## Imperial College London

MEAN FIELD LIMITS OF INTERACTING DIFFUSIONS IN TWO-SCALE POTENTIALS<br>LMS EPSRC DURHAM SYMPOSIUM

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- Mean field limits for interacting diffusions in a two-scale potential (S.N. Gomes and G.A. Pavliotis), Preprint (2017)
- Brownian motion in an N -scale periodic potential (A.B. Duncan and G.A. Pavliotis). Submitted to SIAM J MMS (2016).

O Noise-induced transitions in rugged energy landscapes (A.B. Duncan, S. Kalliadasis, G.A. Pavliotis, M. Pradas). Phys. Rev. E, 94, 032107 (2016).

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## EPSRC



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## Stochastic

 Processes and ApplicationsDiffusion Processes, the Fokker-Planck and Langevin Equations

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We consider a system of weakly interacting diffusions moving in a 2 -scale locally periodic potential:

$$
\begin{equation*}
d X_{t}^{i}=-\nabla V^{\epsilon}\left(X_{t}^{i}\right) d t-\frac{1}{N} \sum_{j=1}^{N} \nabla F\left(X_{t}^{i}-X_{t}^{j}\right) d t+\sqrt{2 \beta^{-1}} d B_{t}^{i}, \quad i=1, . ., \Lambda \tag{1}
\end{equation*}
$$

O where

$$
\begin{equation*}
V^{\epsilon}(x)=V_{0}(x)+V_{1}(x, x / \epsilon) \tag{2}
\end{equation*}
$$

Our goal is to study the combined mean-field/homogenization limits.

- In particular, we want to study bifurcations/phase transitions for the McKean-Vlasov equation in a confining potential with many local minima.


Figure: Bistable potential with (left) separable and (right) nonseparable fluctuations,

$$
V^{\epsilon}(x)=\frac{x^{4}}{4}-\frac{x^{2}}{2}+\delta \cos \left(\frac{x}{\epsilon}\right) \quad \text { and } \quad V^{\epsilon}(x)=\frac{x^{4}}{4}-\left(1-\delta \cos \left(\frac{x}{\epsilon}\right)\right) \frac{x^{2}}{2} .
$$

## MCKEAN-VLASOV DYNAMICS IN A BISTABLE POTENTIAL

Consider a system of interacting diffusions in a bistable potential:

$$
\begin{equation*}
d X_{t}^{i}=\left(-V^{\prime}\left(X_{t}^{i}\right)-\theta\left(X_{t}^{i}-\frac{1}{N} \sum_{j=1}^{N} X_{t}^{j}\right)\right) d t+\sqrt{2 \beta^{-1}} d B_{t}^{i} \tag{3}
\end{equation*}
$$

O The total energy (Hamiltonian) is

$$
\begin{equation*}
W_{N}(\mathbf{X})=\sum_{\ell=1}^{N} V\left(X^{\ell}\right)+\frac{\theta}{4 N} \sum_{n=1}^{N} \sum_{\ell=1}^{N}\left(X^{n}-X^{\ell}\right)^{2} \tag{4}
\end{equation*}
$$

- We can pass rigorously to the mean field limit as $N \rightarrow \infty$ using, for example, martingale techniques, (Dawson 1983, Gartner 1988, Oelschlager 1984).
- Formally, using the law of large numbers we obtain the McKean SDE

$$
\begin{equation*}
d X_{t}=-V^{\prime}\left(X_{t}\right) d t-\theta\left(X_{t}-\mathbb{E} X_{t}\right) d t+\sqrt{2 \beta^{-1}} d B_{t} \tag{5}
\end{equation*}
$$

- The Fokker-Planck equation corresponding to this SDE is the McKean-Vlasov equation

$$
\begin{equation*}
\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}\left(V^{\prime}(x) p+\theta\left(x-\int_{\mathbb{R}} x p(x, t) d x\right) p+\beta^{-1} \frac{\partial p}{\partial x}\right) . \tag{6}
\end{equation*}
$$

O The McKean-Vlasov equation is a gradient flow, with respect to the Wasserstein metric, for the free energy functional
$\mathcal{F}[\rho]=\beta^{-1} \int \rho \ln \rho d x+\int V \rho d x+\frac{\theta}{2} \iint F(x-y) \rho(x) \rho(y) d x d y$,
with $F(x)=\frac{1}{2} x^{2}$.

