

Nonlinear Wave Propagation in Discrete and Continuous Systems

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Outline of the talk

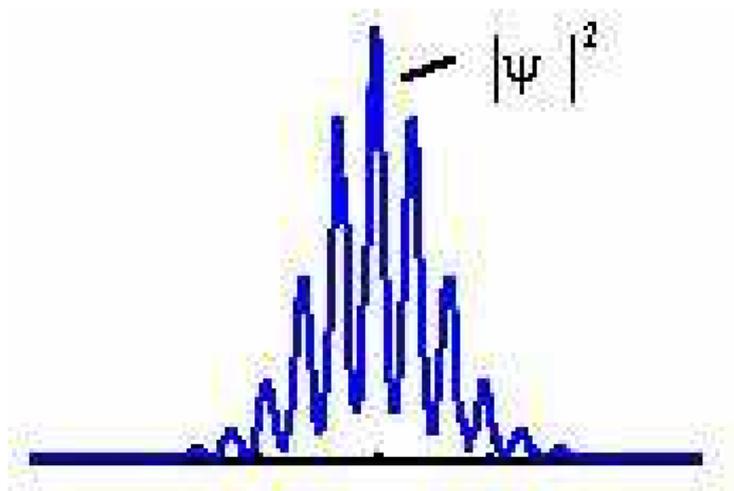
- 1 Nonlinear Lattice
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- 4 Discrete Sine-Gordon
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- 6 Stability of Solitons. Why?
- 7 Nonlinear Schrödinger Equation (NLS)
- 8 Discrete NLS equation
- 9 Conclusions

PART I: NONLINEAR LATTICES

Discrete Solitons

Discrete solitons were first suggested by Davydov in alpha-helix proteins. This model attempted to explain some fundamental issues in biophysics such as for example storage of phonon energy in proteins.

$$i\hbar \frac{d\Psi_n}{dt} + J(\Psi_{n+1} - \Psi_{n-1}) + \sigma |\Psi_n|^2 \Psi_n = 0$$



Integrable vs Non-integrable lattices

sine-Gordon (Integrable) VS Discrete SG (non-integrable)

$$u_{tt} - u_{xx} = \Gamma \sin u, \quad \text{vs} \quad \ddot{u}_n = u_{n+1} - 2u_n + u_{n-1} + \Gamma \sin u_n$$

NSL (integrable) VS Ablowitz-Ladik lattice (Integrable)/DNLS (non-integrable)

$$i u_t = 2|u|^2 u + u_{xx}$$

VS

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

and

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

Klein-Gordon Lattice

Klein-Gordon (KG) lattice models a chain of coupled anharmonic oscillators with nearest-neighbour interactions

$$\ddot{u}_n + V'(u_n) = \varepsilon(u_{n-1} - 2u_n + u_{n+1}).$$

where $\{u_n(t)\}_{n \in \mathbb{Z}} : \mathbb{R} \rightarrow \mathbb{R}^Z$, dot represents time derivative, ε is the coupling constant, and $V : \mathbb{R} \rightarrow \mathbb{R}$ is an on-site potential.



Applications:

- dislocations in crystals (e.g. Frenkel & Kontorova 1938)
- oscillations in biological molecules (e.g. Peyrard & Bishop 1989)

Anharmonic oscillator

We make the following assumptions:

- $V(u) = u \pm u^3 + \mathcal{O}(u^5)$, where $+/-$ corresponds to hard/soft potential;
- $0 < \varepsilon \ll 1$: oscillators are weakly coupled.

In the anti-continuum limit ($\varepsilon = 0$), each oscillator is governed by

$$\ddot{\varphi} + V'(\varphi) = 0, \quad \Rightarrow \quad \frac{1}{2}\dot{\varphi}^2 + V(\varphi) = E,$$

where $\varphi \in H_{per}^2(0, T)$. Period of oscillations T is uniquely defined by the energy level E , according to the following formula:

$$T = \sqrt{2} \int_{-a}^a \frac{d\varphi}{\sqrt{E - V(\varphi)}}.$$

Multi-breathers in the anti-continuum limit

Breathers are spatially localized time-periodic solutions to the Klein-Gordon lattice. Multi-breathers are constructed by parameter continuation in ε from $\varepsilon = 0$. For $\varepsilon = 0$ we take

$$\mathbf{u}^{(0)}(t) = \sum_{k \in S} \sigma_k \varphi(t) \mathbf{e}_k \in \ell^2(\mathbb{Z}, H_{per}^2(0, T)),$$

where $S \subset \mathbb{Z}$ is the set of excited sites and \mathbf{e}_k is the unit vector in $\ell^2(\mathbb{Z})$ at the node k . The oscillators are in phase if $\sigma_k = +1$ and out-of-phase if $\sigma_k = -1$.

Theorem (MacKay & Aubry 1994)

Fix the period $T \neq 2\pi n$, $n \in \mathbb{N}$ and the T -periodic solution $\varphi \in H_{per}^2(0, T)$ of the anharmonic oscillator equation for $T(E) \neq 0$. There exist $\varepsilon_0 > 0$ and $C > 0$ such that $\forall \varepsilon \in (\varepsilon_0, \varepsilon_0)$ there exists a solution $\mathbf{u}^{(\varepsilon)} \in \ell^2(\mathbb{Z}, H_{per}^2(0, T))$, of the Klein-Gordon lattice satisfying

$$\left\| \mathbf{u}^{(\varepsilon)} - \mathbf{u}^{(0)} \right\|_{\ell^2(\mathbb{Z}, H_{per}^2(0, T))} \leq C\varepsilon$$

Stability of discrete breathers

Multibreathers in Klein-Gordon lattices:

- Morgante, Johansson, Kopidakis, Aubry 2002 - numerical results
- Archilla, Cuevas, Sánchez-Rey, Alvarez 2003 - Aubry's spectral band theory
- Koukouloyannis, Kevrekidis 2009 - MacKay's action-angle averaging

Similar works:

