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Modulated Travelling
Waves in Discrete
Reaction Diffusion Systems



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Discrete Reaction-Diffusion Systems

We consider the prototype reaction diffusion system

$$\partial_t y(x, t) = \gamma \partial_{xx} y(x, t) + [L_D y](x, t) + f(y(x, t))$$

with discrete Laplacian

$$[L_D y](x, t) = y(x + 1, t) + y(x - 1, t) - 2y(x, t).$$

- When $\gamma = 0$, we have a pure lattice system
- For $\gamma > 0$, we have a partially discrete reaction-diffusion system
- Useful for models with local and nonlocal interactions
- Allows study of transition continuous \rightarrow discrete (Van Vleck, Elmer, H., Verduyn Lunel) .

Wave trains

We are interested in wave train solutions (periodic travelling waves). Ansatz

$$y(x, t) = u(\omega t - kx)$$

leads to second order MFDE $\mathcal{F}(u, \omega, k) = 0$ with

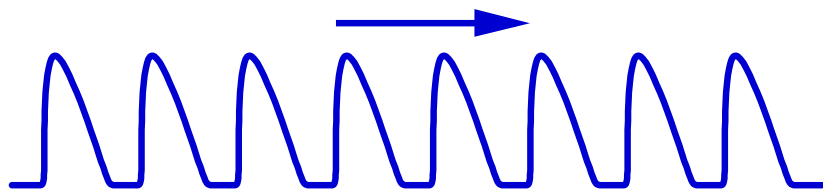
$$\mathcal{F}(u, \omega, k) := -\gamma k^2 u''(\zeta) + \omega u'(\zeta) - [u(\xi - k) + u(\xi + k) - 2u(\xi)] - f(u(\zeta))$$

We require periodicity $u(\zeta) = u(\zeta + 2\pi)$.

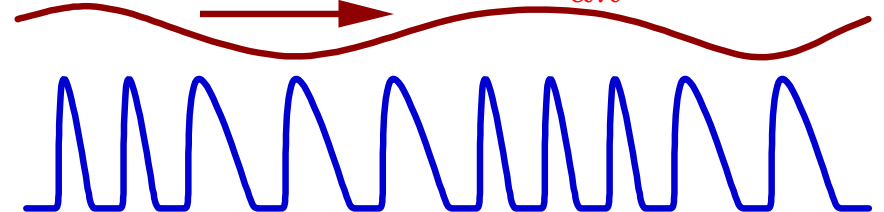
Under generic assumptions, if $\mathcal{F}(u_0, \omega_0, k_0) = 0$, then can construct 1-parameter family of wave-train solutions

$$y(x, t) = u(\omega_{\text{nl}}(k)t - kx; k) \text{ for } k \approx k_0$$

phase velocity $c_p = \frac{\omega}{k}$



group velocity $c_g = \frac{d\omega}{dk}$



Linear stability

To consider the linear stability of the wave train, insert Floquet Ansatz

$$y(x, t) = u(\zeta; k_0) + e^{\lambda t} e^{-\nu \zeta / k_0} w(\zeta),$$

with $\zeta = \omega_0 t - k_0 x$. Ignoring higher order terms, we must have

$$\mathcal{L}_{\text{st}}(\nu)w = \lambda w,$$

with (for $\gamma = 0$)

$$\begin{aligned} \mathcal{L}_{\text{st}}(\nu)w &= [\nu c_p - \omega_0 D]w + [e^\nu w(\cdot - k_0) + e^{-\nu} w(\cdot + k_0) - 2w] \\ &\quad + Df(u(\cdot; k_0))w. \end{aligned}$$

We find a set of curves $\nu \rightarrow \lambda_j(\nu)$ that are analytic except at intersection points.