The finite dimensional dynamics (3) is reversible with respect to the Gibbs measure

$$
\begin{equation*}
\mu_{N}(d x)=\frac{1}{Z_{N}} e^{-\beta W_{N}\left(x^{1}, \ldots x^{N}\right)} d x^{1} \ldots d x^{N}, \quad Z_{N}=\int_{\mathbb{R}^{N}} e^{-\beta W_{N}\left(x^{1}, \ldots x^{N}\right)} \tag{8}
\end{equation*}
$$

o where $W_{N}(\cdot)$ is given by (4).
O the McKean dynamics (5) can have more than one invariant measures, for nonconvex confining potentials and at sufficiently low temperatures (Dawson1983, Tamura 1984, Shiino 1987, Tugaut 2014).

- The density of the invariant measure(s) for the McKean dynamics (5) satisfies the stationary nonlinear Fokker-Planck equation

$$
\begin{equation*}
\frac{\partial}{\partial x}\left(V^{\prime}(x) p_{\infty}+\theta\left(x-\int_{\mathbb{R}} x p_{\infty}(x) d x\right) p_{\infty}+\beta^{-1} \frac{\partial p_{\infty}}{\partial x}\right)=0 \tag{9}
\end{equation*}
$$

- For the quadratic interaction potential a one-parameter family of solutions to the stationary McKean-Vlasov equation (9) can be obtained:

$$
\begin{align*}
p_{\infty}(x ; \theta, \beta, m) & =\frac{1}{Z(\theta, \beta ; m)} e^{-\beta\left(V(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)},(10 \mathrm{a}) \\
Z(\theta, \beta ; m) & =\int_{\mathbb{R}} e^{-\beta\left(V(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)} d x \tag{10b}
\end{align*}
$$

These solutions are subject, to the constraint that they provide us with the correct formula for the first moment:

$$
\begin{equation*}
m=\int_{\mathbb{R}} x p_{\infty}(x ; \theta, \beta, m) d x=: R(m ; \theta, \beta) \tag{11}
\end{equation*}
$$

This is the selfconsistency equation.

- The critical temperature can be calculated from

$$
\begin{equation*}
\left.\operatorname{Var}_{p_{\infty}}(x)\right|_{m=0}=\frac{1}{\beta \theta} \tag{12}
\end{equation*}
$$




Figure: Plot of $R(m ; \theta, \beta)$ and of the straight line $y=x$ for $\theta=0.5$, $\beta=10$, and bifurcation diagram of $m$ as a function of $\beta$ for $\theta=0.5$ for the bistable potential $V(x)=\frac{x^{4}}{4}-\frac{x^{2}}{2}$ and interaction potential $F(x)=\frac{x^{2}}{2}$.

## BROWNIAN PARTICLES IN A TWO-SCALE POTENTIAL

- Dynamics given by Itô SDE:

$$
d X_{t}^{\epsilon}=-\nabla V^{\epsilon}\left(X_{t}^{\epsilon}\right) d t+\sqrt{2 \beta^{-1}} d W_{t}
$$

$\bigcirc$ For $\epsilon \ll 1, V^{\epsilon}$ models a "rough" potential:

$$
V^{\epsilon}(x):=V\left(x, \frac{x}{\epsilon}, \frac{x}{\epsilon^{2}}, \ldots, \frac{x}{\epsilon^{N}}\right)
$$

for a smooth function $V\left(x_{0}, y_{1}, \ldots, y_{N}\right)$.

- $x_{0}$ : slowly-varying structure of potential.
- $y_{1}, \ldots, y_{N}$ : multiscale periodic fluctuations occuring at different scales.


## LONG-TIME BEHAVIOUR OF THE SLOW-FAST DYNAMICS

$X_{t}^{\epsilon}$ is a Markov diffusion process with infinitesimal generator defined by

$$
\mathcal{L}^{\epsilon} f=\beta^{-1} e^{\beta V^{\epsilon}(x)} \nabla \cdot\left(e^{-\beta V^{\epsilon}(x)} \nabla f(x)\right) .
$$

Stationary distribution satisfies the stationary Fokker-Planck equation:

$$
\nabla \cdot\left(e^{-\beta V^{\epsilon}(x)} \nabla\left(\pi^{\epsilon}(x) e^{\beta V^{\epsilon}(x)}\right)=0, \quad x \in \mathbb{R}^{d}\right.
$$

Suppose $Z^{\epsilon}=\int_{\mathbb{R}^{d}} e^{-\beta V^{\epsilon}(x)} d x<\infty$,
$X_{t}^{\epsilon}$ is ergodic, with stationary density $\pi^{\epsilon}(x)=\frac{1}{Z^{\epsilon}} e^{-\beta V^{\epsilon}(x)}$.
$X_{t}^{\epsilon}$ satisfies detailed balance with respect to $\pi^{\epsilon}(x)$, i.e.
Stationary Probability Flux $=\nabla \cdot\left(\pi^{\epsilon}(x) e^{\beta V^{\epsilon}(x)}\right)=0, \quad \forall x \in \mathbb{R}^{d}$.