- Pelinovsky, Kevrekidis, Franzeskakis 2005 - discrete NLS lattice
- Youshimura 2011 - Fermi-Pasta-Ulam bi-atomic lattice
- Youshimura 2012 - KG unharmonic lattice

Floquet Multipliers

Linearize about the breather solution to the dKG by replacing \mathbf{u} with $\mathbf{u} + \mathbf{w}$, where $\mathbf{w} : \mathbb{R} \rightarrow \mathbb{R}^Z$ is a small perturbation, and collect the terms linear in \mathbf{w} :

$$\ddot{\mathbf{w}}_n + V''(\mathbf{u}_n)\mathbf{w}_n = \epsilon(\mathbf{w}_{n+1} - 2\mathbf{w}_n + \mathbf{w}_{n-1}), \quad n \in \mathbb{Z}$$

In the *anti-continuum limit*, it is easy to find the Floquet multipliers:

- on "holes" $n \in \mathbb{Z} \setminus S$,

$$\ddot{\mathbf{w}}_n + \mathbf{w}_n = 0, \quad \begin{pmatrix} \mathbf{w}_n(T) \\ \dot{\mathbf{w}}_n(T) \end{pmatrix} = \begin{pmatrix} \cos T & \sin T \\ -\sin T & \cos T \end{pmatrix} \begin{pmatrix} \mathbf{w}_n(0) \\ \dot{\mathbf{w}}_n(0) \end{pmatrix},$$

Floquet multipliers are $\mu_{1,2} = e^{\pm iT}$

- on excited sites, $n \in S$,

$$\ddot{\mathbf{w}}_n + V''(\varphi)\mathbf{w}_n = 0, \quad \begin{pmatrix} \mathbf{w}_n(T) \\ \dot{\mathbf{w}}_n(T) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ T'(E)(V'(a))^2 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{w}_n(0) \\ \dot{\mathbf{w}}_n(0) \end{pmatrix},$$

Floquet multipliers are $\mu_{1,2} = 1$ of geometric multiplicity 1 and algebraic multiplicity 2.

Floquet Exponent

A Floquet multiplier μ can be written as $\mu = e^{\lambda T}$

Theorem (Pelinovsky '12)

For small $\epsilon > 0$ the linearized stability problem has $2M$ small Floquet exponents $\lambda = \epsilon^{N/2}\Lambda + O(\epsilon^{(N+1)/2})$, where λ is determined from the eigenvalue problem

$$-\frac{T(E)^2}{2T'(E)K_N}\Lambda^2 \mathbf{c} = \mathbf{S}\mathbf{c}, \quad \mathbf{c} \in \mathbb{C}^M$$

with $\mathbf{S} \in \mathbb{R}^{M \times M}$ is a tridiagonal matrix with elements

$$S_{i,j} = -\sigma_j(\sigma_{j-1} + \sigma_{j+1})\delta_{i,j} + \delta_{i,j-1} + \delta_{i,j+1}, \quad 1 \leq i, j \leq M,$$

and K_N is defined by

$$K_N = \int_0^T \dot{\varphi}(t)\dot{\varphi}_{N-1}(t)dt, \quad (\partial_t^2 + 1)\varphi_k = \varphi_{k-1}, \quad \varphi_0 = \varphi.$$

Stability of Multi-breathers

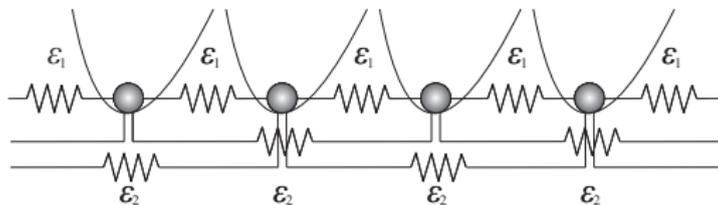
Sandstede (1998) showed that the matrix S has exactly n_0 positive and $M - 1 - n_0$ negative eigenvalues in addition to the simple zero eigenvalue, where $n_0 = (\text{sign changes in } n)$. Hence, stability of multibreathers is determined by the sign $T'(E)K_N(T)$ and the phase parameters $\{\sigma_k\}_{k=1}^{M-1}$.

Theorem

If $T'(E)K_N(T) > 0$ the linearized problem for the multibreathers has exactly n_0 pairs of "stable" Floquet exponents and $M - 1 - n_0$ pairs of "unstable" Floquet exponents counting their multiplicities. If $T'(E)K_N(T) < 0$ the conclusion changes to the opposite.

KG with LRI

The picture *radically* changes when the chain involves interactions with range longer than mere nearest neighbors. The range parameter r will be used to indicate the interaction length between the oscillators of the chain. The next nearest neighbor (NNN) chain the range is $r = 2$. The coupling force between the oscillators of the chain is linear and the coupling constants $\varepsilon_j, j = 1 \dots r$ are not, in general, equal.



The Hamiltonian of a 1D KG chain with long range interactions is:

$$H = \sum_{i=-\infty}^{\infty} \left[\frac{p_i^2}{2} + V(x_i) \right] + \frac{1}{2} \sum_{i=-\infty}^{\infty} \sum_{j=1}^r \varepsilon_j (x_i - x_{i+j})^2 \quad (3.1)$$

which leads to the equations of motion

$$\ddot{x}_i = -V'(x_i) + \sum_{j=1}^r \varepsilon_j (x_{i-j} - 2x_i + x_{i+j})$$

Persistence of Multibreathers in KG with LRI

In the anti-continuum limit $\epsilon = 0$, all the oscillators of the chain at rest except for $n + 1$ “central” ones which move in periodic orbits of frequency w , but arbitrary initial phases. The space localized and time-periodic motion is denoted by $z_0(t)$ and let $\mathbb{S} = \{0, 1, \dots, n\}$ the set of indices corresponding to the central oscillators. Action-angle $(x, p) \mapsto (w, J)$ canonical transformation. Then $H = H(w_i, J_i, x_j, y_j)$ with $i \in \mathbb{S}$ and $j \in \mathbb{Z} \setminus \mathbb{S}$. After that, a second canonical transformation

$$\begin{aligned} \vartheta &= w_0 & A &= \sum_{j=0}^n J_j \\ \phi_i &= w_{i+1} - w_i & l_i &= \sum_{j=i}^n J_j \quad i = 1 \dots n \end{aligned}$$

where ϕ_i denote the n phase differences between the $n + 1$ successive oscillators and l_i are the conjugate generalized momenta.