Linear dispersion relation

Note that $\mathcal{L}_{\text{st}} u'(\cdot; k_0) = 0$. If the eigenvalue $\lambda = 0$ is simple, we find a curve

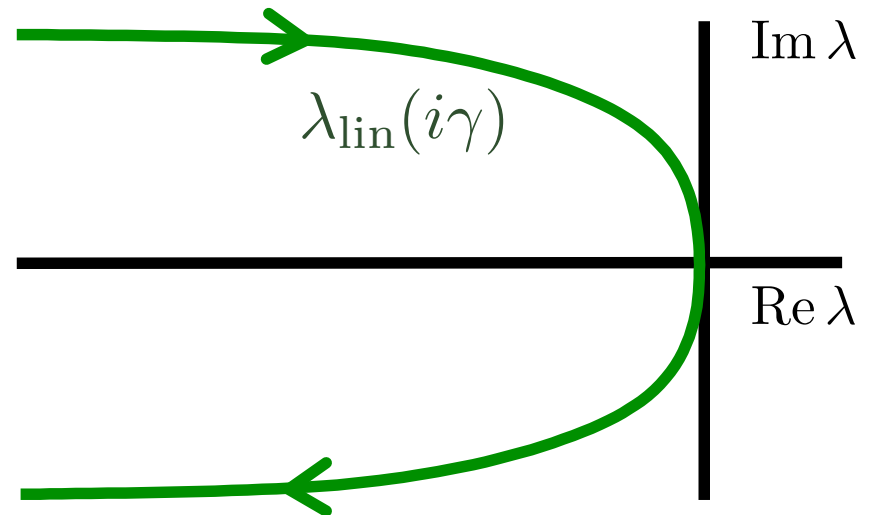
$$\nu \mapsto \lambda_{\text{lin}}(\nu)$$

that is analytic for $\nu \approx 0$, with

$$\lambda_{\text{lin}}(0) = 0, \quad \lambda'_{\text{lin}}(0) = c_p - c_g$$

Spectral stability hypothesis ($d > 0$):

$$\lambda_{\text{lin}}(i\gamma) = i(c_p - c_g)\gamma - d\gamma^2 + \mathcal{O}(\gamma^3)$$



PDE Reaction-Diffusion Systems

Step back for a moment and consider the PDE

$$y_t = y_{xx} + f(y),$$

again with the 1-parameter family of wave-trains $u(\omega_{\text{nl}}(k)t - kx; k)$.

Consider the formal Ansatz

$$y(x, t) = u(kx - \omega t + \phi(X, T); k + \epsilon \phi_X(X, T))$$

where $X = \epsilon(x - c_g t)$, $T = \epsilon^2 t / 2$ and $\epsilon \ll 1$

Wavenumber $q = \phi_X$ formally satisfies the viscous Burgers equation:

$$\frac{\partial q}{\partial T} = \lambda''(0) \frac{\partial^2 q}{\partial X^2} - \omega''_{\text{nl}}(k) (q^2)_X$$

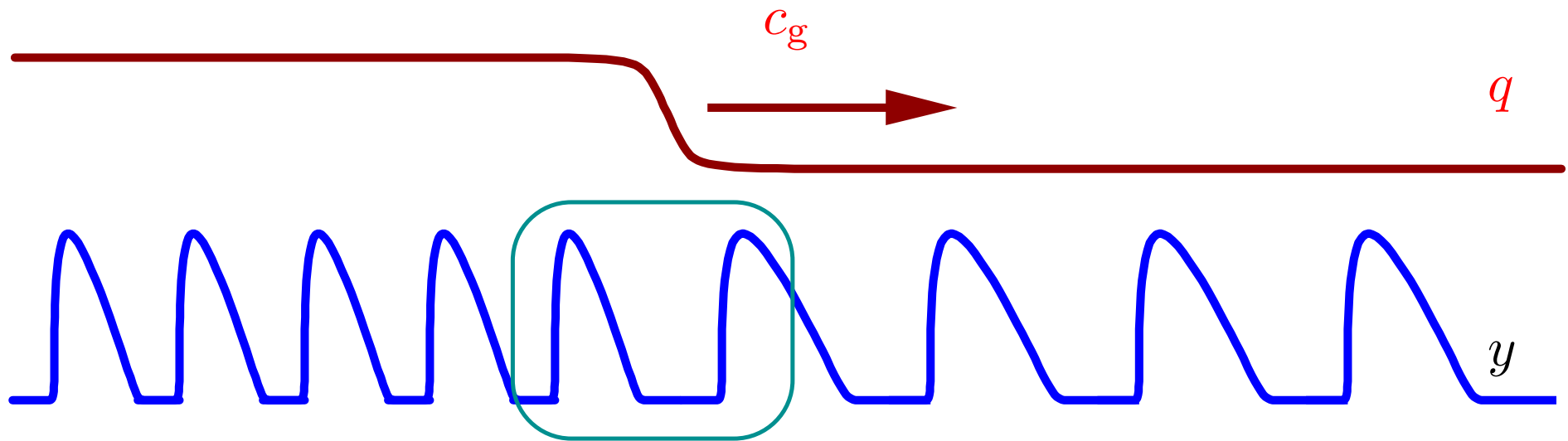
[Howard and Koppel, 1977]

