Travelling kinks in discrete ϕ^4 models

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Joint work with

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Standard discrete ϕ^4 model

ϕ^4 model: $u_{tt} - u_{xx} + \frac{1}{2}u(1-u^2)$ admits kink solutions.

'Standard' discretisation:

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

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Kinks describe

- domain walls in ferroelectrics and ferromagnets,
- topological excitations in biological macromolecules and hydrogen-bonded chains and
- bond-rotation mismatches in polymers.

Exceptional discretizations

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

where $f(u_{n-1}, u_n, u_{n+1}) =$

Speight: $$\frac{1}{12}(2u_n + u_{n+1})\left(1 - \frac{u_n^2 + u_n u_{n+1} + u_{n+1}^2}{3}\right) + \frac{1}{12}(2u_n + u_{n-1})\left(1 - \frac{u_n^2 + u_n u_{n-1} + u_{n-1}^2}{3}\right),$$

Bender/Tovbis: $$\frac{1}{4}\left(u_{n+1} + u_{n-1}\right)\left(1 - u_n^2\right),$$

Kevrekidis: $$\frac{1}{8}\left(u_{n+1} + u_{n-1}\right)\left(2 - u_{n+1}^2 - u_{n-1}^2\right).$$

All support continuous stationary kinks, in contrast to the standard model.

Purpose of this work

We want to answer the questions:

- Does the elimination of the Peierls-Nabarro barrier (in Speight's model) cause the kink's radiation to disappear?
- Does the momentum conservation of the Bender/Tovbis and Kevrekidis models imply the existence of steadily moving kinks?

i.e. does

existence of a translation mode

$\Rightarrow$

kinks can propagate through the lattice without radiative deceleration?

Advance-delay equation

Make the travelling wave ansatz:

$$u_n(t) = \phi(z), \qquad z = h(n-s) - ct,$$

where $\phi(z)$ is assumed to be a twice differentiable function of $z \in \mathbb{R}$. Leads to the advance-delay equation:

$$c^2\phi''(z) = \frac{\phi(z+h) - 2\phi(z) + \phi(z-h)}{h^2} + \frac{1}{2}\phi(z) \\ - Q\left(\phi(z-h), \phi(z), \phi(z+h)\right).$$

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Cubic polynomial

All linear terms can be reduced to $\frac{1}{2}\phi(z)$ by rescaling h.

Regular perturbation expansion

Expand

$$\phi(z \pm h) = \sum_{n=0}^{\infty} \frac{\phi^{(n)}(z)}{n!} h^n \quad \text{and} \quad \phi(z) = \sum_{n=0}^{\infty} h^{2n} \phi_{2n}(z).$$

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$\mathcal{O}(h^0)$:

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

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$\mathcal{O}(h^{2n})$:

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

where $\mathcal{L} = -\frac{d^2}{d\theta^2} + 4 - 6\,\text{sech}^2\,\theta$; $\quad \theta = \frac{z}{2\sqrt{1-c^2}}$.

Radiation?

To all orders, the perturbation expansion exists and $\phi(z)$ decays to ± 1 as $|z| \to \infty$.

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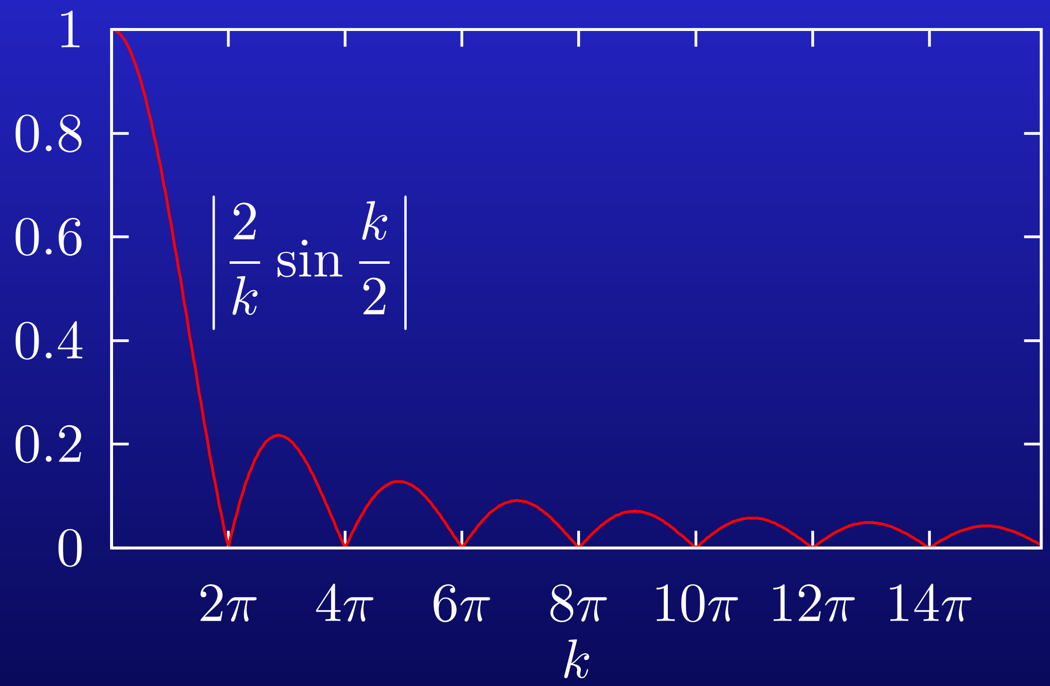
Resonant radiation:

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

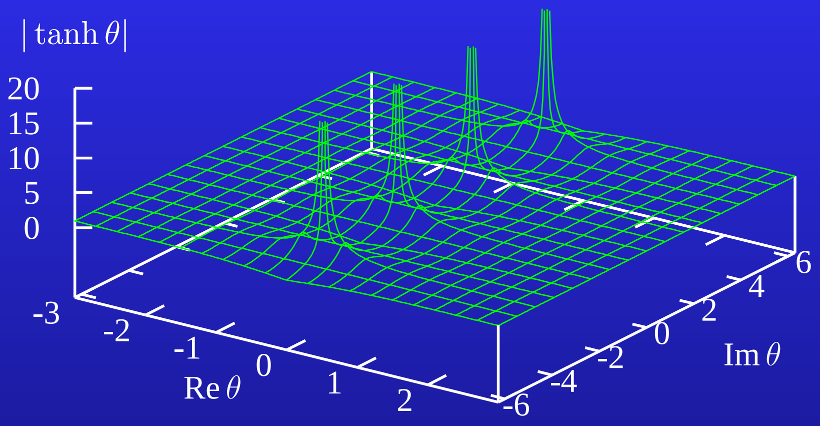
has wavenumber k where

$$\left| \frac{2}{k} \sin \frac{k}{2} \right| = |c| \text{ as } h \to 0.$$



‘Inner’ equation

Idea of Kruskal and Segur: Continue into the complex plane. Strong coupling to radiation near poles of the leading-order solution.



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

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

Inner asymptotic series

We expand the inner solution in powers of h^2 (“inner asymptotic expansion”):

$$\hat{\psi}(\zeta) = \hat{\psi}_0(\zeta) + \sum_{n=1}^{\infty} h^{2n} \hat{\psi}_{2n}(\zeta).$$

Continuation of the first few orders of the outer solution to the inner region motivates the search for the leading-order inner solution as:

$$\hat{\psi}_0(\zeta) = \sum_{n=0}^{\infty} \frac{a_{2n}}{\zeta^{2n+1}}$$

Borel-Laplace transform

Magnitude of the radiation can be determined by Borel-summation of the asymptotic series (Pomeau, Ramani & Grammaticos).

Introduce the Laplace transform $\psi_0(\zeta) = \int_\gamma V_0(p) e^{-p\zeta} dp$. The resulting integral equation,

$$\left(4\sinh^2\frac{p}{2} - c^2p^2\right)V_0(p) = \begin{cases} V_0(p) * V_0(p) * V_0(p) & \text{('standard')} \\ V_0(p)\cosh(p) * V_0(p) * V_0(p) & \text{(Bender-Tovbis)} \\ \text{etc.}\ldots \end{cases}$$