The Hamiltonian becomes $H = H(\phi_j, l_j, \vartheta, A, x_j, p_j)$. We define then

$$H^{\text{eff}}(\phi_i, l_i, A) = \oint H \circ z(t) dt,$$

where $z(t)$ is periodic orbit obtained by a continuation procedure using constant symplectic “area” A .

Persistence Condition

H^{eff} can be written as

$$H^{\text{eff}} = H_0(l_i) + \epsilon \langle H_1 \rangle(\phi_i, l_i) \quad (3.2)$$

where we have omitted constant and higher order terms. The average value of the coupling part of the Hamiltonian is

$$\langle H_1 \rangle(\phi_i, l_i) = \frac{1}{T} \oint H_1(\vartheta, \phi_i, l_i) dt$$

where all the calculations have been made along the unperturbed periodic orbit z_0 . The critical points of the dynamical system associated with H^{eff} are in one-to-one correspondence with the periodic orbits of the original H -system which will be continued for ϵ nonzero but small enough to provide multibreathers. So, by using the form of H^{eff} of (3.2), we obtain the persistence conditions for the existence of $n + 1$ -site multibreathers as

$$\frac{\partial \langle H_1 \rangle}{\partial \phi_i} = 0, \quad i = 1 \dots n, \quad (3.3)$$

Example for LRI in KGlattice

Let $\varepsilon_j = k_j \varepsilon$, with $k_1 = 1$, then the Hamiltonian becomes

$$H = H_0 + \varepsilon H_1 = \sum_{i=-\infty}^{\infty} \left[\frac{p_i^2}{2} + V(x_i) \right] + \frac{\varepsilon}{2} \sum_{i=-\infty}^{\infty} \sum_{j=1}^r k_j (x_i - x_{i+j})^2 \quad (3.4)$$

Now, since the Hamiltonian is written in the form $H = H_0 + \varepsilon H_1$ the persistence conditions (3.3) can be used.

Consider $n + 1$ "central" oscillators and $x_i = \sum_{m=0}^{\infty} A_m \cos(mw_i)$, then

$$\langle H_1 \rangle = -\frac{1}{2} \sum_{m=1}^{\infty} \sum_{j=1}^r \sum_{s=1}^{n-j+1} A_m^2 k_j \cos\left(m \sum_{l=0}^{j-1} \phi_{s+l}\right). \quad (3.5)$$

Then,

$$\frac{\partial \langle H_1 \rangle}{\partial \phi_i} = 0 \Rightarrow \sum_{p=1}^r \sum_{s=z_1}^{z_2} k_p M\left(\sum_{l=0}^{p-1} \phi_{s+l}\right) = 0, \quad (3.6)$$

where $z_1 = \max(1, i - p + 1)$ and $z_2 = \begin{cases} i & \text{for } i + p - 1 \leq n \\ n - p + 1 & \text{for } i + p - 1 > n \end{cases}$.

Stability of Multibreathers in KG with LRI

Theorem (Rothos *et al* 2012)

The characteristic exponents of the multibreather provided by the persistence conditions (3.6) are given,

$$\sigma_{\pm i} = \pm \sqrt{-\varepsilon \frac{\partial w}{\partial J} \chi_{z_i}}, \quad i = 1 \dots n,$$

where χ_{z_i} are the eigenvalues of \mathbf{Z} with

$$\mathbf{Z} = \frac{\partial^2 \langle H_1 \rangle}{\partial \phi_i \partial \phi_j} \cdot \begin{pmatrix} 2 & -1 & 0 & & \\ -1 & 2 & -1 & 0 & \\ & \ddots & \ddots & \ddots & \\ & & 0 & -1 & 2 & -1 \\ & & & 0 & -1 & 2 \end{pmatrix}, \quad i, j = 1 \dots n. \quad (3.7)$$

For linear stability all the characteristic exponents to be purely imaginary. So, if $P = \varepsilon \frac{\partial w}{\partial J} < 0$ we need all the eigenvalues of \mathbf{Z} to be negative, while if $P = \varepsilon \frac{\partial w}{\partial J} > 0$ we need all the eigenvalues of \mathbf{Z} to be positive.

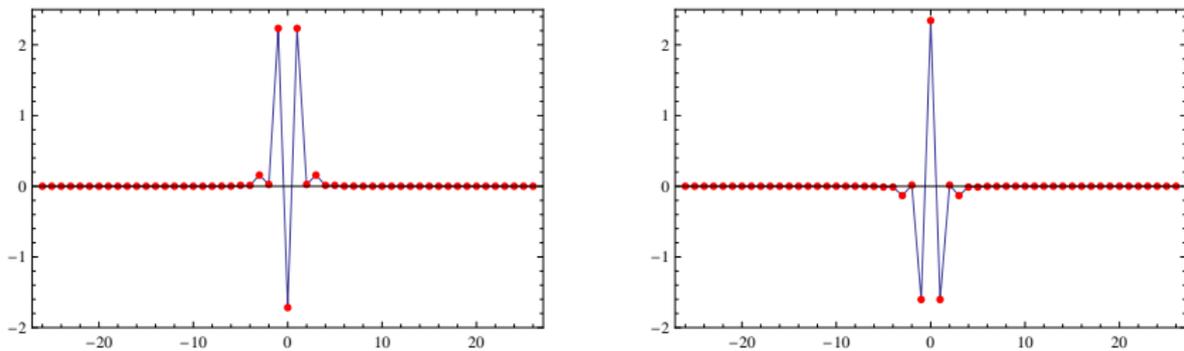
3-site breathers with $r = 2$ 

Figure: [Color online] Two snapshots of a 3-site ($n = 2$), anti-phase ($\phi_1 = \phi_2 = \pi$) multibreather in a range $r = 2$ Klein-Gordon chain with $\varepsilon_1 = \varepsilon_2 = 0.02$ and frequency $\omega = 2\pi/7$.