Predictions from the Burgers equation

- Issue 1: Validity of Burgers equation over natural time scale $[0, \epsilon^{-2}]$:
[Doelman, Sandstede, Scheel, Schneider]

- Issue 2: Predictions from Burger equation

Lax shocks of Burgers equation \longrightarrow Weak defects:



(convex dispersion relation: $\omega''_{nl}(k) > 0$)

Verifying the existence of the lax shock

The shock that we seek is a modulated travelling wave. Write as

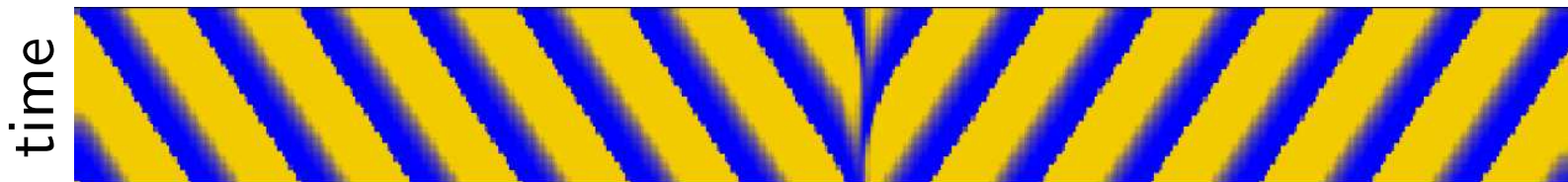
$$y(x, t) = u_*(x - c_*t, \omega_*t)$$

where u_* is 2π periodic in the second variable.

Asymptotics

$$u_*(x - c_*t, \omega_*t) \rightarrow u(\omega_{\pm}t - k_{\pm}x; k_{\pm}) \text{ as } x - c_*t \rightarrow \pm\infty$$

Space-time plot for $\omega_*t \in [0, 2\pi]$:



space (comoving frame)

Since $c_g^- > c_* > c_g^+$, transport occurs towards defect \rightarrow sink.

Construction of lax shock in continuous setting

Introduce new variables $v(\xi, \tau) = u_*(\xi, \tau)$ and $w(\xi, \tau) = \partial_\xi u_*(\xi, \tau)$, with $\xi = x - c_*t$ and $\tau = \omega_*t$.

In the continuous case, we find

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} w \\ -\gamma^{-1}[c_*w - \omega_*\partial_\tau v + f(v)] \end{pmatrix}$$

Following the spatial-dynamics approach due to [Kirchgässner], [Mielke], view as an ODE on the space $H_{per}^2([0, 2\pi]) \times H_{per}^1([0, 2\pi])$.

Fix k_0 and write

$$\begin{aligned} c_* &= c_g(k_0) = \omega'_{nl}(k_0) \\ \omega_* &= \omega_{nl}(k_0) - k_0\omega'_{nl}(k_0) + \bar{\omega} \end{aligned}$$

For small $\bar{\omega}$ with appropriate sign, there exist:

- Wave numbers $k_\pm(\bar{\omega})$ with $k_\pm(\bar{\omega}) \rightarrow k_0$ as $\bar{\omega} \rightarrow 0$.
- Periodic solutions $v_\pm(\xi) = u(-k_\pm\xi + \cdot; k_\pm)$ (with accompanying w_\pm)

Construction of lax shock in continuous setting

For $\bar{w} = 0$, we have the ξ -periodic solution

$$\begin{aligned}v_0(\xi)(\tau) &= u(-k_0\xi + \tau; k_0) \\w_0(\xi)(\tau) &= -k_0u'(-k_0\xi + \tau; k_0)\end{aligned}$$

Idea: construct center manifold around $(v_0, w_0, \bar{w} = 0)$ that captures all solutions that remain **orbitally** close to (v_0, w_0) , for small \bar{w} .