## QUESTIONS AND OBJECTIVES

Questions:

- Can behaviour of $X_{t}^{\epsilon}$ for small $\epsilon$ be approximated by some $X_{t}^{0}$ ?
$X_{t}^{\epsilon}$ ergodic $\Rightarrow X_{t}^{0}$ ergodic?
- Relationship between $\pi^{\epsilon}(\cdot)$ and $\pi^{0}(\cdot)$ ?
- Asymptotic behaviour of other quantities related to $X_{t}^{\epsilon}$,
- Observables of $X_{t}^{\epsilon}$, e.g. reaction coordinates.
- Mean First Passage Time (MFPT), as $\epsilon \rightarrow 0$.

Approach:
O Formal approach: Asymptotic expansions of the Kolmogorov Backward Equation for $X_{t}^{\epsilon}$ in powers of $O\left(\epsilon^{-1}\right)$.
$\bigcirc$ Rigorous Approach: probabilistic techniques for locally-periodic homogenization, [Bensoussans, Lyons, Papanicolau, 1979], [Pardoux, 1999], [Pardoux, Veretennikov, 2001], [Bencherif-Madani, Pardoux, 2003].

## THE HOMOGENIZATION THEOREM

To prove the existence of the limit of $X_{t}^{\epsilon}$ as $\epsilon \rightarrow 0$, we make the following assumptions on $V$.

- There exist confining potentials $M_{0}(x)$ and $M_{1}(x)$ such that

$$
M_{0}(x) \leq V\left(x, y_{1}, \ldots, y_{N}\right) \leq M_{1}(x), \quad \forall x \in \mathbb{R}^{d}, y_{1}, \ldots y_{N} \in \mathbb{T}^{d}
$$

$V\left(x, y_{1}, \ldots, y_{N}\right)$ is smooth in all variables (can be relaxed).
$\bigcirc$ The gradient of the potential is Lipschitz in $x$, i.e.

$$
\left|\nabla V\left(x, y_{1}, \ldots, y_{N}\right)-\nabla V\left(x^{\prime}, y_{1}, \ldots, y_{N}\right)\right| \leq C\left|x-x^{\prime}\right|
$$

$\left|\nabla V\left(x, y_{1}, \ldots, y_{N}\right)\right| \leq C^{\prime}|x|$, for some $C, C^{\prime}$ for all $x, x^{\prime} \in \mathbb{R}$, $y_{1}, \ldots, y_{N} \in \mathbb{T}^{d}$.

## HOMOGENIZATION THEOREM

The limiting dynamics can be characterized by the following Itô SDE:
$d X_{t}^{0}=-\mathcal{K}\left(X_{t}^{0}\right) \nabla \Psi\left(X_{t}^{0}\right) d t+\beta^{-1} \nabla \cdot \mathcal{K}\left(X_{t}^{0}\right) d t+\sqrt{2 \beta^{-1} \mathcal{K}\left(X_{t}^{0}\right)} d W_{t}$, where $\Psi$ is the free energy $\Psi(x)=-\beta^{-1} \log Z(x)$.
O The limiting SDE corresponds to the Klimontovich interpretation of the stochastic integral.
$\bigcirc X_{t}^{0}$ satisfies detailed balance with respect to the invariant measure

$$
\pi^{0}(x)=\frac{1}{\mathcal{Z}} e^{-\Psi(x)}=\frac{Z(x)}{\mathcal{Z}}, \quad \mathcal{Z}=\int Z\left(x^{\prime}\right) d x^{\prime}
$$

For all $e \in \mathbb{R}^{d}$, with $\hat{Z}(x)=\int \cdots \int e^{\beta V\left(x, y_{1}, \ldots, y_{N}\right)} d y_{N} \ldots d y_{1}$ :

$$
\frac{|e|^{2}}{Z(x) \hat{Z}(x)} \leq e \cdot \mathcal{K}(x) e \leq|e|^{2}
$$

## HOMOGENIZATION THEOREM

As $\epsilon \rightarrow 0$, the process $X_{t}^{\epsilon}$ converges weakly in $C\left([0, T], \mathbb{R}^{d}\right)$ to a diffusion process $X_{t}^{0}$ having generator defined by

$$
\mathcal{L}^{0} f(x)=\frac{\beta^{-1}}{Z(x)} \nabla_{x} \cdot\left(Z(x) \mathcal{K}(x) \nabla_{x} f(x)\right), \quad f \in C_{c}^{2}\left(\mathbb{R}^{d}\right)
$$

where $Z(x)=\int \cdots \int e^{-\beta V(x, \ldots)} d y_{N} \ldots d y_{1}$, and

