

# Long-time behaviour and phase transitions for the McKean-Vlasov equation

Grigorios A. Pavliotis

Department of Mathematics  
Imperial College London

**Interactions Between PDEs and Probability, UIMP**

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London

- Joint work with José Carrillo, Susana Gomes, Rishabh Gvalani, Hong Duong, Petr Yatsyshin, Serafim Kalliadasis and André Schlichting (Aachen/Bonn).
- *Phase Transitions for the Desai-Zwanzig model in multiwell and random energy landscapes* (with S.N. Gomes, S. Kalliadasis, G.A. Pavliotis, P. Yatsyshin). Preprint (2018).
- *Long time behaviour and phase transitions for the McKean-Vlasov equation on the torus* (with R. Gvalani, J.A. Carrillo, A. Schlichting) Preprint (2018) <https://arxiv.org/abs/1806.01719>.
- *Mean field limits for interacting diffusions in a two-scale potential* (S.N. Gomes and G.A. Pavliotis), J. Nonlinear Sci. 28(3), pp. 905-941, (2018).
- *Mean field limits for non-Markovian interacting particles: convergence to equilibrium, GENERIC formalism, asymptotic limits and phase transitions* (with M. H. Duong). Preprint (2018). <https://arxiv.org/abs/1805.04959>

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■ Study the mean field limits of weakly interacting diffusions:

■ The Dasai-Swanzing model in a 2-scale potential:

$$dX_i = -V'(X_i, X_i/\varepsilon) dt - \theta \left( X_t^i - \frac{1}{N} \sum_{j=1}^N X_t^j \right) dt + \sqrt{2\beta^{-1}} dW_t^i.$$

■ Noisy Kuramoto oscillators:

$$\dot{x}_i = -\frac{1}{N} \sum_{j=1}^N \cos(x_i - x_j) + \sqrt{2\beta^{-1}} \dot{W}_i.$$

■ Models for opinion formation:

$$\dot{x}_i = \frac{1}{N} \sum_{j=1}^N a_{ij}(|x_i - x_j|)(x_i - x_j) + \sqrt{2\beta^{-1}} \dot{W}_i.$$

- Study the mean field limits of weakly interacting diffusions:
  - Interacting non-Markovian Langevin dynamics

$$\ddot{q}_i = -\frac{\partial V}{\partial q_i} - \frac{1}{N} \sum_{j=1}^N U'(q_i - q_j) - \sum_{j=1}^N \gamma_{ij}(t-s) \dot{q}_j(s) ds + F_i(t), \quad i = 1, \dots, N, \quad (1)$$

- where  $F(t) = (F_1(t), \dots, F_N(t))$  is a mean zero, Gaussian, stationary process with autocorrelation function  $E(F_i(t) F_j(s)) = \beta^{-1} \gamma_{ij}(t-s)$ .
- Langevin dynamics driven by colored noise

$$\dot{x}_i = -V'(x_i) - \frac{1}{N} \sum_{j=1}^N W'(x_i - x_j) + \eta_i, \quad (2a)$$

$$\dot{\eta}_i = -\eta_i + \sqrt{2\beta^{-1}} \dot{B}_i \quad (2b)$$

- applications: Models for systemic risk (Garnier, Papanicolaou...), clustering in the Hegselmann-Krause model (Chazelle, E, .....)

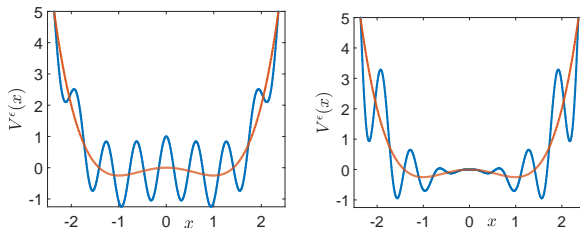
- We consider a system of weakly interacting diffusions moving in a 2-scale locally periodic potential:

$$dX_t^i = -\nabla V^\epsilon(X_t^i)dt - \frac{1}{N} \sum_{j=1}^N \nabla F(X_t^i - X_t^j)dt + \sqrt{2\beta^{-1}}dB_t^i, \quad i = 1, \dots, N, \quad (3)$$

- where

$$V^\epsilon(x) = V_0(x) + V_1(x, x/\epsilon). \quad (4)$$

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

- Consider a system of interacting diffusions in a bistable potential:

$$dX_t^i = \left( -V'(X_t^i) - \theta \left( X_t^i - \frac{1}{N} \sum_{j=1}^N X_t^j \right) \right) dt + \sqrt{2\beta^{-1}} dB_t^i. \quad (5)$$

- The total energy (Hamiltonian) is

$$W_N(\mathbf{X}) = \sum_{\ell=1}^N V(X^\ell) + \frac{\theta}{4N} \sum_{n=1}^N \sum_{\ell=1}^N (X^n - X^\ell)^2. \quad (6)$$

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

$$dX_t = -V'(X_t) dt - \theta(X_t - \mathbb{E}X_t) dt + \sqrt{2\beta^{-1}} dB_t. \quad (7)$$

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

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left( V'(x)p + \theta \left( x - \int_{\mathbb{R}} xp(x, t) dx \right) p + \beta^{-1} \frac{\partial p}{\partial x} \right). \quad (8)$$

- The McKean-Vlasov equation is a gradient flow, with respect to the Wasserstein metric, for the free energy functional

$$\mathcal{F}[\rho] = \beta^{-1} \int \rho \ln \rho dx + \int V \rho dx + \frac{\theta}{2} \int \int F(x - y) \rho(x) \rho(y) dx dy, \quad (9)$$

with  $F(x) = \frac{1}{2}x^2$ .