Crucial ingredient: change of variables $\sigma = \tau - k_0\xi$ into temporal comoving frame yields

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \partial_\sigma v + f(v)] \end{pmatrix}$$

This change of variables turns periodic solution (v_0, w_0) into a ring of equilibria.

Orbitally close in original frame \leftrightarrow close to equilibria-ring in temporal comoving frame

Temporal Comoving Frame

Recall temporal-comoving frame

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\sigma v + f(v)] \end{pmatrix}$$

Center space around equilibrium $\mathbf{u}_0 = (v_0, w_0)$ is **two** dimensional by our choice $c_* = c_g$. Spanned by

$$\mathbf{u}'_0 = (u'(\cdot; k_0), -k_0 u''(\cdot; k_0)), \quad \mathbf{u}_1 = (-\partial_k u(\cdot; k_0), k_0 \partial_k u'(\cdot; k_0) + u'(\cdot; k_0)).$$

Formally insert Ansatz

$$(v, w) = \mathbf{u}_0(\cdot - \theta) - \kappa \mathbf{u}_1(\cdot - \theta) + O(\theta^2 + \kappa^2)$$

and derive ODE

$$\begin{aligned} \partial_\xi \theta &= \kappa + O(|\bar{w}| + |\kappa|^2) \\ \partial_\xi \kappa &= 2\lambda''_{\text{lin}}(0)^{-1} \left(\frac{1}{2} \omega''_{\text{nl}}(k_0) \kappa^2 - \bar{w} \right) + O(|\bar{w}|^2 + |\bar{w}\kappa| + |\kappa|^3) \end{aligned}$$

Read off heteroclinic connections.

Heteroclinic connections

Recall

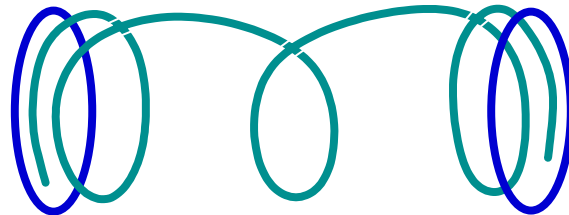
$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\sigma v + f(v)] \end{pmatrix}$$

No general global center manifold result for such mixed hyperbolic - elliptic systems.

To get CM, need to exploit CM result by [Mielke] for original equation

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\tau v + f(v)] \end{pmatrix}$$

Result states that solutions that are **orbitally** close to (v_0, w_0) can be captured.



Discrete Case

In discrete setting, the equation to solve becomes

$$\partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\tau v + [v(\cdot + 1) + v(\cdot - 1) - 2v] + f(v)] \end{pmatrix}$$

This is a functional differential equation of mixed type (MFDE) posed on the space $H_{per}^2([0, 2\pi]) \times H_{per}^1([0, 2\pi])$.

- The center manifold result developed by Mielke no longer works for MFDEs
- The situation was partially remedied in [Hupkes, Verduyn Lunel, 2008], where center manifolds are constructed around periodic solutions to MFDEs
- However, **orbital** closeness is still an unresolved issue.
- In addition, results only for MFDEs posed on \mathbb{C}^n , not general Hilbert spaces

Discrete Case

For simplicity, we choose to work directly in temporal comoving frame and solve

$$\begin{aligned} \partial_\xi \begin{pmatrix} v \\ w \end{pmatrix} &= k_0 \partial_\sigma \begin{pmatrix} v \\ w \end{pmatrix} + \begin{pmatrix} w \\ -\gamma^{-1}[c_* w - \omega_* \partial_\sigma v + f(v)] \end{pmatrix} \\ &\quad + \begin{pmatrix} 0 \\ [v(\cdot + 1)(\cdot - k_0) + v(\cdot - 1)(\cdot + k_0) - 2v] \end{pmatrix} \end{aligned}$$

posed on the space $H_{per}^2([0, 2\pi]) \times H_{per}^1([0, 2\pi])$.