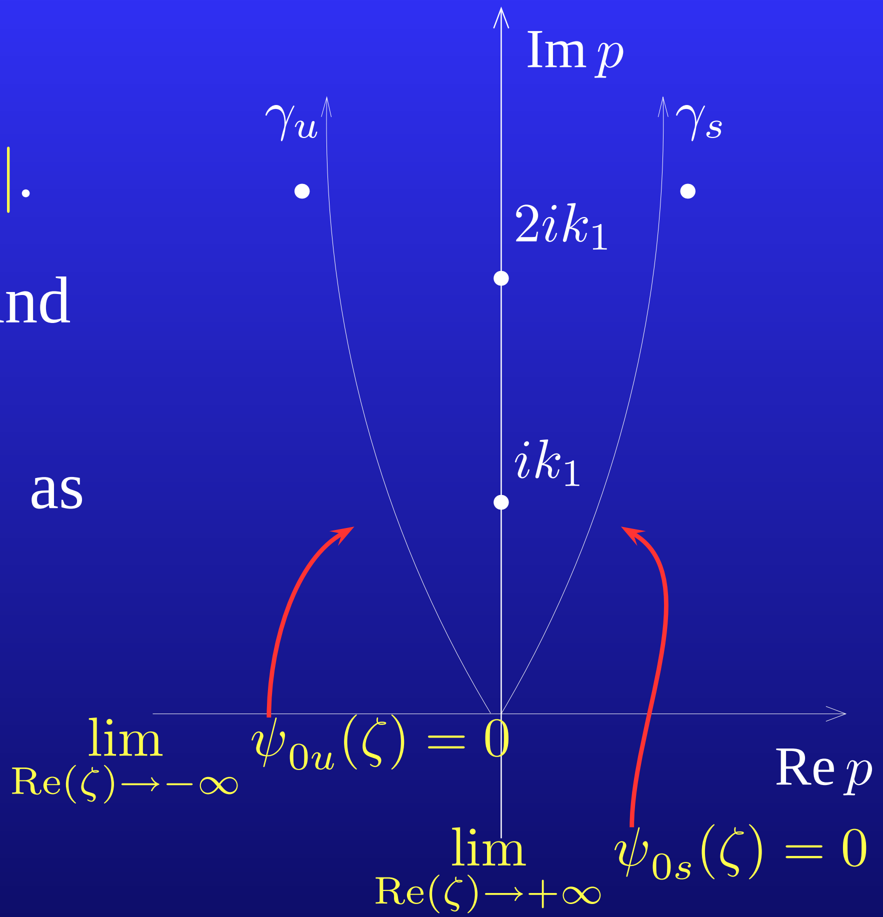
where $V(p) * W(p) = \int_0^p V(p-p_1)W(p_1)dp_1$.

Singularities

Singularities where $\left|\frac{2}{p}\sinh\frac{p}{2}\right| = |c|$.

- Imaginary zeros: Let $p = ik$ and see the previous graph...
- If $c \neq 0$: $p_I \to \pm\frac{2}{c}\cosh\left(\frac{p_R}{2}\right)$ as $p_R \to \infty$.

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



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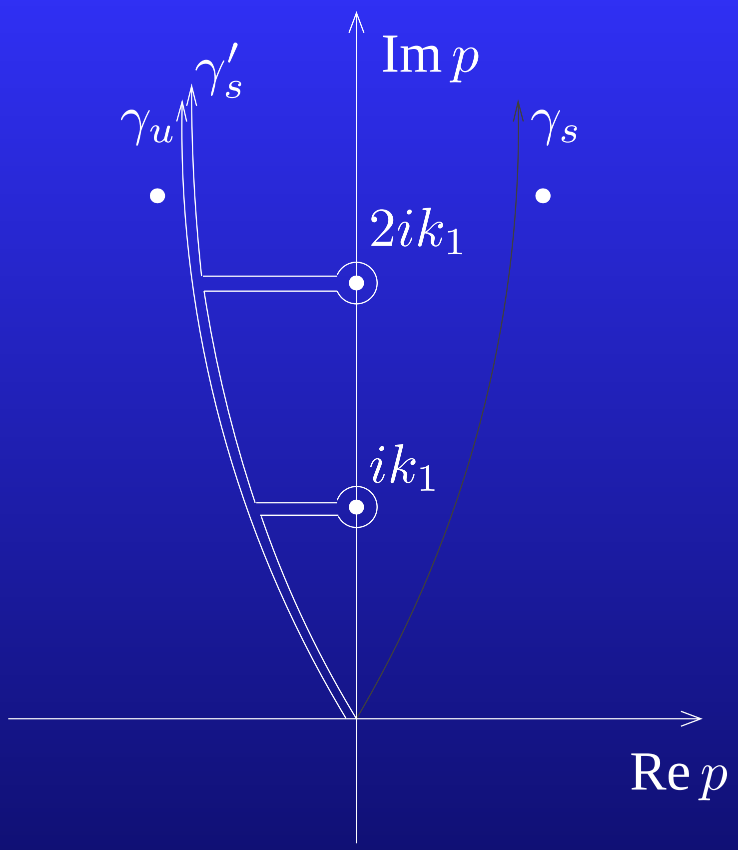


$$\psi_{0s}(\zeta) - \psi_{0u}(\zeta) = 2\pi i \sum \text{res}\ \left[V_0(p) e^{-p\zeta}\right]$$

Singularities of $V_0(p)$

Assume the following leading-order behaviour of $V_0(p)$:

$$V_0(p) \to k_1^2 K_1(c)/(p^2 + k_1^2)$$

Then

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

Virtue of the integral formulation:

Residue of the first pole $p = ik_1$ can be deduced from a power-series solution, which converges for $|p| < k_1$. Allows for efficient numerical computation.

