On the diffusive-mean field limit for weakly interacting diffusions exhibiting phase transitions

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On the Diffusive-Mean Field Limit for Weakly Interacting Diffusions Exhibiting Phase Transitions

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Abstract

The objective of this article is to analyse the statistical behaviour of a large number of weakly interacting diffusion processes evolving under the influence of a periodic interaction potential. We focus our attention on the combined mean field and diffusive (homogenisation) limits. In particular, we show that these two limits do not commute if the mean field system constrained to the torus undergoes a phase transition, that is to say, if it admits more than one steady state. A typical

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Mean Field Limits for Interacting Diffusions in a Two-Scale Potential

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Abstract In this paper, we study the combined mean field and homogenization limits for a system of weakly interacting diffusions moving in a two-scale, locally periodic confining potential, of the form considered in Duncan et al. (Brownian motion in an N-scale periodic potential, arXiv:1605.05854, 2016b). We show that, although the mean field and homogenization limits commute for finite times, they do not, in general, commute in the long time limit. In particular, the bifurcation diagrams for the stationary states can be different depending on the order with which we take the two limits. Furthermore, we construct the bifurcation diagram for the stationary McKean–Vlasov equation in a two-scale potential, before passing to the homogenization limit.

Outline

1. Problems & Motivation
   - Weakly Interacting Diffusions
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2. Two distinguished limits
   - The mean-field limit $N \to +\infty$
3. Qualitative properties
   - The space $\mathcal{P}_{\mathrm{sym}}((\mathbb{R}^d)^N)$ and its limit
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   - The diffusive limit $\varepsilon \to 0$
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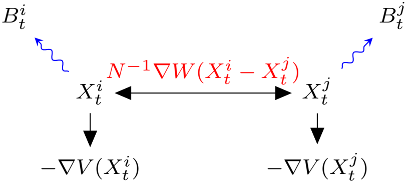
4. The joint limits
   - The limit $N \to \infty$ followed by $\varepsilon \to 0$
   - The limit $\varepsilon \to 0$ followed by $N \to \infty$
   - Non-commutativity
5. Parameter Estimation for Mean Field SDEs

N indistinguishable interacting particles in $\Omega = \mathbb{R}^d$ etc.
$X_t^i \in \Omega$: location of the i^{th} particle, $i = 1, \dots, N$.
X_0^i are i.i.d random variables with law $\nu_0 \in \mathcal{P}(\mathbb{R}^d)$.



$$\mathrm{d}X_t^i = -\nabla V(X_t^i) - \frac{1}{N}\sum_{i \neq j}^{N} \nabla W(X_t^i - X_t^j)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,dB_t^i\,,$$

where $V, W \in C^2(\mathbb{R}^d)$, 1-periodic, even, B_t^i independent Wiener processes.

Some applications:

- Plasma Physics
- Stellar Dynamics
- Collective behaviour of multiagent systems
- Synchronization
- Opinion Dynamics
- Algorithms for sampling/optimization[1]

Extensions:

- Inertia, e.g. underdamped Langevin dynamics.
- Colored, non-Gaussian, multiplicative noise[2].
- non-Markovian dynamics, e.g. the generalized Langevin equation[3] .

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[1] *On stochastic mirror descent with interacting particles: convergence properties and variance reduction* (with A. Borovykh, N. Kantas, P. Parpas). Physica D (2021).

[2] *The Desai-Zwanzig mean field model with colored noise* (with S.N. Gomes and U. Vaes). SIAM J. MMS, 18(3) pp. 1343-1370 (2020)

[3] *Mean field limits for non-Markovian interacting particles: convergence to equilibrium, GENERIC formalism, asymptotic limits and phase transitions* (with M. H. Duong). Comm. Math. Sci. (2018).

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On stochastic mirror descent with interacting particles: Convergence properties and variance reduction

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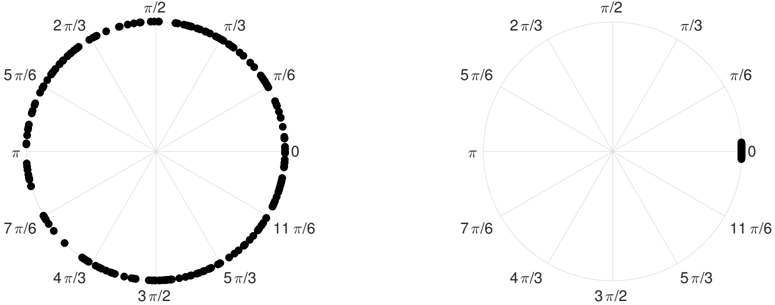
ABSTRACT

An open problem in optimization with noisy information is the computation of an exact minimizer that is independent of the amount of noise. A standard practice in stochastic approximation algorithms is to use a decreasing step-size. This however leads to a slower convergence. A second alternative is to use a fixed step-size and run independent replicas of the algorithm and average these. A third option is to run replicas of the algorithm and allow them to interact. It is unclear which of these options works best. To address this question, we reduce the problem of the computation of an exact minimizer with noisy gradient information to the study of stochastic mirror descent with interacting particles. We study the convergence of stochastic mirror descent and make explicit the tradeoffs between communication and variance reduction. We provide theoretical and numerical evidence to suggest that interaction helps to improve convergence and reduce the variance of the estimate.

1. Introduction

Descent (SMD) (see [5]). SMD can be used to solve constrained and unconstrained problems, and is known to be an optimal

The Kuramoto model: $W(x) = -\sqrt{\frac{2}{L}} \cos\left(2\pi \frac{x}{L}\right)$ with $\Omega = \mathbb{T}$ (the quotiented process)



$\beta < \beta_c$, no phase locking

$\beta > \beta_c$, phase locking

- The Hamiltonian can be written as

$$H_N(x_1,\ldots,x_N) = -\frac{1}{2N}\sum_{i,j}\cos(2\pi(x_i - x_j)) = -\frac{1}{2N}\sum_{i,j} S_i\, S_j, \tag{1}$$

  where $S_i = (\cos(2\pi x_i),\, \sin(2\pi x_i))$.