Goal is to construct global center manifold near ring of equilibria $\left(u(\vartheta + \cdot; k_0), -k_0 u'(\vartheta + \cdot; k_0)\right)$, parametrized by $\vartheta \in [0, 2\pi]$.

Most important issues:

- The ∂_σ derivatives prevent use of bootstrapping methods to get regularity of solutions.
- The Hilbert space setting prevents explicit construction of characteristic equations.

Finite dimensional example

For simplicity, let us consider the planar ODE

$$y' = f(y)$$

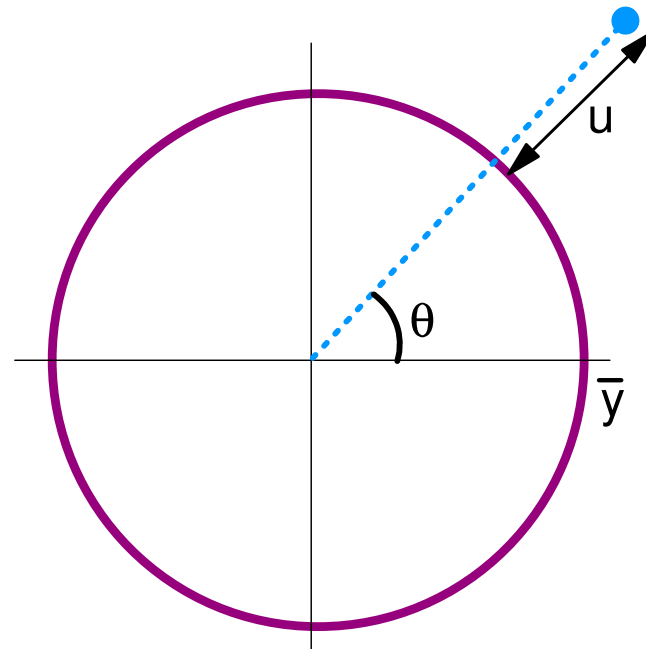
- Write $\rho(\vartheta)$ for rotation with angle ϑ .
- Suppose $f : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ invariant, i.e. $\rho(-\vartheta)f(\rho(\vartheta)v) = f(v)$ for $v \in \mathbb{R}^2$.
- Suppose $f(\bar{y}) = 0$ for $\bar{y} \neq 0$.

Change of variables

$$y(\xi) = \rho(\theta(\xi))[\bar{y} + u(\xi)]$$

with normalization condition

$$\langle D\rho(0)\bar{y}, u(\xi) \rangle = 0.$$



Finite dimensional example - continued

Recall $y' = f(y)$ with

$$y(\xi) = \rho(\theta(\xi))[\bar{y} + u(\xi)], \quad \langle D\rho(0)\bar{y}, u(\xi) \rangle = 0.$$

Differentiation yields

$$u'(\xi) = -\theta'(\xi)D\rho(0)[\bar{y} + u(\xi)] + f(\bar{y} + u(\xi))$$

$$\theta'(\xi) = [\langle D\rho(0)\bar{y}, D\rho(0)\bar{y} \rangle + \langle D\rho(0)\bar{y}, D\rho(0)u(\xi) \rangle]^{-1} \langle D\rho(0)\bar{y}, f(\bar{y} + u(\xi)) \rangle.$$

Variable θ can hence be eliminated from equation for u , allowing use of standard CM theory.

However, turning to our setting $y'(\xi) = f(y(\xi), y(\xi - 1), y(\xi + 1))$, we find:

- Symmetry ρ acts as translation \longrightarrow the term $D\rho(0)u(\xi)$ becomes unbounded.
- Equation for θ no longer decouples.

