Phase transitions for the McKean-Vlasov equation on the torus

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Outline

1. Question and Goal
2. H-stability and basic longtime convergence
3. Bifurcations and local stability
4. Thermodynamics and critical transition

Motivation

Water droplet nucleation from H2O vapor by a molecular dynamics simulations.

[K. K. Tanaka, A. Kawano & H.Tanaka, J. Chem. Phys. 2014]

1. Question and Goal

The McKean–Vlasov equation – Setup

Nonlocal parabolic PDE

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

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

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

The McKean–Vlasov equation – Derivation

Overdamped Langevin equation defined on $\mathbb{T}_L^d$

$$dX_t^i = -\frac{\kappa}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2\beta^{-1}}dW_t^i$$

- Take $\mathrm{law}(X_0) = \varrho_0^{\otimes N}$ and set $\varrho^{(N)}(\mathrm{d}x, t) = \frac{1}{N}\sum_{i=1}^{N} \delta_{X_t^i}(\mathrm{d}x)$
- The mean-field limit governs a weak solution of the McKean–Vlasov equation

$$\mathbb{E}(\varrho^{(N)}(\cdot, t)) \to \varrho(\cdot, t), \qquad \text{as } N \to \infty.$$

Some applications: Finite N or mean-field limit

- Molecules of a gas
- Opinions of individuals
- Collective motion of agents
- Particles in a granular medium
- Nonlinear synchronizing oscillators
- Liquid crystals

The McKean–Vlasov equation – Derivation

Overdamped Langevin equation defined on $\mathbb{T}^d_L$

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Example: The noisy Kuramoto model

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

$\kappa < \kappa_c$, no phase locking

$\kappa > \kappa_c$, phase locking

Goals and Motivation:

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

2. H-stability and basic longtime convergence

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

$$w_k(x) = L^{-d/2}\Theta(k)\prod_{i=1}^{d} w_{k_i}(x_i) \qquad \text{with} \qquad w_{k_i}(x_i) = \begin{cases} \cos\left(\frac{2\pi k_i}{L}x_i\right) & k_i > 0, \\ 1 & k_i = 0, \\ \sin\left(\frac{2\pi k_i}{L}x_i\right) & k_i < 0, \end{cases}$$

$$\Theta(k) = 2^{\#\{i:k_i=0\}/2}$$

Definition (H-stability)

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

$$W_{\mathrm{s}}(x) = \sum_{k\in\mathbb{N}^d} (\langle W, w_k \rangle)_+ w_k(x) \qquad \text{and} \qquad W_{\mathrm{u}}(x) = W(x) - W_s(x)\,.$$

$$\mathcal{E}(\varrho,\varrho) = \iint_{\mathbb{T}_L^d\times\mathbb{T}_L^d} W(x-y)\varrho(x)\varrho(y)\,\mathrm{d}x\,\mathrm{d}y = L^{d/2}\sum_{k\in\mathbb{N}^d}\frac{\widetilde{W}(k)}{\Theta(k)}\sum_{\sigma\in\mathrm{Sym}(\{-1,1\}^d)}|\widetilde{\varrho}(\sigma(k))|^2$$

Functionals for stationary states

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

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

- Disipation: $\mathscr{F}_\kappa$ is Lyapunov-function

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

- Kirkwood-Monroe fixed point mapping

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

Characterization of stationary states: The following are equivalent

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

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

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Exponential stability/convergence in relative entropy

Consider free energy gap wrt. unifrom state

$$\mathscr{F}_\kappa(\varrho) - \mathscr{F}_\kappa(\varrho_\infty) = \beta^{-1}\mathcal{H}(\varrho|\varrho_\infty) + \frac{\kappa}{2}\mathcal{E}(\varrho - \varrho_\infty, \varrho - \varrho_\infty) \,.$$

Theorem

Any solution ϱ of the McKean-Vlasov is exponentially stable in relative entropy

$$\mathcal{H}(\varrho(\cdot,t)|\varrho_\infty) \le \exp\left[\left(-\frac{4\pi^2}{\beta L^2} + 2\kappa\|\Delta W_{\mathrm{u}}\|_\infty\right)t\right] \mathcal{H}(\varrho_0|\varrho_\infty).$$

Especially

- *if $W \in \mathbb{H}_{\mathrm{s}}$, then for any $\beta, \kappa > 0$*
- *if $W \notin \mathbb{H}_{\mathrm{s}}$, then for $\beta\kappa < \frac{2\pi^2}{L^2\|\Delta W_{\mathrm{u}}\|_\infty}$*

it holds exponential convergence to the uniform state.

