Negative Diffusion in High Dimensional Lattice Systems - Travelling Waves

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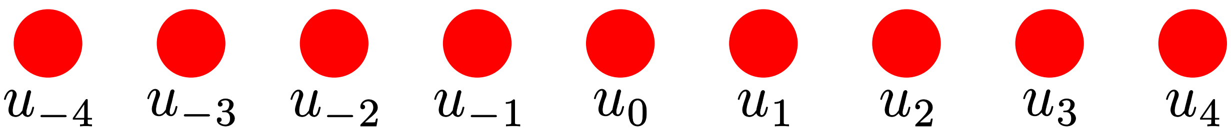
(Joint work with E. van Vleck)

Lattice Differential Equations

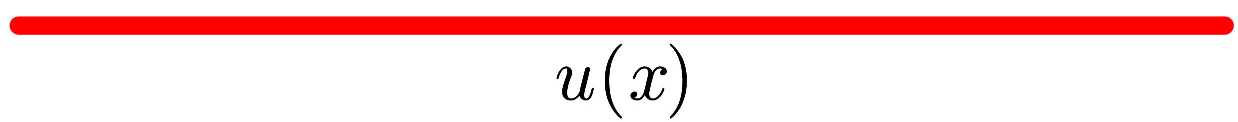
Lattice differential equations (LDEs) are ODEs indexed on a spatial lattice, e.g.

$$\dot{u}_j(t) = \alpha\big(u_{j-1}(t) + u_{j+1}(t) - 2u_j(t)\big) + f\big(u_j(t)\big), \qquad j \in \mathbb{Z}.$$



Picking $\alpha = h^{-2} \gg 1$, LDE can be seen as discretization with distance h of PDE

$$\partial_t u(t,x) = \partial_{xx} u(t,x) + f\big(u(t,x)\big), \qquad x \in \mathbb{R}.$$



- Discrete Laplacian: $u_{j-1} + u_{j+1} - 2u_j$
- Many physical models have a discrete spatial structure $\rightarrow$ LDEs.
- Main theme: qualitative differences between PDEs and LDEs.

Lattice Differential Equations

Recall LDE

$$\dot{u}_j(t) = \alpha\big(u_{j-1}(t) + u_{j+1}(t) - 2u_j(t)\big) + f\big(u_j(t)\big), \qquad j \in \mathbb{Z}.$$

- $\alpha \gg 1$ - semi-discretization of PDE. Useful discretizations should not introduce new behaviour.

- $\alpha \sim 1$ - spatial gaps as energy barriers.

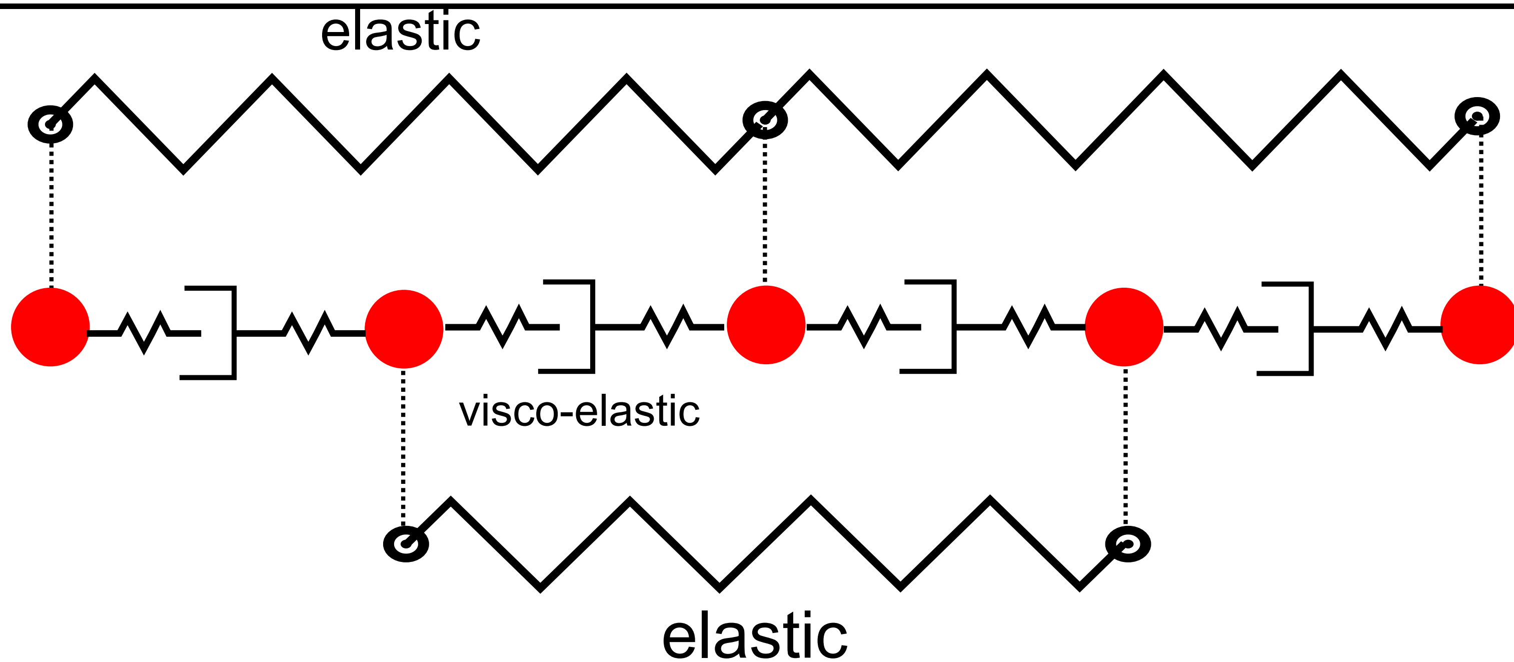
- $\alpha < 0$ - anti-diffusion.

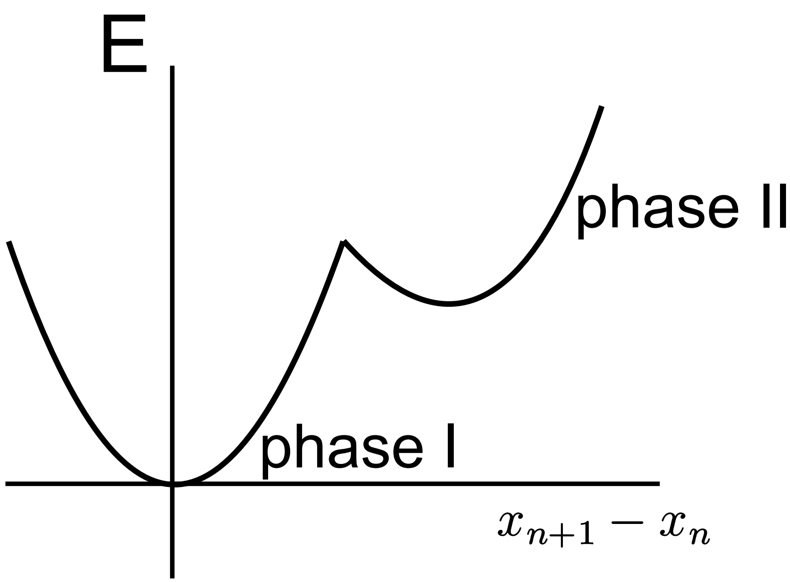
PDE ill-posed.

LDE still well-posed.

Motivation: Phase transition models [Van Vleck, Vainchtein, 2009]

Phase Transition Model

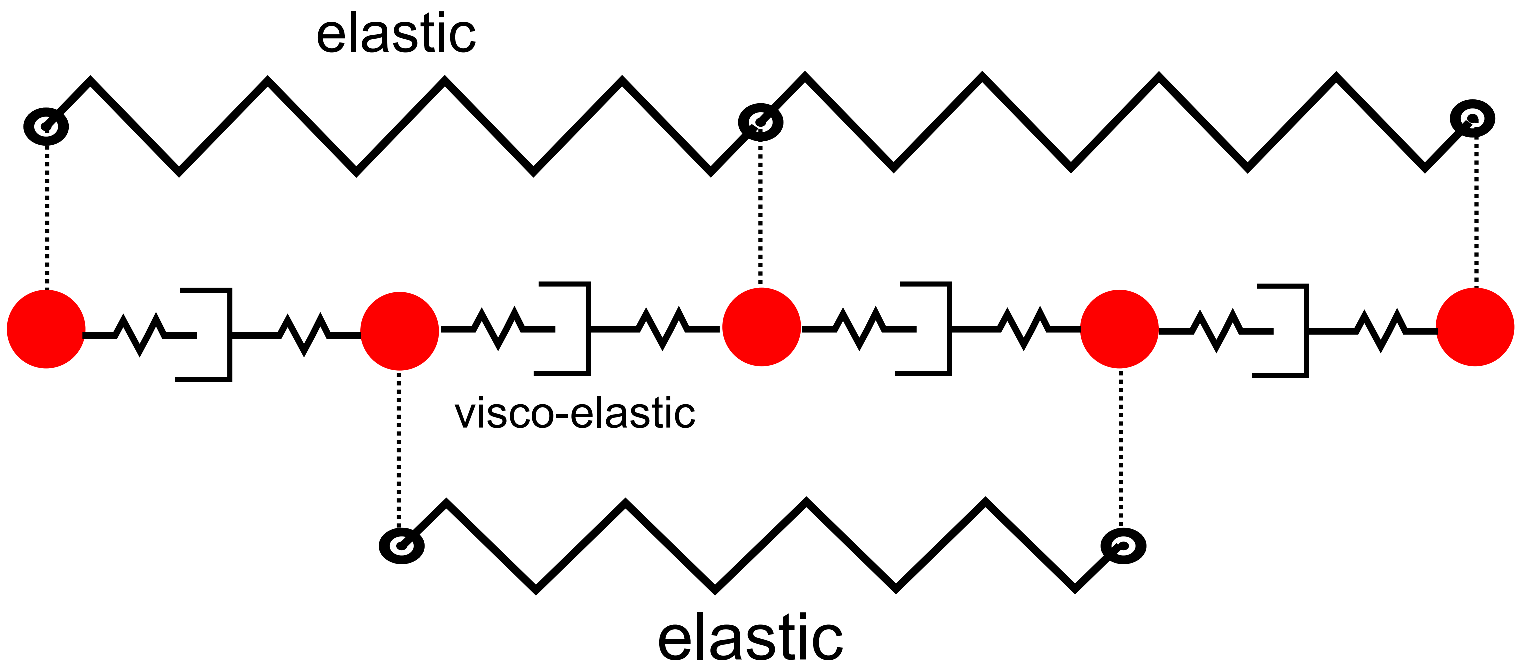




Force between NN depends on $\dot{x}_{n+1} - \dot{x}_n$ (viscous) and $E'(x_{n+1} - x_n)$ (elastic).