Global center manifold

To resolve the unboundedness issue, need to use Ansatz

$$y(\xi) = \rho(\theta(\xi))\bar{y} + u(\xi).$$

We need to obtain CM for the coupled system

$$\begin{aligned} u'(\xi) &= -\theta'(\xi)D\rho(\theta(\xi))\bar{y} + f(\theta_\xi, u_\xi) \\ \theta'(\xi) &= [\langle D\rho(0)\bar{y}, D\rho(0)\bar{y} \rangle + \langle D\rho(\theta(\xi))\bar{y}, u(\xi) \rangle]^{-1} \langle D\rho(\theta(\xi))\bar{y}, f(\theta_\xi, u_\xi) \rangle \end{aligned}$$

in which u is small, but without bound on θ .

$$f(\theta_\xi, u_\xi) = f(\rho(\theta(\xi))\bar{y} + u(\xi), \rho(\theta(\xi - 1))\bar{y} + u(\xi - 1), \rho(\theta(\xi + 1))\bar{y} + u(\xi + 1)).$$

Notice that linearization of equation for u' includes dependence on $\theta(\xi)$, $\theta(\xi \pm 1)$.

Key idea: For small u , the variable θ is **slowly varying**. Linearized equation for u thus has slowly varying coefficients, allowing us to solve for prescribed θ .

Fenichel Theory

Close connection with singularly perturbed systems

$$\begin{aligned}\theta' &= \epsilon g_s(\theta, u, \epsilon) \\ u' &= g_f(\theta, u, \epsilon),\end{aligned}$$

that admit a manifold $\tilde{u}(\vartheta)$ of equilibria

$$g_f(\vartheta, \tilde{u}(\vartheta), 0) = 0.$$

Key question: persistence of invariant manifold as slow flow is turned on ($\epsilon > 0$).

- Fenichel (1970s): in absence of extra center directions (normal hyperbolicity), manifold persists
- Large literature on persistence of center manifolds for general normally-hyperbolic invariant sets
- Some results on situations where normal-hyperbolicity fails [Chow, Liu, Yi]

Analytic techniques

- Almost all results rely on **geometric** Hadamard graph transform techniques
- Need analytic setup for generalization to infinite dimensions
- [Sakamoto, 1990] Analytic proof of first Fenichel theorem by fixed point argument. Idea:
 - For prescribed slowly modulated function θ , construct solution operator $\mathcal{K}(\theta)$ to solve linearized system for u .
 - Solve fixed point system

$$u = \mathcal{K}(\theta[u])G(u),$$

in appropriate weighted function space, where G contains nonlinear terms.

Unfortunately, normal-hyperbolicity is essential.

Construction of global CM

Crucial idea, inspired by technique in [Yi]: use **two** fixed point arguments in succession.

Equation to solve: (E denotes extension from center space to solutions to homogeneous linear system)

$$u = E(\theta[u])\Pi_{ct}u(0) + \mathcal{K}(\theta[u])G(u) \quad (1)$$

- Assume that CM has the form $h : (\kappa, \theta) \rightarrow H$
- Plug in Ansatz

$$u = \rho(\theta)\bar{y} + \kappa\rho(\theta)\mathbf{u}_1 + h(\kappa, \theta)$$

and using center projections and fixed point argument, determine evolution for the center variables (κ, θ) . Evolution depends only on $\kappa(0), \theta(0), h$.

- Pick arbitrary $\kappa(0)$ and $\theta(0)$, determine $\kappa(\xi)$ and $\theta(\xi)$ from this and compute right hand side of (1).
- Evaluating at zero and equating with left hand side of (1) yields fixed point equation for CM function h .

Main Result

Theorem 1 (H., Sandstede, JDDE, to appear). *Consider the partially discrete system*

$$\partial_t y(x, t) = \gamma \partial_{xx} y(x, t) + [L_D y](x, t) + f(y(x, t))$$

with $\gamma > 0$. Suppose that $\omega''_{nl}(k_0) \neq 0$ and $\lambda''_{lin} > 0$. Suppose furthermore that some technical conditions hold for the lattice.

Then for $k_1 \approx k_0$, there exists $k_2 \approx k_0$ and a modulated travelling wave that connects the wavetrain at k_- to the wave train at k_+ , in which $k_- = k_1$ and $k_+ = k_2$ if $\omega''_{nl}(k_0) < 0$ and vice versa if $\omega''_{nl}(k_0) > 0$.

