}t + \sqrt{2}\mathrm{d}B_i \\ m_t &= \mathcal{L}\left(\widetilde{X}_i(t), \widetilde{Y}_i(t)\right) \end{cases}$$

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We are interested in :

- The law m_t that solves the non-linear PDE,
- The non-independent $Z_i = (X_i, Y_i)$ with $Z = (Z_1, \dots, Z_N)$ Markov,
- The independent $\widetilde{Z}_i = \left(\widetilde{X}_i(t), \widetilde{Y}_i\right)$ with law m_t, $\widetilde{Z}$ non Markov.

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- $N \to \infty$: propagation of chaos

- $t \to \infty$: convergence to equilibrium

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  If the $Z_i(0) = \widetilde{Z}_i(0)$ are i.i.d. with law m_0, when $N \to \infty$,

  - $\pi_t^N = \frac{1}{N} \sum \delta_{Z_i}$ should converge to m_t,
  - Z_1 should behave like $\widetilde{Z}_1$,
  - $m_t^{(1,N)} = \mathcal{L}(Z_1(t))$ should converge to m_t.

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Goal : quantitative estimates for the speed of these convergences.

Distances

Coupling of two laws :

$$\Pi(\mu,\nu) \quad = \quad \{(Q,R) \text{ r.v. such that } \mathcal{L}(Q)=\mu,\ \mathcal{L}(R)=\nu\}\,.$$

- Total variation distance :

$$\begin{aligned} d_{VT}(\mu,\nu) &= \inf_{\Pi(\mu,\nu)} \mathbb{P}\left(Q\neq R\right) \\ &= \frac{1}{2}\|\mu-\nu\|_1 \qquad \text{(if density)} \end{aligned}$$

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- Relative entropy (Kullback-Leibler divergence) :

$$\mathcal{H}\left(\mu \mid \nu\right) \quad = \quad \int \ln\left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu}\right) \mathrm{d}\mu$$

Dependency in N

If

- $Q = (Q_1, \ldots, Q_N)$ of law $\mu^{(N)}$ with exchangeable Q_i's
- $R = (R_1, \ldots, R_N)$ of law $\nu^{\otimes N}$ with i.i.d. R_i 's

Then

$$\mathbb{E}\left(|Q - R|^2\right) = \sum_{i=1}^{N} \mathbb{E}\left(|Q_i - R_i|^2\right) = N\mathbb{E}\left(|Q_1 - R_1|^2\right)$$

Hence denoting by $\mu^{(1,N)}$ the law of Q_1,

$$\mathcal{W}_2^2\left(\mu^{(1,N)}, \nu\right) \leq \frac{1}{N}\mathcal{W}_2^2\left(\mu^{(N)}, \nu^{\otimes N}\right).$$

If moreover the Q_i are independent with law μ,

$$\mathcal{W}_2^2\left(\mu, \nu\right) = \frac{1}{N}\mathcal{W}_2^2\left(\mu^{\otimes N}, \nu^{\otimes N}\right).$$

Dependency in N

With again exchangeable Q_i's and i.i.d. R_i's (Csiszár's Inequality) :

$$\mathcal{H}\left(\mu^{(1,N)} \mid \nu\right) \leq \frac{2}{N}\mathcal{H}\left(\mu^{(N)} \mid \nu^{\otimes N}\right)$$

Under our assumptions (to come), there will exist K independent from N such that

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Bad candidate, albeit usual quantity :

$$\mathsf{Var}_\nu(\mu) \quad = \quad \int \left(\frac{\mathsf{d}\mu}{\mathsf{d}\nu} - 1\right)^2 \mathsf{d}\nu$$

$\Rightarrow$ Hilbert norm, spectral theory, long-time convergence... but

$$\mathsf{Var}_{\nu^{\otimes N}}(\mu^{\otimes N}) \quad = \quad (\mathsf{Var}_\nu(\mu) + 1)^N - 1$$

Functional inequalities

- Pinsker's Inequality :