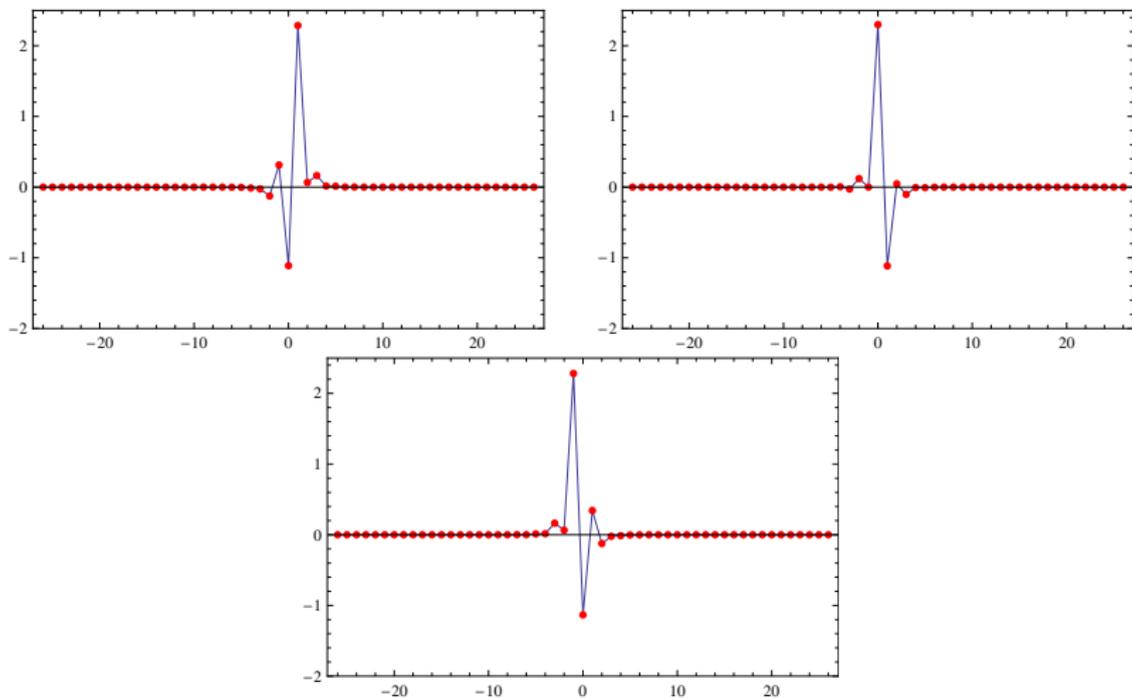


Figure: [Color online] Three snapshots of a 3-site ($n = 2$), phase-shift ($\phi_1 = \phi_2 \neq 0, \pi$) multibreather in a range $r = 2$ Klein-Gordon chain with $\varepsilon_1 = \varepsilon_2 = 0.02$ and frequency $w = 2\pi/7$.

① Periodic solutions in advanced-retarded differential equations

- Periodic Boundary Value Problem for functional differential equations.
- Librational and Periodic travelling waves;
- Multiplicity results.

② Travelling Waves in 2D Lattices: Mathematical Formulation;

③ Applications in travelling waves in nonlinear lattices

④ Travelling Waves in 1D Lattices: Mathematical Formulation;

- Moving Kinks for 1D lattice sine-Gordon
- Numerical Simulations

Travelling Waves in 1D Lattice sine-Gordon

Frenkel Kontorova (FK) lattices have been studied as models for atomic chains, dislocations, charge density waves, magnetic and ferromagnetic domain walls in condensed matter physics and for parallel coupled one-dimensional Josephson junction arrays.

The potentials involved are chosen such that the continuum model supports both stationary and moving defects (kinks or anti-kinks) with topological charge $Q = 1$. That is, the kinks connect 0 to 2π (or vice versa) in the usual dimensionless form of potential adopted in the literature – the so-called sine-Gordon lattice. The discrete sine-Gordon

$$\ddot{u}_n(t) = u_{n+1}(t) - 2u_n(t) + u_{n-1}(t) - \Gamma^2 \sin u_n(t)$$

with solutions

- **Discrete kinks** (stationary solutions)
- **Moving discrete kinks** $u_n(t) = U(n - vt)$
- **Discrete Breathers** a highly spatially localized, time-periodic, stable (or at least very long-lived) excitation in a spatially extended.

Methodology

- The travelling wave equation of the corresponding dSG is formulated as a mixed-type differential equation.
- Applying dynamical system methods (center manifold, normal form) we focus on a 4D dynamical system,
- persistence of periodic solutions for the 4D system implies the existence of travelling waves with non-small amplitude oscillations on infinite nonlinear lattice,
- Analytical results are compared with numerical simulations for a concrete perturbed discrete nonlinear sine-Gordon equation, (*Rothos & Feckan 2005, Aigner, Champneys & Rothos, 2003*).

