Traveling waves in nonlinear lattices

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"Standard" (on-site) discretisation:

$$\ddot{u}_n = \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} + u_n(1 - u_n^2), \quad n \in \mathbb{Z}$$

Does the discrete model have traveling kink solutions?

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where $\omega \in \mathbb{R}_+$ and $(c, s, \theta) \in \mathbb{R}^3$.

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Reductions for traveling waves

Traveling waves

$$u_{1}(t) = u_{0}(t - \tau),$$

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The differential advanced-delay equation

$$c^{2}\phi'' = \frac{\phi(z+h) - 2\phi(z) + \phi(z-h)}{h^{2}} + \phi(1-\phi^{2})$$

Obstacles on existence

Classical solutions $\phi(z)$ on $z \in \mathbb{R}$

- $\phi(z)$ is $C^0(\mathbb{R})$ if c = 0
- $\phi(z)$ is $C^2(\mathbb{R})$ if $c \neq 0$
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Stationary solutions (c = 0) in standard discretizations:

- $\phi(z)$ is piecewise constant on $z \in \mathbb{R}$
- $\phi_n = \phi(nh)$ is odd either about n = 0 or about the midpoint between n = 0 and n = 1
- No continuous deformation exists between two particular solutions (Peierls–Nabarro potential)

Example of stationary solutions

Stationary solutions in the standard discrete NLS model

$$\frac{\phi_{n+1} - 2\phi_n + \phi_{n-1}}{h^2} + \phi_n^3 - \phi_n = 0, \quad n \in \mathbb{Z}$$



General and exceptional discretizations

General discrete ϕ^4 model:

$$\ddot{u}_n = \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2} + f(u_{n-1}, u_n, u_{n+1})$$

where

- P1 (continuity) $f(u, u, u) = u(1 u^2)$
- P2 (symmetry) f(v, u, w) = f(w, u, v)
- P3 f(v, u, w) is independent on h
- P4 f(v, u, w) = u Q(v, u, w), where Q = O(3)

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Exceptional nonlinearities are those that support continuous stationary solutions with c = 0 and $\phi \in C^0(\mathbb{R})$

Examples of exceptional discretizations

Tovbis (1997) $f = (u_{n+1} + u_{n-1}) (1 - u_n^2),$ Speight (1997) $f = (2u_n + u_{n+1}) (3 - u_n^2 - u_n u_{n+1} - u_{n+1}^2) + \{n + 1 \rightarrow n\},$ Kevrekidis (2003) $f = (u_{n+1} + u_{n-1}) (2 - u_{n+1}^2 - u_{n-1}^2).$

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Exceptional stationary solutions:

• The stationary solution has a translation parameter, e.g.

$$u_n = \tanh(a(hn - s)), \quad a = \frac{1}{h} \operatorname{arcsin}(h/2)$$

• Radiation from moving kinks is reduced

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- Q: Can we characterize all possible bifurcations of steadily moving kinks?
- A: YES, when the center manifold is finite-dimensional (when $c \neq 0$).

Families of exceptional discretizations

Consider the second-order difference map for stationary solutions

$$\frac{\phi_{n+1} - 2\phi_n + \phi_{n-1}}{h^2} + f(\phi_{n-1}, \phi_n, \phi_{n+1}) = 0$$

and reduce the problem to the first-order difference map

$$E = \frac{\phi_{n+1} - \phi_n}{h} - g(\phi_n, \phi_{n+1}) = \text{const}$$

Such discretizations with *polynomial* functions $g(\phi_n, \phi_{n+1})$ exist for *exceptional* polynomial functions $f(\phi_{n-1}, \phi_n, \phi_{n+1})$.