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- We say ν satisfies a log-Sobolev inequality if $\exists C$ s.t. $\forall \mu \prec \nu$,

$$\mathcal{H}\left(\mu \mid \nu\right) \quad \leq \quad C\int \left|\nabla \ln \frac{\mathrm{d}\mu}{\mathrm{d}\nu}\right|^2 \mathrm{d}\mu.$$

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- A log-Sobolev inequality implies a Talagrand's T_2 one : $\forall \mu$,

$$\mathcal{W}_2^2\left(\mu, \nu\right) \quad \leq \quad C\mathcal{H}\left(\mu \mid \nu\right).$$

Assumptions

A

- The external potential U is convex ($\nabla^2 U \geq c_1 > 0$) and $\nabla^2 W \geq -c_2$ with $c_2 < \frac{1}{2}c_1$. Moreover $\nabla^2 U$ and $\nabla^2 W$ are bounded.
- The law m_0 has a Lebesgue density, a finite 2nd moment and $\int m_0 \ln m_0 < \infty$.

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Remarks :

- Forbid the Coulomb interaction $W_c(x-y) = \pm\frac{1}{|x-y|}$, but allow $\xi * W_c$ with a smooth kernel, provided U is convex enough.
- $\ll W$ *small enough* $\gg$ not needed (contrary to [Villani 2007, Bolley-Guillin-Malrieu 2010, Hérau-Thomann 2015]).

Results

Theorem (M., 2016)

Under Assumption A, the exist $C, \chi > 0$ which depend neither on t, nor N, nor m_0, and there exists K that depends on m_0 but not on t, N, such that

- For the particle system, $m_\infty^{(N)}$ satisfies a log-Sobolev inequality with constant independent from N and

$$\mathcal{H}\left(m_t^{(N)} \mid m_\infty^{(N)}\right) \leq Ce^{-\chi t}\mathcal{H}\left(m_0^{(N)} \mid m_\infty^{(N)}\right).$$

- The Vlasov-Fokker-Planck PDE admits a unique equilibrium m_∞ and

$$\|m_t - m_\infty\|_1 \leq Ke^{-\chi t}, \qquad \mathcal{W}_2\left(m_t, m_\infty\right) \leq Ke^{-\chi t}.$$

Results

Theorem (M., 2016)

Under Assumption A, there exist $b, \alpha, > 0$ that depend neither on t, nor N, nor m_0, and there exists K that depends on m_0 but not on t, N, such that

- Uniform in time propagation of chaos :

$$W_2\left(m_t^{(1,N)}, m_t\right) \leq K \min\left(\frac{e^{bt}}{N}, \frac{1}{N^\alpha}\right)$$

  and

$$\|m_t^{(1,N)} - m_t\|_1 \leq \frac{K}{N^\alpha}.$$

- Numerical error bound (cf. Bolley-Guillin-Villani 2006) :

$$\mathbb{P}\left(\mathcal{W}_2\left(\pi_t^N, m_\infty\right) \geq \varepsilon\right) \leq \frac{K}{\varepsilon^2}\left(e^{-\chi t} + \frac{1}{N}\right)$$

Coercivity without interaction

$$\begin{cases} \mathrm{d}X &= Y\mathrm{d}t \\ M\mathrm{d}Y &= -\nabla U(X)\mathrm{d}t - Y\mathrm{d}t + \sqrt{2}\mathrm{d}B \end{cases}$$

When the mass $M \to 0$, overdamped Langevin (or Fokker-Planck) diffusion :

$$\mathrm{d}X = -\nabla U(X)\mathrm{d}t + \sqrt{2}\mathrm{d}B$$

with equilibrium $\rho_\infty(\mathrm{d}x) = e^{-U(x)}\mathrm{d}x$ and whose law ρ_t satisfies