$$
\mathcal{K}(x)=I+\frac{1}{Z(x)} \int_{\mathbb{T}^{d}} \cdots \int_{\mathbb{T}^{d}}\left(I+\nabla_{x_{N}} \theta_{N}^{\top}\right) \cdots\left(I+\nabla_{x_{1}} \theta_{1}^{\top}\right) e^{-\beta V} d y_{N} \ldots d y_{1}
$$

and $\theta_{k}$ are mean-zero solutions of the following Poisson equations on $\mathbb{T}^{d}$ :

$$
\nabla_{y_{k}} \cdot\left(\mathcal{K}_{k}\left(\nabla_{y_{k}} \theta_{k}+I\right)\right)=0, \quad y \in \mathbb{T}^{d}
$$

where $\mathcal{K}_{N}\left(x, y_{1}, \ldots, y_{N}\right)=e^{-\beta V\left(x, y_{1}, \ldots, y_{N}\right)} /$ and
$\mathcal{K}_{k}\left(x, y_{1}, \ldots, y_{k}\right)=\int\left(I+\nabla_{N} \theta_{N}^{\top}\right) \cdots\left(I+\nabla_{k+1} \theta_{k+1}^{\top}\right) e^{-\beta V} d y_{N} \ldots d y_{k+1}$.

## PROOF OF THE HOMOGENIZATION THEOREM

Slight generalisation of classical martingale approach to homogenization, applied to SDEs with locally-periodic coefficients having $N$-scales.

## Rough idea:

1. The slow-fast system is the solution to the following martingale problem:

$$
\mathbb{E}_{X}\left[\phi^{\epsilon}\left(X_{t}^{\epsilon}\right)-\int_{s}^{t} \mathcal{L}^{\epsilon} \phi^{\epsilon}\left(X_{u}^{\epsilon}\right) d u \mid \mathcal{F}_{s}\right]=\phi^{\epsilon}\left(X_{s}^{\epsilon}\right), \quad \forall \phi^{\epsilon} \in \mathcal{D}\left(\mathcal{L}^{\epsilon}\right)
$$

Construct a test function
$\phi^{\epsilon}(x)=\phi_{0}(x)+\epsilon \phi_{1}(x, x / \epsilon)+\ldots+\epsilon^{N} \phi_{N}\left(x, x / \epsilon, \ldots, x / \epsilon^{N}\right)+\ldots$
such that

$$
\mathcal{L}^{\epsilon} \phi^{\epsilon}(x)=\mathcal{L}^{0} \phi_{0}(x)+\epsilon R^{\epsilon}(x)
$$

where $E_{x}\left[\epsilon R^{\epsilon}\left(X_{u}^{\epsilon}\right)\right] \rightarrow 0$, as $\epsilon \rightarrow 0$.

## PROOF OF THE HOMOGENIZATION THEOREM CTD.

1. If the set of measures $\mathbb{P}^{\epsilon}$ on $C\left([0, T], \mathbb{R}^{d}\right)$ corresponding to the processes $\left\{X_{t}^{\epsilon}, t \in[0, T]\right\}$ possesses a limit point $X_{t}^{0}$ then it is the unique solution of the following martingale problem

$$
\mathbb{E}_{X}\left[\phi_{0}\left(X^{0}\right)-\int_{s}^{t} \mathcal{L}^{0} \phi_{0}\left(X_{u}^{\epsilon}\right) d u \mid \mathcal{F}_{s}\right]=\phi_{0}\left(X_{s}^{\epsilon}\right), \quad \forall \phi \in \mathcal{D}\left(\mathcal{L}^{0}\right) .
$$

2. Show that $\left\{X_{t}^{\epsilon}\right\}_{\epsilon>0}$ possesses an accumulation point. i.e. Establish tightness of the family of processes in $\left\{X_{t}^{\epsilon}\right\}_{\epsilon>0}$.

## CRITICAL POINTS OF THE INVARIANT DISTRIBUTION

- we want to calculate the critical points of the stationary distribution:

$$
\nabla Z(x ; \beta)=0
$$

- Multiplicative noise can change the location and number of the critical points.
- We distinguish between two cases:

1. Separable Potential: the fluctuations and large scale parts of the potential are uncoupled:

$$
V^{\epsilon}(x)=V_{0}(x)+V_{1}\left(x / \epsilon, x / \epsilon^{2}, \ldots x / \epsilon^{N}\right) .
$$

In this case:

$$
Z(x) \propto \int \cdots \int e^{-\beta V\left(x, y_{1}, \ldots y_{N}\right)} d y_{N} \ldots d y_{1} \propto e^{-V_{0}(x)} .
$$

and $\mathcal{K}$ is independent of $x$. Rapid fluctuations do not alter stationary behaviour, but only speed of convergence to equilibrium and effective diffusion tensor.
2. Nonseparable potential. In this case

$$
Z(x) \nprec e^{-V_{0}(x)}, \quad \text { in general. }
$$

Rapid fluctuations can change the critical points of the stationary distribution.