Negative diffusion comes from viscous terms in overdamped limit.

Phase Transition Model



Writing $u_n = x_{n+1} - x_n$, in overdamped limit we get system

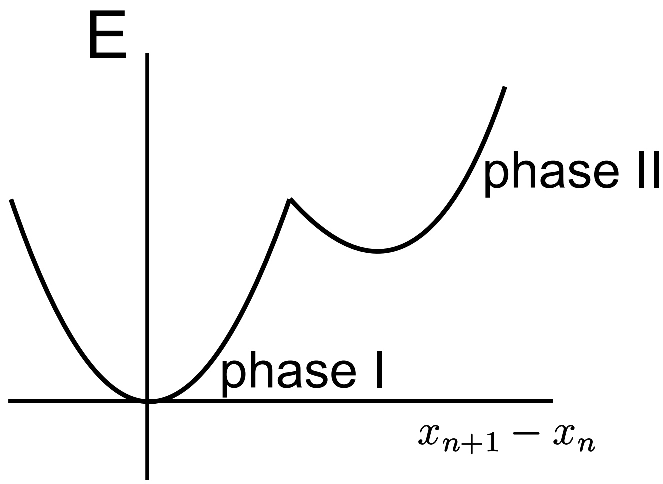
$$\dot{u}_n(t) = -d[u_{n+1}(t) + u_{n-1}(t) - 2u_n(t)] + E'\big(u_n(t)\big), \qquad d > 0.$$

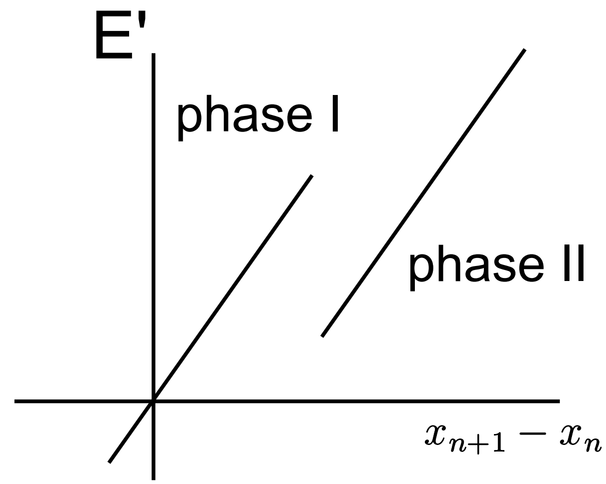
Phase Transition Model

Recall dynamics

$$\dot{u}_n(t) = -d[u_{n+1}(t) + u_{n-1}(t) - 2u_n(t)] + E'\big(u_n(t)\big), \qquad d > 0.$$

Note that E' is cartoon of cubic.





Negative diffusion 'encourages' interactions near phase boundary instead of smoothing them all out.

Negative Diffusion

Main interest here: 2d lattices

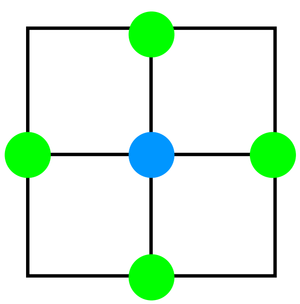
$$\dot{u}_{ij}(t) = -d[\Delta_+ u(t)]_{ij} + g\big(u_{ij}(t); a\big), \qquad d > 0.$$

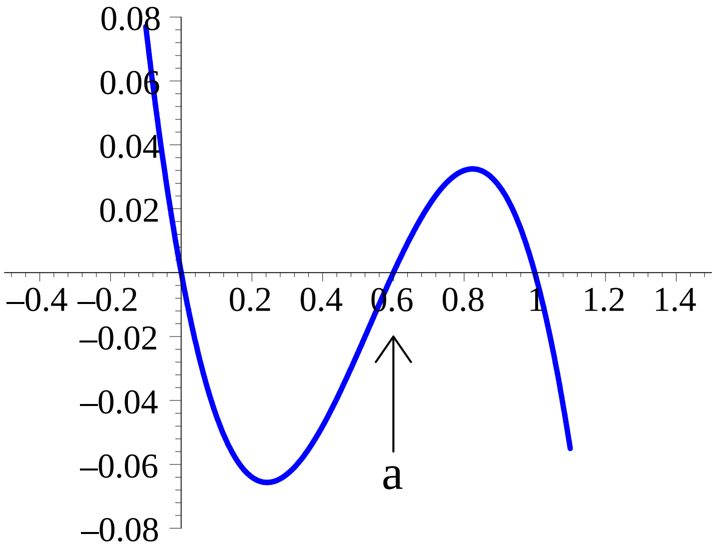
Plus-shaped discrete Laplacian:

$$[\Delta_+ u]_{ij} = u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1} - 4u_{ij}.$$

Bistable nonlinearity g given by

$$g(u; a) = u(a-u)(u-1).$$





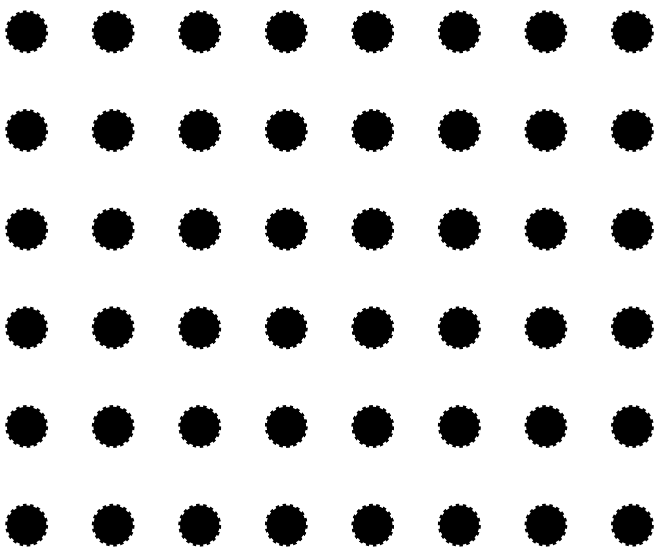
Negative Diffusion

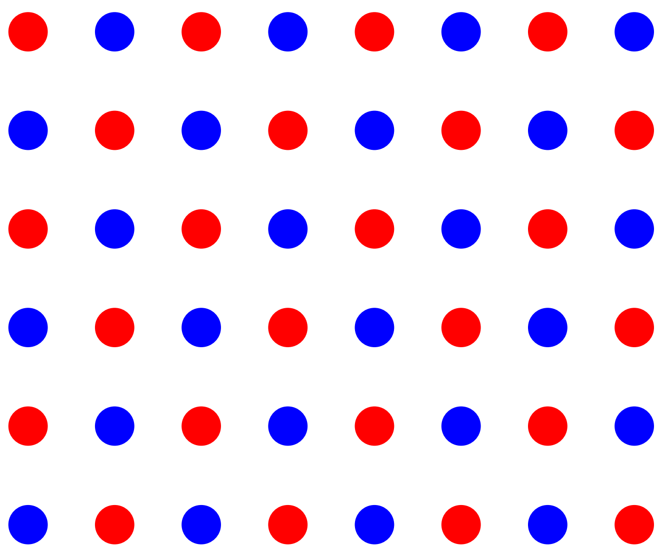
Recall negative diffusion equation

$$\dot{u}_{ij}(t) = -d[\Delta_+ u]_{ij}(t) + g\big(u_{ij}(t); a\big), \qquad d > 0.$$

Looking for travelling wave $u_{ij}(t) = \Psi\Big((\cos\theta, \sin\theta) \cdot (i, j) - ct\Big)$ will not get you very far.

Main idea: split lattice into even and odd sites.





Negative Diffusion

Writing $u_{ij}(t)$ for odd sites and $v_{ij}(t)$ for even sites, system rewrites as

$$\begin{aligned}\frac{d}{dt}u_{ij} &= -d[v_{i,j+1}+v_{i,j-1}+v_{i-1,j}+v_{i+1,j}-4u_{ij}]+g\big(u_{ij};a\big),\\ \frac{d}{dt}v_{ij} &= -d[u_{i,j+1}+u_{i,j-1}+u_{i-1,j}+u_{i+1,j}-4v_{ij}]+g\big(v_{ij};a\big)\end{aligned}$$

Equilibria $(\overline{u},\overline{v})$ must satisfy

$$\begin{aligned}4d(\overline{v}-\overline{u}) &= g(\overline{u};a),\\ 4d(\overline{u}-\overline{v}) &= g(\overline{v};a).\end{aligned}$$

Besides three 'constant' equilibria $(0,0)$, (a,a) and $(1,1)$, also 'periodic' equilibria $\overline{u}\neq\overline{v}$. In particular, eliminating $\overline{u}$ gives

$$-g(\overline{v};a)=g\Big(\overline{v}+(4d)^{-1}g(\overline{v};a);a\Big).$$

Since g was a cubic; we get a ninth-degree polynomial expression in $\overline{v}$.

Negative Diffusion

Recall ninth-order system

$$-g(\overline{v};a) = g\Big(\overline{v} + (4d)^{-1} g(\overline{v};a); a\Big).$$

Studied in detail by [Brucal, Van Vleck]. For appropriate choices of parameters, exists equilibrium $(\overline{u}_*, \overline{v}_*)$ with $\overline{u}_* \overline{v}_* < 0$ (opposite sign).

Idea: look for waves that connect $(0,0)$ to $(\overline{u}_*, \overline{v}_*)$.

Idea: rescale u and v so connection is from $(0,0) \to (1,1)$.

$$\begin{aligned}
\tfrac{d}{dt} u_{ij} &= d_o[v_{i,j+1} + v_{i,j-1} + v_{i-1,j} + v_{i+1,j} - 4u_{ij}] + g_o\big(u_{ij}; a\big), \\
\tfrac{d}{dt} v_{ij} &= d_e[u_{i,j+1} + u_{i,j-1} + u_{i-1,j} + u_{i+1,j} - 4v_{ij}] + g_e\big(v_{ij}; a\big)
\end{aligned}$$

Now we have $d_o > 0$ and $d_e > 0$; typically different. Also g_o and g_e typically different.