## **Critical Dynamics and Fluctuations for a Mean-Field Model of Cooperative Behavior**

**Donald A. Dawson**<sup>1,2</sup>

*Received September 20, 1982*

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The main objective of this paper is to examine in some detail the dynamics and fluctuations in the critical situation for a simple model exhibiting bistable macroscopic behavior. The model under consideration is a dynamic model of a collection of anharmonic oscillators in a two-well potential together with an attractive mean-field interaction. The system is studied in the limit as the number of oscillators goes to infinity. The limit is described by a nonlinear partial differential equation and the existence of a phase transition for this limiting system is established. The main result deals with the fluctuations at the critical point in the limit as the number of oscillators goes to infinity. It is established that these fluctuations are non-Gaussian and occur at a time scale slower than the noncritical fluctuations. The method used is based on the phase transition for the McKendrick-Vlasov process developed by Papanicolaou, Stroock, and Varadhan adapted to the context of probability-measure-valued processes.

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# Dynamical behavior of stochastic systems of infinitely many coupled nonlinear oscillators exhibiting phase transitions of mean-field type: $H$ theorem on asymptotic approach to equilibrium and critical slowing down of order-parameter fluctuations

Masatoshi Shiino

*Department of Applied Physics, Faculty of Science, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo 152, Japan*

(Received 29 September 1986)

It is shown that statistical-mechanical properties as well as irreversible phenomena of stochastic systems, which consist of infinitely many coupled nonlinear oscillators and are capable of exhibiting phase transitions of mean-field type, can be successfully explored on the basis of nonlinear Fokker-Planck equations, which are essentially nonlinear in unknown distribution functions. Results of two kinds of approaches to the study of their dynamical behavior are presented. Firstly, a problem of asymptotic approaches to stationary states of the infinite systems is treated. A method of Lyapunov functional is employed to conduct a global as well as a local stability analysis of the systems. By constructing an  $H$  functional for the nonlinear Fokker-Planck equation, an  $H$  theorem is proved, ensuring that the Helmholtz free energy for a nonequilibrium state of the system decreases monotonically until a stationary state is approached. Calculations of the second-order variation of the  $H$  functional around a stationary state yield a stability criterion for bifurcating solutions of the nonlinear Fokker-Planck equation, in terms of an inequality involving the second moment of the stationary distribution function. Secondly, the behavior of critical dynamics is studied within the framework of linear-response theory. Generalized dynamical susceptibilities are calculated rigorously from linear responses of the order parameter to externally driven fields by linearizing the nonlinear Fokker-Planck equation. Correlation functions, together with spectra of the fluctuations of the order parameter of the system, are also obtained by use of the fluctuation-dissipation theorem for stochastic systems. A critical slowing down is shown to occur in the form of the divergence of relaxation time for the fluctuations, in accordance with the divergence of the static susceptibility, as a phase transition point is approached.

## I. INTRODUCTION

The study of dynamical behavior of systems exhibiting thermodynamic phase transitions has been of considerable

interest for many years. Phase transitions for the Ising-Vlasov thermodynamic system undergoing phase transitions critical anomaly such as critical slowing down is generally expected to occur at its transition points. Recently, the con-

tained by omitting the random force  $f(t)$  in Eq. (1.1) can exhibit a bifurcation at  $\gamma=0$ , the stochastic differential equation (1.1) has nothing to do with bifurcations nor phase transitions in that a stationary distribution for the random variable  $x$  is always uniquely determined irrespective of the values of  $\gamma$  and  $\sigma$ . This is because the corresponding linear Fokker-Planck equation

- The finite dimensional dynamics (5) is reversible with respect to the Gibbs measure

$$\mu_N(dx) = \frac{1}{Z_N} e^{-\beta W_N(x^1, \dots, x^N)} dx^1 \dots dx^N, \quad Z_N = \int_{\mathbb{R}^N} e^{-\beta W_N(x^1, \dots, x^N)} dx^1 \dots dx^N \quad (10)$$

- where  $W_N(\cdot)$  is given by (6).
- the McKean dynamics (7) 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 (7) satisfies the stationary nonlinear Fokker-Planck equation

$$\frac{\partial}{\partial x} \left( V'(x) p_\infty + \theta \left( x - \int_{\mathbb{R}} x p_\infty(x) dx \right) p_\infty + \beta^{-1} \frac{\partial p_\infty}{\partial x} \right) = 0. \quad (11)$$

- For the quadratic interaction potential a one-parameter family of solutions to the stationary McKean-Vlasov equation (11) can be obtained:

$$p_{\infty}(x; \theta, \beta, m) = \frac{1}{Z(\theta, \beta; m)} e^{-\beta(V(x) + \theta(\frac{1}{2}x^2 - xm))}, \quad (12a)$$

$$Z(\theta, \beta; m) = \int_{\mathbb{R}} e^{-\beta(V(x) + \theta(\frac{1}{2}x^2 - xm))} dx. \quad (12b)$$

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

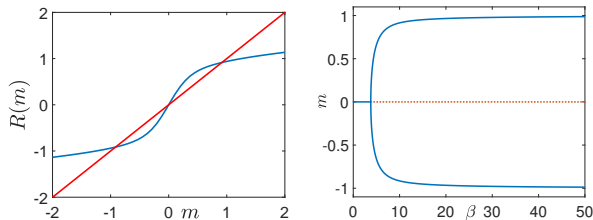
$$m = \int_{\mathbb{R}} x p_{\infty}(x; \theta, \beta, m) dx =: R(m; \theta, \beta). \quad (13)$$

- This is the **selfconsistency** equation:

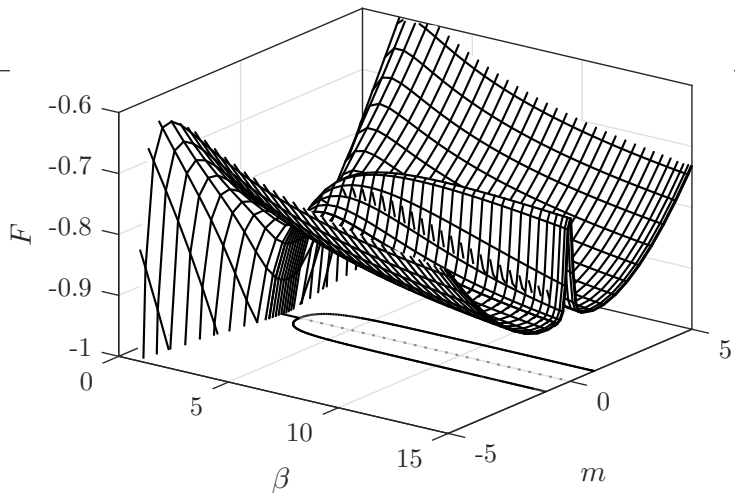
$$m = R(m; \theta, \beta).$$

- The critical temperature can be calculated from

$$\text{Var}_{p_\infty}(x) \Big|_{m=0} = \frac{1}{\beta\theta}. \quad (14)$$



**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  $F(x) = \frac{x^2}{2}$ .

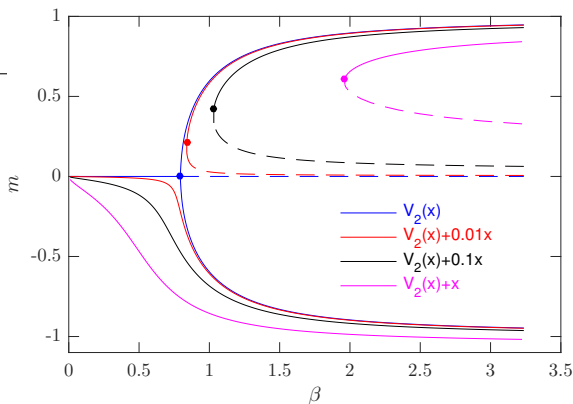


**Figure:** Free energy surface corresponding to the bistable potential, as a function of the inverse temperature  $\beta$  and the first moment  $m$  with  $\theta = 0.5$ .

- We can study the effect of breaking the symmetry of polynomial potentials by adding a tilt to a bistable potential.
- We consider potentials of the form

$$V(x) = \frac{1}{a_0} \left( \frac{x^4}{4} - \frac{x^2}{2} \right) + \kappa x. \quad (15)$$





**Figure:** Bifurcation diagrams of  $m$  as a function of  $\beta$  for tilted bistable potentials with  $a_0 = 0.25$ , and  $\kappa = 0, 0.01, 0.1, 1$  (see legend). Here, we used  $\theta = 2.5$ . The symmetric pitchfork bifurcation is broken at any  $\kappa > 0$ . Note that the locus of the critical points forms a distinct critical line.

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

$$dX_t^i = -\nabla V^\epsilon(X_t^i)dt - \frac{1}{N} \sum_{j=1}^N \nabla F(X_t^i - X_t^j)dt + \sqrt{2\beta^{-1}}dB_t^i, \quad i = 1, \dots, N, \quad (16)$$

- where

$$V^\epsilon(x) = V_0(x) + V_1(x, x/\epsilon).$$

- The full  $N$ -particle potential is

$$U(x_1, \dots, x_N, y_1, \dots, y_N) = \sum_{i=1}^N V_0(x_i) + \frac{1}{2N} \sum_{i=1}^N \sum_{j=1}^N F(x_i - x_j) + \sum_{i=1}^N V_1(x_i, y_i).$$

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

- The homogenized equation is

$$dX_t^i = -M(X_t^i) \left( \nabla V_0(X_t^i) + \frac{1}{N} \sum_{i \neq j} \nabla F(X_t^j - X_t^i) + \nabla \psi(X_t^i) \right) dt + \beta^{-1} \nabla \cdot M(X_t^i) dt + \sqrt{2\beta^{-1} M(X_t^i)} dW_t^i, \quad (17)$$

- for  $i = 1, \dots, N$ , where

$$\psi(x) = -\beta^{-1} \nabla \ln Z(x), \quad \text{with } Z(x) = \int_{\mathbb{T}^d} e^{-\beta V_1(x,y)} dy.$$

- The stochastic integral in (17) can be interpreted in the Klimontovich sense:

$$dX_t = -M(X_t) \nabla U(X_t) dt + \sqrt{2\beta^{-1} M(X_t)} \circ^{\text{Klim}} dW_t.$$

The dynamics is ergodic with respect to the Gibbs measure

$$\mu_\beta(dx) = \frac{1}{Z} e^{-\beta U(x)} dx.$$

- The diffusion tensor  $M : \mathbb{R}^d \rightarrow \mathbb{R}_{sym}^{d \times d}$  is defined by

$$M(x) = \frac{1}{Z(x)} \int_{\mathbb{T}^d} \int (I + \nabla_y \theta(x, y)) e^{-\beta V_1(x, y)} dy, \quad x \in \mathbb{R}^d,$$

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

$$\nabla \cdot (e^{-\beta V_1(x, y)} (I + \nabla_y \theta(x, y))) = 0, \quad y \in \mathbb{T}^d, \quad (18)$$

- We can pass to the mean field limit  $N \rightarrow +\infty$  using the results from e.g. Dawson (1983), Oelschläger (1984) to obtain the McKean-Vlasov-Fokker-Planck equation:

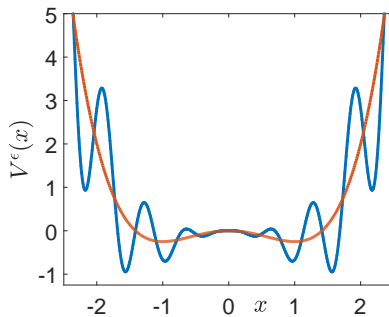
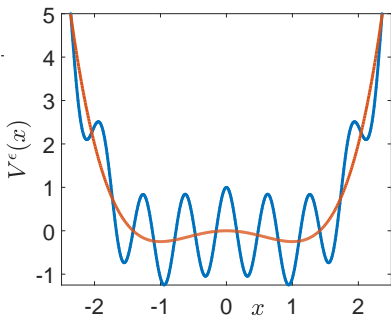
$$\frac{\partial p}{\partial t} = \nabla \cdot \left( M(\nabla V_0 p + \nabla \Psi p + (\nabla F * p)p) + \beta^{-1} \nabla \cdot M p + \beta^{-1} \nabla \cdot (M p) \right). \quad (19)$$