## TOY EXAMPLE: ID DOUBLE WELL POTENTIAL

Consider the ODE in $\mathbb{R}$ :

$$
\dot{x}(t)=-\frac{d}{d x} V_{0}(x ; \alpha), \quad t>0
$$

where $V_{0}(x ; \alpha)=-\frac{\alpha}{2} x^{2}+\frac{1}{4} x^{4}$, corresponding to the invariant density $e^{-\beta V(x)}$.

- Normal form for supercritical pitchfork bifurcation.$\alpha<0$ : One stable equilibrium at $x=0$.
○ $\alpha>0$ : Stable equilibria at $x= \pm \sqrt{\alpha}$. Unstable
 equilibrium at $x=0$.


## 1D DOUBLE WELL POTENTIAL

Consider the ODE in $\mathbb{R}$ :

$$
\dot{x}(t)=-\frac{d}{d x} V_{0}(x ; \alpha), \quad t>0,
$$

where $V_{0}(x ; \alpha)=-\frac{\alpha}{2} x^{2}+\frac{1}{4} x^{4}$.
Add multiscale fluctuations $V^{\epsilon}(x ; \alpha)=V(x, x / \epsilon ; \alpha)$, where

$$
V(x, y ; \alpha)=\frac{1}{4} x^{4}-\left(\frac{\alpha+\sin (2 \pi y)}{2}\right) x^{2} .
$$

Thermal motion in potential:

$$
d X_{t}^{\epsilon}=-\frac{d V^{\epsilon}}{d x}\left(X_{t}^{\epsilon}\right) d t+\sqrt{2 \beta^{-1}} d W_{t} .
$$

## 1D DOUBLE WELL POTENTIAL

By previous theory, $X_{t}^{\epsilon} \Rightarrow X_{t}^{0}$, as $\epsilon \rightarrow 0$, where $X_{t}^{0}$ is ergodic with stationary distribution

$$
\pi^{0}(d x) \propto Z(x) d x
$$

Can show that

$$
\pi^{0}(x) \propto \underbrace{e^{\beta\left(\frac{\alpha^{2} x^{2}}{2}-\frac{x^{4}}{4}\right)}}_{\pi_{0}(x)} / \underbrace{\left(0, \frac{x^{2}}{2 \beta^{-1}}\right)}_{\text {correction }}
$$

where $I$ is the modified Bessel function of the first kind.
Varying the intensity of the noise can alter the equilibrium properties of the system, i.e. the critical points of the stationary distribution.

## 1D DOUBLE WELL POTENTIAL

The strength of the noise now plays an interesting role in the dynamics.


Figure: $\beta^{-1}=1.0$

## 1D DOUBLE WELL POTENTIAL

The strength of the noise now plays an interesting role in the dynamics.


Figure: $\beta^{-1}=10^{-1}$

## 1D DOUBLE WELL POTENTIAL

The strength of the noise now plays an interesting role in the dynamics.


Figure: $\beta^{-1}=5 \cdot 10^{-2}$

## 1D DOUBLE WELL POTENTIAL

More generally: consider an $N$-scale potential

$$
V^{\epsilon}(x ; \alpha)=V_{0}(x ; \alpha)-\frac{1}{2} \sum_{n=1}^{N} \sin \left(\frac{2 \pi x}{\epsilon^{n}}\right) x^{2}
$$



Figure: Bifurcation diagram for a different number $N$ of microscopic scales in the potential

## 1D DOUBLE WELL POTENTIAL

Stationary PDF of homogenized dynamics is:

$$
Z_{N}(x ; \alpha) \propto e^{-\beta V_{0}(x ; \alpha)} /\left(0, \frac{x^{2}}{2 \beta^{-1 / 2}}\right)^{N}
$$




Figure: Phase diagram for $\alpha$ and $\sigma$

## EFFECT OF NUMBER OF SCALES ON DIFFUSIVITY TENSOR

As the number of scales increase, the effective diffusivity $K(x)$ decreases.
Must increase temperature $\beta^{-1}$ to overcome "trapping effect" of regions of slow diffusivity. Consider separable $N$-scale potential

$$
V^{\epsilon}(x)=S(x / \epsilon)+\ldots+S\left(x / \epsilon^{N}\right)
$$

where

$$
S(x)= \begin{cases}2 x & \text { if } x \bmod 1 \in\left[0, \frac{1}{2}\right) \\ 2-2 x & \text { if } x \bmod 1 \in\left[\frac{1}{2}, 1\right)\end{cases}
$$

## EFFECT OF NUMBER OF SCALES ON DIFFUSIVITY TENSOR



## EFFECT OF NUMBER OF SCALES ON DIFFUSIVITY TENSOR

As $\epsilon \rightarrow 0, X_{t}^{\epsilon} \Rightarrow X_{t}^{0}$, where

$$
d X_{t}^{0}=\sqrt{\frac{2 \sigma}{K(\sigma)^{N}}} d W_{t}
$$

where $\sigma=\beta^{-1}$, for $K(\sigma)=2 \sigma^{2}\left(\cosh \left(\frac{1}{\sigma}\right)-1\right)$.