Power-series expansions

- Expanding the expressions for the poles of $V_0(p)$ as $p \to \pm i k_1$:

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

- This coincides with the $n \to \infty$ behaviour of a power-series solution $V_0(p) = \sum_{n=0}^{\infty} v_{2n} p^{2n}$ (convergent for $|p| < k_1$).
- v_{2n} are obtained by substituting the power-series into the integral equation and deriving a recurrence relation between its coefficients.
- Then $K_1(c)$ can be obtained as a numerical limit.

Computation of Stokes constants

$$K_1(c) = \lim_{n\to\infty} w_n \quad \text{where} \quad w_n = (-1)^n k_1^{2n} v_{2n}.$$

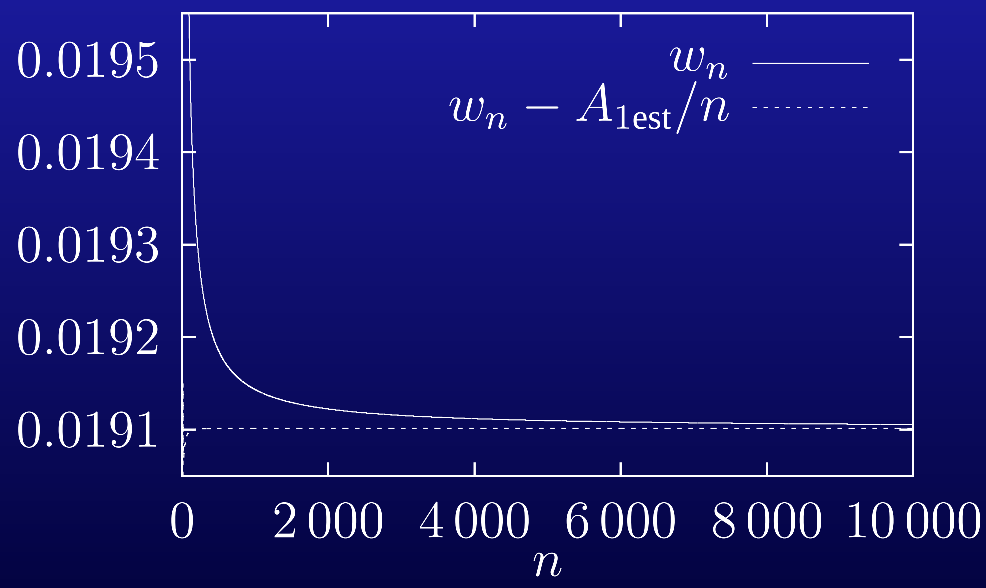
Convergence of w_n is very slow:

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

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

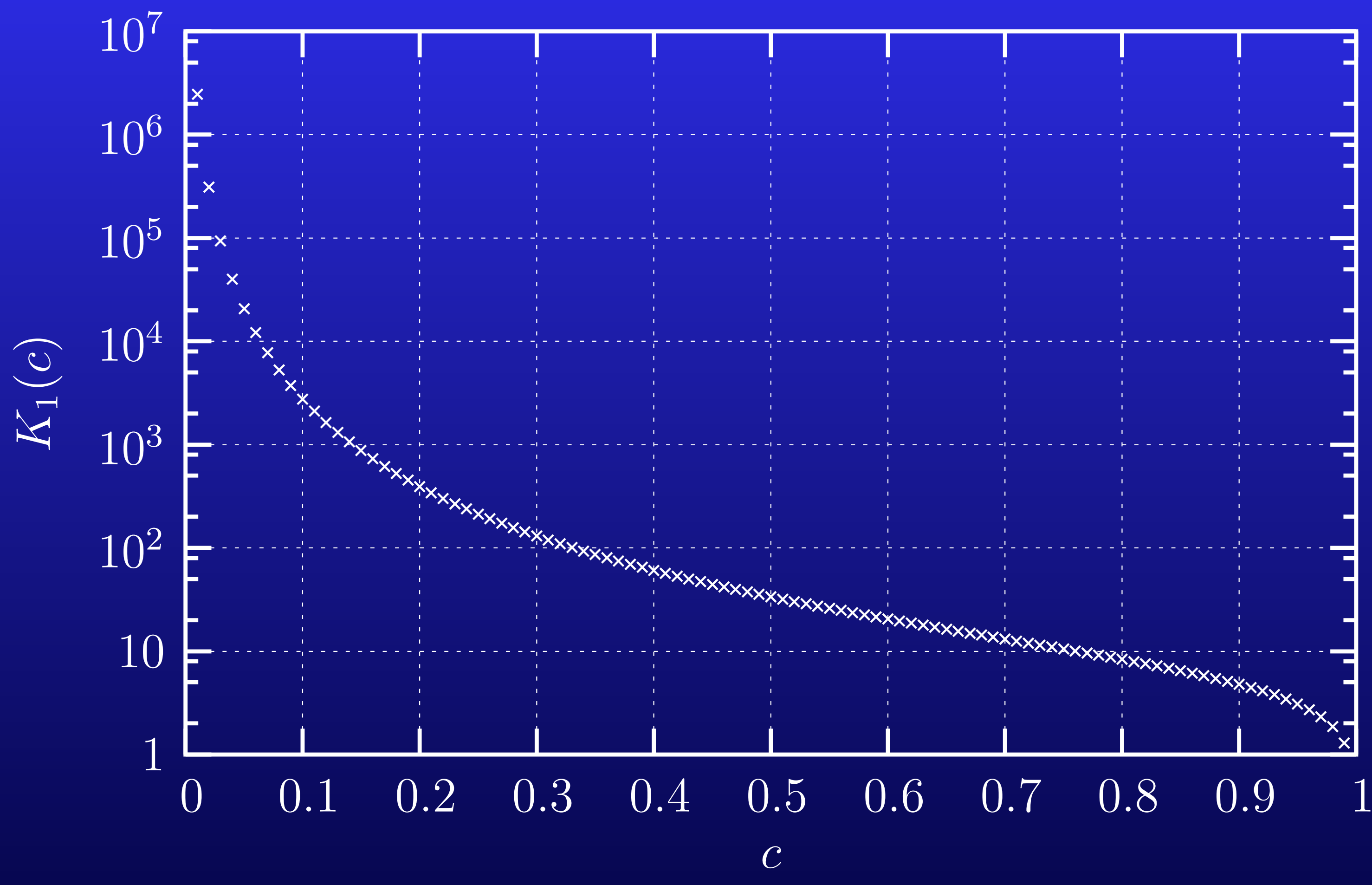
We use A_{est}/n as an error estimate for the numerical limit.

Kevrekidis' model with $c = 0.5$:



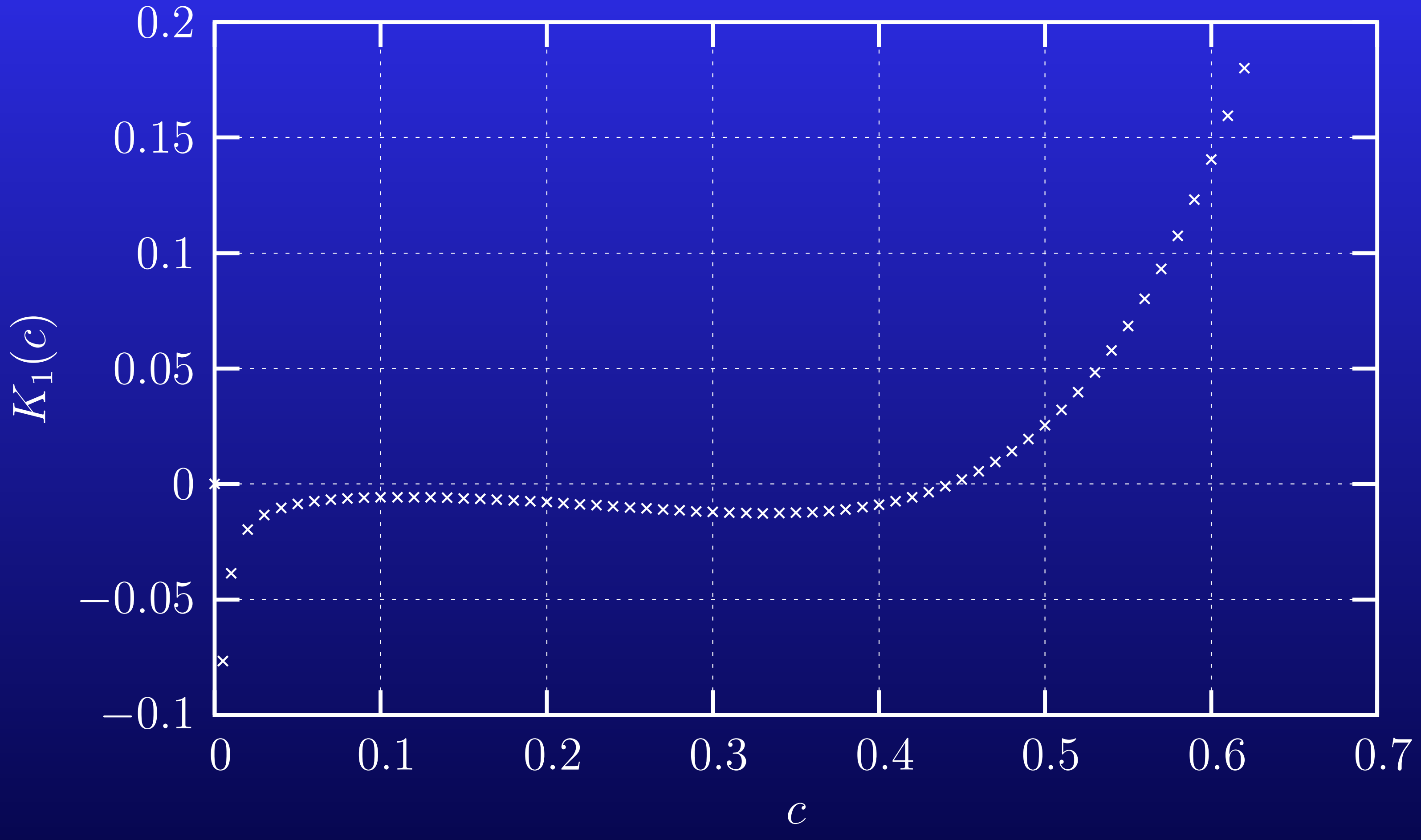
Stokes Constant

Standard nonlinearity



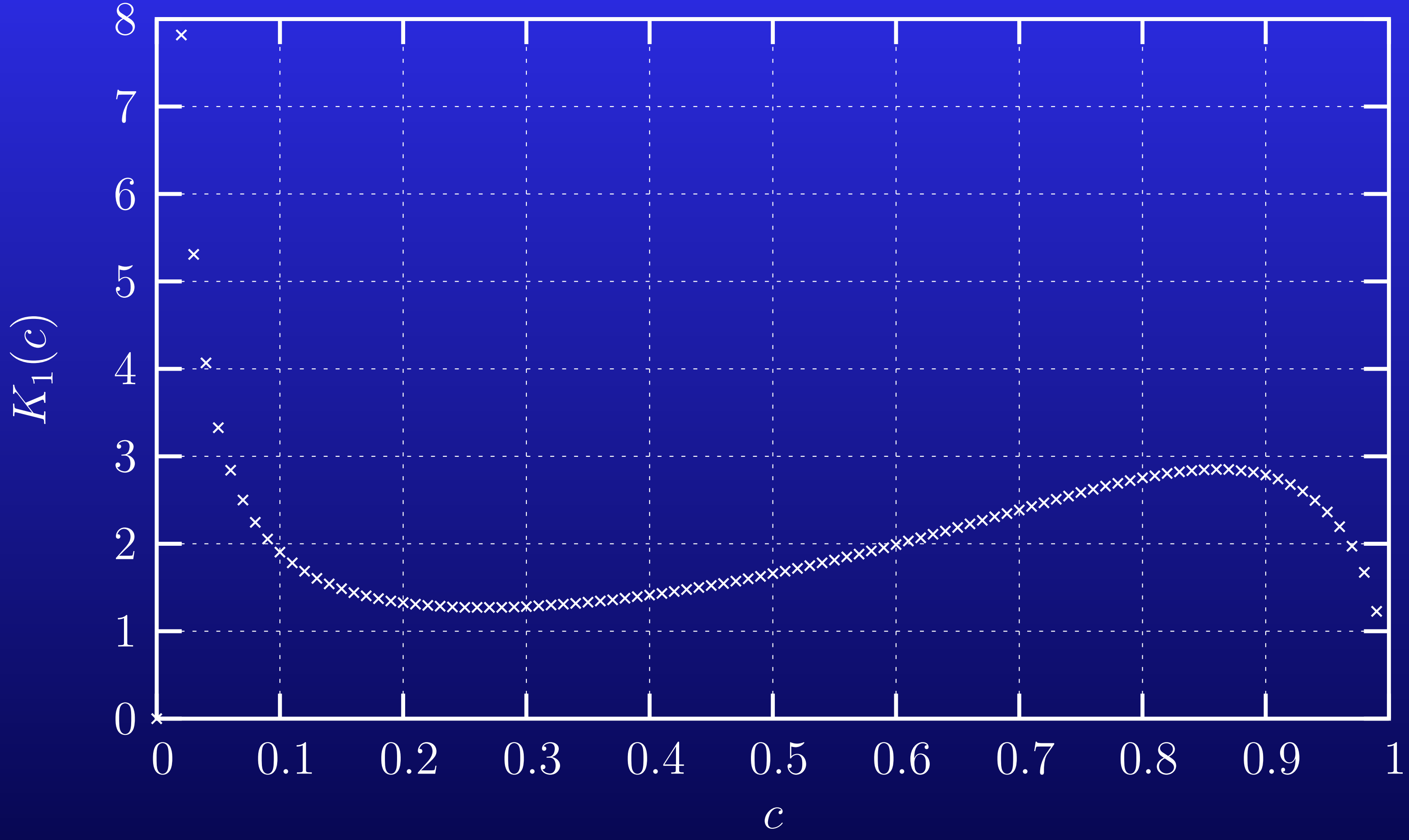
Stokes Constant

Speight's discretization