Continuous stationary solutions

Theorem[Speight, 1999]: Let $g(\phi_n, \phi_{n+1})$ be a polynomial such that $g(\phi, \phi) = \frac{1}{2}(1 - \phi^2)$. Then, for any $-1 < \phi_0 < 1$, there exists a unique monotonic sequence $\{\phi_n\}_{n \in \mathbb{Z}}$ such that

$$\phi_n < \phi_{n+1}, \quad \lim_{n \to \pm \infty} \phi_n = \pm 1$$

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Corollary: There exists a $C^0(\mathbb{R})$ monotonic kink solution $\phi(z - s)$ of the advance-delay equation

$$\frac{\phi(z-h) - 2\phi(z) + \phi(z+h)}{h^2} + f(\phi(z-h), \phi(z), \phi(z+h)) = 0,$$

such that $\lim_{z \to \pm \infty} \phi(z) = \pm 1$ and $\phi_0 = \phi(-s)$.

Traveling solutions with $c \neq 0$ **?**

Solutions $\phi(z) = e^{\lambda z}$ of the linearized equation at $\phi = 0$:

$$c^{2}\phi''(z) = \frac{\phi(z+h) - 2\phi(z) + \phi(z-h)}{h^{2}} + \phi(z)$$

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Dispersion relation for $\Lambda = \lambda h$:

$$D(\Lambda; c, h) = 2\left(\cosh \Lambda - 1\right) + h^2 - c^2 \Lambda^2 = 0$$

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Roots on the imaginary axis $\Lambda = 2iK, K \in \mathbb{R}$

$$\sin^2 K = \frac{h^2}{4} + c^2 K^2$$

Parameter plane (*c*, *h*) and bifurcations



Three bifurcations: $c = 0, \ 0 < h < 2$ $h = 0, \ 0 < c < 1$ $h = h_*(c), \ 0 < c < 1$

- c = 0, 0 < h < 2: All roots of K are real and simple.
- h = 0, 0 < c < 1: Double zero coexists with finitely many pairs of real roots *K*.
- $h = h_*(c), \ 0 < c < 1$: One pair of double real (non-zero) roots K exist (1:1 resonant Hopf bifurcation).

Bifurcation at h = 0

Differential advance-delay equation:

$$c^{2}\phi''(z) = \frac{\phi(z+h) - 2\phi(z) + \phi(z-h)}{h^{2}} + \phi(z) - Q\left(\phi(z-h), \phi(z), \phi(z+h)\right)$$

Formal perturbation expansion:

$$\phi(z+h) - 2\phi(z) + \phi(z+h) = h^2 \phi''(z) + \sum_{n=2}^{\infty} \frac{2}{(2n)!} \phi^{(2n)}(z) h^{2n}$$

and

$$\phi(z) = \sum_{n=0}^{\infty} h^{2n} \phi_{2n}(z)$$

At the leading order $\mathcal{O}(h^0)$:

$$(1-c^2)\phi_0''+\phi_0(1-\phi_0^2)=0; \quad \Rightarrow \quad \phi_0(z)=\tanh\theta, \quad \theta=\frac{z}{2\sqrt{1-c^2}}.$$

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At the higher orders $\mathcal{O}(h^{2n})$:

 $\mathcal{L}\phi_{2n} = (\text{odd inhomogeneous terms})$

where $\mathcal{L} = -\frac{d^2}{d\theta^2} + 4 - 6 \operatorname{sech}^2 \theta$ with $\mathcal{L}\operatorname{sech}^2 \theta = 0$.

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To all orders, the perturbation expansion exists and

$$\phi(z) \rightarrow \pm 1$$
 as $|z| \rightarrow \infty$.

Does it exist beyond all orders of the perturbation expansion?

Fourier oscillatory modes:

$$\phi(z) = \pm 1 + \epsilon e^{ikz/h}$$

has wavenumber k where

$$\sin^2 k = c^2 k^2 \text{ as } h \to 0.$$





 \rightarrow Fourier modes do not occur in power series of *h*.

