Traveling Waves for Lattice Equations

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Acknowledgements

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Collaborators: Tony Humphries, Robert McLachlan, Reinout Quispel, Erik Van Vleck

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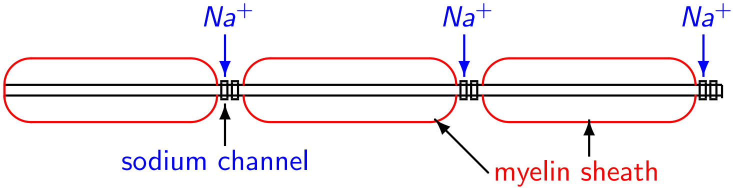
Metaphor

"There are many other things I have found myself saying about poetry, but the chiefest of these is that it is metaphor. . . saying one thing in terms of another. . . . Poetry is simply made of metaphor. So also is philosophy–and science, too, for that matter, if it will take the soft impeachment from a friend."

- Robert Frost

Our Nervous System



The nervous cells live inside the myelin sheath.

Ionized sodium causes electric impulse to jump from node to node.

Multiple Sclerosis destroys myelin, which inhibits conduction.

Questions

- When/Where does conduction stop due to demyelination?
- How much demeylination is required to make it stop?

Bistable Equation with Inhomogeneous Diffusion

$$\frac{d}{dt}u_j = \alpha_j(u_{j+1} - u_j) - \alpha_{j-1}(u_j - u_{j-1}) - f(u_j)$$

with

$$\alpha_j = \alpha \quad \text{for} \quad j < -m \text{ or } j > n$$

$$\alpha_j \neq \alpha \quad \text{for} \quad -m \leq j \leq n, \qquad \text{for} \quad m, n \in \{0\} \cup \mathbb{N}$$

Boundary Conditions
for Fronts $\lim_{j \to -\infty} u_j = 0, \qquad \lim_{j \to \infty} u_j = 1$
for Pulses $\lim_{j \to \pm\infty} u_j = 0$

The nonlinearity is the derivative of a double-well potential,

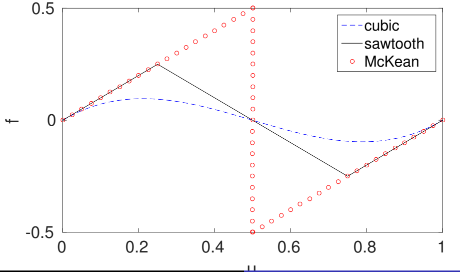
$$\text{typically} \quad f(u) = u(u-a)(u-1) \quad \text{with} \quad a \in (0,1).$$

Nonlinearities

Cubic: $f(u) = u(u-a)(u-1)$, with $a \in (0,1)$

McKean: $f(u) = u - h(u-a)$ $\qquad h(x) = \begin{cases} 1 & x > 0 \\ [0,1] & x = 0 \\ 0 & x < 0 \end{cases}$

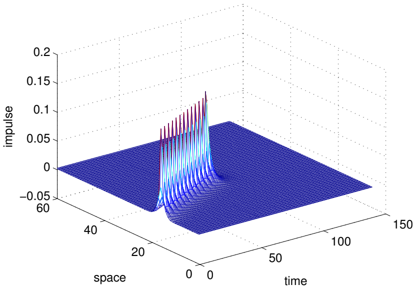
Sawtooth: $f(u) = \begin{cases} u, & u \leq a/2 \\ a-u, & a/2 < u < (a+1)/2 \\ u-1, & u \geq (a+1)/2 \end{cases}$