Travelling Wave

Recall lattice system

$$\begin{aligned}
\frac{d}{dt}u_{ij} &= d_o[v_{i,j+1} + v_{i,j-1} + v_{i-1,j} + v_{i+1,j} - 4u_{ij}] + g_o\big(u_{ij};a\big), \\
\frac{d}{dt}v_{ij} &= d_e[u_{i,j+1} + u_{i,j-1} + u_{i-1,j} + u_{i+1,j} - 4v_{ij}] + g_e\big(v_{ij};a\big)
\end{aligned}$$

Travelling wave Ansatz

$$u_{ij}(t) = \Psi_u\Big((\cos\theta, \sin\theta)\cdot(i,j) - ct\Big), \qquad v_{ij}(t) = \Psi_v\Big((\cos\theta, \sin\theta)\cdot(i,j) - ct\Big),$$

leads to system with both advances and delays:

$$\begin{aligned}
-c\Psi_u'(\xi) &= d_o[\Psi_v(\xi \pm \cos\theta) + \Psi_v(\xi \pm \sin\theta) - 4\Psi_u(\xi)] \\
&\quad + g_o\big(\Psi_u(\xi);a\big), \\
-c\Psi_v'(\xi) &= d_e[\Psi_u(\xi \pm \cos\theta) + \Psi_u(\xi \pm \sin\theta) - 4\Psi_v(\xi)] \\
&\quad + g_e\big(\Psi_v(\xi);a\big)
\end{aligned}$$

Notation: $\Psi(\xi \pm \cos\theta)$ means $\Psi(\xi + \cos\theta) + \Psi(\xi - \cos\theta)$.

Setting

Notice that any solution to

$$\begin{aligned} -c\Psi_u'(\xi) &= d_o[\Psi_v(\xi \pm \cos\theta) + \Psi_v(\xi \pm \sin\theta) - 4\Psi_u(\xi)] \\ &\quad + g_o\big(\Psi_u(\xi); a\big), \\ -c\Psi_v'(\xi) &= d_e[\Psi_u(\xi \pm \cos\theta) + \Psi_u(\xi \pm \sin\theta) - 4\Psi_v(\xi)] \\ &\quad + g_e\big(\Psi_v(\xi); a\big) \end{aligned}$$

is in fact ALSO a travelling wave solution to the non-local system

$$\begin{aligned} \partial_t u(x,t) &= d_o[v(x \pm \cos\theta, t) + v(x \pm \sin\theta) - 4u(x,t)] \\ &\quad + g_o\big(u(x,t); a\big), \\ \partial_t v(x,t) &= d_e[u(x \pm \cos\theta, t) + u(x \pm \sin\theta, t) - 4v(x,t)] \\ &\quad + g_e\big(v(x,t); a\big). \end{aligned}$$

Notice: $x \in \mathbb{R}$ so this system now has only one spatial variable.

Main System

Our focus is on travelling wave solutions to the system

$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,; a\big).$$

- Non-scalar system: $u(x,t) \in \mathbb{R}^n$ for some $n \geq 2$.
- Matrices $A_j \geq 0 \in \mathbb{R}^{n\times n}$.
- Matrix $\mathcal{A} := \sum_{j=0}^{N} A_j$ is irreducible; i.e. all components of u are mixed.
- Off-diagonal derivatives non-zero:

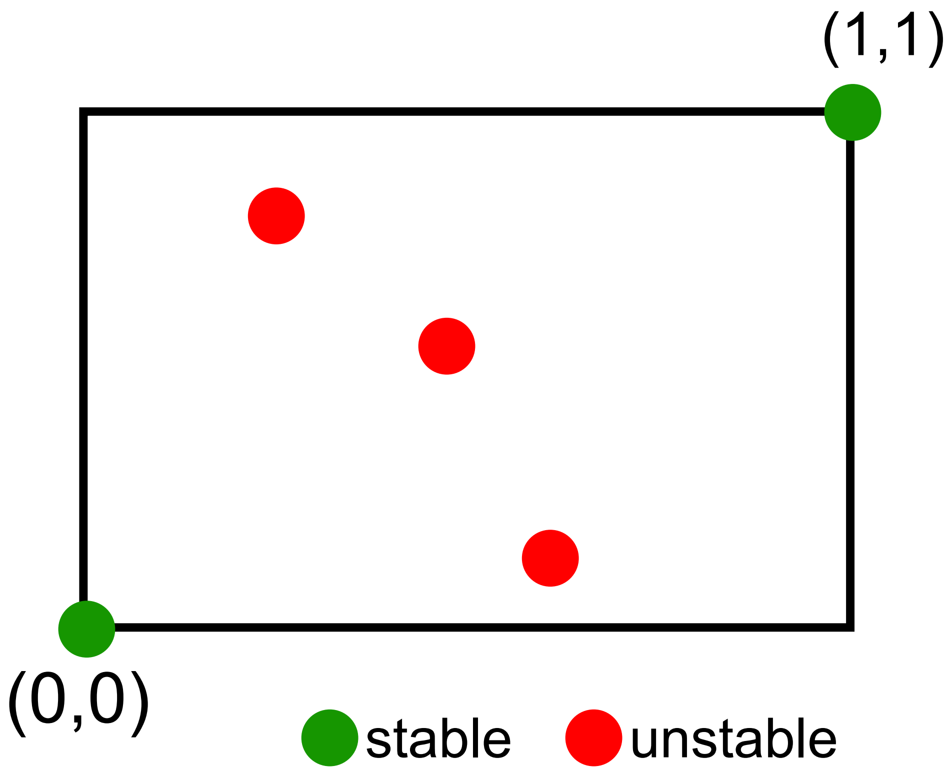
$$\partial_{u_j} g_i(u;a) \geq \mathcal{A}_{ij}, \qquad\qquad i \neq j.$$

- Extra smoothing term $\gamma \geq 0$.

Main System

Requirements on zeroes of $g(\cdot; a)$ for fixed parameter a:

$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big).$$



Stability refers to ODE $u' = g(u; a)$.

Main Results

Chiefly interested in transition $\gamma \downarrow 0$:

$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big). \qquad (1)$$

Thm. [H., Van Vleck] For each $\gamma > 0$, (1) has unique travelling wave solution $u = \Psi(x - ct)$ connecting $\mathbf{0}$ to $\mathbf{1}$, which depends smoothly on parameter a.

Thm. [H., Van Vleck] Consider sequence $\gamma_k \downarrow 0$ and corresponding waves $u_k = \Psi_k(x - c_k t)$. After passing to a subsequence, we have

$$\Psi_k(x) \to \Psi_*(x), \qquad c_k \to c_*$$

and (Ψ_*, c_*) is travelling wave at $\gamma = 0$ that connects $\mathbf{0}$ and $\mathbf{1}$.

These results generalize earlier scalar equation results [H., Verduyn-Lunel, 2004].

Main Results: $\gamma = 0$

When $\gamma = 0$, we recover nonlocal system

$$u_t(x,t) = \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big). \tag{2}$$

Thm. [...] Unique wave speed c for which (2) has travelling waves that connect $\mathbf{0}$ to $\mathbf{1}$. If $c \neq 0$, then profile is unique and (Ψ, c) depend smoothly on a. If $c = 0$, profiles exist but no longer unique.

This generalizes scalar ($u(x,t) \in \mathbb{R}$) equation results [Mallet-Paret, 1998].

Existence of travelling waves for (2) with rationally related r_j can be found as a byproduct in [Chen, Guo, Wu, 2008], where periodic $1d$-lattices were considered. Lattice-based approach; cannot easily consider $\gamma > 0$.

Our focus is on dependence on a and γ; closely follow [Mallet-Paret] ideas.

Mallet-Paret: Fredholm theory

Focus in [Mallet-Paret, 1998] and [H., Verduyn Lunel] is on scalar mixed type equation

$$-\gamma\Psi''(\xi) - c\Psi'(\xi) = \sum_{j=0}^{N} A_j[\Psi(\xi + r_j) - \Psi(x)] + g\big(\Psi(\xi); a\big).$$

that wave profiles must satisfy.

- **Continuation of waves:** Relies on studying Fredholm operator

$$\mathcal{L} : \Phi \mapsto \gamma\Phi''(\xi) + c\Phi'(\xi) + \sum_{j=0}^{N} A_j[\Phi(\xi + r_j) - \Phi(\xi)] + Dg(\overline{\Psi}(\xi); a)\Phi(\xi)$$

  related to linearization around wave $\overline{\Psi}$. Important for stability, gluing waves together, singular perturbations. Natural to generalize to systems.

- **Existence of waves:** Relies on embedding system into a **normal family**, with very specific rules on how $g(\cdot; a)$ depends on a. Homotopy to reference system. Unclear how to lift to systems.

Continuation of Waves: Fredholm theory

Main task: understand Fredholm properties of

$$\mathcal{L} : \Phi \mapsto \gamma\Phi''(\xi) + c\Phi'(\xi) + \sum_{j=0}^{N} A_j[\Phi(\xi + r_j) - \Phi(\xi)] + Dg(\overline{\Psi}(\xi); a)\Phi(\xi)$$

related to linearization around wave $\overline{\Psi}$.

Need to show: kernel $\mathcal{L}$ is one-dimensional ($\overline{\Psi}' > 0$) and same for adjoint $\mathcal{L}^*$.
Krein-Rutman type result.

Main issue: matrices A_j not necessarily invertible; in contrast with scalar case.

Main consequence: 2d stability of waves; see [Aaron's talk].

Secondary consequence: can understand perturbations [Van Vleck, Zhang]; e.g. (1d)

$$\begin{aligned} \dot{u}_n(t) &= -d[u_{n+1}(t) + u_{n-1}(t) - 2u_n(t)] + g\big(u_n(t); a\big) \\ &\quad + \epsilon \textstyle\sum_{k\in\mathbb{Z}} \frac{1}{k^2}(-1)^k u_{n+k}(t). \end{aligned}$$

Existence of Waves

Second task is focus on existence of travelling waves with $\gamma > 0$ for

$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big).$$

Degenerate situation $\gamma = 0$ handled afterwards by limit $\gamma \downarrow 0$.