Proof

- Use log-Sobolev on $\mathbb{T}_L^d$, constant $\frac{L^2}{4\pi^2}$
- H-stability and Fourier representation of interaction energy
- Young convolution inequality and Pinsker inequality to compare with $\mathcal{H}(\varrho|\varrho_\infty)$

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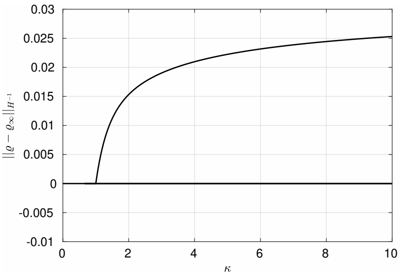
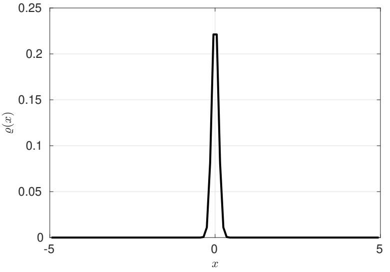
3. Bifurcations and local stability

- $W \notin \mathbb{H}_s$ needs to be a necessary condition
- Numerical experiments indicate one, multiple, or possibly infinite solutions
- What determines the number of nontrivial solutions?
- Birfurcation 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 ϱ_∞.

Local bifurcation result

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

Theorem

Consider $\hat{F} : L^2_s(\mathbb{T}^d_L) \times \mathbb{R}_{>0} \to L^2_s(\mathbb{T}^d_L)$ *with* $\hat{F}(u,\kappa) = F_\kappa(u + \varrho_\infty)$ *and* $W \in L^2_s(\mathbb{T}^d_L)$ *with* $L^2_s(\mathbb{T}^d_L)$ *the subspace of coordinate-wise even functions. Assume there exists* $k^* \in \mathbb{N}^d$*, such that:*

1. $\operatorname{card}\{k \in \mathbb{N}^d : \widetilde{W}(k) = \widetilde{W}(k^*)\} = 1$
2. $\widetilde{W}(k^*) < 0$

Then, $(0,\kappa_*)$ *is a bifurcation point of* $\hat{F}(u,\kappa) = 0$*, where,*

$$\kappa_* = -\frac{L^{\frac{d}{2}}\Theta(k^*)}{\beta\widetilde{W}(k^*)} \,.$$

The branch of solutions has the following form

$$\varrho^*_s = \varrho_\infty + s w_{k^*} + o(s) \,.$$

Examples of birfucations results

- Kuramoto-type of models: $W(x) = -w_k(x)$ in $d = 1$

$$\widetilde{W}(k) = -1,$$

satisfying both conditions. Thus we have that $\kappa_* = \frac{\sqrt{2L}}{\beta}$

- For $W(x) = \frac{x^2}{2}$ holds

$$\widetilde{W}(k) = \frac{L^{5/2}\cos(\pi k)}{2\sqrt{2}\pi k^2}$$

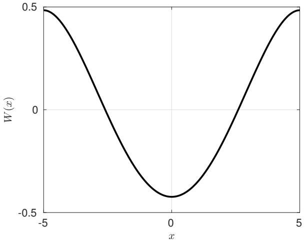
satisfying both conditions for odd values of k. Hence, every odd k is birfucation point $\kappa_* = \frac{4k^2}{\beta L^2}$.

- $W^s(x) = -\sum_{k=1}^{\infty} \frac{1}{k^{2s+2}} w_k(x)$

  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



4. Thermodynamics and critical transition

Transition points: Qualitative change of minimizers

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

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

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

Definition (Continuous and discontinuous transition point)

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

1. For $\kappa = \kappa_c$: ϱ_∞ is the unique minimiser of $\mathscr{F}_\kappa(\varrho)$
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.