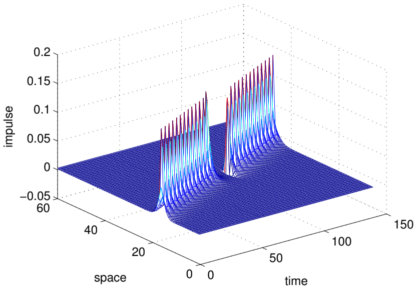


Computer Simulations

Case: McKean and a single defect

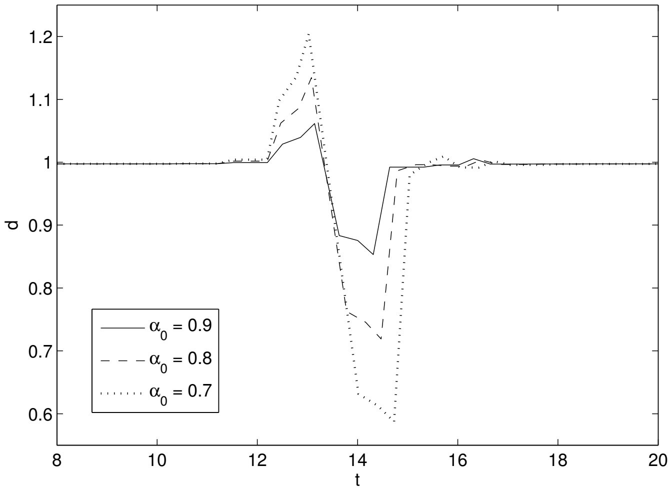
$$\alpha_j = \begin{cases} 0.6 & j = 30 \\ 1 & j \neq 30 \end{cases}$$





A slightly faster impulse is able to pass through the defect.

Change in wave speed passing through the defect



Set-up

We seek solutions that satisfy

for Fronts

$$u_j < a \quad \text{for} \quad j < j^* \qquad u_j > a \quad \text{for} \quad j > j^*,$$

which implies

$$h(u_{j^*} - a) = h(j - j^*) =: g_j$$

for Pulses

$$u_j > a \quad \text{for} \quad j^* < j < j^{**} \qquad \text{and} \quad u_j < a \quad \text{otherwise.}$$

which implies

$$h(u_{j^*} - a) = h(j - j^*) - h(j - j^{**}) =: g_j$$

In both cases, the steady-state equation becomes

$$\alpha_j u_{j+1} - (1 + \gamma + \alpha_j + \alpha_{j-1}) u_j + \alpha_{j-1} u_{j-1} = g_j$$

Solutions Using the Method of Undetermined Coefficients

General Solution = Homogeneous Solution + Particular Solution

$$u_j = u_{j^*}\rho_j + u_{j^*+1}\sigma_j + \begin{cases} -\sum_{k=j^*+1}^{j} \frac{g_k}{\alpha_k}\sigma_{j-k} & j > j^* \\ 0 & j = j^* \\ \frac{g_{j^*}}{\alpha_{j^*}}\sigma_{j-j^*} & j < j^* \end{cases}$$

Fundamental solutions satisfy
$(\rho_{j^*}, \rho_{j^*+1}) = (1, 0)$, and $(\sigma_{j^*}, \sigma_{j^*+1}) = (0, 1)$.

The particular solution can be found in Teschl (2000).

The coefficients are determined by the boundary conditions.

