Phase transitions for the McKean-Vlasov equation on the torus

André Schlichting

Institute for Applied Mathematics, University of Bonn (on leave)
Department of Mathematics I, RWTH Aachen University

joint work with JOSÉ CARRILLO, RISHABH S. GVALANI, GREG PAVLIOTIS

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Outline

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

- $\varrho(\cdot,t) \in \mathcal{P}(\mathbb{T}_L^d)$ 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

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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

H-stability

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)

An even 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

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

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

Functionals for stationary states

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

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

- Dissipation: $\mathscr{F}_\kappa$ 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 $\mathbb{T}^d_L$, 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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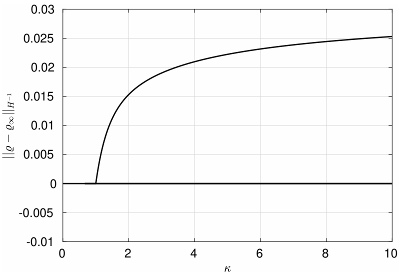
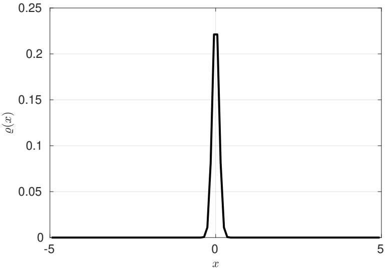
3. Bifurcations and local stability

Nontrivial solutions to the stationary McKean–Vlasov equation?

- $W \notin \mathbb{H}_s$ 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

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

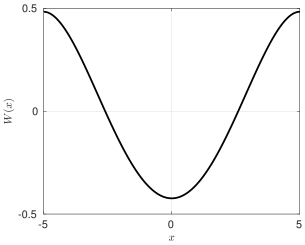
  satisfying both conditions for odd values of k. Hence, every odd k is birfucation point $\kappa_* = \frac{4k^2}{\beta L^2}$.

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

  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

Lehrstuhl I für Mathematik RWTH AACHEN UNIVERSITY

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

  If $k_\sharp = \arg\min \widetilde{W}(k)$ is unique, 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_∞ is no longer global minimizer at $\kappa_\sharp$.
- To proof a continuous transition:
  If $\kappa_* = \kappa_\sharp$, sufficient to show that ϱ_∞ at $\kappa_\sharp$ is the unqiue global minimizer.

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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*

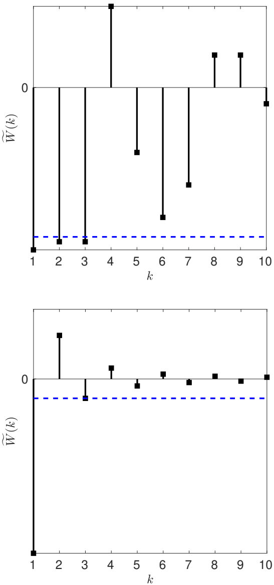
  $$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \frac{\widetilde{W}(k')}{\Theta(k')} \leq \min_{k \in \mathbb{N}^d} \frac{\widetilde{W}(k)}{\Theta(k)} + \delta \right\}$$

  satisfying $k^a = k^b + k^c$, *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*

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

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



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

Let $\varepsilon > 0$ be sufficiently small such that

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

Then, it holds

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

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

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

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

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

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

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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More details on relative entropy bound

Dual formulation of the entropy:

$$\mathcal{H}(f\mu|\mu) = \sup_{g\in L^2(\Omega,\mu)} \left\{ \int f g \,\mathrm{d}\mu : \int e^g \,\mathrm{d}\mu \le 1 \right\}.$$

From here a lower bound is obtain by choosing for $b \in \mathbb{R}$ arbitrary

$$g(x) = b\langle f, w_k\rangle_\mu w_k(x) - \log \int \exp\bigl(b\langle f, w_k\rangle_\mu w_k(x)\bigr)\,\mathrm{d}\mu.$$

Then $\int e^g \,\mathrm{d}\mu = 1$ and hence the lower bound

$$\mathcal{H}(f\mu|\mu) \ge -\log \int \exp\bigl(b\langle f, w_k\rangle_\mu w_k(x)\bigr)\,\mathrm{d}\mu + b|\langle f, w_k\rangle_\mu|^2.$$

Special case $\Omega = U$ and $\mu = \varrho_\infty$, setting $f = \frac{\varrho}{\varrho_\infty}$ then

$$\mathcal{H}(\varrho|\varrho_\infty) \ge -\log \int \exp(b\widetilde{\varrho}(k) w_k(x))\varrho_\infty \,\mathrm{d}x + b|\widetilde{\varrho}(k)|^2.$$

Pick $b = \alpha L^d$ for some $\alpha > 0$ and set $y = L^{d/2} 2^{n/2} \widetilde{\varrho}(k)$ to obtain

$$\mathcal{H}(\varrho|\varrho_\infty) \ge \frac{\alpha y^2}{2^n} - \log\left(\varrho_\infty \int_{\mathbb{T}_L^d} e^{\alpha y \prod_{i=1}^n \cos(2\pi k_i x_i/L)} \,\mathrm{d}x \right),$$

with $n \ge 1$ representing the number of $k_i \ne 0$.

Even more details on relative entropy bound

Setting $x_i = \frac{L}{2\pi k_i}\theta_i$ for all $k_i \neq 0$, we arrive at

$$\mathcal{H}(\varrho|\varrho_\infty) \geq \frac{\alpha y^2}{2^n} - \log\left(\frac{1}{2^n\pi^n}\int_{[0,2\pi]^n} \exp\left(\alpha y \prod_{i=1}^n \cos(\theta_i)\right) \prod_{j=1}^n \mathrm{d}\theta_j\right) .$$

We introduce the function

$$\mathcal{I}_n(z) = \frac{1}{2^n\pi^n}\int_{[0,2\pi]^n} \exp\left(z \prod_{i=1}^n \cos(\theta_i)\right) \prod_{j=1}^n \mathrm{d}\theta_j = \sum_{l=0}^\infty \frac{z^{2l}}{(2l)!}\left(\frac{1}{\pi}\int_0^\pi \cos(\theta)^{2l}\,\mathrm{d}\theta\right)^n$$

$$= \sum_{l=0}^\infty z^{2l}\frac{((2l)!)^{n-1}}{(l!)^{2n}2^{2ln}}$$

and are going to show that

$$\widetilde{\mathcal{G}}(z) = \frac{\lambda z^2}{2^{n+1}} - \log \mathcal{I}_n(z) \qquad \text{with} \qquad \lambda = \lambda(n) = \begin{cases} 1 & , n \in \{1,2\} \\ \frac{(n-1)^{n-1}}{(n/2)^n} & , n > 2 \end{cases} .$$

is strictly increasing in z with $\widetilde{\mathcal{G}}(0) = 0$. Then, the proof concludes

$$\mathcal{H}(\varrho|\varrho_\infty) - \widetilde{\mathcal{G}}(\alpha y) \geq \frac{\alpha y^2}{2^n} - \frac{\lambda\alpha^2 y^2}{2^{n+1}} = (2-\alpha\lambda)\alpha\frac{y^2}{2^{n+1}} \overset{\alpha=\lambda^{-1}}{=} \frac{y^2}{\lambda\, 2^{n+1}}.$$

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.