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Large-time convergence, assuming a log-Sobolev inequality holds :

$$\partial_t \left(\mathcal{H}\left(\rho_t \mid \rho_\infty\right)\right) = -\int \left| \nabla \ln \frac{\mathrm{d}\rho_t}{\mathrm{d}\rho_\infty} \right|^2 \mathrm{d}\rho_t \leq -\frac{1}{C}\mathcal{H}\left(\rho_t \mid \rho_\infty\right)$$

$$\Rightarrow \qquad \mathcal{H}\left(\rho_t \mid \rho_\infty\right) \leq e^{-\frac{t}{C}}\mathcal{H}\left(\rho_0 \mid \rho_\infty\right).$$

Hypoercivity without interaction

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The entropy dissipation may vanish outside of equilibrium :

$$\partial_t \left(\mathcal{H}\left(m_t \mid m_\infty\right)\right) = -\int \left|\nabla_y \ln \frac{\mathrm{d}m_t}{\mathrm{d}m_\infty}\right|^2 \mathrm{d}m_t.$$

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$$\partial_t \left(\mathcal{H}\left(m_t \mid m_\infty \right) \right) = - \int \left| \nabla_y \ln \frac{dm_t}{dm_\infty} \right|^2 dm_t.$$

Modified entropy (Hérau 2006, Villani 2007) : set $h_t = \frac{dm_t}{dm_\infty}$ and

$$\mathcal{N}(h) := \int h \ln h dm_\infty + \int |P \nabla \ln h|^2 h dm_\infty.$$

With a well-chosen P and log-Sobolev inequality,

$$\partial_t \left(\mathcal{N}\left(h_t \right) \right) \leq -c \int |\nabla \log h_t|^2 dm_t \leq -c' \mathcal{N}\left(h_t \right)$$

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$$\Rightarrow \mathcal{H}\left(m_t \mid m_\infty\right) \leq \mathcal{N}\left(h_t\right) \leq e^{-\frac{(t-t_0)}{c'}} \mathcal{N}\left(h_{t_0}\right) \overset{regul.}{\leq} Ce^{-\frac{t}{c'}} \mathcal{H}\left(m_0 \mid m_\infty\right)$$

The McKean-Vlasov equation

Overdamped mean-field particles : for $i \in [\![1, N]\!]$,

$$\begin{aligned} \mathrm{d}X_i &= -\nabla U(X_i)\mathrm{d}t - \frac{1}{N}\sum_{j=1}^{N} \nabla W(X_i - X_j)\mathrm{d}t + \sqrt{2}\mathrm{d}B_i \\ \mathrm{d}\widetilde{X}_i &= -\nabla U\left(\widetilde{X}_i\right)\mathrm{d}t - \int \nabla W\left(\widetilde{X}_i - u\right)\rho_t(u)\mathrm{d}u\mathrm{d}t + \sqrt{2}\mathrm{d}B_i \\ \rho_t &= \mathcal{L}\left(\widetilde{X}_1\right). \end{aligned}$$

Elliptic but non-linear EDP :

$$\partial_t \rho_t = \nabla \cdot \left(\nabla \rho_t + \left(\nabla U + \nabla W * \rho_t\right)\rho_t\right).$$

Parallel coupling : same Brownian motions B_i for both X_i and $\widetilde{X}_i$.

Propagation of chaos

Denote by

$$\alpha(t) = \mathbb{E}\left(\left|X_1(t) - \widetilde{X}_1(t)\right|^2\right) = \frac{1}{N}\mathbb{E}\left(\left|X(t) - \widetilde{X}(t)\right|^2\right).$$

Parallel coupling and convexity assumption (Malrieu 2001) :

$$\alpha'(t) \quad \leq \quad -c\alpha(t) + \frac{K}{\sqrt{N}}\sqrt{\alpha(t)}$$

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Consequences :

$$\begin{aligned} \mathcal{W}_2^2\left(\rho_t^{(1,N)}, \rho_t\right) \quad &\leq \quad \frac{K}{N} \\ \mathcal{W}_2^2\left(\rho_\infty^{(1,N)}, \rho_\infty\right) \quad &\leq \quad \frac{K}{N} \end{aligned}$$