- 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 (19) 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:

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

- 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:

$$p^\epsilon(x; m, \theta, \beta) = \frac{1}{Z^\epsilon} e^{-\beta(V^\epsilon(x) + \theta(\frac{1}{2}x^2 - x m))}, \quad Z^\epsilon = \int e^{-\beta(V^\epsilon(x) + \theta(\frac{1}{2}x^2 - x m))} dx,$$

- where

$$m = \int x p^\epsilon(x; m, \theta, \beta) dx. \quad (20)$$

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

$$p(x; m, \theta, \beta) = \frac{1}{Z} e^{-\beta(V_0(x) + \psi(x) + \theta(\frac{1}{2}x^2 - x m))}, \quad Z = \int e^{-\beta(V_0(x) + \psi(x) + \theta(\frac{1}{2}x^2 - x m))} dx,$$

- where

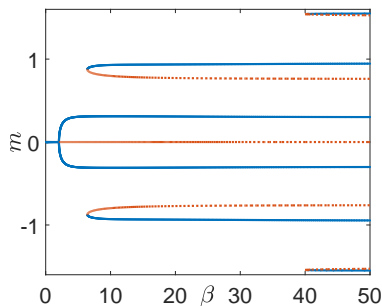
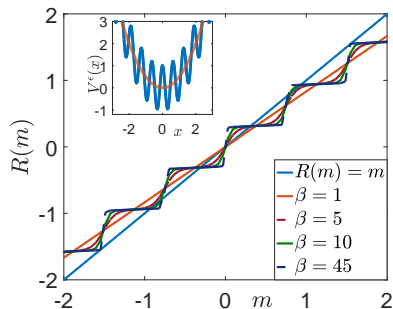
$$m = \int x p(x; m, \theta, \beta) dx. \quad (21)$$

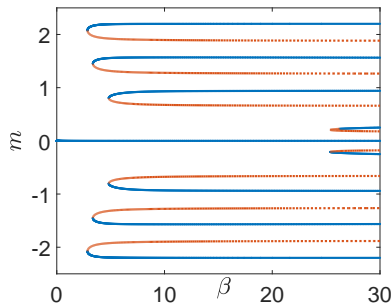
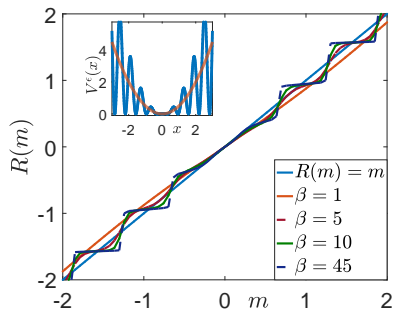


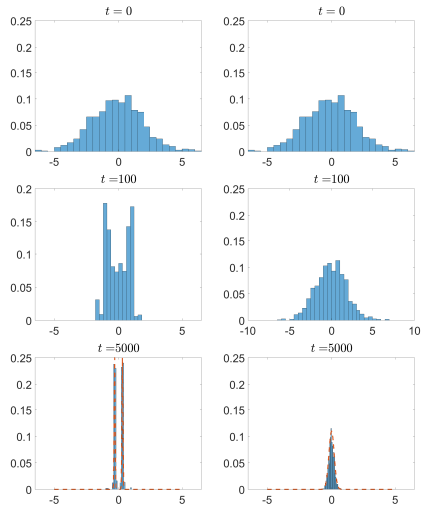
- The number of invariant measures is given by the number of solutions to the self-consistency equations (20) and (21).
- Separable fluctuations  $V_0(x) + V_1(x/\varepsilon)$  do not change the structure of the phase diagram, since they lead to additive noise. Nonseparable fluctuations  $V_0(x) + V_1(x, x/\varepsilon)$  lead to multiplicative noise and change the bifurcation diagram.
- Rigorous results for the  $\varepsilon \rightarrow 0$ ,  $N \rightarrow +\infty$  limits, formal asymptotics for the opposite limit.

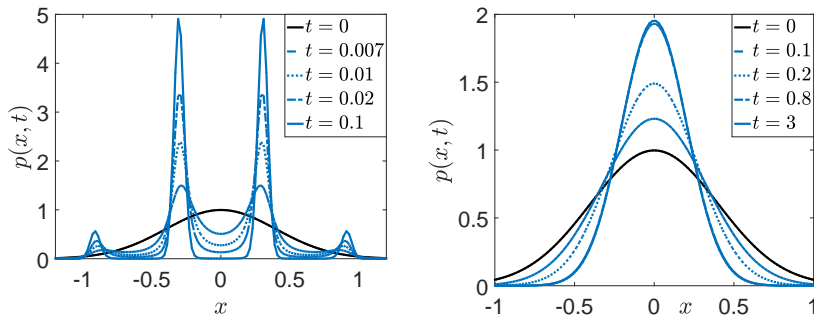
- The structure of the bifurcation diagram for the homogenized dynamics is similar to the one for the dynamics in the absence of fluctuations.
- The critical temperature is different, but there are no additional branches and their stability is the same as in the case  $V_1 = 0$ .
- This is the case both for additive and multiplicative oscillations.
- We can study the stability of the different branches using the formula for the free energy

$$\mathcal{F}[\rho_\infty] = -\beta^{-1} \ln Z_{\beta, \theta, m} + \frac{\theta}{2} m^2.$$