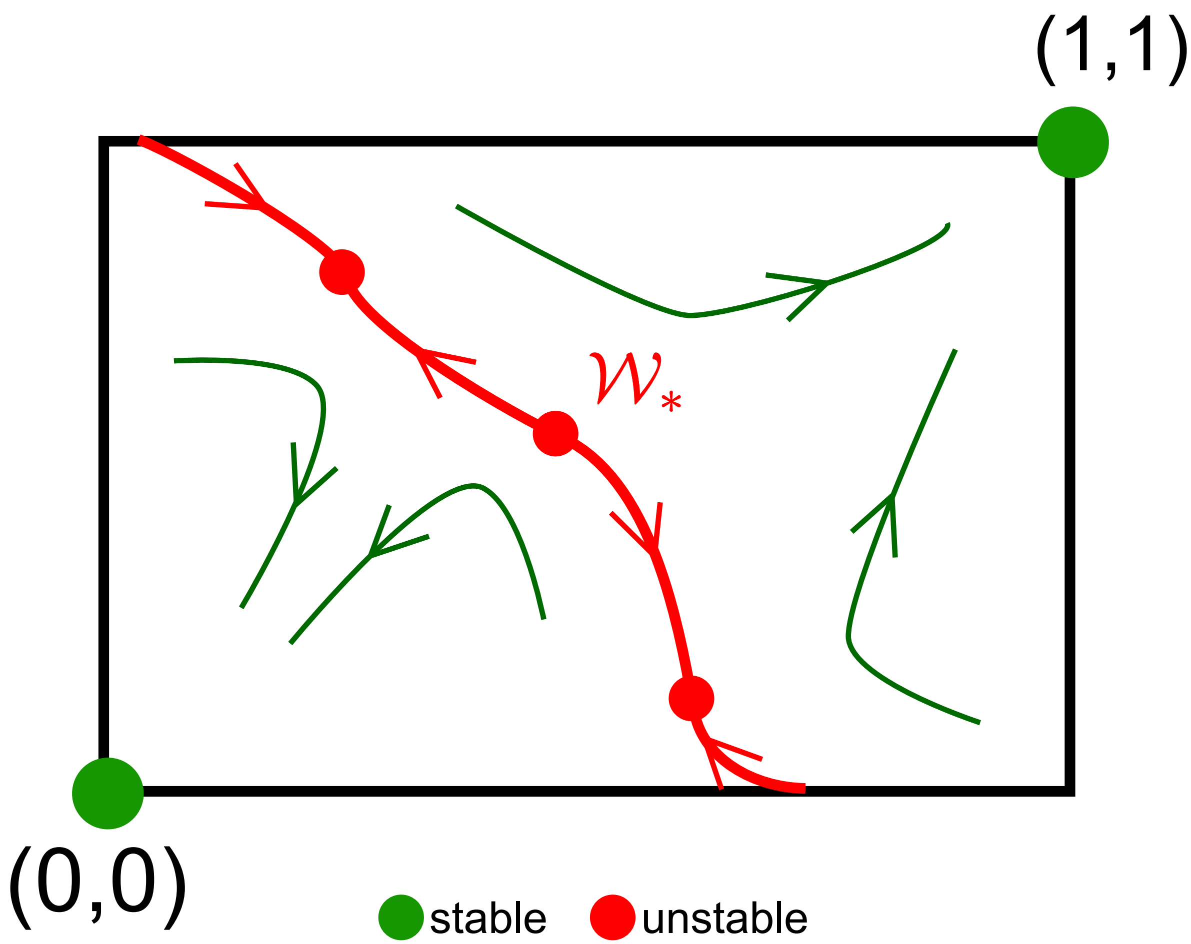
If $A_j = 0$ for all $0 \leq j \leq n$, then can use standard theory [Volpert, Volpert, Volpert] (see also [Crooks, Toland] for convective terms). Methods rely on topological arguments (index theory; homotopies).

In [Chen, 1991] scalar non-local PDEs are considered. Waves constructed using only comparison principles. Basis for our approach.

Main System

Focus on spatially invariant solutions, which satisfy ODE

$$u'(t) = g\big(u(t)\,;a\big).$$



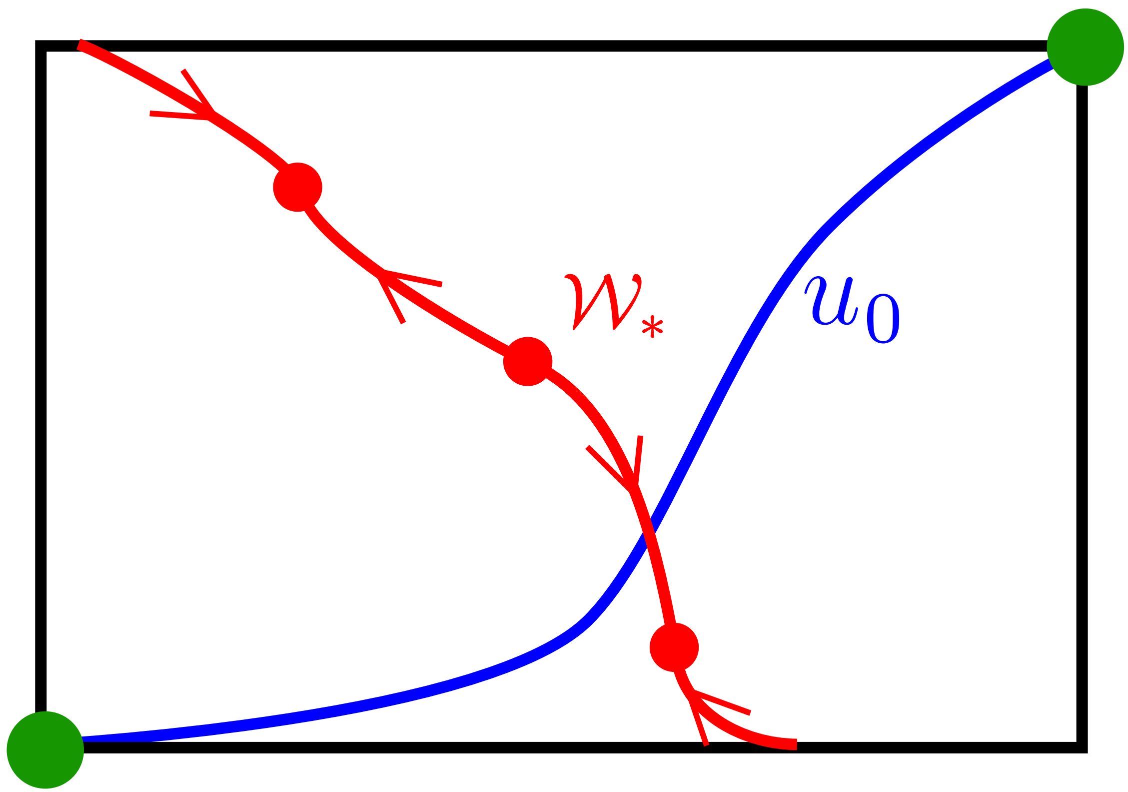
Separatrix $\mathcal{W}_*$ splits basins of attraction.

Based on [Hirsch, 1982] (cooperative systems): no points on $\mathcal{W}_*$ related by $\leq$.

Existence of travelling wave

Pick smooth non-decreasing initial condition $u(x,0) = u_0(x)$ and evolve

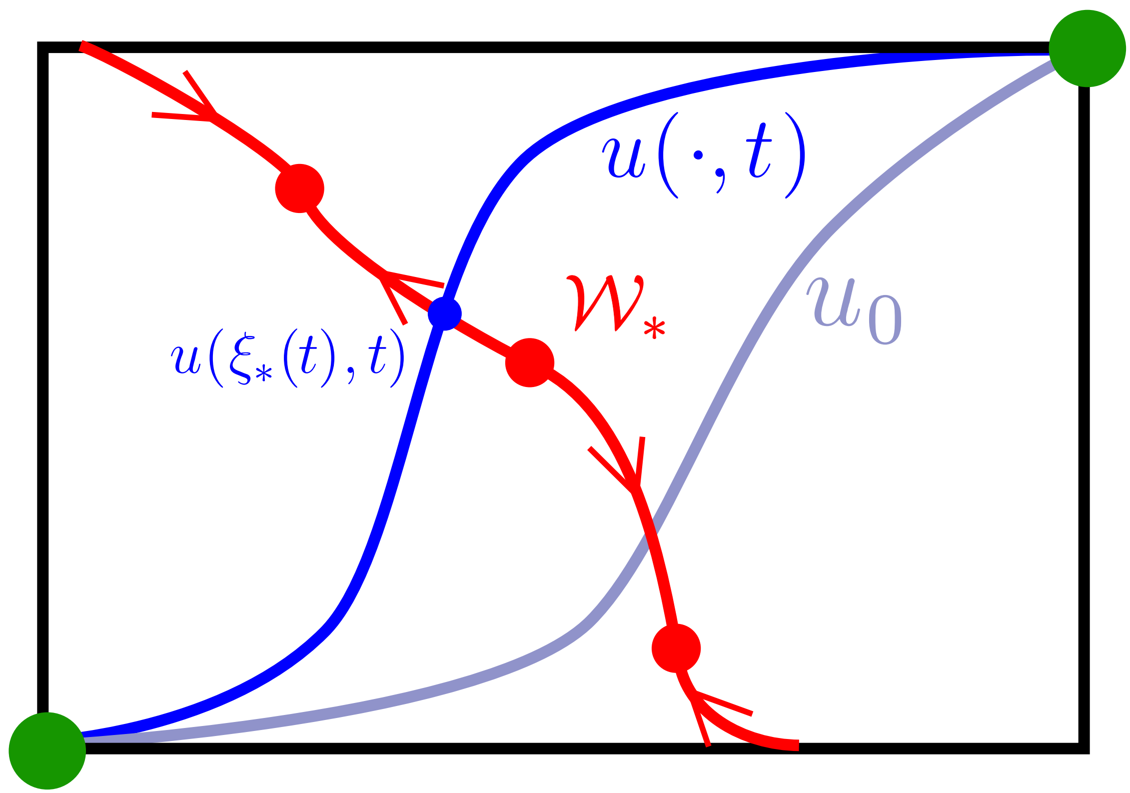
$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big).$$



Existence of travelling wave

Note that $u(\cdot, t)$ must always intersect $\mathcal{W}_*$ once; say at $x = \xi_*(t)$.