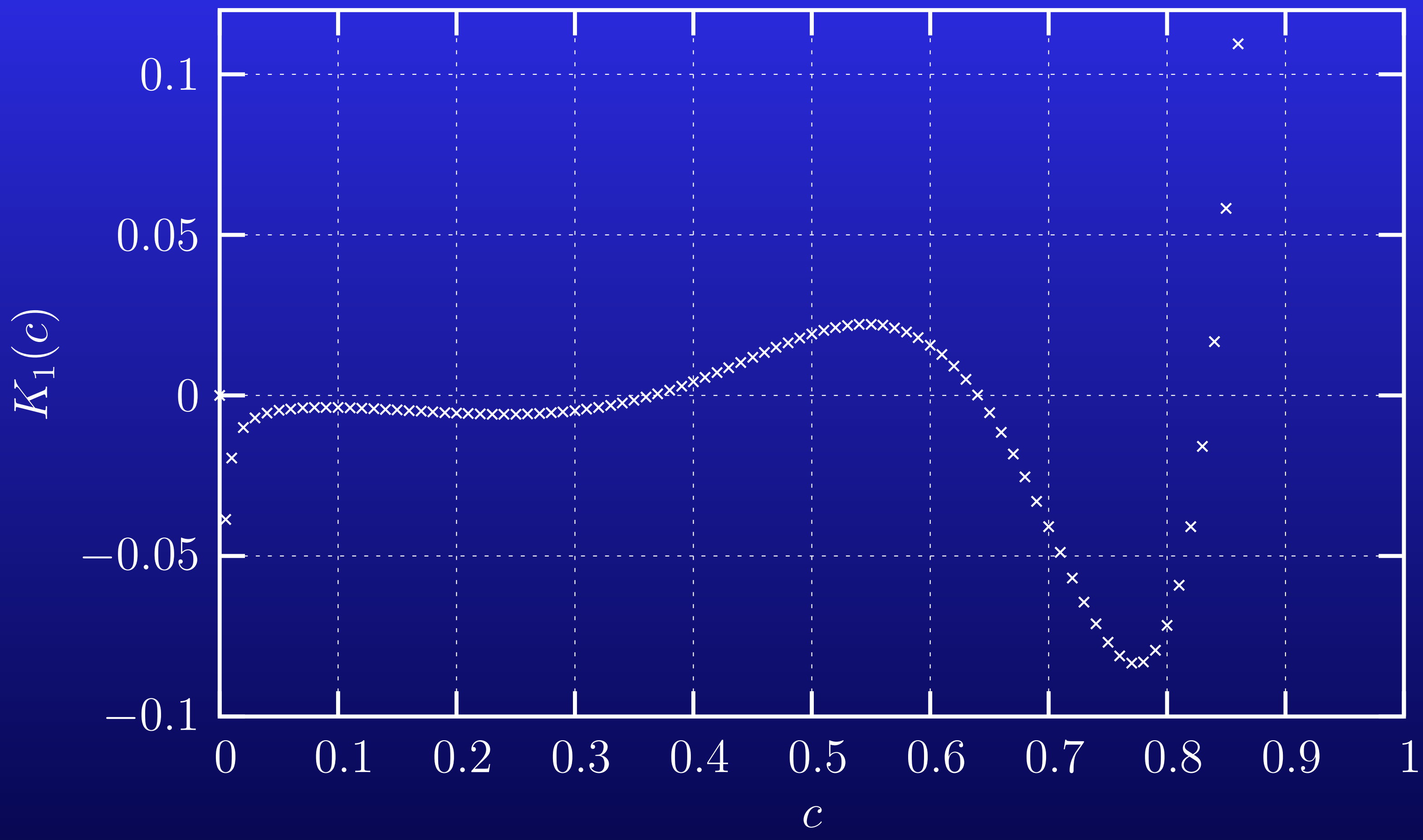
Stokes Constant

Bender & Tovbis' discretization



Stokes Constant

Kevrekidis' discretization



Radiationless travelling kinks?