Interval of Propagation Failure

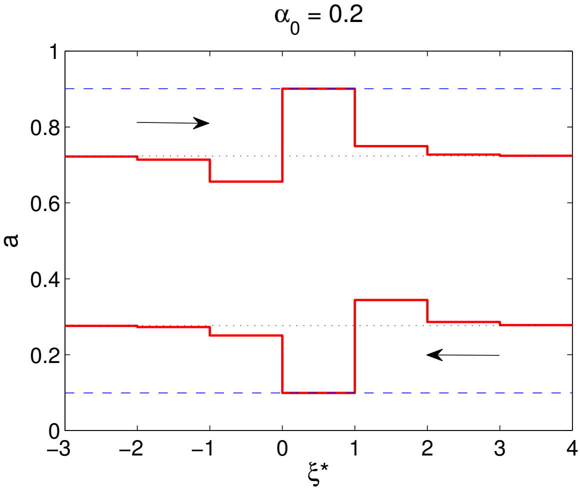
Theorem

If a yields a traveling front for $\alpha_0 = \alpha$, then

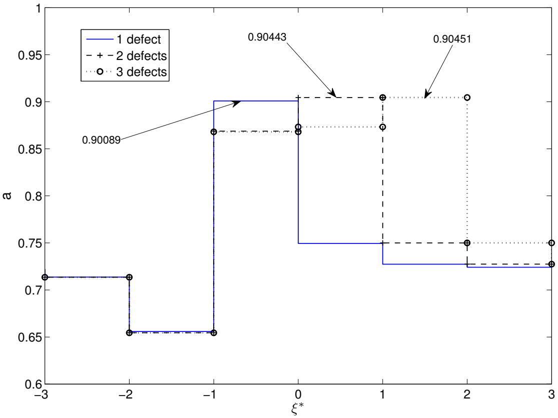
- Either $a \in (0, 1/(\lambda+2))$ or $a \in ((\lambda+1)/(\lambda+2), 1)$ with $\lambda = (1+\sqrt{1+4\alpha})/2\alpha$
- There are no corresponding standing fronts for $\alpha_0 < \alpha$ and $j^* \neq 0$, nor for $\alpha_0 > \alpha$ and $j^* = 0$.
- There exist standing fronts for $\alpha_0 < \alpha$ and $j^* = 0$, and for $\alpha_0 > \alpha$ and $j^* \neq 0$, provided

$$a \in \left[\frac{\alpha_0/\alpha}{\lambda + 2(\alpha_0/\alpha)}, \frac{\lambda + \alpha_0/\alpha}{\lambda + 2(\alpha_0/\alpha)}\right].$$

Interval of Propagation Failure, $\alpha = 1$

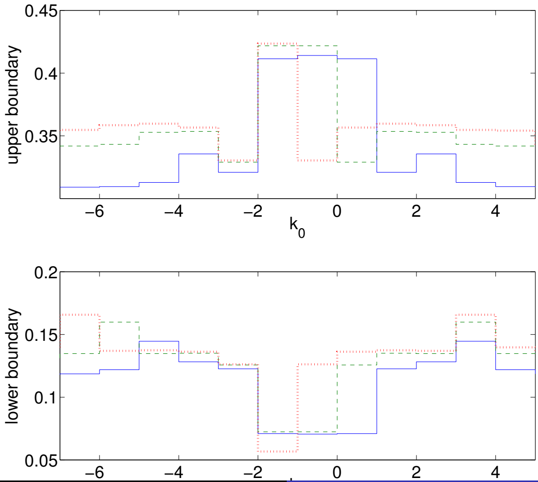


Interval of Propagation Failure

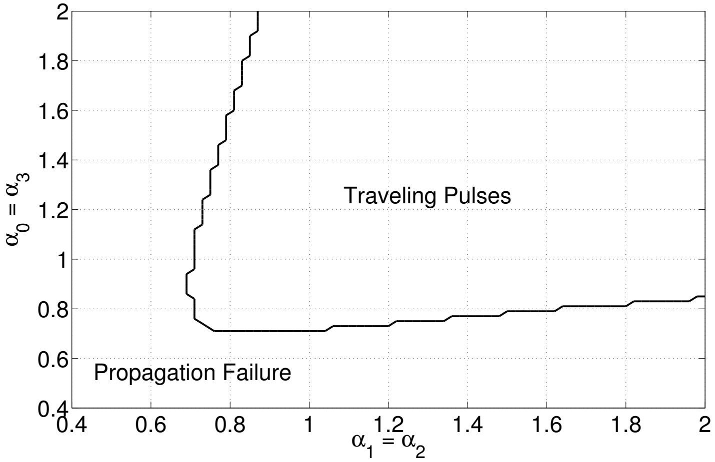


Propagation Failure for Pulses of Various Widths

$\alpha = 2$, and $\alpha_j = 1/2$ for $j \in [-2, 2]$



Multiple Defect with $\alpha = 2$



Sawtooth Steady-State Equation

$$-\alpha_k u_{k+1} + (v_k + \alpha_k + \alpha_{k-1})u_k - \alpha_{k-1}u_{k-1} = w_k, \qquad \forall k \in \mathbb{Z}$$

$$v_k = \begin{cases} 1, & k < k^* + 1 \\ -1, & k^* + 1 \leq k \leq k^* + n \\ 1, & k > k^* + n \end{cases}$$

$$w_k = \begin{cases} 0, & k < k^* + 1 \\ -a, & k^* + 1 \leq k \leq k^* + n \\ 1, & k > k^* + n \end{cases}$$

infinite tridiagonal system of equations

$(\mathbf{M} + \mathbf{y}\mathbf{z}^T)\mathbf{u} = \mathbf{w}$, where $\mathbf{y} = -2\mathbf{e}_{k^*+1}$, $\mathbf{z} = \mathbf{e}_{k^*+1}$,

$$\mathbf{u} = [\ldots u_{k-1} \;\; u_k \;\; u_{k+1} \ldots]^T, \qquad \mathbf{w} = [\ldots w_{k-1} \;\; w_k \;\; w_{k+1} \ldots]^T,$$