$$u_t(x,t) = \gamma u_{xx}(x,t) + \sum_{j=0}^{N} A_j[u(x+r_j,t) - u(x)] + g\big(u(x,t)\,;a\big).$$

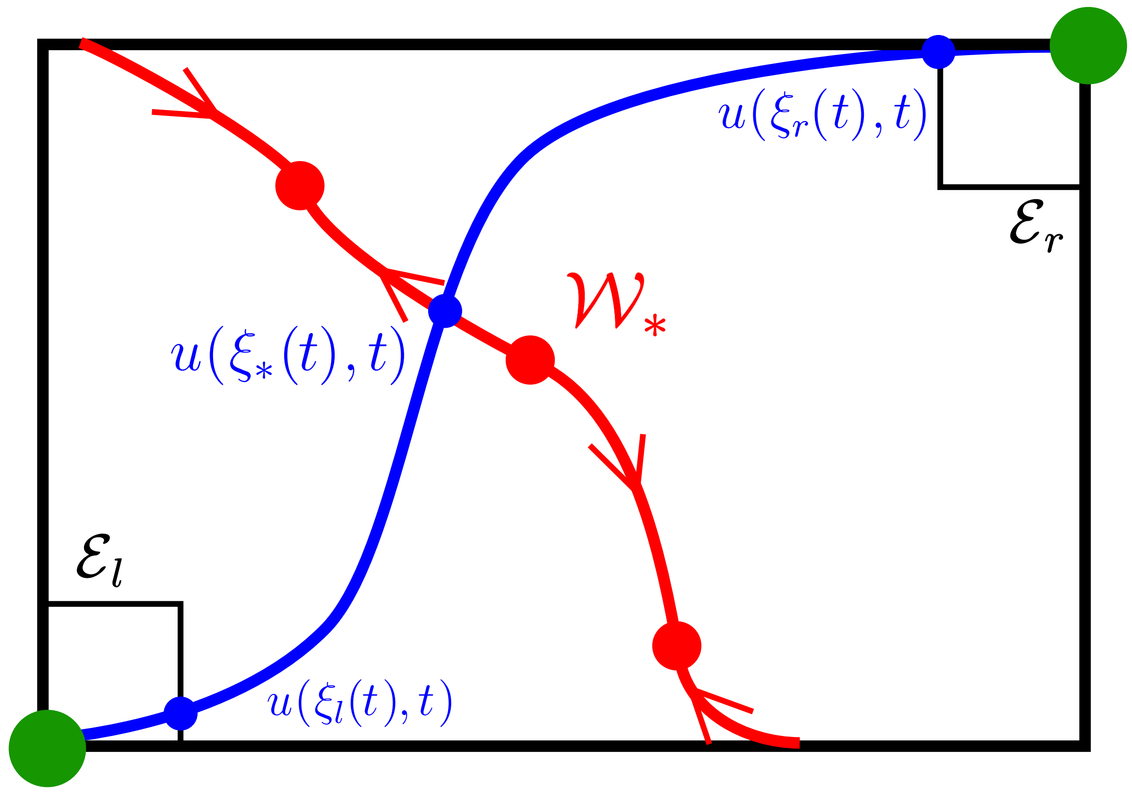


Main goal: show that $u(x - \xi_*(t), t) \to U(x)$ as $t \to \infty$ in some sense.

Existence of travelling wave

Pick two squares $\mathcal{E}_l$ and $\mathcal{E}_r$ near $(0,0)$ and $(1,1)$

$u(\cdot,t)$ intersects squares at $x = \xi_l(t)$, $x = \xi_r(t)$.

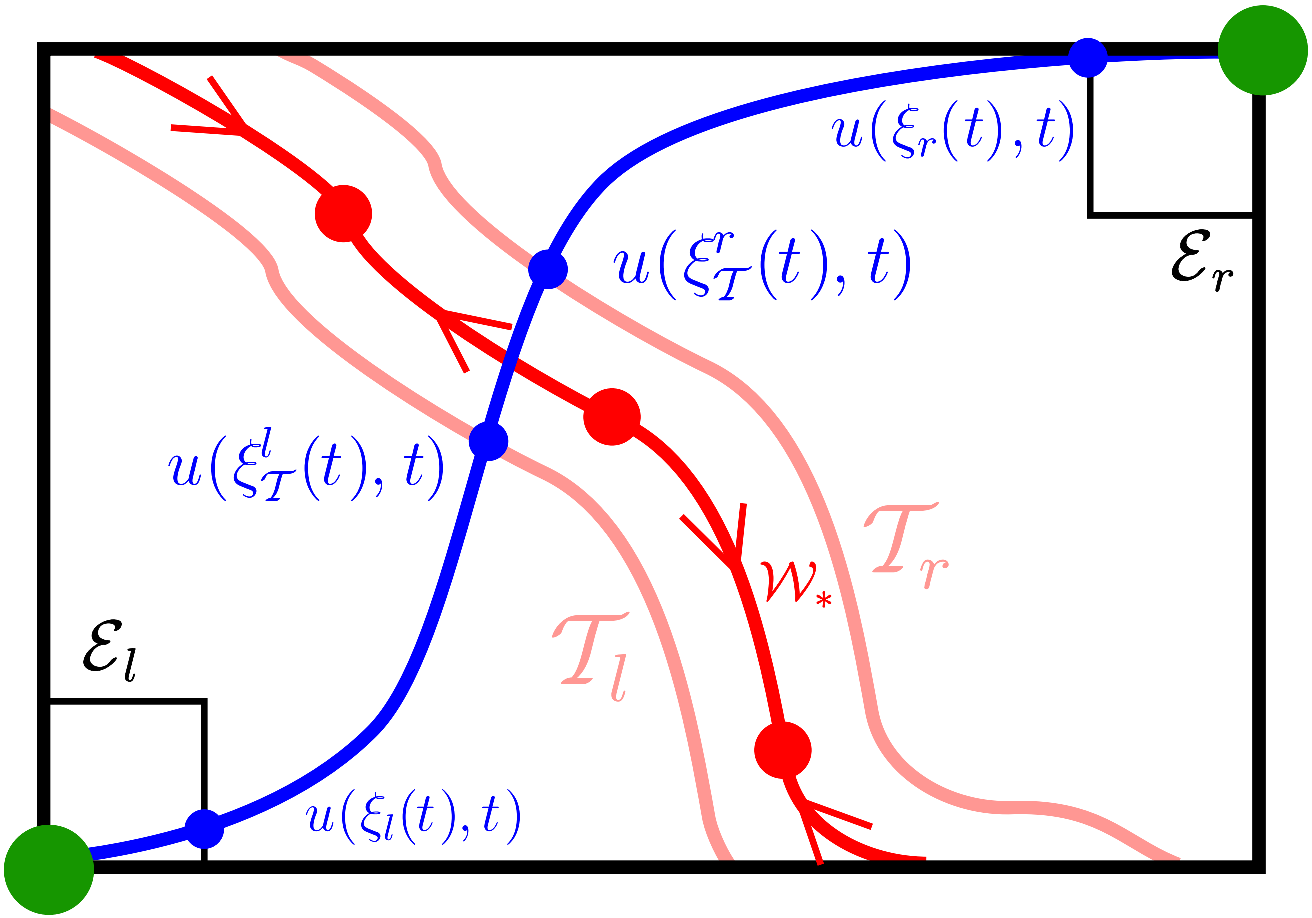


Must show: $\xi_r(t) - \xi_l(t)$ bounded for convergence $u(x - \xi_*(t), t) \to U(x)$ to be useful.

Existence of travelling wave

Build a tube around separatrix: build $\mathcal{T}_r$ and $\mathcal{T}_l$ by shifting $\mathcal{W}_*$ left and right.

Intersections with $\mathcal{T}_l$, $\mathcal{T}_r$ at $x = \xi^l_{\mathcal{T}}(t)$, $x = \xi^r_{\mathcal{T}}(t)$.



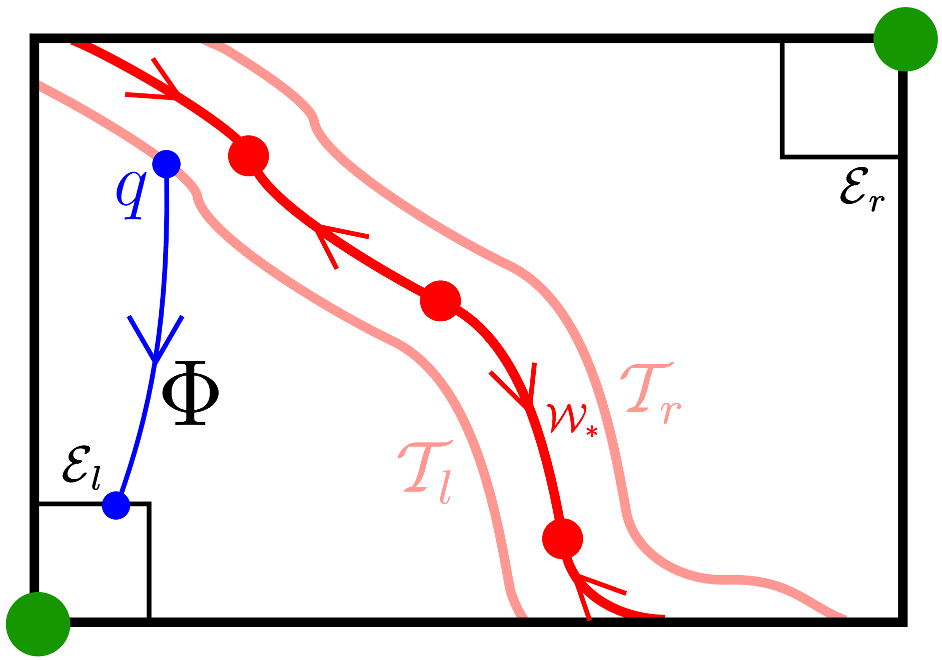
Idea: bound $\xi^l_{\mathcal{T}}(t) - \xi_l(t)$, $\xi^r_{\mathcal{T}}(t) - \xi^l_{\mathcal{T}}(t)$ and $\xi_r(t) - \xi^r_{\mathcal{T}}(t)$ separately.

Existence of travelling wave

Step I: Bound for $\xi^l_{\mathcal{T}}(t) - \xi_l(t)$.