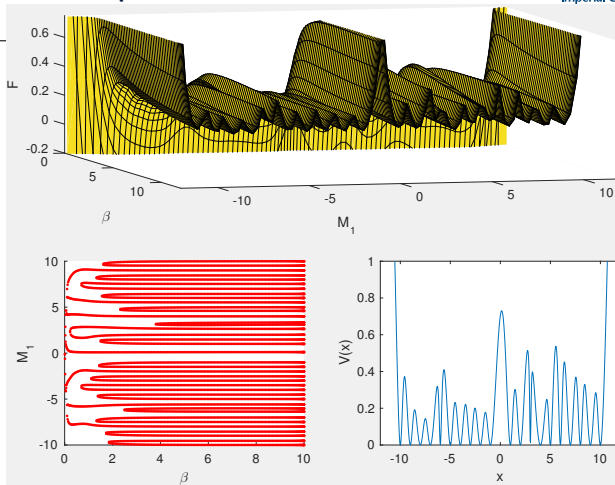








**Figure:** Time evolution of  $p(x, t)$  for  $V_0(x) = \frac{x^2}{2} + \delta \cos\left(\frac{x}{\epsilon}\right)$ . Parameters used were  $\theta = 2$ ,  $\beta = 8$ ,  $\delta = 1$ . Left:  $\epsilon = 0.1$ . Right: homogenized system.



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

# The McKean-Vlasov equation on the torus



Nonlocal parabolic PDE

$$\frac{\partial \varrho}{\partial t} = \beta^{-1} \Delta \varrho + \kappa \nabla \cdot (\varrho \nabla W \star \varrho) \quad \text{in } \mathbb{T}_L^d \times (0, T]$$

with periodic boundary conditions,  $\varrho(\cdot, 0) = \varrho_0 \in \mathcal{P}(\mathbb{T}_L^d)$ ,  $\mathbb{T}_L^d \hat{=} \left(-\frac{L}{2}, \frac{L}{2}\right)^d$

- $\varrho(\cdot, t) \in \mathcal{P}(\mathbb{T}_L^d)$  probability density of particles
- $W$  coordinate-wise even interaction potential
- $\beta > 0$  inverse temperature (fixed)
- $\kappa > 0$  interaction strength (parameter)

## Example: The noisy Kuramoto model

The Kuramoto model:  $W(x) = -\sqrt{\frac{2}{L}} \cos\left(2\pi k \frac{x}{L}\right), k \in \mathbb{Z}$

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Figure: \*

$\kappa < \kappa_c$ , no phase locking

Figure: \*

$\kappa > \kappa_c$ , phase locking

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## Goals and Motivation:

- Classification of continuous and discontinuous transitions.
- Better understanding of the free energy landscape.
- Study dynamical properties related to nucleation/coarsening of clustered states.

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

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

$$\widetilde{W}(k) = \langle W, w_k \rangle \geq 0, \quad \forall k \in \mathbb{Z}^d,$$

- Decomposition of potential  $W$  into *H*-stable and *H*-unstable part

$$W_s(x) = \sum_{k \in \mathbb{N}^d} (\langle W, w_k \rangle)_+ w_k(x) \quad \text{and} \quad W_u(x) = W(x) - W_s(x).$$

- **Free energy functional  $\mathcal{F}_\kappa$ :** Driving the  $W_2$ -gradient flow

$$\mathcal{F}_\kappa(\varrho) = \beta^{-1} \int_{\mathbb{T}_L^d} \varrho \log \varrho \, dx + \frac{\kappa}{2} \iint_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y) \varrho(x) \varrho(y) \, dx \, dy .$$

- **Dissipation:**  $\mathcal{F}_\kappa$  is Lyapunov-function

$$\mathcal{J}_\kappa(\varrho) = -\frac{d}{dt} \mathcal{F}_\kappa(\varrho) = \int_{\mathbb{T}_L^d} \left| \nabla \log \frac{\varrho}{e^{-\beta \kappa W \star \varrho}} \right|^2 \varrho \, dx ,$$

- **Kirkwood-Monroe** fixed point mapping

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

## Characterization of stationary states: The following are equivalent

- $\varrho$  is a stationary state:  $\beta^{-1} \Delta \varrho + \kappa \nabla \cdot (\varrho \nabla W \star \varrho) = 0$ .
- $\varrho$  is a root of  $F_\kappa(\varrho)$ .
- $\varrho$  is a global minimizer of  $\mathcal{J}_\kappa(\varrho)$ .
- $\varrho$  is a critical point of  $\mathcal{F}_\kappa(\varrho)$ .

$\Rightarrow \varrho_\infty \equiv L^{-d}$  is a stationary state for all  $\kappa > 0$ .

## Theorem

*Under appropriate assumptions on the potential, for  $\varrho_0 \in H^{3+d}(U) \cap \mathcal{P}_{\text{ac}}(U)$ , there exists a unique classical solution  $\varrho$  of the McKean-Vlasov equation such that  $\varrho(\cdot, t) \in \mathcal{P}_{\text{ac}}(U) \cap C^2(\overline{U})$  for all  $t > 0$ . Additionally,  $\varrho(\cdot, t)$  is strictly positive and has finite entropy, i.e,  $\varrho(\cdot, t) > 0$  and  $S(\varrho(\cdot, t)) < \infty$ , for all  $t > 0$ .*

## Theorem

*(Convergence to equilibrium) Let  $\varrho(x, t)$  be a classical solution of the McKean–Vlasov equation with smooth initial data and smooth, even, interaction potential  $W$ . Then we have:*

1. *If  $0 < \kappa < \frac{2\pi}{3\beta L \|\nabla W\|_\infty}$ , then  $\left\| \varrho - \frac{1}{L} \right\|_2 \rightarrow 0$ , exponentially, as  $t \rightarrow \infty$ ,*
2. *If  $\hat{W}(k) \geq 0$  for all  $k \in \mathbb{Z}$  or  $0 < \kappa < \frac{2\pi^2}{\beta L^2 \|\Delta W\|_\infty}$ , then  $\mathcal{H}\left(\varrho \middle| \frac{1}{L}\right) \rightarrow 0$ , exponentially, as  $t \rightarrow \infty$ ,*