# MEAN FIELD LIMITS FOR INTERACTING DIFFUSIONS IN A TWO-SCALE POTENTIAL 

We consider a system of weakly interacting diffusions moving in a 2 -scale locally periodic potential:

$$
\begin{equation*}
d X_{t}^{i}=-\nabla V^{\epsilon}\left(X_{t}^{i}\right) d t-\frac{1}{N} \sum_{j=1}^{N} \nabla F\left(X_{t}^{i}-X_{t}^{j}\right) d t+\sqrt{2 \beta^{-1}} d B_{t}^{i}, \quad i=1, . ., \Lambda \tag{13}
\end{equation*}
$$

O where

$$
\begin{equation*}
V^{\epsilon}(x)=V_{0}(x)+V_{1}(x, x / \epsilon) \tag{14}
\end{equation*}
$$

The full $N$-particle potential is

$$
\begin{align*}
U\left(x_{1}, \ldots, x_{N}, y_{1}, \ldots, y_{N}\right)= & \sum_{i=1}^{N} V_{0}\left(x_{i}\right)+\frac{1}{2 N} \sum_{i=1}^{N} \sum_{j=1}^{N} F\left(x_{i}-x_{j}\right) \\
& +\sum_{i=1}^{N} V_{1}\left(x_{i}, y_{i}\right) \tag{15}
\end{align*}
$$

The homogenization theorem applies to the $N$-particle system.

The homogenized equation is

$$
\begin{align*}
d X_{t}^{i}=- & M\left(X_{t}^{i}\right)\left(\nabla V_{0}\left(X_{t}^{i}\right)+\frac{1}{N} \sum_{i \neq j} \nabla F\left(X_{t}^{j}-X_{t}^{i}\right)+\nabla \psi\left(X_{t}^{i}\right)\right) d t \\
& +\beta^{-1} \nabla \cdot M\left(X_{t}^{i}\right) d t+\sqrt{2 \beta^{-1} M\left(X_{t}^{i}\right)} d W_{t}^{i} \tag{16}
\end{align*}
$$

for $i=1, \ldots, N$, where $M: \mathbb{R}^{d} \rightarrow \mathbb{R}_{\text {sym }}^{d \times d}$ is defined by

$$
\begin{equation*}
M(x)=\frac{1}{Z(x)} \int_{\mathbb{T}^{d}} \int\left(I+\nabla_{y} \theta(x, y)\right) e^{-\beta V_{1}(x, y)} d y, \quad x \in \mathbb{R}^{d} \tag{17}
\end{equation*}
$$

and

$$
\begin{equation*}
\psi(x)=-\beta^{-1} \nabla \log Z(x) \tag{18}
\end{equation*}
$$

for (this is the free energy only with respect to $V_{1}(x, y)$ )

$$
Z(x)=\int_{\mathbb{T}^{d}} e^{-\beta V_{1}(x, y)} d y
$$

and where, for fixed $x \in \mathbb{R}^{d}, \theta$ is the unique mean zero solution to

$$
\begin{equation*}
\nabla \cdot\left(e^{-\beta V_{1}(x, y)}\left(I+\nabla_{y} \theta(x, y)\right)=0, \quad y \in \mathbb{T}^{d}\right. \tag{19}
\end{equation*}
$$

- We can pass to the mean field limit $N \rightarrow+\infty$ using the results from e.g. Dawson (1983), Oelschlager (1984) to obtain the McKean-Vlasov-Fokker-Planck equation:
$\frac{\partial p}{\partial t}=\nabla \cdot\left(M\left(\nabla V_{0} p+\nabla \Psi p+(\nabla F * p) p\right)+\beta^{-1} \nabla \cdot M p+\beta^{-1} \nabla \cdot(M p)\right)$.
$\bigcirc$ The mean field $N \rightarrow+\infty$ and the homogenization $\epsilon \rightarrow 0$ limits commute over finite time intervals.
- This is a nonlinear equation and more than one invariant measures can exist, depending on the temperature. Eqn (20) can exhibit phase transitions.
- The number of invariant measures depends on the number of solutions of the self-consistency equation.
- The phase/bifurcation diagrams can be different depending on the order with which we take the limits. For example:

$$
V^{\epsilon}(x)=\frac{x^{2}}{2}+\cos (x / \epsilon)
$$

O The homogenization process tends to "convexify" the potential.