- Zeros $c = c_*$ of $K_1(c)$ lie in the region $c > 0.22$, where there is only one resonance, $p = \pm i k_1$.
- Probably means that a family of travelling kinks exists along a one-parameter curve on the (h, c) plane that passes through the point $(0, c_*)$.

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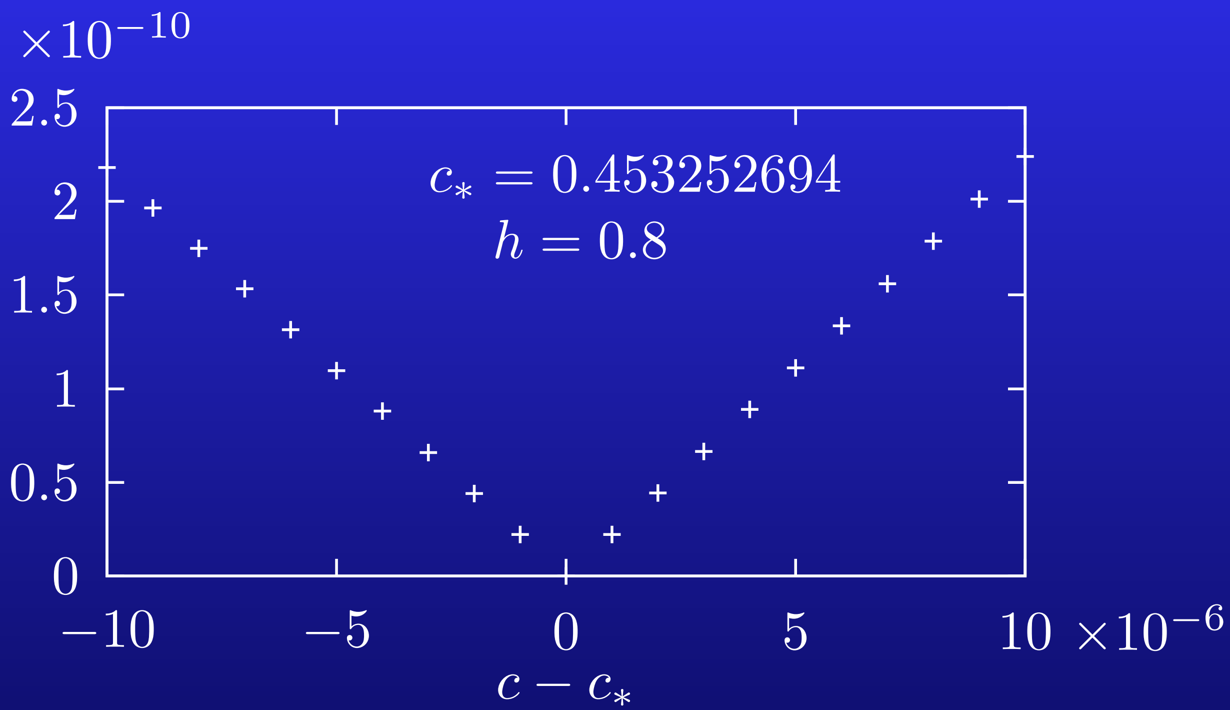
- To verify: solve the differential advance-delay equation numerically: Interval length $2L = 200$; anti-periodic boundary conditions $\phi(L) = -\phi(-L)$; iterative Newton's method with the continuum kink as starting guess; eigth-order finite-difference approximation to the second derivative, step size $h/10$.

Radiationless travelling kinks

Speight's model



$\longrightarrow$ Plotting the average of $[\phi(z) - \phi_{\text{ave}}]^2$ over the last 20 units of the interval.

Conclusions

- "Effective translation invariance" is not enough to ensure that kinks can travel without the emission of radiation, although it does seem to reduce the radiation drastically.
- There are some isolated velocities in Speight's and Kevrekidis' models at which kinks can travel without losing energy to radiation.
- Problematic to consider beyond-all-orders expansion in powers of c^2.