- The technical conditions on the lattice are absent in the continuous case.
- They arise due to the fact that the θ equation is an MFDE.
- Equation is scalar, but many eigenfunctions can in principle appear.
- To make sure flow on CM depends only on $\theta(0)$ and $\kappa(0)$, need to ensure that there are no resonances.
- In the limit $\gamma \rightarrow 0$ one cannot avoid these resonances.

Technical conditions on the lattice

Characteristic equation (for $c_* = c_g$) is given by

$$\mathcal{L}_{\text{ch}}(z)v = [-\mathcal{L}_{\text{st}}(z) + z(c_p - c_g)]v$$

Associated operator

$\mathcal{T}(z) : H_{\text{per}}^2([0, 2\pi]) \times H_{\text{per}}^1([0, 2\pi]) \rightarrow H_{\text{per}}^1([0, 2\pi]) \times H_{\text{per}}^0([0, 2\pi])$ given by

$$\mathcal{T}(z) \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -(z + \frac{1}{\gamma}c_g - k_0D) & 1 \end{pmatrix} \begin{pmatrix} -\gamma z + \gamma k_0D & \gamma \\ \mathcal{L}_{\text{ch}}(z) & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix},$$

- We have $\langle \mathbf{u}'_0, \mathcal{T}'(0)\mathbf{u}'_0 \rangle \neq 0$ and $\langle \mathbf{u}'_0, \mathcal{T}(i\kappa)\mathbf{u}'_0 \rangle \neq 0$ for $\kappa \in \mathbb{R} \setminus \{0\}$. [The MFDE for normalization θ is well-defined after fixing $\theta(0)$]
- We have $\Delta(i\kappa) \neq 0$ for $\kappa \in \mathbb{R} \setminus \{0\}$ and $\Delta''(0) \neq 0$, for

$$\begin{aligned} \Delta(z) = & -\gamma z \|\mathbf{u}_1\|_{H^1 \times H^0}^2 \langle \mathbf{u}'_0, \mathcal{T}(z)\mathbf{u}'_0 \rangle - \langle \mathbf{u}_1, \mathcal{T}'(0)\mathbf{u}'_0 \rangle \langle \mathbf{u}'_0, \mathcal{T}(z)\mathbf{u}'_0 \rangle \\ & + \langle \mathbf{u}'_0, \mathcal{T}'(0)\mathbf{u}'_0 \rangle \langle \mathbf{u}_1, \mathcal{T}(z)\mathbf{u}'_0 \rangle, \end{aligned}$$

[Evolution on center manifold defined after fixing $\kappa(0)$ and $\theta(0)$].

The limit $\gamma \rightarrow 0$.

To get a further idea what goes wrong in $\gamma \rightarrow 0$ limit, study the characteristic equation (for $\gamma = 0$)

$$\begin{aligned}\mathcal{L}_{\text{ch}}(z)v &= [-\mathcal{L}_{\text{st}}(z) + z(c_p - c_g)]v \\ &= [zc_g - (\omega_* + k_0c_g)D]v + [e^z v(\cdot - k_0) + e^{-z} v(\cdot + k_0) - 2v] \\ &\quad + Df(u(\cdot; k_0))v.\end{aligned}$$

Consider $\ell \in \mathbb{Z}$ and $\Delta k \in \mathbb{Z}$, and

$$\begin{aligned}\tilde{v} &= \exp[i\Delta k \cdot]v \\ \tilde{z} &= z + ik_0\Delta k + 2\pi\ell\end{aligned}$$

We get

$$\exp[-i\Delta k \cdot]\mathcal{L}_{\text{ch}}(\tilde{z})\tilde{v} = \mathcal{L}_{\text{ch}}(z)v + i(2\pi c_g \ell - \omega_* \Delta k)v$$

If πc_g and ω_* are not rationally related, there is no hope of getting a uniform bound on $\mathcal{L}_{\text{ch}}(z)$ in vertical strips if $\mathcal{L}_{\text{ch}}(z_0)$ has eigenvalue with $\text{Re } \lambda = \text{Re } z_0$.