Figure: Bistable potential with additive (left) and multiplicative (right) fluctuations.

Consider the case $F(x)=\theta \frac{x^{2}}{2}$, take $N \rightarrow+\infty$ and keep $\epsilon$ fixed. The invariant distribution(s) are:

$$
\begin{align*}
p^{\epsilon}(x ; m, \theta, \beta) & =\frac{1}{Z^{\epsilon}} e^{-\beta\left(V^{\epsilon}(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)}  \tag{21a}\\
Z^{\epsilon} & =\int e^{-\beta\left(V^{\epsilon}(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)} d x \tag{21b}
\end{align*}
$$

O where

$$
\begin{equation*}
m=\int x p^{\epsilon}(x ; m, \theta, \beta) d x \tag{22}
\end{equation*}
$$

$\bigcirc$ Take first $\epsilon \rightarrow 0$ and then $N \rightarrow+\infty$. The invariant distribution(s) are

$$
\begin{aligned}
p(x ; m, \theta, \beta) & =\frac{1}{Z} e^{-\beta\left(V_{0}(x)+\psi(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)} \\
Z & =\int e^{-\beta\left(V_{0}(x)+\psi(x)+\theta\left(\frac{1}{2} x^{2}-x m\right)\right)} d y,(23 \mathrm{~b})
\end{aligned}
$$

O where

$$
\begin{equation*}
m=\int x p(x ; m, \theta, \beta) d x \tag{24}
\end{equation*}
$$

- The number of invariant measures is given by the number of solutions to the self-consistency equations (22) and (24).
Separable fluctuations $V_{0}(x)+V_{1}(x / \epsilon)$ do not change the structure of the phase diagram, since they lead to additive noise. Nonseparable fluctuations $V_{0}(x)+V_{1}(x, x / \epsilon)$ lead to multiplicative noise and change the bifurcation diagram.
Rigorous results for the $\epsilon \rightarrow 0, N \rightarrow+\infty$ limits, formal asymptotics for the opposite limit.

O The structure of the bifurcation diagram for the homogenized dynamics is similar to the one for the dynamics in the absence of fluctuations.
O The critical temperature is different, but there are no additional branches and their stability is the same as in the case $V_{1}=0$.
This is the case both for additive and multiplicative oscillations.


Figure: $R_{\text {hom }}(m ; \theta, \beta)$ compared to $y=x$ for $\theta=0.5, \delta=1$ and various values of $\beta$ for the homogenized bistable potentials with separable and nonseparable fluctuations. Bifurcation diagram of $m$ as a function of $\beta$ for the additive (full line) and multiplicative (dashed line) fluctuations.

## COMMUTATIVITY FOR SEPARABLE POTENTIALS




Figure: Plot of $R(m ; \theta, \beta)=m$ and $R\left(m^{\epsilon} ; \theta, \beta\right)$ for $\theta=5, \beta=30, \delta=1$ and various values of $\epsilon$ for separable fluctuations. Convex potential $V_{0}(x)$ and Bistable potential $V_{0}(x)$.

## NONCOMMUTATIVITY FOR SEPARABLE POTENTIALS




Figure: Plot of $R(m ; \theta, \beta)=m$ and $R(m ; \epsilon)$ for $\theta=5, \beta=30, \delta=1$ and various values of $\epsilon$ where the fluctuations are nonseparable. Convex potential $V_{0}(x)$ and Bistable potential $V_{0}(x)$.

## FINITE $\epsilon$ : SEPARABLE FLUCTUATIONS I




Figure: Results for case 1: convex $V_{0}^{c}$ with separable fluctuations, for $\theta=5, \delta=1, \epsilon=0.1$. $R\left(m^{\epsilon} ; \theta, \beta\right)$ for various values of $\beta$, with the potential $V^{\epsilon}(x)$ (full line) compared with $V_{0}^{c}(x)$ (dashed line) in the inside panel. Bifurcation diagram of $m$ as a function of $\beta$. Full lines correspond to stable solutions, while dashed lines represent unstable ones.

## FINITE $\epsilon$ : NONSEPARABLE FLUCTUATIONS I




Figure: Results for case 2: convex $V_{0}$ with nonseparable fluctuations, for $\theta=5, \delta=1, \epsilon=0.1 . R(m ; \theta, \beta)$ for various values of $\beta$, with the potential $V^{\epsilon}(x)$ (full line) compared with $V_{0}^{c}(x)$ (dashed line) in the inside panel. Bifurcation diagram of $m$ as a function of $\beta$. Full lines correspond to stable solutions, while dashed lines represent unstable ones.