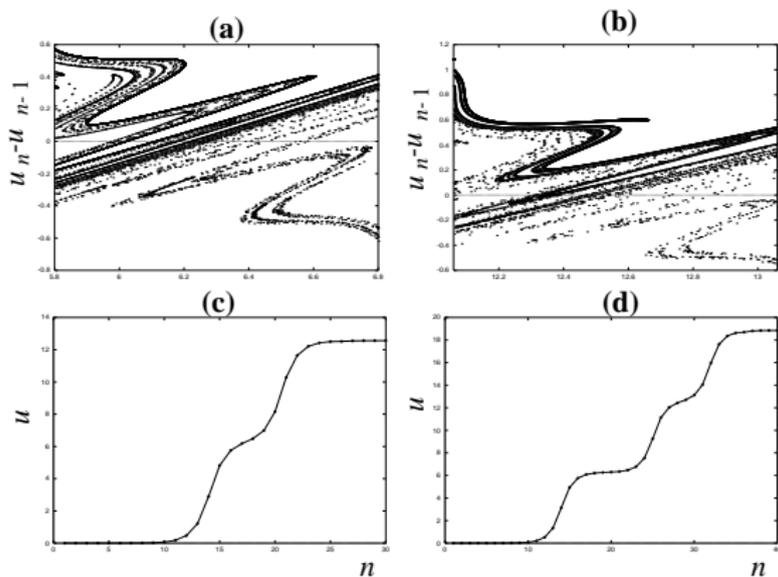


Figure: Construction of stationary kinks

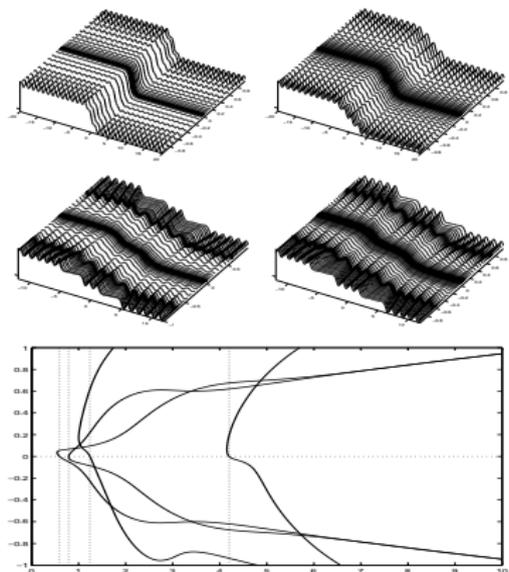


Figure: Travelling Kinks with tails

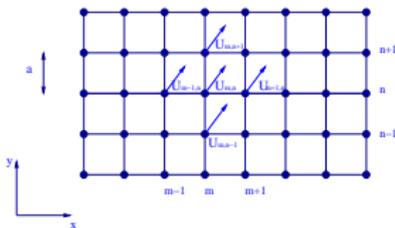
2D nonlinear lattices

An isotropic two dimensional planar model where rigid molecules rotate in the plane of a square lattice of spacing a .

At site (n, m) the angle of rotation is $u_{n,m}$ each molecule interacts linearly with its first nearest neighbors and with a nonlinear periodic substrate potential.

The equation of motion of the rotator at site (n, m) is

$$\ddot{u}_{n,m} = G[u_{n+1,m} + u_{n-1,m} + u_{n,m+1} + u_{n,m-1} - 4u_{n,m}] + \omega_0^2 \sin u_{n,m}$$



where G the linear coupling coefficient and ω_0^2 square of the frequency of small oscillations in the bottom of the potential wells.

Due to the symmetry imposed by the lattice \mathbb{Z}^2 , the existence and speed of a wave generally will depend on the direction $e^{i\theta}$ of motion.

Let $\theta \in \mathbb{R}$ be given, consider solution of lattice

$$u_{n,m}(t) = U(ncos\theta + m\sin\theta - \nu t)$$

for some $\nu \in \mathbb{R}$ and $U : \mathbb{R} \rightarrow \mathbb{R}$.

Mixed-Type functional differential Equation $\nu \neq 0$:

$$\begin{aligned} \nu^2 U''(z) &= U(z + \cos\theta) + U(z - \cos\theta) + U(z + \sin\theta) + U(z - \sin\theta) \\ &\quad - 4U(z) - f(U(z)) \end{aligned}$$

with $z = n\cos\theta + m\sin\theta - \nu t$ and $U(-\infty) = 0$, $U(+\infty) = 2\pi$

Theorem (Rothos & Feckan '07)

For any $\omega > 16$ and $1.17196 < T < 1.7579$, $2d$ discrete sine-Gordon equation

$$u_{n,m} - u_{n+1,m} - u_{n-1,m} - u_{n,m+1} - u_{n,m-1} + 4u_{n,m} + \omega \sin u_{n,m} = 0$$

possesses 4 nontrivial/nonconstant travelling wave solutions of the form

$$u_{n,m}(t) = \pi + U\left(\frac{1}{\sqrt{2}}\left(n + m\right) - \frac{1}{2}t\right)$$

or $U(z)$ satisfying periodical conditions

$$U(z + T) = U(z) + 2\pi, U(-z) = -U(z), T > 0, \text{ or}$$

$$U(z + T) = -U(z) + 2\pi, \text{ or } U(z + T) = -U(z), \text{ or, } U(z + T) = U(z), U(-z) = -U(z)$$

Theorem (Rothos & Feckan '07)

① Let $\nu > 1$ and $f'(0) > 0$. Moreover, suppose

$$\text{e1) } \nu^2 \neq g_\theta\left(\frac{\pi}{T}k\right) + \frac{T^2}{4\pi^2 k^2} f'(0) \quad \forall k \in \mathbb{N},$$

$$\text{e2) } \#\left\{k \in \mathbb{N} \mid \nu^2 < g_\theta\left(\frac{\pi}{T}k\right) + \frac{T^2}{4\pi^2 k^2} f'(0)\right\} \geq \left\lfloor \frac{T\sqrt{L}}{2\pi\sqrt{\nu^2-1}} \right\rfloor \geq 2, \text{ where}$$

$[\cdot]$ is the integer part function.

Then the advance-delay equation has at least 2 nonzero odd T -periodic solutions.

② Let $\nu_1 < \nu < 1$. Then the advance-delay equation for $\theta = \pi/4$ has infinitely many odd π/r_ν -periodic solutions $\{U_n(z)\}_{n \in \mathbb{N}}$ with

$$|U_n(z) - c_n \sin 2r_\nu z| \leq \tilde{K}|\epsilon|$$

for $c_n \rightarrow \infty$ as $n \rightarrow \infty$ and a constant $\tilde{K} > 0$.