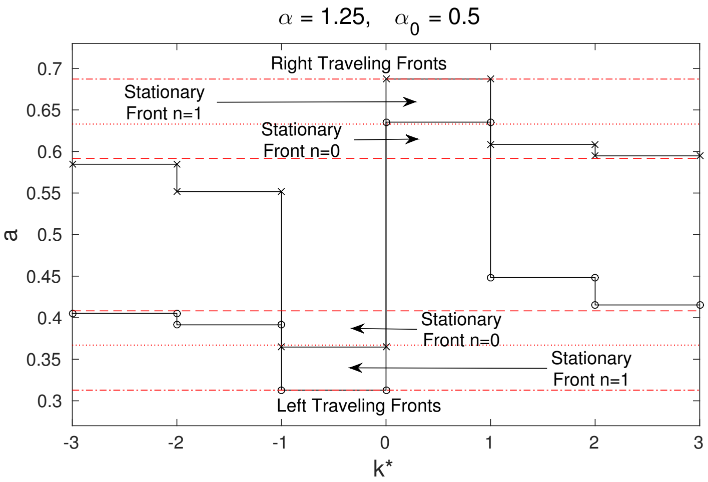
$$M_{ij} = \begin{cases} -\alpha_{i-1} & i = j+1 \\ (1 + \alpha_i + \alpha_{i-1}) & i = j \\ -\alpha_i & i = j-1 \\ 0 & \text{otherwise} \end{cases}$$

Using the Sherman-Morrison formula

$$\mathbf{u} = (\mathbf{M}_0 + \mathbf{y}_0\mathbf{z}_0^T)^{-1}\mathbf{w} = \mathbf{M}^{-1}\mathbf{w} - \frac{\mathbf{M}^{-1}\mathbf{y}_0\mathbf{z}_0^T\mathbf{M}^{-1}\mathbf{w}}{1 + \mathbf{z}_0^T\mathbf{M}^{-1}\mathbf{y}_0}.$$

$\mathbf{M}^{-1}\mathbf{x}$ is the solution provided by Teschl (2000).

Stationary Fronts for $\alpha_0 \neq \alpha$



Algorithm for solving $(\mathbf{M} + \mathbf{y}_0\mathbf{z}_0^T + \ldots + \mathbf{y}_{n-1}\mathbf{z}_{n-1}^T)\mathbf{u}_n = \mathbf{w}$

1. Input: α_k, a, n, k^*
2. Construct $\mathbf{w}$, $\mathbf{M}$, $\mathbf{y}_i$, $\mathbf{z}_i$ for $i = 0, 1, \ldots, n-1$
3. Solve $\mathbf{M}\mathbf{u}_0 = \mathbf{w}$
4. For $i = 0$ to $n - 1$
5.   Solve $\mathbf{M}\mathbf{x}_{i,0} = \mathbf{y}_i$
6.   For $j = 1$ to i
7.   Compute $\mathbf{x}_{i,j} = \mathbf{x}_{i,j-1} - \frac{\mathbf{x}_{j-1,j-1}\mathbf{z}_{j-1}^T\mathbf{x}_{i,j-1}}{1+\mathbf{z}_{j-1}^T\mathbf{x}_{j-1,j-1}}$
8.   End For
9.   Compute $\mathbf{u}_{i+1} = \mathbf{u}_i - \frac{\mathbf{x}_{i,i}\mathbf{z}_i^T\mathbf{u}_i}{1+\mathbf{z}_i^T\mathbf{x}_{i,i}}$
10. End For
11. Output: $\mathbf{u}_n$

Problem on a 2-dimensional lattice

Semi-linear wave equation: $u_{tt} = u_{xx} - V'(u)$

5-point central difference scheme:

$$\frac{1}{(\Delta t)^2}\left(u_i^{n+1} - 2u_i^n + u_i^{n-1}\right) - \frac{1}{(\Delta x)^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right) = -V'(u_i^n)$$