(for a unique ρ_∞ ; moreover a log-Sobolev inequality for $\rho_\infty^{(N)}$ independently from N, and for ρ_∞)

Without interaction

$$\begin{cases} \mathrm{d}X &= Y\mathrm{d}t \\ \mathrm{d}Y &= -\nabla U(X)\mathrm{d}t - Y\mathrm{d}t + \sqrt{2}\mathrm{d}B. \end{cases}$$

Denoting by γ the standard Gaussian density, the equilibrium is

$$\begin{aligned} m_\infty(\mathrm{d}x,\mathrm{d}y) &= \left(e^{-U(x)}\mathrm{d}x\right) \otimes \gamma(\mathrm{d}y) \\ &= \rho_\infty(\mathrm{d}x) \otimes \gamma(\mathrm{d}y) \end{aligned}$$

where ρ_∞ is the invariant measure of

$$\mathrm{d}X = -\nabla U(X)\mathrm{d}t + \sqrt{2}\mathrm{d}B.$$

With interaction

$$\begin{cases} \mathrm{d}\widetilde{X} &= \widetilde{Y}\mathrm{d}t \\ \mathrm{d}\widetilde{Y} &= -\nabla U\left(\widetilde{X}\right)\mathrm{d}t - (\nabla W * m_t)\left(\widetilde{X}\right) - \widetilde{Y}\mathrm{d}t + \sqrt{2}\mathrm{d}B \\ m_t &= \mathcal{L}\left(\widetilde{X}(t), \widetilde{Y}(t)\right). \end{cases}$$

Then (Duong-Tugaut 2016)

$$m_\infty(\mathrm{d}x, \mathrm{d}y) = \rho_\infty(\mathrm{d}x) \otimes \gamma(\mathrm{d}y)$$

is a bijection between the equilibria m_∞ and the equilibria ρ_∞ of

$$\mathrm{d}\widetilde{X} = -\nabla U\left(\widetilde{X}\right)\mathrm{d}t - \int \nabla W\left(\widetilde{X} - u\right)\rho_t(u)\mathrm{d}u\mathrm{d}t + \sqrt{2}\mathrm{d}B.$$

Large time for the particle system

- The system $Z = (X, Y) \in \mathbb{R}^{2dN}$ satisfies a Langevin SDE

$$\begin{cases} \mathrm{d}X &= Y \mathrm{d}t \\ \mathrm{d}Y &= -\nabla U_N(X)\mathrm{d}t - Y\mathrm{d}t + \sqrt{2}\mathrm{d}B \end{cases}$$

with $U_N(x) = \frac{1}{2N}\sum_{i,j=1}^{N}\left(U(x_i) + U(x_j) + W(x_i - x_j)\right)$,

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with C, χ, K independent from t and N.

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- $+$ Talagrand Inequality independent from N,

$$\mathcal{W}_2^2\left(m_t^{(N)},m_\infty^{(N)}\right)\leq KNe^{-\chi t}.$$

Crude propagation of chaos

Parallel coupling between

$$\left\{ \begin{array}{rcl} \mathrm{d}X_i & = & Y_i \mathrm{d}t \\ \mathrm{d}Y_i & = & -\nabla U(X_i)\mathrm{d}t - \frac{1}{N}\sum_{j=1}^N \nabla W(X_i - X_j)\mathrm{d}t - Y_i\mathrm{d}t + \sqrt{2}\mathrm{d}B_i \end{array} \right.$$

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If the forces were close to be linear (Bolley-Guillin-Malrieu 2010) we could have a coercive drift. Here we simply say

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If the forces were close to be linear (Bolley-Guillin-Malrieu 2010) we could have a coercive drift. Here we simply say

$$\alpha'(t) \leq b\alpha(t) + \frac{K}{\sqrt{N}}\sqrt{\alpha(t)}$$

$$\Rightarrow \quad \mathbb{E}\left(\left|Z_1(t) - \widetilde{Z}_1(t)\right|^2\right) \leq \frac{Ke^{bt}}{N}.$$