Write $\Phi(t; q)$ for solution to ODE initial value problem:

$$u'(t) = g(u), \qquad u(0) = q.$$

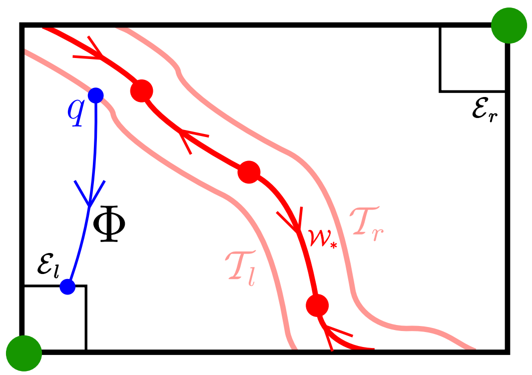


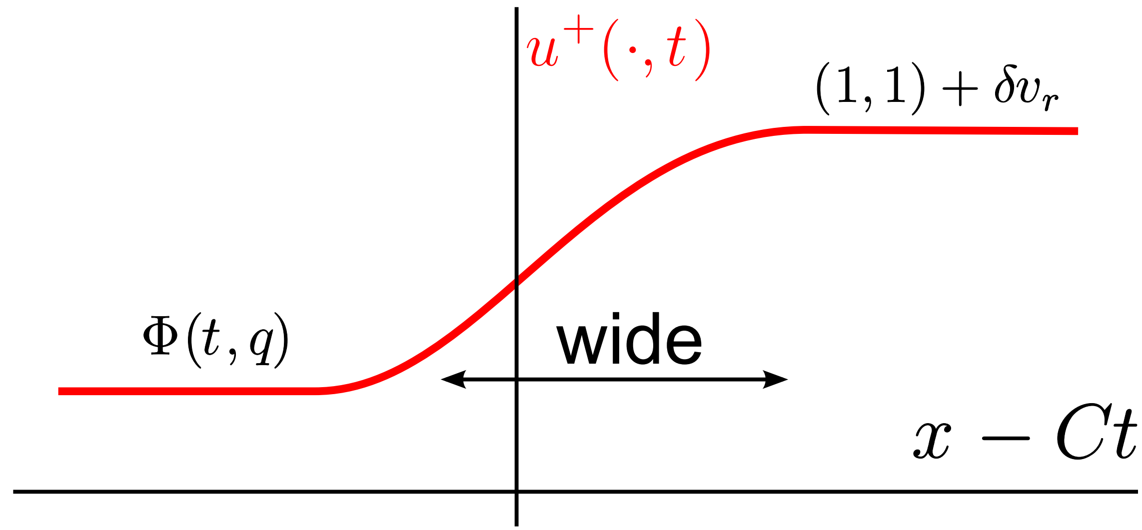
For any $q \in \mathcal{T}_l$, note that under flow Φ q is transferred through $\mathcal{E}_l$.

Transfer time can be uniformly bounded in q.

Existence of travelling wave: Step I: Bound for $\xi_{\mathcal{T}}^{l}(t) - \xi_l(t)$

Construct supersolution u^+ by picking $C \gg 1$ and connecting $\Phi(t;q)$ with $(1,1) + \delta v_r$, where $v_r > 0$ is eigenvector for $Df(1,1)$.





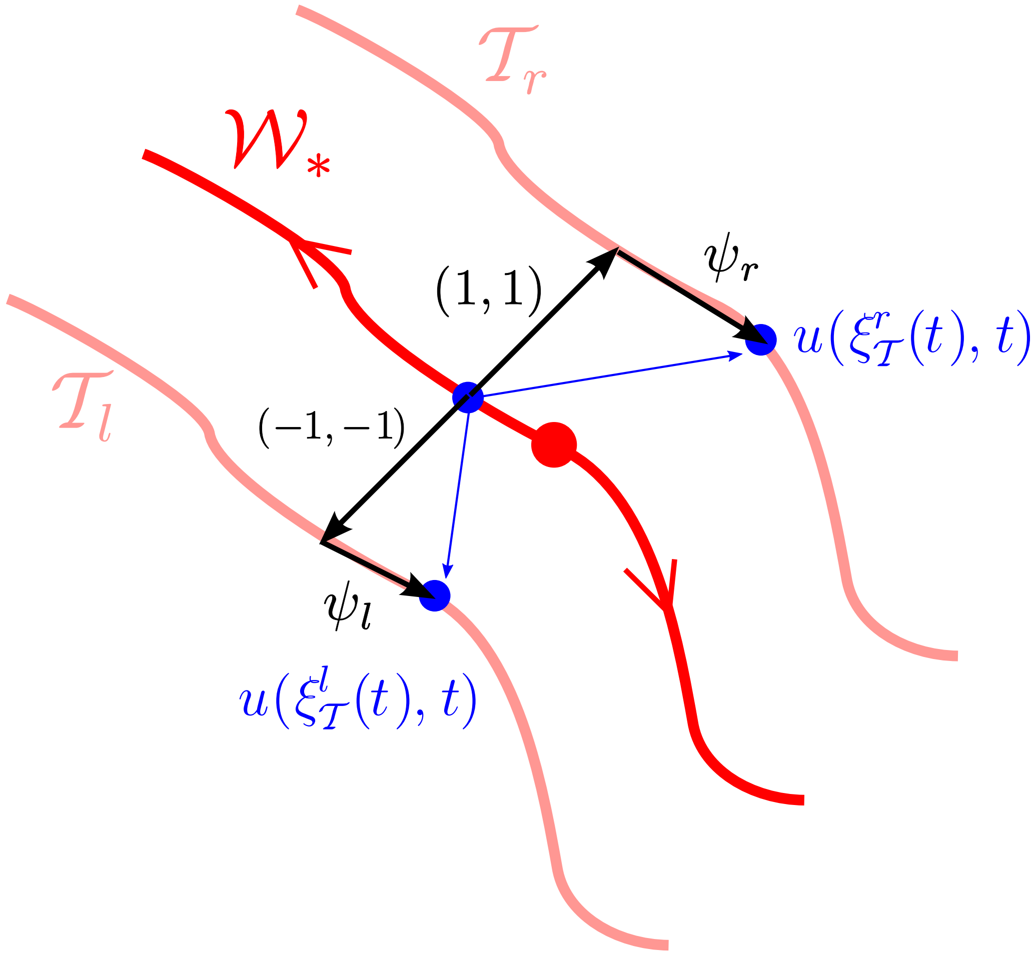
Remember: super solutions satisfy

$$\partial_t u^+ - \gamma \partial_{xx} u^+ - \sum_{j=0}^{N} A_j[u^+(\cdot + r_j) - u^+(\cdot)] - g(u^+) \geq 0.$$

Our choice ensures $\xi_l(t+T) - \xi_{\mathcal{T}}^{l}$ is bounded from below; where T was maximal transfer time.

Existence of travelling wave

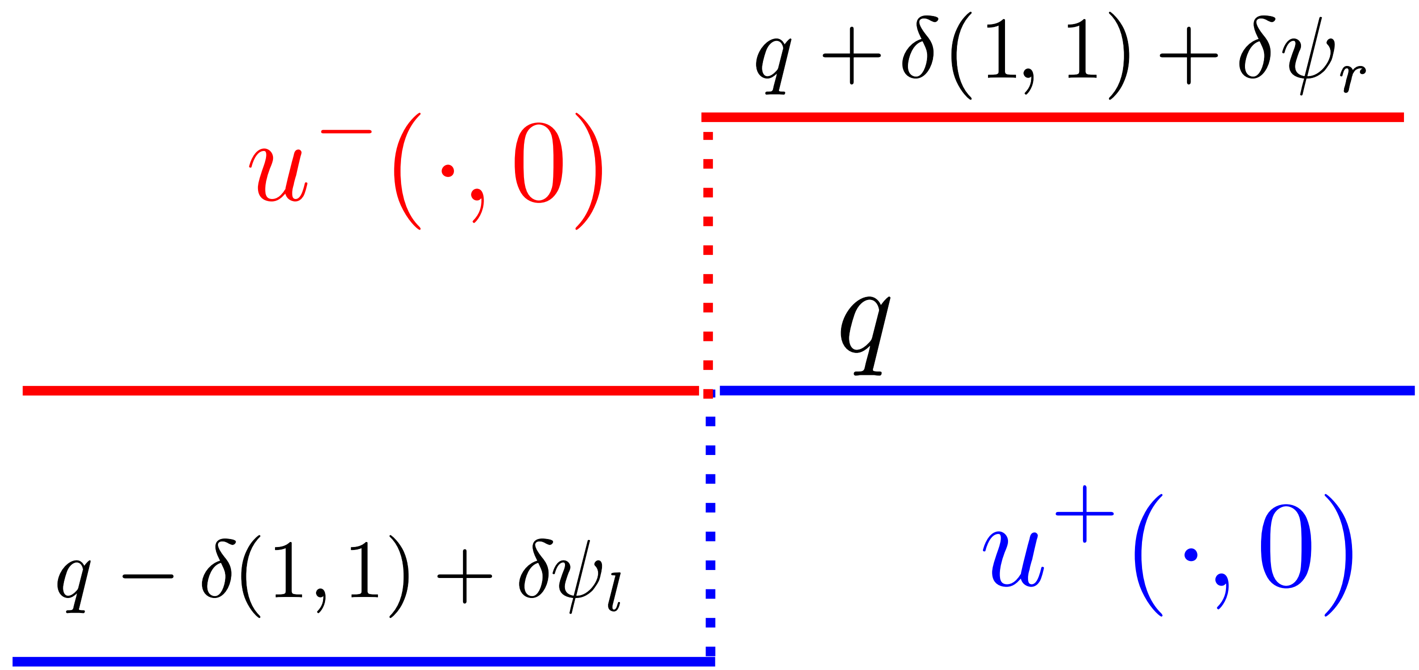
Step II: Bound for $\xi^r_{\mathcal{T}}(t) - \xi^l_{\mathcal{T}}(t)$.



Idea: decompose crossings vectors as $(1,1)+\psi_r$ and $(-1,-1)+\psi_l$, where ψ_l and ψ_r lie in tangent bundle of $\mathcal{W}_*$.

Existence of travelling wave

Step II: Bound for $\xi^r_{\mathcal{T}}(t) - \xi^l_{\mathcal{T}}(t)$.