Traveling wave ansatz:

$$u_i^n = \varphi(x_i - ct_n) = \varphi(i\Delta x - cn\Delta t) = \varphi(i\sigma - n\kappa) = \varphi(\xi)$$

where $\sigma = \Delta x$, $\kappa = c\Delta t$, and $\xi = i\sigma - n\kappa$

Resulting functional equation:

$$\frac{c^2}{\kappa^2}\left(\varphi(\xi+\kappa) - 2\varphi(\xi) + \varphi(\xi-\kappa)\right) \qquad (1)$$

$$-\frac{1}{\sigma^2}\left(\varphi(\xi+\sigma) - 2\varphi(\xi) + \varphi(\xi-\sigma)\right) = -V'(\varphi(\xi))$$

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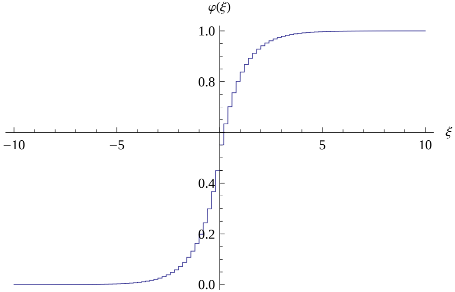
Resulting functional equation:

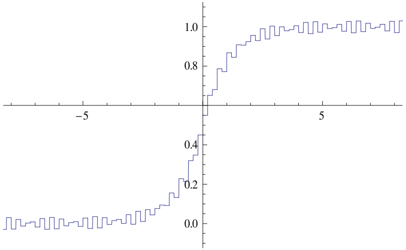
$$\frac{c^2}{\kappa^2}\left(\varphi(\xi+\kappa) - 2\varphi(\xi) + \varphi(\xi-\kappa)\right) \qquad (1)$$
$$- \frac{1}{\sigma^2}\left(\varphi(\xi+\sigma) - 2\varphi(\xi) + \varphi(\xi-\sigma)\right) = -V'(\varphi(\xi))$$

McKean: heteroclinic solutions by Fourier transform

For rational values of $\frac{\sigma}{\kappa}$ solutions may be

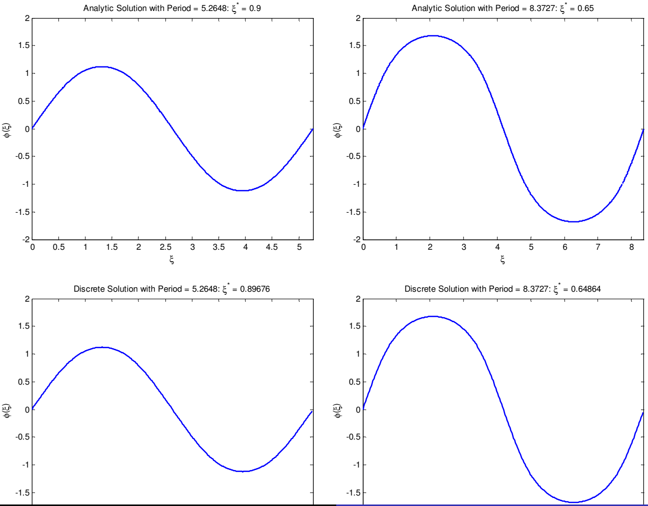
- piecewise constant, monotonic, without wiggles
- piecewise constant, nonmonotonic, with $\mathcal{O}(\kappa^2)$ wiggles





Sawtooth: solutions by Fourier transform

Periodic TWs persist for both rational and irrational $\frac{\sigma}{\kappa}$.

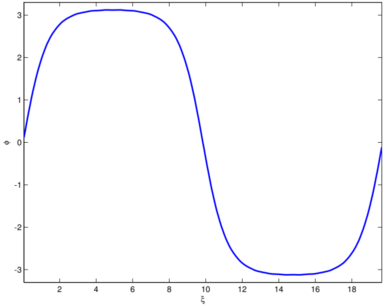


Case Study: Sine-Gordon, $V'(\varphi) = \sin(\varphi)$

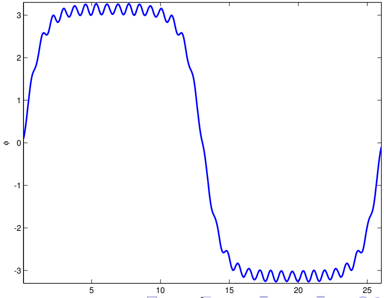
We solve $\mathcal{F}^{-1}D\mathcal{F}\varphi + \sin(\varphi) = 0$ using Newtons Method, where $\mathcal{F}$ is the discrete Fourier transform, and $D = diag(d_n)$.