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Basic properties of transition points

Summary of critical points:

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

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

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

- $\mathscr{F}_\kappa$ has a transition point κ_c iff $W \notin \mathbb{H}_s$
- $\min \mathscr{F}_\kappa$ is non-increasing as a function of κ
- If for some κ' : ϱ_∞ is no longer the unique minimiser, then $\forall \kappa > \kappa'$: ϱ_∞ is no longer a minimizer
- If κ_c is continuous, then $\kappa_c = \kappa_\sharp$

Conclusion:

- To proof a discontinous transition: Show ϱ_∞ at $\kappa_\sharp$ is no longer global minimizer
- To proof a continuous transition:
  If $\kappa_* = \kappa_\sharp$, sufficient to show that ϱ_∞ at $\kappa_\sharp$ is the only global minimizer and

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Conditions for continuous and discontinous phase transition

Theorem

Let $W(x) \in \mathbb{H}_s^c$.

- *If there exist (near)-resonating dominant modes: That is for δ small enough*

$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \frac{\widetilde{W}(k')}{\Theta(k')} \leq \min_{k \in \mathbb{N}^d} \frac{\widetilde{W}(k)}{\Theta(k)} + \delta \right\} \quad \textit{satisfy} \quad k^a + k^b = k^c ,$$

  then there exists a discontinous transition point $\kappa_c \leq \kappa_\sharp$.

- *If there is only one dominant unstable mode k^* : For $\alpha > 0$ small enough holds*

$$\alpha \widetilde{W}(k^\sharp) \leq \widetilde{W}(k) \qquad \textit{for all } k \neq k^\sharp : \widetilde{W}(k) < 0 ,$$

  then the transition point $\kappa_c = \kappa_\sharp = \kappa_*$ is continuous.

Proof: Need estimates on free energy difference $\mathcal{F}_{\kappa_\sharp}(\varrho) - \mathcal{F}_{\kappa_\sharp}(\varrho_\infty)$!

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  then the transition point $\kappa_c = \kappa_\sharp = \kappa_*$ *is continuous.*

Proof: Need estimates on free energy difference $\mathcal{F}_{\kappa_\sharp}(\varrho) - \mathcal{F}_{\kappa_\sharp}(\varrho_\infty)$!

Argument for resonating dominant modes ($\delta = 0$)

Let $\varepsilon > 0$ and set

$$\varrho = \varrho_\infty \Big(1 + \varepsilon \sum_{k \in K^\delta} w_k \Big) \in \mathcal{P}_{\mathrm{ac}}^+(U).$$

Then, it holds

$$\beta^{-1} S(\varrho) = \beta^{-1} \left(S(\varrho_\infty) + \frac{|K^\delta|}{2} \varrho_\infty \varepsilon^2 - \frac{\varrho_\infty}{3} \int_{\mathbb{T}_L^d} \varepsilon^3 \Big(\sum_{k \in K^\delta} w_k \Big)^3 \mathrm{d}x + O(\varepsilon^4) \right)$$

$$\frac{\kappa_\sharp}{2} \mathcal{E}(\varrho, \varrho) = \frac{\kappa_\sharp}{2} \mathcal{E}(\varrho_\infty, \varrho_\infty) + \frac{\kappa_\sharp \varepsilon^2 |K^\delta| \varrho_\infty^2}{2} \min_{k \in \mathbb{N}^d} \frac{\widetilde{W}(k)}{\Theta(k)} L^{d/2}$$

Combining both estimates, recalling $\kappa_\sharp = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$, yields

$$\mathscr{F}_{\kappa_\sharp}(\varrho) - \mathscr{F}_{\kappa_\sharp}(\varrho_\infty) \le -\frac{\varepsilon^3 \varrho_\infty}{3\beta} \int_{\mathbb{T}_L^d} \Big(\sum_{k \in K^\delta} w_k \Big)^3 \mathrm{d}x + O(\varepsilon^4).$$

The resonance condition $k^a + k^b = k^c$ ensures that

$$\int_{\mathbb{T}_L^d} \Big(\sum_{k \in K^{\delta *}} w_k \Big)^3 \mathrm{d}x > 0\,.$$