- The corresponding Gibbs measure is

$$\mu_{N,\theta}(d\mathbf{x}) = \frac{1}{Z_{N,\theta}} e^{-\beta\theta H_N(\mathbf{x})}\lambda_N(d\mathbf{x}), \quad Z_{N,\theta} = \int_{\mathbb{T}^N} e^{-\beta\theta H_N(\mathbf{x})}\lambda_N(d\mathbf{x}). \tag{2}$$

- Let $F \in C^2(\mathbb{T})$, denote by $\mu_t^N(d\mathbf{x})$, write $W(x) = -\cos(2\pi x)$ the empirical measure and apply Itô's formula to obtain

$$\begin{aligned}
&\int_{\mathbb{T}} F(\mathbf{x})\mu_t^N(d\mathbf{x}) - \int_{\mathbb{T}} F(\mathbf{x})\mu_0^N(d\mathbf{x}) \\
&= -\theta\int_0^t\int_{\mathbb{T}^2} F'(\mathbf{x})W'(\mathbf{x}-\mathbf{y})\mu_s^N(d\mathbf{x})\mu_s^N(d\mathbf{y})\,ds \\
&= \beta^{-1}\int_0^t\int_{\mathbb{T}} F''(\mathbf{x})\mu_s^N(d\mathbf{x})\,ds + M_{N,F}(t),
\end{aligned}$$

- where $M_{N,F}(t)$ is a continuous martingale with quadratic variation $\langle M_{N,F}\rangle(t) = \frac{1}{N}\int_0^t\int_{\mathbb{T}}(F'(\mathbf{x}))^2\mu_s^N(d\mathbf{x})\,ds$.

- By Doob's martingale inequality we have that

$$\mathcal{F}\left(\sup_{t\in[0,T]} M_{N,F}(t)\right) \leq \langle M_{N,F}\rangle(t) \leq \frac{T}{N}\|F\|^2_{L^\infty}.$$

- Therefore, the stochastic term vanishes in the limit as $N \to +\infty$ so that the limit of the empirical measure, if it exists, is deterministic.
- We study the limit in the space $C^0([0,T];\mathcal{M}_1(\mathbb{T}))$ where $\mathcal{M}_1(\mathbb{T})$ is the space of probability measures on $\mathbb{T}$ equipped with the topology of weak convergence.
- Proving tightness of the family of empirical (probability) measures, assuming chaotic initial conditions and proving uniqueness of the limiting equation, we can pass rigorously to the limit to obtain the mean field PDE

$$\frac{\partial \rho}{\partial t} = \beta^{-1}\frac{\partial^2 \rho}{\partial x^2} + \theta\frac{\partial}{\partial x}\left((W' \star \rho)\rho\right), \tag{3}$$

- where $\mu_t(dx) = \rho(t,x)\,dx$.

The Fokker–Planck equation

- Hamiltonian: $H^N(x_1, \dots, x_N) := \frac{1}{2N} \sum_{i,j} W(x_i - x_j) + \sum_i V(x_i)$
- The generator of the process is
$$\mathcal{L} = -\nabla H^N \cdot \nabla + \beta^{-1} \Delta.$$
- Associated Fokker–Planck/forward Kolmogorov equation for the law $\nu^N = \mathrm{Law}(X_t^1, \dots, X_t^N)$:
$$\begin{cases} \partial_t \nu^N & = \beta^{-1} \Delta \nu^N + \nabla \cdot (\nabla H^N \nu^N), \quad (t, x) \in (0, \infty) \times (\mathbb{R}^d)^N \\ \nu^N(0) & = \nu_0^N = \nu_0^{\otimes N} \in \mathcal{P}((\mathbb{R}^d)^N) \end{cases}$$
- Initial data i.i.d.

The mean-field limit $N \to +\infty$

Consider the empirical measure : $\nu^{(N)} := \frac{1}{N}\sum_{i=1}^{N} \delta_{X_t^i} \in \mathcal{P}(\mathbb{R}^d)$. Easier to study $\mathbb{E}\left[\nu^{(N)}\right]$:

Theorem (The mean-field limit/propagation of chaos)

As $N \to \infty$, $\mathbb{E}\left[\nu^{(N)}\right]$ converges in weak-$\star$ to $\nu(t, \mathrm{d}x) = \nu(t,x)\,\mathrm{d}x$, which solves (weakly):

$$\partial_t \nu = \beta^{-1}\Delta\nu + \nabla\cdot(\nu(\nabla W \star \nu + \nabla V)) \qquad \text{(McKean–Vlasov equation)}$$

with initial datum $\nu_0 \in \mathcal{P}(\mathbb{R}^d)$.

Another interpretation: $\nu^N \to \nu^{\otimes N}$ as $N \to \infty$.

1. The McKean–Vlasov equation:
   1. Classical: McKean '66, Oelschläger '84, Gärtner '88, Sznitman '91 (coupling)
   2. Rates of convergence: Sznitman '91, Mouhot–Mischler '13, Hauray–Mischler '14, Eberle et al. '17 (coupling), Delgadino, Gvalani, P. (in preparation).
   3. Variational/$\Gamma-$convergence approaches (Messer-Spohn 1982, J.C. Carrillo, M. Delgadino, P., J. Func. analysis 2020).

The space $\mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N)$

Due to the indistinguishability assumption on the particles their joint law is invariant under relabelling of the particles. In probability this is known as exchangeability, i.e., the law $\nu^N \in \mathcal{P}_{\text{sym}}\big((\mathbb{R}^d)^N\big)$.
Question: Given some $\{\rho^N\}_{n\in\mathbb{N}} \in \mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N)$ what does $\lim_{N\to\infty} \rho^N$ mean?