We obtain 2 types of periodic solutions, non-resonant and resonant.

$T = 2(\pi + 6.7)$



$T = 2(\pi + 9.9)$



Backward Error Analysis (BEA)

Problem: Finding discrete traveling waves means solving an infinite dimensional functional equation.

Idea: Find a differential equation that is satisfied (to higher order) by the discrete traveling wave.

Technique:

1. Write the discrete traveling wave equation as $L_{\kappa,\sigma}\varphi = f(\varphi)$.
2. Invert $L_{\kappa,\sigma}$ and differentiate to get $\dot{\varphi} = DL^{-1}_{\kappa,\sigma}f(\varphi)$.
3. Expand $L^{-1}_{\kappa,\sigma}$ in a Taylor series to get a modified equation

$$\dot{\varphi} = f(\varphi) + \mu_1(\kappa,\sigma)f_1(\varphi) + \mu_2(\kappa,\sigma)f_2(\varphi) + \dots$$

Benefit: This approach is applicable to many Multi-symplectic methods for many PDEs and provides considerable insight.

Result for equation (1): Modified equation is a planar Hamiltonian system; its solutions represent the discrete traveling waves.

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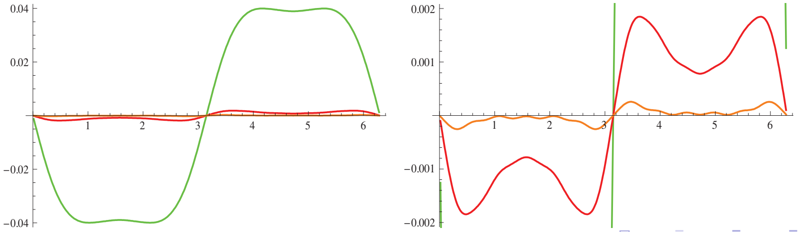
BEA: Solution error for modified equations of Sine-Gordon

Plots of $\varphi - \hat{\varphi}$, where φ is the DTW computed using Fourier series and $\hat{\varphi}$ is the solution of the modified equation.

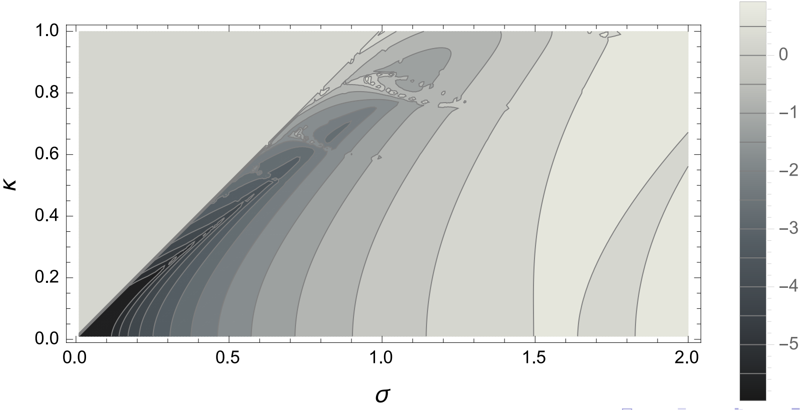
Plots show results for 0, 1, and 2 modifications, with $\sigma = \kappa = 1/2$.



BEA: Solution error for modified equations of Sine-Gordon

Plot of $\log_{10} \|\varphi - \hat{\varphi}\|$ where φ is DTW and $\hat{\varphi}$ is solution of modified equation truncated after one term.

Small anomalies signify resonances.