Conclusions

- ▷ Overview of our recent theoretical and numerical activity in the theme of solitary nonlinear waves that arise in lattice system.
- ▷ The existence of localized traveling waves (sometimes called “moving discrete breathers” or “discrete solitons”) in Klein-Gordon Lattices and discrete sine-Gordon
- ▷ We study the existence and bifurcation of discrete solitons in lattices with local and nonlocal interactions (Long range interactions).
- ▷ LS reduction method, perturbation method, dynamical systems method, topological and variational methods. Pseudospectral method, Numerical Bifurcation results.
- ▷ Application in nonlinear metamaterial lattices, DNA, liquid crystals etc

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PART II: NONLINEAR PDEs

Stability of solutions

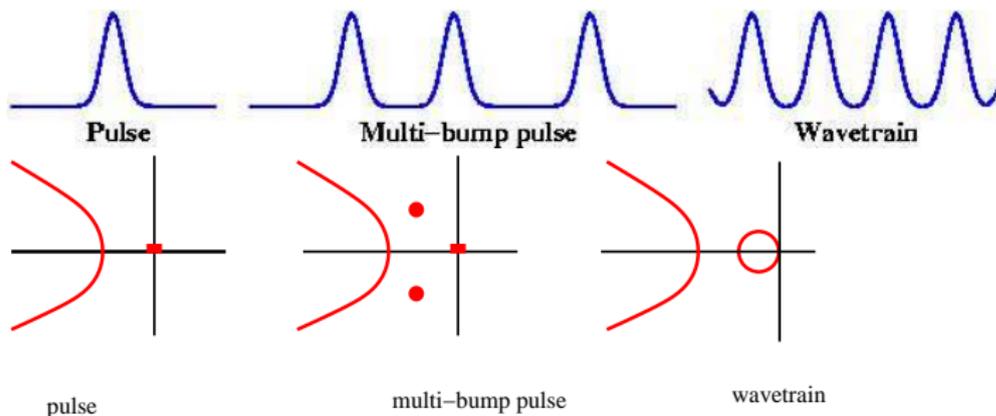
Consider PDE of the form

$$U_t = \mathcal{A}(\partial_x)U + \mathcal{N}(U), \quad x \in \mathbb{R}, \quad U \in \mathcal{X}$$

$\mathcal{A}(z)$ is a vector-valued polynomial in z , \mathcal{X} Banach space consisting of functions $U(x)$, $x \in \mathbb{R}$, $\mathcal{A}(\partial_x)$ closed dense, \mathcal{N} nonlinear operator. Travelling waves: $U(x, t) = Q(x - ct)$, $\xi = x - ct$

- In (ξ, t) the PDE reads $U_t = \mathcal{A}(\partial_x)U + c\partial_\xi U + \mathcal{N}(U)$, $\xi \in \mathbb{R}$, $U \in \mathcal{X}$;
- Travelling wave is a stationary solution $Q(\xi)$: $\mathcal{A}(\partial_x)U + c\partial_\xi U + \mathcal{N}(U) = 0$;
- Linearization about steady state $Q(\xi)$ is $U_t = \mathcal{A}(\partial_x)U + c\partial_\xi U + \partial_U \mathcal{N}(Q)U := \mathcal{L}U$. The stability of pulses is obtained by the spectrum of operator \mathcal{L} .

Type of Solutions



Pulse $Q(\xi)$.

Multi-bump pulses: finite number of well-separated copies of the primary pulses.

Periodic Wave Trains with spatial period L $Q(\xi + L) = Q(\xi)$.

Fronts (kinks, anti-kinks) $\lim_{|\xi| \rightarrow \infty} Q(\xi) = Q_{\pm}$.



- The study of the dynamics associated with the propagation of information (*nonlinear optics, phase transitions in materials* etc)
- Only waves that are stable can be reasonably expected to be physically realizable.
- The presence of any instability and understanding its source can be crucial if the goal is to control the wave to a stable configuration.
- The key information for stability is contained in the linearization of the PDE about the wave. In many cases, **location of the spectrum suffices to determine the stability**, i.e., spectrum in the left half plane corresponds to stable directions and that in the right half plane corresponds to unstable directions.
- One tool in particular has come to stand out as central in stability investigations of nonlinear waves. The *Evans function* is an analytic function whose zeroes give the eigenvalues of the linearized operator, with the order of the zero and the multiplicity of the eigenvalue matching.

Evans Function, set-up 1

Consider the scalar reaction-diffusion equation

$$u_t = u_{xx} - u + 2u^3, \quad (x, t) \in \mathbb{R} \times \mathbb{R}^+$$

a pulse solution is given by

$$u(x) = U(x), \quad \text{where } U(x) = \operatorname{sech}(x)$$

Linearizing the PDE yields the following eigenvalue problem

$$p'' - (1 - 6U^2(x))p = \lambda p, \quad ' = \frac{d}{dx}$$

$\lambda = 0$ is an eigenvalue with eigenfunction $U'(x)$.

Evans Function, set-up 2

Upon setting $\mathbf{Y} = (p, q)^\top$, write the eigenvalue problem as

$$\mathbf{Y}' = (M(\lambda) + R(x))\mathbf{Y}$$

where

$$M(\lambda) = \begin{pmatrix} 0 & 1 \\ 1 + \lambda & 0 \end{pmatrix}, \quad R(x) = \begin{pmatrix} 0 & 0 \\ -6U^2(x) & 0 \end{pmatrix}$$

$\lim_{|x| \rightarrow \infty} |R(x)| = 0$. We will assume $\text{Re} \lambda > -1$. The eigenvalues and associated eigenfunctions of $M(\lambda)$ are given by

$$\mu^\pm(\lambda) = \pm \sqrt{\lambda + 1}, \quad \eta^\pm(\lambda) = (1, \mu^\pm(\lambda))^\top$$

The solutions $\mathbf{Y}^\pm(\lambda, x)$ which satisfy

$$\lim_{|x| \rightarrow \infty} \mathbf{Y}^\pm(\lambda, x) e^{-\mu^\mp(\lambda)x} = \eta^\mp(\lambda), \quad \text{note!} \quad \lim_{|x| \rightarrow \infty} |\mathbf{Y}^\pm(\lambda, x)| = 0$$