Definition (The limit of of $\mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N)$)

Given a family $\{\rho^N\}_{N\in\mathbb{N}}$ such that $\rho^N \in \mathcal{P}_{\text{sym}}((\mathbb{R}^d)^N)$ we say that

$$\rho^N \to \boldsymbol{X} \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d)), \quad \text{as } N \to \infty,$$

if for every $n \in \mathbb{N}$ we have

$$\rho_n^N \rightharpoonup^* \boldsymbol{X}^n \in \mathcal{P}_{\text{sym}}\big((\mathbb{R}^d)^n\big), \quad \text{as } N \to \infty,$$

where $\boldsymbol{X}^n \in \mathcal{P}_{\text{sym}}\big((\mathbb{R}^d)^n\big)$ is defined by duality as follows

$$\langle \boldsymbol{X}^n, \varphi\rangle = \int_{\mathcal{P}(\mathcal{P}(\mathbb{R}^d))} \int \varphi \,\mathrm{d}\rho^{\otimes n} \;\mathrm{d}\boldsymbol{X}(\rho),$$

for all $\varphi \in C_b((\mathbb{R}^d)^n)$ and $\rho_n^N = \int_{(\mathbb{R}^d)^{N-n}} \rho^N \;\mathrm{d}x_{N-n+1}...dx_N \in \mathcal{P}_{\text{sym}}\big((\mathbb{R}^d)^n\big)$ is the n^{th} marginal of ρ^N

Another interpretation:

Definition (Empirical measure)

Given some $\rho^N \in \mathcal{P}_{\rm sym}((\mathbb{R}^d)^N)$ we define its empirical measure $\hat{\rho}^N \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ as follows:

$$\hat{\rho}^N := T_N \# \rho^N \, ,$$

where $T^N : (\mathbb{R}^d)^N \to \mathcal{P}(\mathbb{R}^d)$ is the measurable mapping $(x_1, \ldots, x_N) \mapsto N^{-1} \sum_{i=1}^N \delta_{x_i}$.
Futhermore, given a family $\{\rho^N\}_{N \in \mathbb{N}}$, we have that $\rho^N \to \boldsymbol{X} \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ if and only if $\hat{\rho}^N \rightharpoonup^* \boldsymbol{X}$, i.e tested against $C_b(\mathcal{P}(\mathbb{R}^d))$.

Lemma (de Finneti–Hewitt–Savage)

Given a sequence $\{\rho^N\}_{N \in \mathbb{N}}$, such that $\rho^N \in \mathcal{P}_{\rm sym}\left((\mathbb{R}^d)^N\right)$ for every N, assume that the sequence of the first marginals $\{\rho_1^N\}_{N \in \mathbb{N}} \in \mathcal{P}(\mathbb{R}^d)$ is tight. Then, up to subsequence, not relabelled, there exists $\boldsymbol{X} \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ such that $\rho^N \to \boldsymbol{X}$.

Conclusion: The limit of the space $\mathcal{P}_{\rm sym}((\mathbb{R}^d)^N)$ is $\mathcal{P}(\mathcal{P}(\mathbb{R}^d))$. Similarly the limit of $\mathcal{P}_{\rm sym}((\mathbb{T}^d)^N)$ is $\mathcal{P}(\mathcal{P}(\mathbb{T}^d))$.

Gradient flows

N-particle free energy, $E^N : \mathcal{P}_{\rm sym}((\mathbb{R}^d)^N) \to (-\infty,+\infty]$:

$$E^N[\rho^N] := \frac{1}{N}\left(\beta^{-1}\int_{(\mathbb{R}^d)^N} \rho^N \log \rho^N \, \mathrm{d}x + \int_{(\mathbb{R}^d)^N} H^N(x)\, \mathrm{d}\rho^N(x)\right),$$

ν^N is a gradient flow of E^N w.r.t rescaled 2-Wasserstein distance $\frac{1}{\sqrt{N}} d_2$ on $\mathcal{P}_{\rm sym}((\mathbb{R}^d)^N)$ (cf. Jordan–Kinderlehrer–Otto '98, Ambrosio–Gigli-Savare '08).
Mean field free energy $E_{MF} : \mathcal{P}(\mathbb{R}^d) \to (-\infty,+\infty]$:

$$E_{MF}[\rho] = \beta^{-1}\int_{\mathbb{R}^d} \rho \log(\rho)\, \mathrm{d}x + \int_{\mathbb{R}^d} V(x)\, \mathrm{d}\rho(x) + \frac{1}{2}\iint_{\mathbb{R}^d\times\mathbb{R}^d} W(x-y)\, \mathrm{d}\rho(y)\, \mathrm{d}\rho(x).$$

ν is a gradient flow of E_{MF} w.r.t 2-Wasserstein distance d_2 on $\mathcal{P}(\mathbb{R}^d)$.

Lemma (Messer–Spohn '82)

The N-particle free energy E^N Γ-converges to $E^\infty : \mathcal{P}(\mathcal{P}(\mathbb{R}^d)) \to (-\infty,+\infty]$, where

$$E^\infty[\boldsymbol{X}] = \int_{\mathcal{P}(\mathbb{R}^d)} E_{MF}[\rho]\, \mathrm{d}\boldsymbol{X}(\rho).$$

Gradient flow reformulation of the mean field limit

Similar analysis can be carried out for the quotiented system: $\tilde{E}^N$, $\tilde{E}_{MF}$ with particles living in $\mathbb{T}^d$. We consider the periodic N-particle energy $\tilde{E}^N$ and the periodic mean field energy $\tilde{E}_{MF}$. Then:

Lemma (Messer–Spohn '82)

The N-particle free energy $\tilde{E}^N$ Γ-converges to $\tilde{E}^\infty : \mathcal{P}(\mathcal{P}(\mathbb{T}^d)) \to (-\infty, +\infty]$, where

$$\tilde{E}^\infty[\boldsymbol{X}] = \int_{\mathcal{P}(\mathbb{T}^d)} \tilde{E}_{MF}[\rho] \, \mathrm{d}\boldsymbol{X}(\tilde{\nu}) \, .$$

As a consequence, if $\{M_N\}_{N\in\mathbb{N}}$ is the sequence of minimisers of $\tilde{E}^N$ (namely the sequence of Gibbs measures), then any accumulation point $\boldsymbol{X} \in \mathcal{P}(\mathcal{P}(\mathbb{T}^d))$ of this sequence is a minimiser of $\tilde{E}^\infty$.