*where  $\hat{W}(k)$  represents the Fourier transform and  $\mathcal{H}\left(\varrho \middle| \frac{1}{L}\right)$  represents the relative entropy.*



# *Free energy and the convergence of distributions of diffusion processes of McKean type*

By YOZO TAMURA<sup>\*)</sup>

(Communicated by S. Kusuoka)

## § 1. Introduction.

In this paper, we investigate the convergence of the probability distribution  $p(t)$  of a diffusion process of McKean type at time  $t$  to an invariant probability measure as  $t$  goes to  $\infty$  by using the free energy function. The process we consider is given by the following stochastic differential equation of McKean type on  $R^d$ :

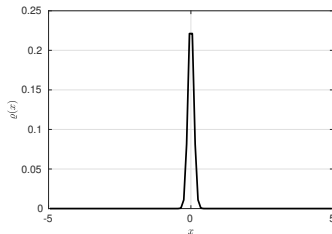
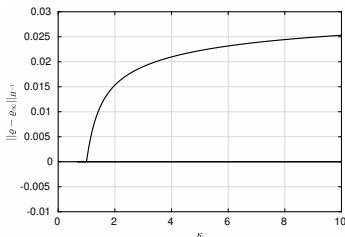
$$(1.1) \quad \begin{cases} dX(t) = dB(t) - \text{grad } \Phi_1(X(t))dt + \text{grad } \Phi_2[X(t), p(t)]dt, \\ p(t) \text{ is the probability distribution of } X(t), \\ \text{the initial distribution is } p_0, \end{cases}$$

where  $\Phi_2[x, p] = \int \Phi_2(x, y)p(dy)$  for any probability measure  $p$  on  $R^d$ ,  
Phase transitions for the McKean-Vlasov eqn

$\{B(t); t \geq 0\}$  is a standard Brownian motion. We assume that the potentials  $\Phi_1$  and  $\Phi_2$  satisfy the following:

- $W \notin \mathbb{H}_s$  is a necessary condition for the existence of nontrivial steady states.
- Numerical experiments indicate one, multiple, or possibly infinite solutions
- What determines the number of nontrivial solutions?
- Bifurcation analysis of  $\varrho \mapsto F_\kappa(\varrho)$ .

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



$\Rightarrow$  1-cluster solution and uniform state  $\varrho_\infty$ .

## Theorem

*(Local bifurcations) Let  $W$  be smooth and even and let  $(1/L, \kappa)$  represent the trivial branch of solutions. Then every  $k^* \in \mathbb{Z}, k > 0$  such that*

1.  $\text{card}\{k \in \mathbb{Z}, k > 0 : \hat{W}(k) = \hat{W}(k^*)\} = 1$ ,
2.  $\hat{W}(k) < 0$ ,

*corresponds to a bifurcation point of the stationary McKean–Vlasov equation through the formula*

$$\kappa_* = -\frac{\sqrt{L}}{\beta \hat{W}(k^*)}, \quad (22)$$

*with  $(1/L, \kappa_*)$  the bifurcation point.*

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# On asymptotic behaviors of the solution of a non-linear diffusion equation<sup>\*)</sup>

By YOZO TAMURA

(Communicated by Y. Okabe)

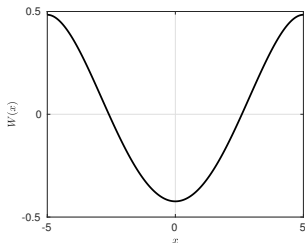
## § 1. Introduction

M. Kac [2] discovered the propagation of chaos for Kac's caricature of the Boltzmann equation for Maxwellian gas. In an analogy of this, H. P. McKean, Jr. [3] showed that a certain class of non-linear parabolic equations are derived from a system of  $n$ -particle diffusion processes through the propagation of chaos; if the initial distribution of the  $n$ -particle diffusion is  $u_0^{\otimes n}$ , then for any  $m \in N$  and any  $t > 0$ , the  $m$ -marginal distribution of the  $n$ -particle diffusion at time  $t$  converges to  $m$ -fold direct product of  $u(t)$ , where  $u(t)$  is a weak solution of the non-linear parabolic equation with the initial data  $u_0$ .

In this paper we consider a system of some class of  $nd$ -dimensional diffusion processes  $X^{(n)}$  ( $n \in N$ ) treated in H. P. McKean, Jr. [3]. For fixed  $n \in N$ ,  $X^{(n)}(t) = (X^{(n,1)}(t), \dots, X^{(n,n)}(t))$  is described by the following stochastic differential equation:

- Kuramoto-type of models:  $W(x) = -w_k(x)$  in  $d = 1$  with  $\widetilde{W}(k) = -1$ , satisfying both conditions. Thus we have that  $\kappa_* = \frac{\sqrt{2L}}{\beta}$ .
- For  $W(x) = \frac{x^2}{2}$  holds  $\widetilde{W}(k) = \frac{L^{5/2} \cos(\pi k)}{2\sqrt{2}\pi k^2}$  satisfying both conditions for odd values of  $k$ . Hence, every odd  $k$  is bifurcation point  $\kappa_* = \frac{4k^2}{\beta L^2}$ .