Inner equation

Kruskal–Segur (1991): Continue the solution into the complex plane and study Fourier modes near the poles of the regular perturbation expansion



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Scaling transformation $z = h\zeta + i\pi\sqrt{1-c^2}$ and $\phi(z) = \frac{1}{h}\psi(\zeta)$ leads to the inner equation:

$$c^{2}\psi''(\zeta) = \psi(\zeta+1) - 2\psi(\zeta) + \psi(\zeta-1) - Q(\psi(\zeta-1), \psi(\zeta), \psi(\zeta+1)) + \frac{h^{2}}{2}\psi(\zeta).$$

Inner asymptotic series

Let the solution $\psi(\zeta)$ be expanded in powers of h^2 :

$$\psi(\zeta) = \psi_0(\zeta) + \sum_{n=1}^{\infty} h^{2n} \psi_{2n}(\zeta).$$

Let the leading-order solution $\psi_0(\zeta)$ be expanded in inverse power series of ζ :

$$\psi_0(\zeta) = \sum_{n=0}^{\infty} \frac{a_{2n}}{\zeta^{2n+1}}, \qquad a_0 = 2\sqrt{1-c^2}.$$

<u>Theorem</u> (Tovbis, 2000): If the inverse power series for $\psi_0(\zeta)$ diverges, the formal perturbation expansion for $\phi(z)$ diverges and some Fourier modes are non-zero beyond the formal expansion.

Borel-Laplace transform

Let $\psi_0(\zeta)$ be the Laplace transform of $V_0(p)$:

$$\psi_0(\zeta) = \int_{\gamma} V_0(p) e^{-p\zeta} dp$$

The resulting integral equation,

numerical coefficients

 $\overline{c^2}$

$$\left(4\sinh^2\frac{p}{2} - c^2p^2\right)V_0(p) = \sum_{\alpha_1,\alpha_2,\alpha_3} a_{\alpha_1,\alpha_2,\alpha_3} e^{\alpha_1 p}V_0(p) * e^{\alpha_2 p}V_0(p) * e^{\alpha_3 p}V_0(p) + e^{\alpha_3 p}V_0(p) * e^{\alpha_3 p}V_0(p) + e^{\alpha_3 p}V_0(p) * e^{\alpha_3 p}V_0(p) + e^{\alpha_3 p}V_0(p) +$$

Power series solution:

$$V_0(p) = \sum_{n=0}^{\infty} v_{2n} p^{2n}, \qquad v_0 = 2\sqrt{1-1}$$

Singularities of $V_0(p)$



Singularities of $V_0(p)$

The distance between the stable and unstable manifold:

$$\psi_{0s}(\zeta) - \psi_{0u}(\zeta) = 2\pi i \sum \operatorname{Res} \left[V_0(p) e^{-p\zeta} \right]$$



The first pole of $V_0(p)$

Let $p = ik_1$ be the nearest singularity to p = 0. Then, $V_0(p)$ has the leading order behavior near $p = ik_1$:

$$V_0(p) \to rac{k_1^2 K_1(c)}{(p^2 + k_1^2)},$$

where $K_1(c)$ is referred to as the *Stokes constant*.

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where $K_1(c)$ is referred to as the *Stokes constant*. Then

$$\psi_{0s}(\zeta) - \psi_{0u}(\zeta) = [\pi k_1 K_1(c) + \mathcal{O}(1/\zeta)]e^{-ik_1\zeta}$$

Residue of the first pole $p = ik_1$ can be deduced from a power-series solution for $V_0(p)$ at p = 0, which converges for $|p| < k_1$.