Theorem (Mean field limit, Carrillo–Delgadino–P. J. Func. Analysis 2020)

Fix some $t > 0$, then, $\lim_{N\to\infty} \nu^N(t) = \boldsymbol{X} \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ Furthermore, we have that the curve $\boldsymbol{X} : [0,\infty) \to \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ is a gradient flow of E^∞ under the 2-Wasserstein metric $\mathfrak{D}_2$. Moreover, $\boldsymbol{X}_t = S_t \# X_0$, where $X_0 = \lim_{N\to\infty} \rho_0^{\varepsilon,N}$ and $S_t : \mathcal{P}(\mathbb{R}^d) \to \mathcal{P}(\mathbb{R}^d)$ is the solution semigroup associated to the nonlinear McKean–Vlasov evolution equation

$$\partial_t \nu = \beta^{-1} \Delta \nu + \nabla \cdot (\nu(\nabla W \star \nu + \nabla V)).$$

The diffusive limit $\varepsilon \to 0$

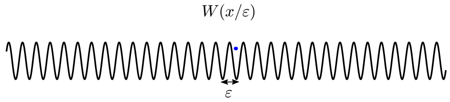
We consider the following system of weakly interacting diffusions with a periodic interaction potential:

$$\mathrm{d}X_t^{i,\varepsilon} = -\nabla V(\varepsilon^{-1} X_t^{i,\varepsilon}) - \frac{1}{N} \sum_{i \neq j}^{N} \nabla W(\varepsilon^{-1}(X_t^{i,\varepsilon} - X_t^{j,\varepsilon}))\, \mathrm{d}t + \sqrt{2\beta^{-1}}\, dB_t^i$$

with W, V chosen to be 1-periodic.
Let $\rho^{\varepsilon,N} = \mathrm{Law}(X_t^{1,\varepsilon}, \dots, X_t^{N,\varepsilon})$ and consider the diffusive rescaling

$$\rho^{\varepsilon,N}(x,t) := \varepsilon^{-Nd} \nu^N(\varepsilon^{-1} x, \varepsilon^{-2} t) \in \mathcal{P}((\mathbb{R}^d)^N)\,.$$

Interpretation: zooming out in space and looking at sufficiently long (diffusive) times.



Can pass to the limit:

- Bensoussan–Lions–Papanicolaou (1978), P.-Stuart (2008) (PDE approach)
- Kipnis–Varadhan 1986 (Probabilistic approach)

The 1d problem (Freidlin, Lifson-Jackson, 1962)

- Consider a single particle moving in a periodic potential

$$dX_t = -\sin(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t$$

- From the martingale central limit theorem it follows that the rescaled process converges weakly to a Brownian motion

$$\varepsilon X_{t/\varepsilon^2} \to \sqrt{2D_\beta}\,W_t$$

- where

$$D_\beta = \frac{\beta^{-1}}{Z_+\,Z_-}, \quad Z_\pm = \frac{1}{2\pi}\int_0^{2\pi} e^{\mp\cos(x)}\,dx.$$

- This formula was obtained by Lifson-Jackson (J. Chem. Phys., 1962) by doing a mean exit time calculation.
- Similar result in the multidimensional case. Upper and lower bounds on the covariance matrix of the effective Brownian motion

$$\frac{\beta^{-1}}{Z_+\,Z_-}\|\xi\|^2 \leq \langle D_\beta\xi,\xi\rangle \leq \beta^{-1}\|\xi\|^2, \quad \forall\,\xi\in\mathbb{R}^d.$$

- The analysis is based on the study of an appropriate Poisson equation.

The quotiented N-particle system

$$\mathrm{d}\dot{X}_t^i = -\nabla V(\dot{X}_t^i) - \frac{1}{N}\sum_{i\neq j}^{N} \nabla W(\dot{X}_t^i - \dot{X}_t^j)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,d\dot{B}_t^i\,,$$

$\dot{X}_t^i \in \mathbb{T}^d$ and $\dot{B}_t^i$ are $\mathbb{T}^d$-valued Wiener processes.
This is a reversible process with respect to the N-particle Gibbs measure

$$M_N(x) = \frac{e^{-H^N(x)}}{\int\limits_{\mathbb{T}^{dN}} e^{-H^N(y)}\,\mathrm{d}y}\,,$$

and the law $\tilde{\nu}^N$ evolves according to

$$\begin{cases} \partial_t \tilde{\nu}^N &= \beta^{-1}\Delta\tilde{\nu}^N + \nabla\cdot(\nabla H^N \tilde{\nu}^N), \quad (t,x)\in(0,\infty)\times(\mathbb{T}^d)^N \\ \tilde{\nu}^N(0) &= \tilde{\nu}_0^N := \sum_{k\in\mathbb{Z}^d} \nu_0^N(k+x) \in \mathcal{P}((\mathbb{T}^d)^N) \end{cases}$$

Periodic rearrangement of ν^N.

$\varepsilon \to 0$

Theorem (The diffusive limit)

Consider $\rho^{\varepsilon,N}$ *the solution to the rescaled Fokker–Planck equation with initial data* $\rho_0^{\varepsilon,N} \in \mathcal{P}((\mathbb{R}^d)^N)$. *Then, for all* $t > 0$ *the limit*

$$\rho^{N,*}(t) = \lim_{\varepsilon \to 0} \rho^{\varepsilon,N}(t)$$

exists. Furthermore, the curve of measures $\rho^{N,*} : [0,\infty) \to \mathcal{P}_{\mathrm{sym}}((\mathbb{R}^d)^N)$ *satisfies the heat equation*

$$\partial_t \rho^{N,*} = \nabla \cdot \left(A^{\mathrm{eff},N} \nabla \rho^{N,*}\right),$$

with initial data $\rho^{N,*}(0) = \lim_{\varepsilon \to 0} \rho_0^{\varepsilon,N}$ *and where the covariance matrix is given by the Kipnis–Varadhan formula*

$$A^{\mathrm{eff},N} = \beta^{-1} \int_{(\mathbb{T}^d)^N} \left(I + \nabla \Psi^N(y)\right) M_N(y) \; \mathrm{d}y ,$$

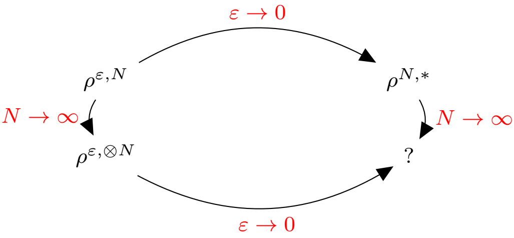
with M_N *the Gibbs measure of the quotiented* N *particle system and* $\Psi^N : \left(\mathbb{T}^d\right)^N \to \left(\mathbb{R}^d\right)^N$ *the unique mean zero solution to the associated corrector problem*

$$\nabla \cdot \left(M_N \nabla \Psi^N\right) = -\nabla M_N .$$

The diffusive limit is affected by the properties of the quotiented system on the torus!