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Figure: Convex $V_{0}$ with nonseparable fluctuations, for $\theta=5, \delta=1, \epsilon=0.1 . R(m ; \theta, \beta)$, bifurcation diagram of $m$ as a function of $\beta$. Full lines correspond to stable solutions, while dashed lines represent unstable ones. Values of the free energy of the steady state in each branch of the bifurcation diagram for $\beta=45$. Free energy of each branch of the bifurcation diagram.

## FINITE $\epsilon$ : SEPARABLE FLUCTUATIONS II




Figure: Bistable $V_{0}^{b}$ with separable fluctuations, for
$\theta=5, \delta=1, \epsilon=0.1$. $R\left(m^{\epsilon} ; \theta, \beta\right)$ for various values of $\beta$. Bifurcation diagram of $m$ as a function of $\beta$. Full lines correspond to stable solutions, while dashed lines represent unstable ones.

## FINITE $\epsilon$ : NONSEPARABLE FLUCTUATIONS II




Figure: Bistable $V_{0}^{b}$ with nonseparable fluctuations, for $\theta=5, \delta=1, \epsilon=0.1 . R(m \epsilon ; \theta, \beta)$ for various values of $\beta$. Bifurcation diagram of $m$ as a function of $\beta$. Full lines correspond to stable solutions, while dashed lines represent unstable ones.

- We can study the dependence of the critical temperature $\beta_{C}$ on $\epsilon$.

We study solutions of the equation

$$
\begin{equation*}
\theta^{-1} \beta^{-1}=\int x^{2} p_{\infty}(x ; m=0) d x \tag{25}
\end{equation*}
$$



Figure: Critical temperature $\beta_{C}$ as a function of $\epsilon$ for the multiscale Fokker-Planck equation with $\theta=5$ for $1-V^{\epsilon}(x)=\frac{x^{2}}{2}+\delta \cos \left(\frac{x}{\epsilon}\right), 2-$ $V^{\epsilon}(x)=\frac{x^{4}}{4}-\frac{x^{2}}{2}+\delta \cos \left(\frac{x}{\epsilon}\right)$, and $3-V^{\epsilon}(x)=\frac{x^{4}}{4}-\frac{x^{2}}{2}\left(1-\delta \cos \left(\frac{x}{\epsilon}\right)\right)$.

## NONCOMMUTATIVITY: PARTICLE SIMULATIONS



Figure: Histogram of $N=1000$ particles for a MC simulation of a convex potential with separable fluctuations. Parameters used were $\theta=2$, $\beta=8, \delta=1$. Left: $\epsilon=0.1$. Right: homogenized system.


Figure: Histogram of $N=500$ particles for an MC simulation of a bistable potential with nonseparable fluctuations. Parameters used were $\theta=0.5, \beta \approx 5.6, \delta=1$. Left: $\epsilon=0.1$. Right: homogenized system.


Figure: Time evolution of the mean $\bar{X}_{t}$ of $N=500$ particles for an MC simulation of a bistable potential with separable fluctuations. Parameters used were $\theta=0.5, \beta \approx 5.6, \delta=1$. Left: $\epsilon=0.1$. Right: homogenized system.

## NONCOMMUTATIVITY: MCKEAN-VLASOV EVOLUTION




Figure: Time evolution of $p(x, t)$ for $V_{0}(x)=\frac{x^{2}}{2}+\delta \cos \left(\frac{x}{\epsilon}\right)$. Parameters used were $\theta=2, \beta=8, \delta=1$. Left: $\epsilon=0.1$. Right: homogenized system.


Figure: Time evolution of $p(x, t)$ when $V_{0}^{b}(x)$ is a bistable potential and with nonseparable fluctuations. Parameters used were $\theta=0.5, \beta \approx 5.6$, $\delta=1$. Left: $\epsilon=0.1$. Right: homogenized system.



Figure: Potential and solution of self-consistency equation for the potential $V(q)=\frac{1}{\sum_{\ell=-N}^{N}\left|q-q_{\ell}\right|^{-2}}$ (used in the Thesis of Dr Z. Trstanova).

## NON-PERIODIC MULTIWELL POTENTIALS



Figure: Bifurcation diagram for for the potential $V(q)=\frac{1}{\sum_{\ell=-N}^{N}\left|q-q_{\ell}\right|^{-2}}$
for the order parameter $m$ as a function of $\beta^{-1}$ for $N=6$ and $N=8$.

## NON-PERIODIC MULTIWELL POTENTIALS



Figure: Free energy surface as a function of $\beta$ and the first moment $m$ for potential $V(q)=\frac{1}{\sum_{\ell}^{N}\left|q-q_{\ell}\right|^{-2}}$, but the energy barriers are