Numerical computations of $K_1(c)$

• Expand $V_0(p)$ near the pole $p \to \pm ik_1$:

$$V_0(p) \to K_1(c) \sum_{n=0}^{\infty} (-1)^n k_1^{-2n} p^{2n}$$

• Expand $V_0(p)$ in the power series at p = 0:

$$V_0(p) = \sum_{n=0}^{\infty} v_{2n} p^{2n}, \qquad v_0 = 2\sqrt{1-c^2}.$$

where the coefficients are obtained from a recurrence relation. • Then $K_1(c)$ can be obtained as a numerical limit:

$$K_1(c) = \lim_{n \to \infty} w_n, \qquad w_n = (-1)^n k_1^{2n} v_{2n}$$

Convergence of the algorithm

Convergence of w_n is slow:

$$w_n = K_1(c) + \frac{A(c)}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)$$

The error estimate of the numerical limit:

$$A_{\rm est} = -n^2(w_n - w_{n-1})$$





Standard nonlinearity



Speight's discretization



Tovbis' discretization



Kevrekidis' discretization



Bifurcations of traveling kinks on (c, h)

• Zeros $c = c_*$ of $K_1(c)$ lie in the region c > 0.22, where only one pair $p = \pm ik_1$ is purely imaginary.

- One can expect a bifurcation of the one-parameter curve on the (h, c) plane that passes through the point $(0, c_*)$.
- Numerical analysis of the bifurcation:
 - solve the differential advance-delay equation on $z \in [-L, L]$ where L = 100
 - subject to the anti-periodic boundary conditions $\phi(L) = -\phi(-L)$
 - by using the iterative Newton's method with the continuum kink as starting guess,
 - the eight-order finite-difference approximation to the second derivative with the step size $\Delta z = h/10$.

Numerical analysis of the bifurcation



The average of $[\phi(z) - \phi_{ave}]^2$ is computed over the the interval $z \in [L - 20, L]$ for fixed values of parameter c

Bifurcation at h = 0, c = 1

Differential advance-delay equation (inner form):

 $c^{2}\phi'' = \phi(\zeta+1) - 2\phi(\zeta) + \phi(\zeta-1) + h^{2}\phi - h^{2}Q(\phi(\zeta-1), \phi(\zeta), \phi(\zeta+1)),$

where $\zeta = z/h$.

Near the point h = 0, c = 1: $c^2 = 1 + \epsilon \gamma$ $h^2 = \epsilon^2 \tau$ $\zeta_1 = \sqrt{\epsilon} \zeta$



Truncated normal form for bifurcation:

$$\frac{1}{12}\phi^{(\mathrm{iv})}(\zeta_1) - \gamma\phi''(\zeta_1) + \tau\phi(\zeta_1)(1 - \phi^2(\zeta_1)) = 0.$$

Numerical analysis of heteroclinic orbits

Truncated normal form:

$$\phi^{(\mathrm{iv})} + \sigma \phi'' + \phi - \phi^3 = 0,$$

where $\sigma = -\sqrt{12}\gamma/\sqrt{\tau}$ and $\phi = \phi(t)$.

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Linearization at $\phi = \pm 1$ gives pairs of eigenvalues $(\lambda_0, -\lambda_0)$ and $(i\omega_0, -i\omega_0)$ with the one-dimensional unstable manifold:

$$\lim_{t \to -\infty} \phi_u(t) = -1, \qquad \lim_{t \to -\infty} \left(\phi_u(t) + 1 \right) e^{-\lambda_0 t} = C_0$$

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The kink solution is odd in $t \in \mathbb{R}$ (up to translational invariance). Iterating the initial-value problem along the unstable manifold from t = 0 to $t = t_0$ where $\phi(t_0) = 0$, one can compute the split function $K(\sigma) = \phi''(t_0)$, which may depend on numerical factors C_0 and Δt .

Numerical results on $K(\sigma)$





No bifurcations of kinks occur from the point h = 0, c = 1.

Conclusions

- Existence of continuous stationary kinks at c = 0 is not sufficient for existence of traveling kinks at c ≠ 0
- Bifurcations of traveling kinks may occur at isolated velocities with 0 < c < 1 (e.g. in the numerical analysis of the Speight's and Kevrekidis' exceptional nonlinearities)
- No bifurcations of traveling kinks occur from the point c = 1
- It is problematic to consider asymptotic expansions in powers of c^2 and the bifurcation of traveling kinks from the point c = 0