$N \to \infty + \varepsilon \to 0$?

Question: $\lim_{N\to\infty} \rho^{N,*} = ?$.
We already know $\rho^{\varepsilon,N} \to \rho^{\varepsilon,\otimes N}, \quad N \to \infty$ where ρ^ε solves the rescaled McKean–Vlasov equation.
Another question : $\lim_{\varepsilon\to 0} \rho^{\varepsilon,\otimes N} \to ?$.



Theorem (Delgadino–Gvalani–P. ’20)

Assume that the quotiented system has a phase transition at some β_c. Then for $\beta < \beta_c$

$$\lim_{N\to\infty} \lim_{\varepsilon\to 0} \rho^{\varepsilon,N} = \lim_{\varepsilon\to 0} \lim_{N\to\infty} \rho^{\varepsilon,N} .$$

On the other hand if $\beta > \beta_c$, there exists initial data $\rho_0^{\varepsilon,\otimes N}$ such that

$$\lim_{N\to\infty} \lim_{\varepsilon\to 0} \rho^{\varepsilon,N} \neq \lim_{\varepsilon\to 0} \lim_{N\to\infty} \rho^{\varepsilon,N} .$$

Consider the periodic McKean–Vlasov equation:

$$\begin{cases} \partial_t \tilde{\nu} = \beta^{-1} \Delta \tilde{\nu} + \nabla \cdot (\tilde{\nu}(\nabla W \star \tilde{\nu} + \nabla V)) & (t,x) \in (0,\infty) \times \mathbb{T}^d \\ \tilde{\nu}(0) = \tilde{\nu}_0 = \sum_{k \in \mathbb{Z}^d} \nu_0(k+x)\,. \end{cases}$$

Definition (Phase transition)

The periodic mean field McKean–Vlasov equation is said to undergo a phase transition at some $0 < \beta_c < \infty$ if

1. For $\beta < \beta_c$, there exists a unique steady state.
2. For $\beta > \beta_c$, there exist at least two steady states.

The temperature β_c is referred to as the point of phase transition or the critical temperature.

Example (noisy Kuramoto model)

Let $d = 1$, $W = -\cos(2\pi x)$, *and* $V = 0$. *Then for* $\beta \leq 2$, $\tilde{\nu}_\infty \equiv 1$ *is the unique minimiser of* $\tilde{E}_{MF}$ *and steady state. For* $\beta > 2$, *the steady states are given by* $\tilde{\nu}_\infty \equiv 1$ *and the family of translates of some measure* $\tilde{\nu}_\beta^{\min}$. *Moreover for* $\beta > 2$, $\tilde{\nu}_\beta^{\min}$ *(and its translates) are the only minimisers of the periodic mean field energy* $\tilde{E}_{MF}$. *Thus,* $\beta_c = 2$ *is the critical temperature.*

see Carrillo–Gvalani–P.–Schlichting, ARMA, 235 (2020) 635-690 for a detailed study.

H-stability

Fourier representation $\tilde{f}(k) = \langle f, w_k \rangle_{L^2(T^d)}$ with $k \in \mathbb{Z}^d$

- A function $W \in L^2(T^d)$ is H**-stable**, $W \in \mathcal{H}_s$, if

$$\tilde{W}(k) = \langle W, w_k \rangle_{L^2(T^d)} \geq 0, \quad \forall k \in \mathbb{Z}^d \, ,$$

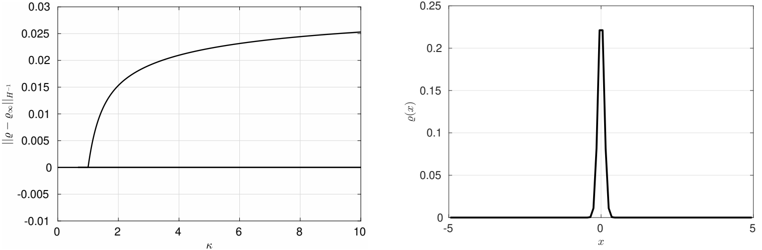
- We can characterize stationary states by studying the **Kirkwood-Monroe** fixed point mapping

$$F_\kappa(\varrho) = \varrho - \mathcal{T}\varrho = \varrho - \frac{1}{Z(\varrho, \kappa)} e^{-\beta\kappa W \star \varrho} \, , \quad \text{with} \quad Z(\varrho, \kappa) = \int_{T^d} e^{-\beta\kappa W \star \varrho} \, \mathrm{d}x \, .$$

- The uniform distribution is always a stationary state for the McKean-Vlasov equation on the torus.
- $W \in \mathcal{H}_s$ is a necessary condition for the existence of nontrivial steady states.

Nontrivial solutions to the stationary McKean–Vlasov equation?

Example: Kuramoto model: $W(x) = -\sqrt{\frac{2}{L}}\cos(2\pi x/L)$



$\Rightarrow$ 1-cluster solution and uniform state ϱ_∞.

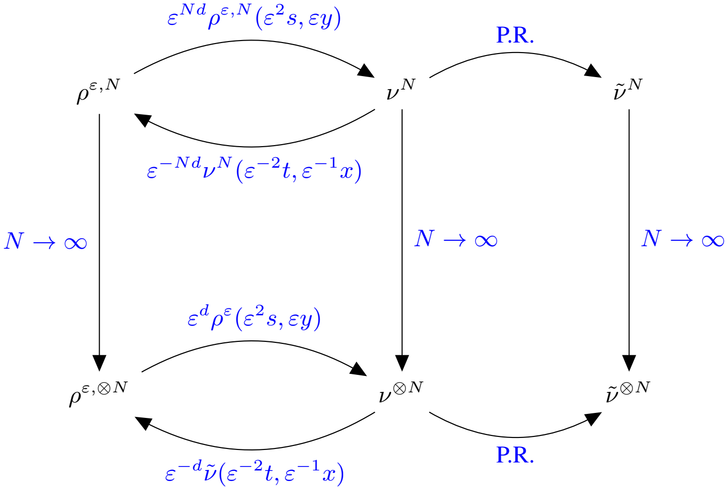
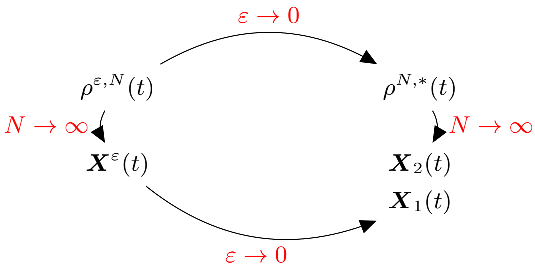


Figure: A schematic of the notation. The P.R. denotes periodic rearrangement.