- $W^s(x) = - \sum_{k=1}^{\infty} \frac{1}{k^{2s+2}} w_k(x)$   
 For  $s \geq 1$  :  $W^s(x) \in H^s(\mathbb{T}_L^d)$   
 $\forall k > 0$  : conditions (1) and (2) ok  
 Infinitely many bifurcation points



### Definition (Transition point [Chayes & Panferov '10])

A parameter value  $\kappa_c > 0$  is said to be a **transition point** of  $\mathcal{F}_\kappa$  if it satisfies the following conditions,

1. For  $0 < \kappa < \kappa_c$ :  $\varrho_\infty$  is the unique minimiser of  $\mathcal{F}_\kappa(\varrho)$
2. For  $\kappa = \kappa_c$ :  $\varrho_\infty$  is a minimiser of  $\mathcal{F}_\kappa(\varrho)$ .
3. For  $\kappa > \kappa_c$ :  $\exists \varrho_\kappa \neq \varrho_\infty$ , such that  $\varrho_\kappa$  is a minimiser of  $\mathcal{F}_\kappa(\varrho)$ .

## Definition (Continuous and discontinuous transition point)

A transition point  $\kappa_c > 0$  is a **continuous transition point** of  $\mathcal{F}_\kappa$  if

1. For  $\kappa = \kappa_c$ :  $\varrho_\infty$  is the unique minimiser of  $\mathcal{F}_\kappa(\varrho)$ .
2. For any family of minimizers  $\{\varrho_\kappa \neq \varrho_\infty\}_{\kappa > \kappa_c}$  it holds

$$\limsup_{\kappa \downarrow \kappa_c} \|\varrho_\kappa - \varrho_\infty\|_1 = 0.$$

A transition point  $\kappa_c > 0$  which is not continuous is **discontinuous**.

# Thermodynamics

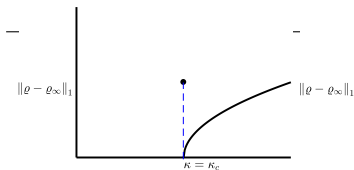


Figure: (M1)

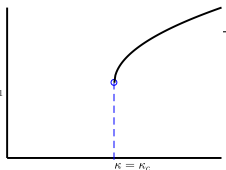


Figure: (M2)

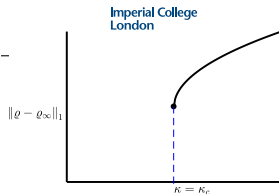


Figure: (M1)+(M2)

**Figure:** Ways in which a discontinuous transition can occur. The horizontal line represents the uniform solution



Summary of critical points:

- $\kappa_c$  transition point.
- $\kappa_*$  bifurcation point.
- $\kappa_\#$  point of linear stability, i.e.,  $\kappa_\# = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$  with  $k_\# = \arg \min \widetilde{W}(k)$ .

If there is exactly one  $k_\#$ , then  $\kappa_\# = \kappa_*$  is a bifurcation point.

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Results from [Gates & Penrose 1970] and [Chayes & Panferov '10]

- $\mathcal{F}_\kappa$  has a transition point  $\kappa_c$  iff  $W \notin \mathbb{H}_s$ .
- $\min \mathcal{F}_\kappa$  is non-increasing as a function of  $\kappa$ .
- If for some  $\kappa' : \varrho_\infty$  is no longer the unique minimiser, then  $\forall \kappa > \kappa' : \varrho_\infty$  is no longer a minimizer.
- If  $\kappa_c$  is continuous, then  $\kappa_c = \kappa_\#$ .
- (M2)  $\implies$  (M1)+(M2).
- For  $L$  sufficiently large,  $d \geq 2$ , and  $W(x) \in \mathbb{H}_s^c$ , radially symmetric, the transition point is discontinuous.

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## Conclusion:

- To prove a discontinuous transition: Show  $\varrho_\infty$  at  $\kappa_\sharp$  is no longer global minimizer.
- To prove a continuous transition:  
If  $\kappa_* = \kappa_\sharp$ , sufficient to show that  $\varrho_\infty$  at  $\kappa_\sharp$  is the only global minimizer and investigate a resonance condition.

## Theorem

*(Discontinuous and continuous phase transitions) Let  $W$  be smooth and even and assume the free energy  $\mathcal{F}_{\kappa,\beta}$  exhibits a transition point,  $\kappa_c < \infty$ . Then we have the following two scenarios:*

1. *If there exist strictly positive  $k^a, k^b, k^c \in \mathbb{Z}$  with  $\hat{W}(k^a) = \hat{W}(k^b) = \hat{W}(k^c) = \min_k \hat{W}(k) < 0$  such that  $k^a = k^b + k^c$  or  $k^a = 2k^b$ , then  $\kappa_c$  is a discontinuous transition point.*
  2. *Let  $k^\sharp = \arg \min_k \hat{W}(k)$  be well-defined with  $\hat{W}(k^\sharp) < 0$ . Let  $W_\alpha$  denote the potential obtained by multiplying all the negative  $\hat{W}(k)$  except  $\hat{W}(k^\sharp)$  by some  $\alpha \in (0, 1]$ . Then if  $\alpha$  is made small enough, the transition point  $\kappa_c$  is continuous.*
-

### Proposition

*The generalised Kuramoto model  $W(x) = -w_k(x)$ , for some  $k \in \mathbb{N}, k \neq 0$  exhibits a continuous transition point at  $\kappa_c = \kappa_\sharp$ . Additionally, for  $\kappa > \kappa_c$ , the equation  $F(\varrho, \kappa) = 0$  has only two solutions in  $L^2(U)$  (up to translations). The nontrivial one,  $\varrho_\kappa$  minimises  $\mathcal{F}_\kappa$  for  $\kappa > \kappa_c$  and converges in the narrow topology as  $\kappa \rightarrow \infty$  to a normalised linear sum of equally weighted Dirac measures centred at the minima of  $W(x)$ .*

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- The noisy Hegselmann–Krause system models the opinions of  $N$  interacting agents such that each agent is only influenced by the opinions of its immediate neighbours. The interaction potential is

$$W_{\text{hk}}(x) = -\frac{1}{2} \left( \left( |x| - \frac{R}{2} \right)_- \right)^2$$

- for some  $R > 0$ . The ratio  $R/L$  measures the range of influence of an individual agent with  $R/L = 1$  representing full influence.
- The Fourier transform of  $W_{\text{hk}}(x)$  is

$$\widetilde{W}_{\text{hk}}(k) = \frac{\left(-\pi^2 k^2 R^2 + 2L^2\right) \sin\left(\frac{\pi k R}{L}\right) - 2\pi k L R \cos\left(\frac{\pi k R}{L}\right)}{4\sqrt{2}\pi^3 k^3 \sqrt{\frac{1}{L}}}, \quad k \in \mathbb{N}, k \neq 0. \quad (23)$$

- the model has infinitely many bifurcation points for  $R/L = 1$ .