Argument for dominant unstable mode

By using $\kappa_\sharp = -\frac{L^{\frac{d}{2}}}{\beta \min_k \widetilde{W}(k)/\Theta(k)}$, we obtain the lower bound

$$
\begin{aligned}
\mathscr{F}(\varrho) - \mathscr{F}(\varrho_\infty) &= \beta^{-1}\mathcal{H}(\varrho|\varrho_\infty) + \frac{\kappa_\sharp}{2}\mathcal{E}(\varrho - \varrho_\infty, \varrho - \varrho_\infty) \\
&= \beta^{-1}\mathcal{H}(\varrho|\varrho_\infty) + \frac{\kappa_\sharp}{2} L^{d/2} \frac{\widetilde{W}(k^\sharp)}{\Theta(k^\sharp)} \sum_{\sigma \in \mathrm{Sym}(\Lambda)} |\widetilde{\varrho}(\sigma(k^\sharp))|^2 \\
&\quad + \frac{\kappa_\sharp}{2} L^{d/2} \sum_{k \in \mathbb{N}^d, k \neq k^\sharp} \frac{\widetilde{W}(k)}{\Theta(k)} \sum_{\sigma \in \mathrm{Sym}(\Lambda)} |\widetilde{\varrho}(\sigma(k))|^2 \\
&\geq \beta^{-1}\Bigg(\underbrace{\mathcal{H}(\varrho|\varrho_\infty) - \frac{L^d}{2}|\widetilde{\varrho}(k^\sharp)|^2}_{>0???} - \frac{\alpha L^d}{2}\|\varrho\|_2^2\Bigg) .
\end{aligned}
$$

By dual formulation of relative entropy follows for any $b \in \mathbb{R}$

$$
\mathcal{H}(\varrho|\varrho_\infty) \geq b|\widetilde{\varrho}(k^\sharp)|^2 - \log \int_{\mathbb{T}_L^d} \exp\Big(b\widetilde{\varrho}(k^\sharp) w_{k^\sharp}(x)\Big)\varrho_\infty \, \mathrm{d}x.
$$

Optimization over b provides desired positive lower bound.

Conclusions and future work

- Improve conditions on continuous and discontinous transitions
- Symmetries of critical points
- Extend results to $\mathbb{R}^d$ and a class of confining potentials $V(x)$
  $\Rightarrow$ use appropriate orthonormal system
- Global/local stability results for nontrivial solutions beyond criticality
- The structure of global bifurcations
- Dynamical metastability and coarsening for discontinous transitions

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Thank you for your attention!

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Sketch of the bifurcation result

Proof: Relies on the Crandall–Rabinowitz theorem. Need to show that conditions imply $D_\varrho \hat{F}$ has a 1D kernel. We have,

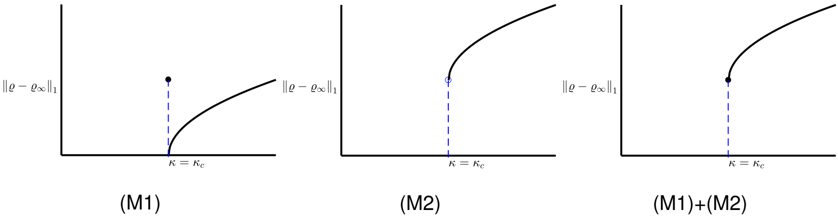
$$D_\varrho(\hat{F}(0,\kappa))[w_1] = w_1 + \beta\kappa\varrho_\infty(W \star w_1) - \beta\kappa\varrho_\infty^2 \int_U (W \star w_1)(x)\,\mathrm{d}x$$

We can diagonalise $D_\varrho \hat{F}(0,\kappa)$ using the orthonormal basis, $w_k(x)$ to obtain,

$$D_\varrho \hat{F}(0,\kappa)[w_k(x)] = \begin{cases} \left(1 + \beta\kappa \frac{\widetilde{W}_k}{(2L)^{d/2}}\right) w_k(x) & k_i > 0, \text{ for some } i = 1 \dots d \\ w_k(x) & k_i = 0, \forall i = 1 \dots d \end{cases}$$

Then condition (1) tells us when the $\dim \ker D_\varrho \hat{F}(0,\kappa) = 1$ and condition (2) ensures that the corresponding κ_* is positive. The results about the structure of the branch are obtained by looking at higher order Frechét derivatives.

Discontinuous transitions in the birfucation diagram



Ways in which a discontinuous transition can occur.