- Question: Is $\boldsymbol{X}_1 = \boldsymbol{X}_2$?
- Non-commutativity observed numerically in Gomes–P. '18 based on numerics in slightly different setting (Dasai-Zwanzing in a two-scale confining potential).

Theorem (Delgadino–Gvalani–P. '20)

Consider the set of initial data given by $\{\rho_0^\varepsilon\}_{\varepsilon>0} \subset \mathcal{P}(\mathbb{R}^d)$*, and consider the periodic rearrangement at scale* $\varepsilon > 0$ *, i.e.*

$$\tilde{\nu}_0^\varepsilon(A) = \varepsilon^d \sum_{k\in\mathbb{Z}^d} \rho_0^\varepsilon(\varepsilon(A+k)) \qquad \text{for } \varepsilon > 0\,.$$

Assume that there exists $C > 0$*,* $p > 1$ *and* $\tilde{\nu}^* \in \mathcal{P}(\mathbb{T}^d)$ *such that* $\tilde{\nu}^\varepsilon(t)$*, with initial data* $\tilde{\nu}_0^\varepsilon(x)$*, satisfies*

$$\sup_{\varepsilon>0} d_2^2(\tilde{\nu}^\varepsilon(t), \tilde{\nu}^*) \leq Ct^{-p}\,.$$

Then,

$$\lim_{\varepsilon\to 0} d_2^2(S_t^\varepsilon \rho_0^\varepsilon, S_t^* \rho_0^*) = 0,$$

where S_t^ε *is the solution semigroup associated to the rescaled PDE on* $\mathbb{R}^d$*,* $\rho_0^* \in \mathcal{P}(\mathbb{R}^d)$ *is the weak-$*$ limit of* ρ_0^ε*, and* S_t^* *is the solution semigroup of the heat equation*

$$\partial_t \rho = \nabla\cdot(A_*^{\text{eff}}\nabla\rho),$$

where the covariance matrix

$$A_*^{\text{eff}} = \beta^{-1}\int_{\mathbb{T}^d}(I + \nabla\Psi^*(y))\ \mathrm{d}\tilde{\nu}^*(y)\,.$$

$N \to \infty$ then $\varepsilon \to 0$

Theorem (Delgadino–Gvalani–P. '20)

$\Psi^* : \mathbb{T}^d \to \mathbb{R}^d$ *is the solution to the associated corrector problem*

$$\nabla \cdot (\tilde{\nu}^* \nabla \Psi^*) = -\nabla \tilde{\nu}^* .$$

Furthermore, assume that $\boldsymbol{X}^\varepsilon(t)$ *is the mean field limit and that* $\lim_{N\to\infty} \rho_0^{\varepsilon,N} = \boldsymbol{X}_0^\varepsilon = \delta_{\rho_0^\varepsilon}$. *Then it holds that:*

$$\boldsymbol{X}_1(t) = \lim_{\varepsilon\to 0} \lim_{N\to\infty} \rho^{\varepsilon,N} = \lim_{\varepsilon\to 0} \boldsymbol{X}(t)^\varepsilon = S_t^* \# \boldsymbol{X}_0 \,,$$

where $\boldsymbol{X}_0 = \delta_{\rho_0^*}$.

Theorem (Delgadino–Gvalani–P. '20)

Assume that the periodic mean field energy $\tilde{E}_{MF}$ admits a unique minimiser $\tilde{\nu}^{\min}$, then we have that $\rho^{N,*}$ satisfies, for any fixed $t > 0$,

$$\lim_{N\to\infty} \rho^{N,*}(t) = \boldsymbol{X}_2(t) = S_t^{\min}\#\boldsymbol{X}_0,$$

where $\boldsymbol{X}_0 \in \mathcal{P}(\mathcal{P}(\mathbb{R}^d))$ is the limit of $\rho^{N,*}(0)$, and $S_t^{\min} : \mathcal{P}(\mathbb{R}^d) \to \mathcal{P}(\mathbb{R}^d)$ is the solution semigroup of the heat equation

$$\partial_t \rho = \nabla \cdot (A_{\min}^{\mathrm{eff}} \nabla \rho),$$

where the covariance matrix

$$A_{\min}^{\mathrm{eff}} = \beta^{-1} \int_{\mathbb{T}^d} (I + \nabla \Psi^{\min}(y)) \, \mathrm{d}\tilde{\nu}^{\min}(y)\,,$$

with $\Psi^{\min} : \mathbb{T}^d \to \mathbb{R}^d$, the solution to the associated corrector problem

$$\nabla \cdot (\tilde{\nu}^{\min} \nabla \Psi^{\min}) = -\nabla \tilde{\nu}^{\min}\,.$$

It follows then, that for any fixed $t > 0$, the solution $\rho^{\varepsilon,N}(t)$ satisfies

$$\boldsymbol{X}_2(t) = \lim_{N\to\infty} \lim_{\varepsilon\to 0} \rho^{\varepsilon,N}(t) = \lim_{N\to\infty} \rho^{N,*}(t) = S_t^{\min}\#X_0\,.$$

- The limit $\boldsymbol{X}_1(t)$ sees the long time behaviour of $\tilde{\nu}$ and thus steady states.
- The limit $\boldsymbol{X}_2(t)$ sees minimisers of $\tilde{E}_{MF}$.

Thus we can break commutativity ahead of the phase transition.