Evans Function, set-up 3

Using hypergeometric series, the solutions $\mathbf{Y}^\pm = (u^\pm, u_x^\pm)$ are found to be

$$u^\pm(x; \lambda) = e^{\mp\sqrt{1+\lambda}x} \left[1 + \frac{\lambda}{3} \pm \sqrt{1+\lambda} \tanh(x) - \operatorname{sech}^2(x) \right]$$

which decays to 0 as $x \rightarrow -\infty$ for $\operatorname{Re}\lambda > -1$ and decays to 0 as $x \rightarrow \infty$ for $\operatorname{Re}\lambda > -1$. The Evans Function $E(\lambda)$ is defined to be the Wronskian:

$$E(\lambda) = \det \begin{pmatrix} u^-(0; \lambda) & u^+(0; \lambda) \\ u_x^-(0; \lambda) & u_x^+(0; \lambda) \end{pmatrix} = -\frac{2}{9}\lambda(\lambda - 3)\sqrt{1+\lambda}$$

A complex number λ is a root of Evans function $E(\lambda)$ precisely when

$p'' - (1 - 6U^2(x))p = \lambda p$, $' = \frac{d}{dx}$ has a bounded nonzero solution for that value of λ ; indeed the solutions $u^-(x; \lambda)$ and $u^+(x; \lambda)$ are then linearly dependent and generate a bounded nonzero solution of $p'' - (1 - 6U^2(x))p = \lambda p$.

NLS: Introduction

The Nonlinear Schrödinger (NLS) equation

$$iu_t + u_{xx} + 2\sigma |u|^2 u = 0, \quad \text{where } \sigma = \pm 1 \quad (7.1)$$

governs the dynamics of the envelopes of wavepackets in the dispersive media, and arises in many different contexts (nonlinear optics, water waves, etc.)

Zakharov and Shabat published the IST for the NLS equation. Then they extended the technique (**ZS scheme**) to some other equations (1973-1974). At about the same time, Ablowitz, Kaup, Newell and Segur (**AKNS**) developed an equivalent scheme, which generalizes the method, described earlier for the KdV equation (AKNS, 1974).

Lie symmetries of the NLS equation

In the following we use the following **one-parameter groups of symmetries**, admitted by the NLS equation (7.1):

- shift in t

$$t \rightarrow t + t_0, \quad x \rightarrow x, \quad u \rightarrow u$$

- shift in x

$$t \rightarrow t, \quad x \rightarrow x + x_0, \quad u \rightarrow u$$

- Galilean transformation

$$t \rightarrow t, \quad x \rightarrow x - ct, \quad u \rightarrow u \exp \left[i \frac{c}{2} \left(x - \frac{c}{2} t \right) \right]$$

- scaling

$$t \rightarrow a^2 t, \quad x \rightarrow ax, \quad u \rightarrow \frac{u}{a}$$

For example, if $u(x; t)$ is a solution of (7.1), then due to the Galilean invariance so are

$$u(x - ct, t) \exp \left[i \frac{c}{2} \left(x - \frac{c}{2} t \right) \right],$$

and so on.

Solitary waves of the NLS equation

We look for a solution of the NLS equation (7.1) of the form

$$u(x, t) = a(x)e^{i\phi(t)}, \quad (7.2)$$

Substituting (7.2) into (7.1), we derive

$$-a\phi_t + a_{xx} + 2\sigma a^3 = 0. \quad (7.3)$$

Separating variables in (7.3) gives $\phi_t = \frac{a_{xx}}{a} + 2\sigma a^2 = \text{const}$. Then, integrating, we obtain (up to the scaling and the shift in t):

$$\phi = st$$

(we can assume that $s = \pm 1$), and

$$a_{xx} = -2\sigma a^3 + sa. \quad (7.4)$$

Multiplying (7.4) by a_x and integrating, we arrive at

$$(a_x)^2 = -\sigma a^4 + sa^2 + C.$$

It turns out that the form of solitary waves depends on the sign of (the sign of the nonlinear term in the NLS equation).

Focusing NLS: bright solitons

Case I ($\sigma = 1$, focusing NLS in the context of optics-"anomalous dispersion")

$$iu_t + u_{xx} + 2|u|^2 u = 0,$$

In this case, $(a_x)^2 = -a^4 + sa^2 + C$. If $a, a_x \rightarrow 0$ as $x \rightarrow \pm\infty$, then $C = 0$, and

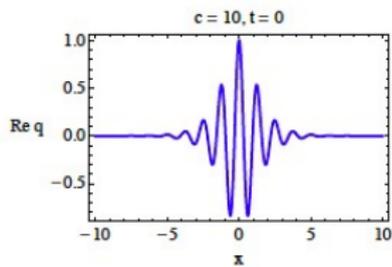
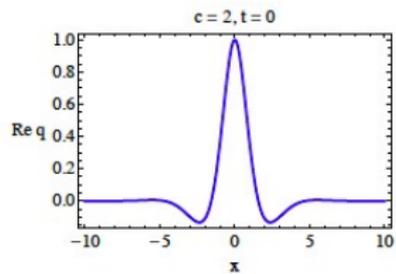
$$\int \frac{da}{a\sqrt{s-a^2}} = \int dx.$$

For $s = 1$ we obtain the simplest form of the so-called **bright soliton** $a = \operatorname{sech}x$, $\phi = t$, yielding $u = e^{it}\operatorname{sech}x$. (Consider the second case, $s = -1$.) Using the scaling and Galilean symmetries, we immediately obtain **the two-parameter family of bright solitons**:

$$u = A\operatorname{sech}A(x - ct)\exp\left[i\left(\frac{c}{2}x + A\left(A^2 - \frac{c^2}{4}\right)t\right)\right].$$

Note that A and c are independent parameters. (Two more parameters can be added using shifts in x and t , but these parameters are insignificant.)