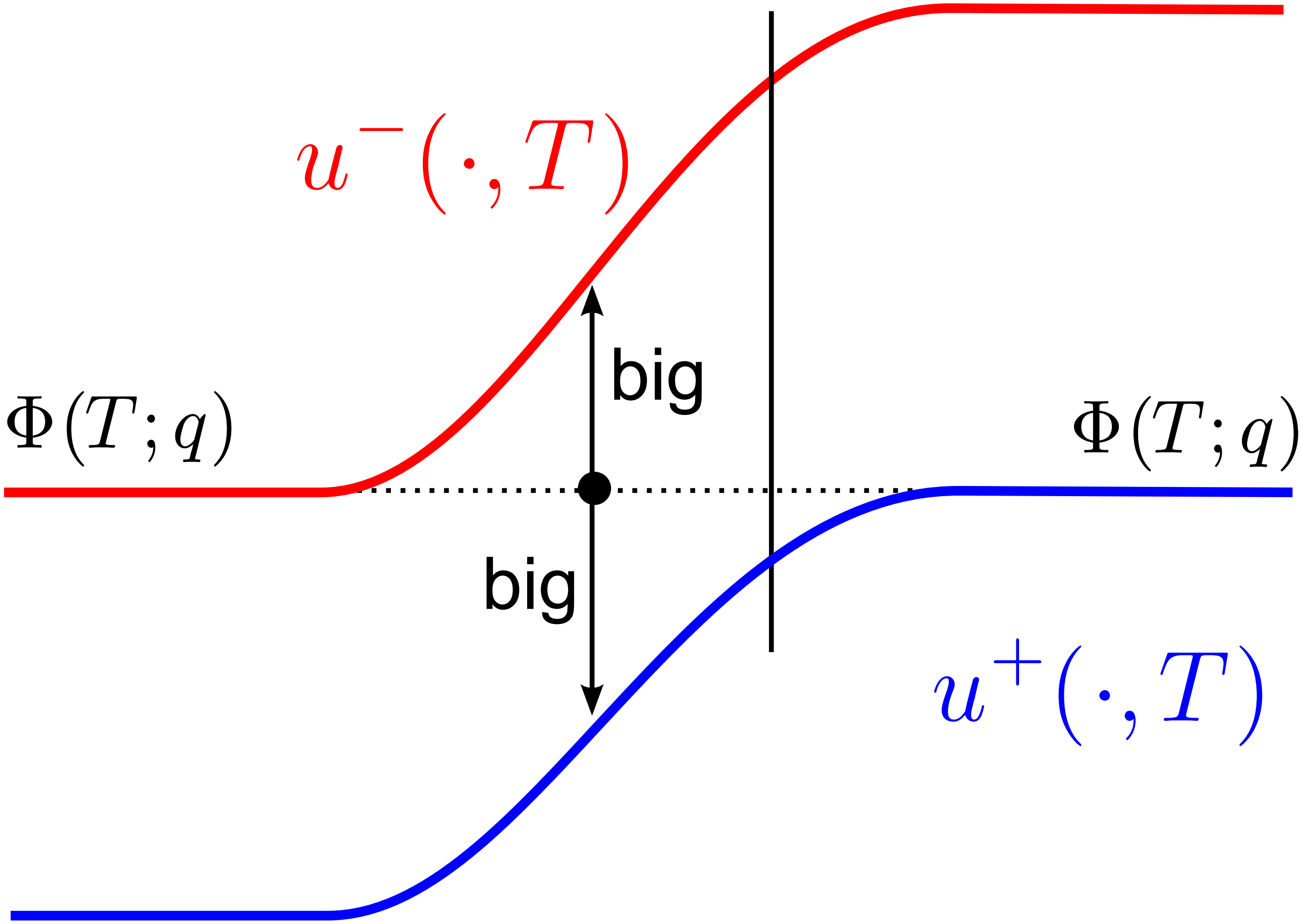
Shorthand: $q = u(\xi_*(t), t) \in \mathcal{W}_s$; intersection with separatrix.

Construct super solution u^+ and subsolution u^- that are step functions at $t = 0$ and solve system for $t > 0$.

Use: $(1, 1)$ direction will grow faster than parallel directions ψ_r and ψ_l.

Existence of travelling wave

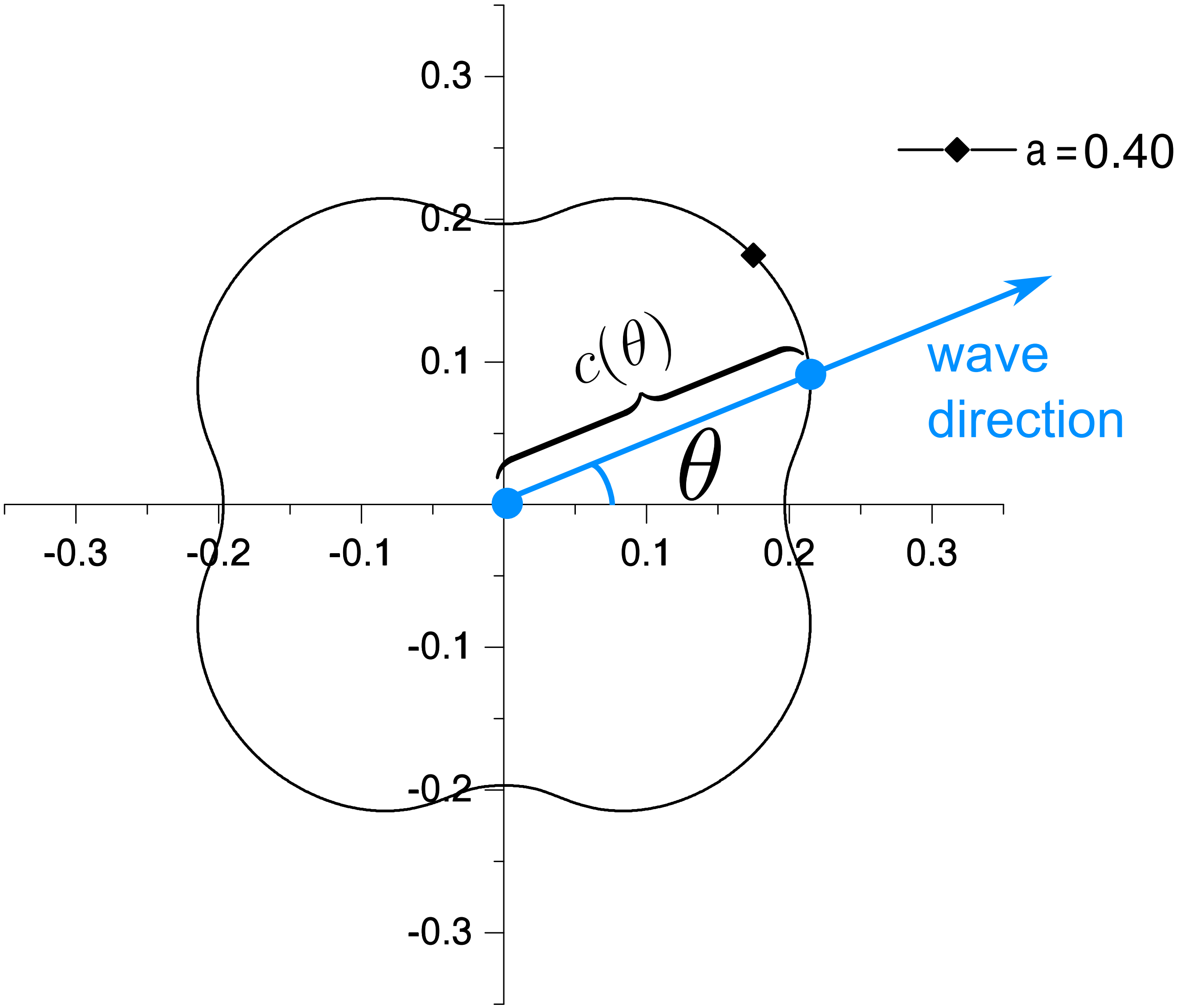
Step II: Bound for $\xi^r_{\mathcal{T}}(t) - \xi^l_{\mathcal{T}}(t)$.

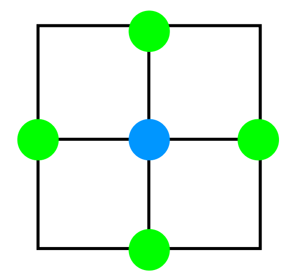


Similar to heat-flow; solutions spread out. $(1,1)$ direction expands. Can push both $u^\pm$ out of tube $\mathcal{T}$ at same x-value after T time steps.

Spatially Periodic Diffusion - Anisotropy

Wavespeed c depends on the angle of propagation θ.