Example (A biased Kuramoto model)

Consider the model with $V = -\eta\cos(2\pi x), W = -\cos(2\pi x)$ *with* $\eta \in (0,1)$*. Then the mean field model on the torus has a phase transition at some* $0 < \beta_c < \infty$*. It has at least two steady states for* $\beta > \beta_c$*,* $\tilde{\nu}^*$ *and* $\tilde{\nu}^{\min}$ *the minimiser of* $\tilde{E}_{MF}$*.*

Additionally, for $\beta > \beta_c$ *and* $\rho_0^{\varepsilon,N} = (\rho_0^\varepsilon)^{\otimes N}$ *such that* $\tilde{\nu}^* = \sum_{k\in\mathbb{Z}^d} \varepsilon^d \rho_0^\varepsilon(\varepsilon x)$ *we have that*

$$\lim_{\varepsilon\to 0}\lim_{N\to\infty} \rho^{\varepsilon,N}(t) = \boldsymbol{X}_1(t) = S_t^* \# \boldsymbol{X}_0 \neq S_t^{\min} \# \boldsymbol{X}_0 = \boldsymbol{X}_2(t) = \lim_{N\to\infty}\lim_{\varepsilon\to 0} \rho^{\varepsilon,N}(t)\,.$$

Lemma

Consider the quotiented Kuramoto model for a fixed $\eta \in (0,1)$. Then there exists a $\beta = \beta_c$ such that:

- *For $\beta < \beta_c$, there exists a unique steady state given by*

$$\tilde{\nu}^{\min}(x) = Z_{\min}^{-1} e^{a^{\min}\cos(2\pi x)}\,, \qquad Z_{\min} = \int_{\mathbb{T}} e^{a^{\min}\cos(2\pi x)}\, \mathrm{d}x\,, \tag{4}$$

  for some $a^{\min} = a^{\min}(\beta), a^{\min} > 0$, which is the unique minimiser of the periodic mean field energy $\tilde{E}_{MF}$.

- *For $\beta > \beta_c$, there exist at least 2 steady states given by*

$$\tilde{\nu}^{\min}(x) = Z_{\min}^{-1} e^{a^{\min}\cos(2\pi x)}\,, \qquad Z_{\min} = \int_{\mathbb{T}} e^{a^{\min}\cos(2\pi x)}\, \mathrm{d}x\,, \tag{5}$$

$$\tilde{\nu}^{*}(x) = Z_{*}^{-1} e^{a^{*}\cos(2\pi x)}\,, \qquad Z_{*}^{-1} = \int_{\mathbb{T}} e^{a^{*}\cos(2\pi x)}\, \mathrm{d}x\,, \tag{6}$$

  where $a^* < 0 < a^{\min}$ and both constants depend on β. Here $\tilde{\nu}^{\min}$ is the unique minimiser and $\tilde{\nu}^*$ is a non-minimising critical points of the periodic mean field energy $\tilde{E}_{MF}$. Moreover, $a^* \neq -a^{\min}$.

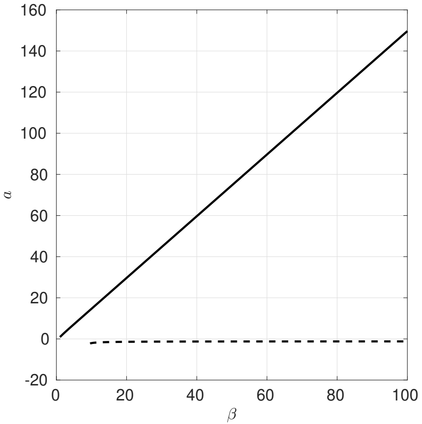


Figure: $a^{\min}$ (solid line) and a^* (dotted line) for $\eta = 0.5$. The two effective diffusion coefficients are $A_*^{\text{eff}} = \frac{\beta^{-1}}{I_0(-a^*)^2}$ and $A_{\min}^{\text{eff}} = \frac{\beta^{-1}}{I_0(a^{\min})^2}$.

Sketch of proof for $N \to \infty$ followed by $\varepsilon \to 0$

- Pass to the mean field limit to obtain $\boldsymbol{X}^{\varepsilon}(t)$.
- For the associated mean field SDE on the torus consider a moving corrector problem:

$$\nabla \cdot (\tilde{\mu}^{\varepsilon}(t) \nabla \chi) = -\nabla(\tilde{\mu}^{\varepsilon}) , \quad \tilde{\mu}^{\varepsilon}(t) \sim \exp(-\beta(W \star \tilde{\nu}(t) - V))$$

  and obtain time-dependent estimates:

$$\|\chi_i\|_{C^m(\mathbb{T}^d)} \lesssim 1$$
$$\|\partial_t \chi_i\|_{C^m(\mathbb{T}^d)} \lesssim \sum_{m=1}^{k} d_2^m(\tilde{\nu}(t), \tilde{\nu}^*) .$$

- Using coupling techniques (a' la Eberle et al.) prove an initial data dependent version of the martingale CLT.
- Pass to the limit as $\varepsilon \to 0$.

Sketch of proof for $\varepsilon \to 0$ followed by $N \to \infty$

- Need to pass to the limit in the diffusion matrix $A^{\mathrm{eff,N}}$:

$$A^{\mathrm{eff},N} = \beta^{-1} \int_{(\mathbb{T}^d)^N} (I + \nabla \Psi^N(y))\, M_N(y)\, \mathrm{d}y\,.$$

- Key idea $M_N \approx M_{N-1}(M_N)_1$ as $N \to \infty$ + natural uniform in N estimate on Ψ^N:

$$\begin{aligned}
&\int_{(\mathbb{T}^d)^N} (I + \nabla \Psi^N(y))\, \left(M_N - M_{N-1}(M_N)_1\right)\, \mathrm{d}y \\
&= \int_{(\mathbb{T}^d)^N} (I + \nabla \Psi^N(y))\, \left(\frac{M_N}{M_{N-1}} - (M_N)_1\right) M_{N-1}\, \mathrm{d}y \\
&\leq \left\| I + \nabla \Psi^N \right\|_{L^2(M_{N-1})} \left\| \left(\frac{M_N}{M_{N-1}} - (M_N)_1\right) \right\|_{L^2(M_{N-1})}\,.
\end{aligned}$$

- The function $M_N/(M_{N-1})$ is symmetric in all but one of its variables. Use techniques due to Lions pass to $N \to \infty$ on $C(\mathcal{P}(\mathbb{T}^d))$. Similarly pass to $N \to \infty$ to obtain $M_{N-1} \to \delta_{\tilde{\nu}^{\min}} \in \mathcal{P}(\mathcal{P}(\mathbb{T})^d)$.
- Enough information to pass to the limit in the PDE.