Large-time in $\mathcal{W}_2$ for the non-linear process

At fixed t and for all N,

$$\mathcal{W}_2\left(m_t, m_\infty\right)$$

$$\leq \quad \mathcal{W}_2\left(m_t, m_t^{(1,N)}\right) + \mathcal{W}_2\left(m_t^{(1,N)}, m_\infty^{(1,N)}\right) + \mathcal{W}_2\left(m_\infty^{(1,N)}, m_\infty\right)$$

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&\leq \frac{Ke^{bt}}{N} + Ke^{-\chi t} + \frac{K}{N} \\
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\end{aligned}
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Uniform propagation of chaos in $\mathcal{W}_2$

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For $t \leq \varepsilon \ln N$, parallel coupling :

$$\mathcal{W}_2^2\left(m_t^{(1,N)}, m_t\right) \leq \frac{Ke^{bt}}{N} \leq \frac{K}{N^{1-b\varepsilon}}.$$

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&\leq Ke^{-\chi t} + \frac{K}{N} + Ke^{-\chi t} \\
&\leq \frac{3K}{N^{\varepsilon\chi}}
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\end{aligned}$$

Conclusion, for all time, $\mathcal{W}_2\left(m_t^{(1,N)}, m_t\right) \leq \frac{K}{N^\alpha}$.

Total variation

Based on Malrieu's 2001 guideline,

$$\partial_t \left(\mathcal{H}\left(m_t^{(N)} \mid m_t^{\otimes N} \right) \right) \leq KN\mathcal{W}_2\left(m_t^{(1,N)}, m_t \right) \leq KN^{1-\alpha}$$

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Not uniform, but sufficient :

$$\begin{aligned} & \| m_t - m_\infty \|_1 \\ \leq \quad & \| m_t - m_t^{(1,N)} \|_1 + \| m_t^{(1,N)} - m_\infty^{(1,N)} \|_1 + \| m_\infty^{(1,N)} - m_\infty \|_1 \end{aligned}$$

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&\leq\ \ \frac{\sqrt{Kt}}{N^{\frac{\alpha}{2}}}+\sqrt{KN}e^{-\frac{1}{2}\chi t}+\frac{K}{\sqrt{N}}
\end{aligned}$$

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Not uniform, but sufficient : for N of order $e^{\frac{\chi t}{\alpha+1}}$.

$$\begin{aligned} & \| m_t - m_\infty \|_1 \\ \leq \; & \| m_t - m_t^{(1,N)} \|_1 + \| m_t^{(1,N)} - m_\infty^{(1,N)} \|_1 + \| m_\infty^{(1,N)} - m_\infty \|_1 \\ \leq \; & \frac{\sqrt{Kt}}{N^{\frac{\alpha}{2}}} + \sqrt{KN} e^{-\frac{1}{2}\chi t} + \frac{K}{\sqrt{N}} \leq K e^{-\chi' t}. \end{aligned}$$

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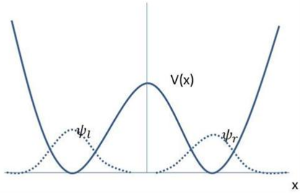
\end{aligned}$$

($\Rightarrow$ uniform in time propagation of chaos in the total variation sense...)

Without convexity

If U has several minima and the interaction is attractive, in the small noise regime, the non-linear PDE has several distinct equilibria, but there is unicity for a large enough noise



- If uniqueness, uniform estimates, with respect to t or N ?
- Without uniqueness, replace THE invariant measure by quasi-stationary ones ? Are there two regimes

$$t \ll e^{aN} \ \Rightarrow \ \mathcal{W}_2\left(m_t^{(1,N)}, m_t\right) \ \leq \ \frac{K}{N}$$
$$t \gg e^{aN} \ \Rightarrow \ \mathcal{W}_2\left(m_t^{(1,N)}, m_t\right) \ \geq \ K$$

and convergence of the QSD towards the equilibria of the PDE ?

- toy model (Curie-Weiss).

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