BEA: Preissmann box scheme for $i\psi_t + \psi_{xx} + |\psi|^2\psi = 0$

Define $\psi = p + iq$, $\psi_x = v + iw$, and

$$D_\xi^\kappa \varphi(\xi) = -\frac{c(\varphi(\xi) - \varphi(\xi - \kappa))}{\kappa}, \qquad D_\xi^\sigma \varphi(\xi) = \frac{\varphi(\xi + \sigma) - \varphi(\xi)}{\sigma},$$

$$A_\xi^\kappa \varphi(\xi) = \frac{\varphi(\xi) + \varphi(\xi - \kappa)}{2}, \qquad A_\xi^\sigma \varphi(\xi) = \frac{\varphi(\xi) + \varphi(\xi + \sigma)}{2}$$

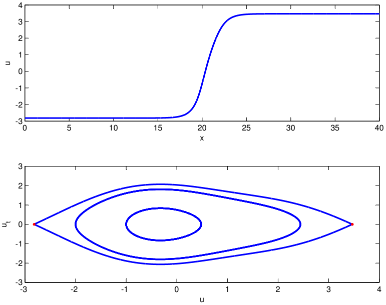
The modified equation is

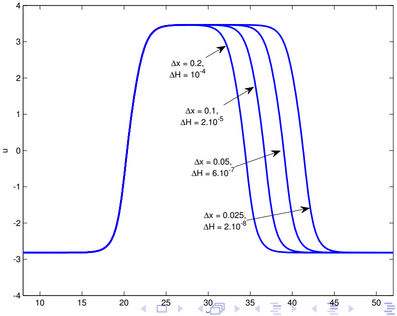
$$\begin{bmatrix} \dot{p} \\ \dot{q} \\ \dot{v} \\ \dot{w} \end{bmatrix} = D \begin{bmatrix} 0 & 0 & \frac{1}{D_\xi^\sigma A_\xi^\kappa} & 0 \\ & 0 & 0 & \frac{1}{D_\xi^\sigma A_\xi^\kappa} \\ \frac{-1}{D_\xi^\sigma A_\xi^\kappa} & 0 & 0 & \frac{D_\xi^\kappa A_\xi^\sigma}{(D_\xi^\kappa A_\xi^\sigma)^2} \\ 0 & \frac{-1}{D_\xi^\sigma A_\xi^\kappa} & \frac{-D_\xi^\kappa A_\xi^\sigma}{(D_\xi^\kappa A_\xi^\sigma)^2} & 0 \end{bmatrix} \begin{bmatrix} |A_\xi^\kappa A_\xi^\sigma \psi|^2 A_\xi^\kappa A_\xi^\sigma p \\ |A_\xi^\kappa A_\xi^\sigma \psi|^2 A_\xi^\kappa A_\xi^\sigma q \\ A_\xi^\kappa A_\xi^\sigma v \\ A_\xi^\kappa A_\xi^\sigma w \end{bmatrix}$$

which is a noncannonical Hamiltonian system with rotational invariance and TWs are preserved.

Comparison of discretizations for steady state solutions

- Multi-symplectic:
  - Modified equations: periodic, hetero/homoclinic orbits persist
  - Leapfrog: orbits approximate continuous solutions
- Non-Symplectic
  - Non-symmetric: destroy periodic and hetero/homoclinic orbits
  - Symmetric: do not preserve non-symmetric waves





Conclusion

"Unless you are at home in the metaphor, unless you have had your proper poetical education in the metaphor, you are not safe anywhere. Because you are not at ease with figurative values: you don't know the metaphor in its strength and its weakness. You don't know how far you may expect to ride it and when it may break down with you. You are not safe with science; you are not safe in history."

- Robert Frost

Relevant Publications

- A.R. Humphries, B.E. Moore, and E.S. Van Vleck, Front Solutions for Bistable Differential-Difference Equations with Inhomogeneous Diffusion, *SIAM Journal on Applied Mathematics*, 71(4):1374-1400, 2011.
- B.E. Moore and J.M. Segal, Stationary Bistable Pulses in Discrete Inhomogeneous Media, *Journal of Difference Equations and Applications*, 20(1):1-23, 2014.
- F. McDonald, R.I. McLachlan, B.E. Moore, and G.R.W. Quispel, Traveling Wave Solutions of Multisymplectic Discretizations of Nonlinear Wave Equations, *Journal of Difference Equations and Applications*, 22(7):913-940, 2016.
- E. Lydon and B.E. Moore, Propagation Failure of Fronts in Discrete Inhomogeneous Media with a Sawtooth Nonlinearity, *Journal of Difference Equations and Applications*, 22(12):1930-1947, 2016.