PHASE TRANSITIONS, LOGARITHMIC SOBOLEV INEQUALITIES, AND UNIFORM-IN-TIME PROPAGATION OF CHAOS FOR WEAKLY INTERACTING DIFFUSIONS

BY MATÍAS G. DELGADINO[1], RISHABH S. GVALANI[2], GRIGORIOS A. PAVLIOTIS[3] AND SCOTT A. SMITH[4]

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Abstract In this article, we study the mean field limit of weakly interacting diffusions for confining and interaction potentials that are not necessarily convex. We explore the relationship between the large N limit of the constant in the logarithmic Sobolev inequality (LSI) for the N-particle system and the presence or absence of phase transitions for the mean field limit. The non-degeneracy of the LSI constant is shown to have far reaching consequences,

We consider $\{X_t^i\}_{i=1,\dots,N} \subset \mathbb{R}^d$, the positions of N indistinguishable interacting particles at time $t \geq 0$, satisfying the following system of SDEs:

$$\begin{cases} dX_t^i = -\nabla V(X_t^i)\,\mathrm{d}t - \dfrac{1}{N}\displaystyle\sum_{j=1}^{N} \nabla_1 W(X_t^i, X_t^j)\,\mathrm{d}t + \sqrt{2\beta^{-1}}dB_t^i \\ \mathrm{Law}(X_0^1, \dots, X_0^N) = \rho_{\mathrm{in}}^{\otimes N} \in \mathcal{P}_{2,\mathrm{sym}}((\mathbb{R}^d)^N), \end{cases} \tag{7}$$

where $V : \mathbb{R}^d \to \mathbb{R}$, $W : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $\beta^{-1} > 0$ is the inverse temperature, $B_t^i, i = 1, \dots, N$ are independent d-dimensional Brownian motions, and the initial position of the particles is i.i.d with law ρ_{in}.

Assumption

The confining potential V is lower semicontinuous, bounded below, K_V-convex for some $K_V \in \mathbb{R}$ and there exists $R_0 > 0$ and $\delta > 0$, such that $V(x) \geq |x|^\delta$ for $|x| > R_0$.

Assumption

The interaction potential W is lower semicontinuous, K_W-convex for some $K_W \in \mathbb{R}$, bounded below, symmetric $W(x,y) = W(y,x)$, vanishes along the diagonal $W(x,x) = 0$, and there exists C such that

$$|\nabla_1 W(x,y)| \leq C(1 + |W(x,y)| + V(x) + V(y)) \tag{8}$$

Theorem

Under A1,A2, we have

$$\limsup_{N\to\infty} \lambda_{\mathrm{LSI}}^N \le \lambda_{\mathrm{LSI}}^\infty. \tag{9}$$

Moreover, if the mean field energy $E^{MF} : \mathcal{P}(\Omega) \to \mathbb{R} \cup \{+\infty\}$ *given by*

$$E^{MF}[\rho] := \beta^{-1} \int_\Omega \rho \log(\rho) \, \mathrm{d}x + \frac{1}{2} \int_{\Omega^2} W(x,y) \, \mathrm{d}\rho(x) \, \mathrm{d}\rho(y) + \int_\Omega V(x) \, \mathrm{d}\rho(x) \,, \tag{10}$$

admits a critical point that is not a minimiser, then $\lambda_{\mathrm{LSI}}^\infty = 0$*, and there exists* $C > 0$ *such that*

$$\lambda_{\mathrm{LSI}}^N \le \frac{C}{N}. \tag{11}$$

- We often need to learn parameters in SDEs from data.
- For multiscale diffusions standard inference methodologies are biased due to the incompatibility between the homogenized model and the data at small scales (P.-Stuart '07, P.-Papavasiliou-Stuart '09).
- Maximum likelihood, together with appropriate filtering/subsampling of the data leads to unbiased estimators (Abdulle et al 2021).
- Alternative approach based on eigenfunction estimators.
- Goal: learn parameters in (multiscale) mean field SDEs using data from single trajectories.
- Fluctuations around the mean field limit play in important role in the analysis of these estimators.

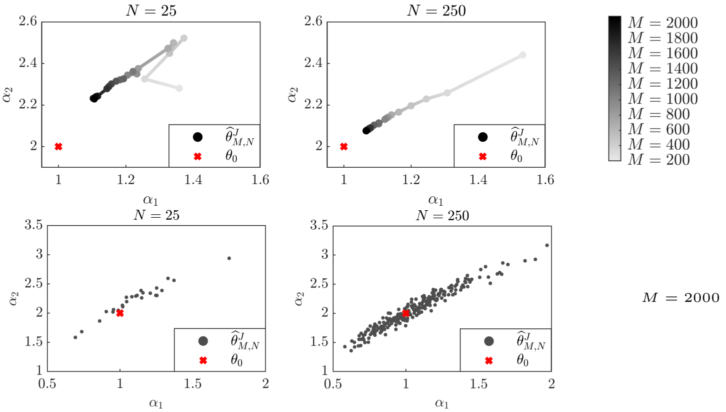
- *Drift estimation of multiscale diffusions based on filtered data* A Abdulle, G Garegnani, GA Pavliotis, AM Stuart, A Zanoni Foundations of Computational Mathematics, 1-52 4 2021
- *Parameter Estimation for the McKean Stochastic Differential Equation* L Sharrock, N Kantas, P Parpas, GA Pavliotis arXiv preprint arXiv:2106.13751 2021
- *Eigenfunction martingale estimating functions and filtered data for drift estimation of discretely observed multiscale diffusions* A Abdulle, GA Pavliotis, A Zanoni, Preprint (2021).

Eigenfunction martingale estimator

Problem: estimate parameters of interacting particle systems given discrete observations of one single particle

Idea: employ martingale estimating functions based on eigenfunctions and eigenvalues of the linearized generator of the *mean field limit*

Example: bistable confining potential and quadratic interaction



Top of fig:bistable: evolution of the estimator varying the number of observations M for $N = 25$ and $N = 250$, the estimator approaches the correct drift coefficient α as the number