- We define a rescaled version of the potential

$$W_{\text{hk}}^R(x) = -\frac{1}{2R^3} \left( \left( |x| - \frac{R}{2} \right)_- \right)^2,$$

which does not lose mass as  $R \rightarrow 0$ .

### Proposition

*For  $R$  small enough, the rescaled noisy Hegselmann–Krause model possesses a discontinuous transition point.*

- The Onsager/Maiers–Saupe model is described by the interaction potential

$$W_\ell(x) = \left| \sin\left(\frac{2\pi}{L}x\right) \right|^\ell \in L_s^2(U) \cap C^\infty(\bar{U})$$

- with  $\ell \in \mathbb{N}, \ell \geq 1$ , so that the Onsager and Maiers–Saupe potential correspond to the cases  $\ell = 1$  and  $\ell = 2$ , respectively.
- The Fourier transform of  $W_\ell(x)$  is

$$\widetilde{W}_\ell(k) = \frac{\sqrt{\pi} 2^{\frac{1}{2}-\ell} \cos\left(\frac{\pi k}{2}\right) \Gamma(\ell+1)}{\Gamma\left(\frac{1}{2}(-k+\ell+2)\right) \Gamma\left(\frac{1}{2}(k+\ell+2)\right)}. \quad (24)$$

- Any nontrivial solutions to the stationary dynamics correspond to the so-called nematic phases of the liquid crystals.



## Proposition

1. *The trivial branch of the Onsager model,  $W_1(x)$ , has infinitely many bifurcation points.*
2. *The trivial branch of the Maier–Saupe model,  $W_2(x)$ , has exactly one bifurcation point.*
3. *The trivial branch of the model  $W_\ell(x)$  for  $\ell$  even has at least  $\frac{\ell}{4}$  bifurcation points if  $\frac{\ell}{2}$  is even and  $\frac{\ell}{4} + \frac{1}{2}$  bifurcation points if  $\frac{\ell}{2}$  is odd.*
4. *The trivial branch of the model  $W_\ell(x)$  for  $\ell$  odd has infinitely many bifurcation points if  $\frac{\ell-1}{2}$  is even and at least  $\frac{\ell+1}{4}$  bifurcation points if  $\frac{\ell-1}{2}$  is odd.*

- The Keller–Segel model is used to describe the motion of a group of bacteria under the effect of the concentration gradient of a chemical stimulus, whose distribution is determined by the density of the bacteria.
- For this system,  $\varrho(x, t)$  represents the particle density of the bacteria and  $c(x, t)$  represents the availability of the chemical resource.
- The dynamics of the system are then described by the following system of coupled PDEs:

$$\begin{aligned} \partial_t \varrho &= \nabla \cdot (\beta^{-1} \nabla \varrho + \kappa \varrho \nabla c) & (x, t) \in U \times (0, \infty), \\ -(-\Delta)^s c &= \varrho & (x, t) \in U \times [0, \infty), \\ \varrho(x, 0) &= \varrho_0 & x \in U \times \{0\}, \\ \varrho(\cdot, t) &\in C^2(\overline{U}) & t \in [0, \infty), \end{aligned} \tag{25}$$

- for  $s \in (\frac{1}{2}, 1]$ .

- The stationary Keller–Segel equation is given by,

$$\nabla \cdot (\beta^{-1} \nabla \varrho + \kappa \varrho \nabla \Phi^s \star \varrho) = 0 \quad x \in U, \quad (26)$$

- with  $\varrho \in C^2(\bar{U})$  and where  $\Phi^s$  is the fundamental solution of  $-(-\Delta)^s$ .

## Theorem

*Consider the stationary Keller–Segel equation (26). For  $d \leq 2$  and  $s \in (\frac{1}{2}, 1]$ , it has smooth solutions and its trivial branch  $(\varrho_\infty, \kappa)$  has infinitely many bifurcation points.*

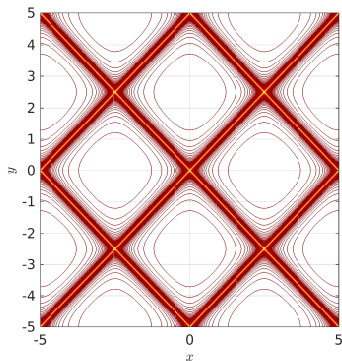


Figure: \*

(a)

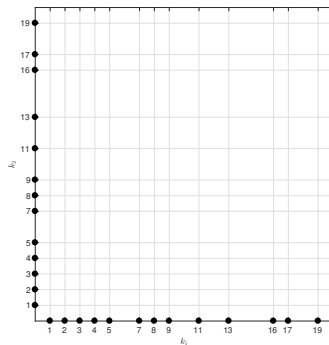


Figure: \*

(b)

**Figure:** (a). Contour plot of the Keller–Segel interaction potential  $\Phi^s$  for  $d = 2$  and  $s = 0.51$ . The orange lines indicate the positions at which the potential is singular (b). The associated wave numbers which correspond to bifurcation points of the stationary system.

- Studied the combined homogenization mean-field limits; the limits do not necessarily commute.
- Complete analysis of local and global bifurcations for the McKean-Vlasov equation on the torus.
- Study the effect of memory, colored noise/non-gradient structure, hypoellipticity etc.
- Study dynamical metastability phenomena.
- Predicting phase transitions, linear response theory, optimal control.