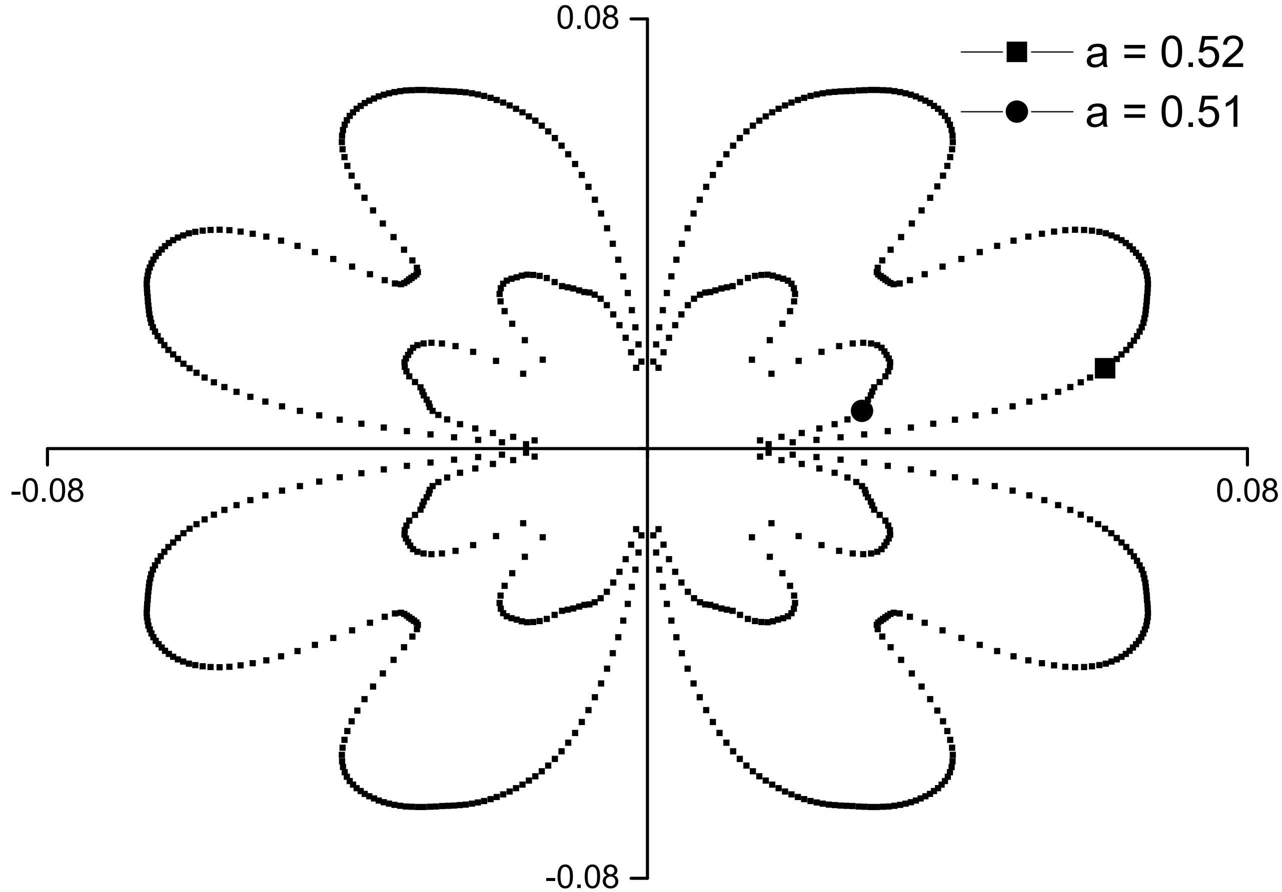




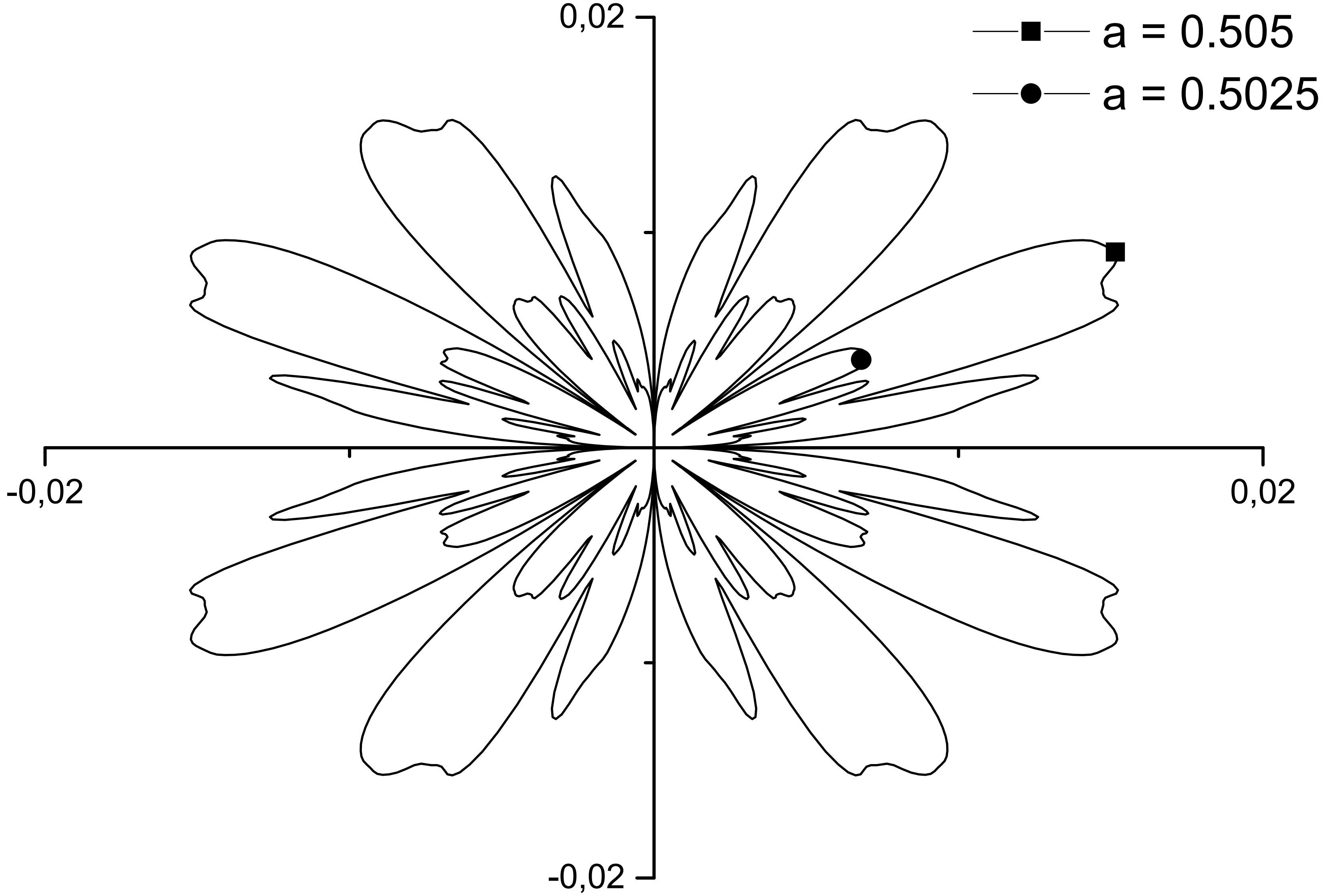
Spatially Periodic Diffusion - Anisotropy

Wavespeed plot for system

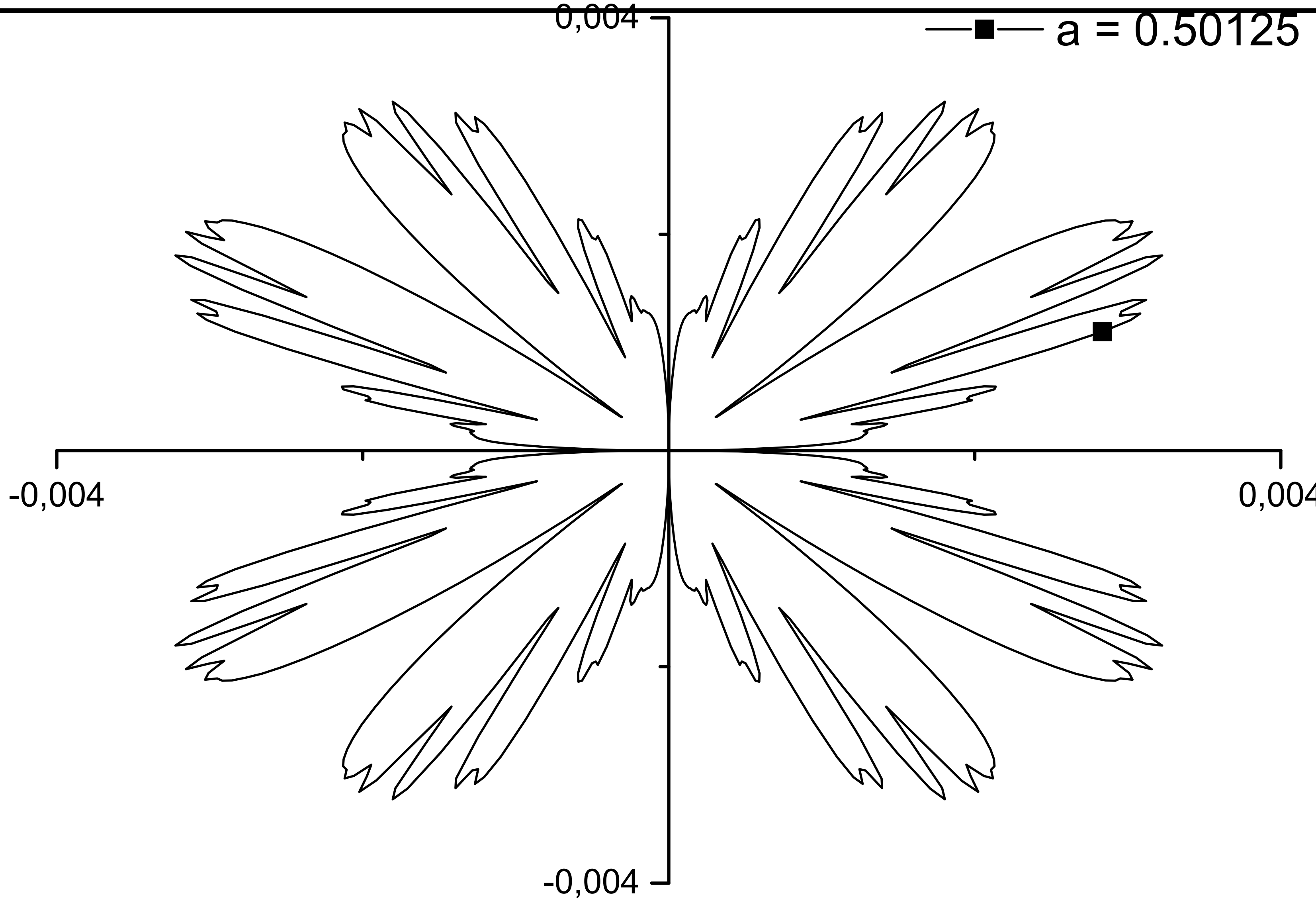
$$\frac{d}{dt}u_{ij} = 0.9[v_{i,j+1} + v_{i,j-1} + v_{i-1,j} + v_{i+1,j} - 4u_{ij}] + u_{ij}(u_{ij} - a)(1 - u_{ij}),$$
$$\frac{d}{dt}v_{ij} = 1.1[u_{i,j+1} + u_{i,j-1} + u_{i-1,j} + u_{i+1,j} - 4v_{ij}] + v_{ij}(v_{ij} - a)(1 - v_{ij}).$$



Spatially Periodic Diffusion - Anisotropy



Spatially Periodic Diffusion - Anisotropy



Crystallographic pinning: 1-component [Hoffman, Mallet-Paret], [Cahn, V.Vleck, Mallet-Paret].