Bright Soliton of NLS



Defocusing NLS: dark solitons

Case II ($\sigma = -1$, defocusing NLS, in the context of optics-"normal dispersion")

$$iu_t + u_{xx} - 2|u|^2 u = 0,$$

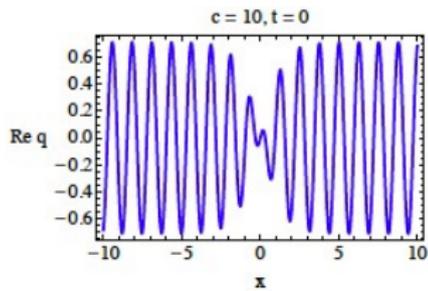
In this case, $(a_x)^2 = a^4 + sa^2 + C$, and solitary waves are rather different from those in Case I. For $s = -1$, choosing $C = 1/4$ (when the polynomial has repeated roots) we obtain the simplest form of the so-called **dark soliton** $a = \frac{1}{\sqrt{2}} \tanh \frac{x}{\sqrt{2}}$, $\phi = -t$, yielding

$$u = e^{-it} \frac{1}{\sqrt{2}} \tanh \frac{x}{\sqrt{2}}$$

(Consider the second case, $s = 1$.) Again, using symmetries, we obtain **the two-parameter family of dark solitons**:

$$u = \frac{A}{\sqrt{2}} \tanh \frac{A(x-ct)}{\sqrt{2}} \exp \left[i \left(\frac{c}{2} x - \left(A^2 + \frac{c^2}{4} \right) t \right) \right].$$

Dark Soliton of NLS



Focusing NLS: Breathers

The focusing NLS equation models the evolution of one-dimensional packets of surface gravity waves on sufficiently deep water (Zakharov 1968). Recently, there has been renewed interest in the so-called "breather" solutions of this equation, which have been suggested as models for so-called "freak" waves (also, "rogue" waves). Loosely speaking, a "freak" wave is a single wave or a very short- and short-lived group with a significantly larger steepness than the surrounding waves.

NLS breather

The first breather type solution for the focusing NLS equation was found by Ma (1979). Ma solved the IVP for this equation, where the initial condition was a perturbed plane wave with boundary conditions $|q(x, t)| \rightarrow |q_0|$ as $x \rightarrow \pm\infty$. Ma has found that the asymptotic state for his problem consisted of a series of breathers (Ma-breathers), given below, and small dispersive radiation:

$$u_M = \frac{\cos(\Omega t - 2ik) - \cosh(k)\cosh(px)}{\cos(\Omega t) - \cosh(\phi)\cosh(px)} e^{2it}$$

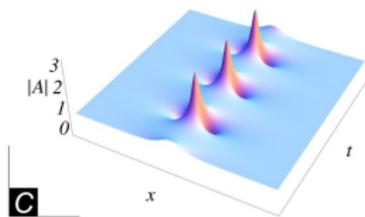
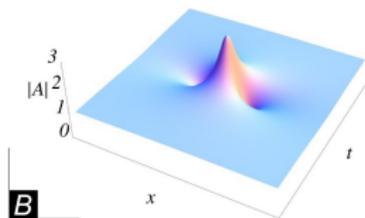
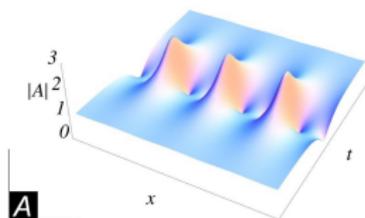
Here, k is the real valued parameter, $\Omega = 2\sinh(2k)$ and $p = 2\sinh(k)$.

Taking the limit $k \rightarrow 0$ (i.e. when the breathing period tends to zero), Peregrine (1983) has obtained

$$u_P = \lim_{k \rightarrow 0} q_M = \left[1 - \frac{4(1 + 4it)}{1 + 4x^2 + 16t^2} \right] e^{2it}$$

Other breather-type solutions have been found by Akhmediev et al. (1987) and Ablowitz and Herbst (1990).

(A) The Akhmediev breather, (B) the Peregrine breather and (C) the Kuznetsov-Ma breather



Discretize spatial variable:

$$x \rightarrow nh, \quad \mathbf{u} = \{u_n(t)\}_{n \in \mathbb{Z}}.$$

Discrete second order difference operator:

$$\partial_x^2 u(x, t) \rightarrow \frac{1}{h^2} \left(\delta^2 \mathbf{u}(t) \right)_n \equiv \frac{1}{h^2} [u_{n+1}(t) + u_{n-1}(t) - 2u_n(t)]$$

NLS becomes the discrete nonlinear Schrödinger equation:

$$i \partial_t u_n(t) = -\frac{1}{h^2} \left(\delta^2 \mathbf{u}(t) \right)_n - |u_n(t)|^2 u_n(t), \quad n \in \mathbb{Z}$$

(Infinite coupled system discrete nonlinear oscillators)

Application of DNLS

The existence of localized waves in DNLS lattices has shown itself to be a delicate question of fundamental interest. This interest is largely due to the experimental realization of solitons in discrete media, such as waveguide arrays, optically induced photorefractive crystals, Bose-Einstein condensates coupled to an optical wave trap, DNA

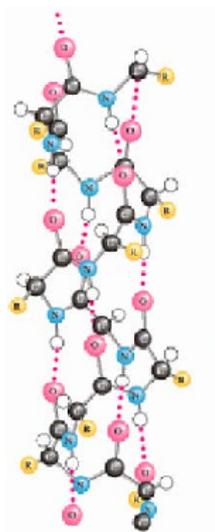


Figure: A. S. Davydov, *J. Theor. Biol.* 38, 559 (1973); *Biology and Quantum Mechanics*, Pergamon, Oxford, 1982.

The prototypical equation that emerges to explain the experimental observations is the DNLS equation the form

$$i\dot{u}_n = \frac{1}{\hbar^2}(u_{n+1} - 2u_n + u_{n-1}) + f(u_{n+1}, u_n, u_{n-1}), \quad u_n : \mathbb{R}_+ \rightarrow \mathbb{C}, n \in \mathbb{Z} \quad (8.1)$$

The nonlinear term F can take a number of different forms:

- ▷ DNLS $f_{\text{DNLS}} = |u_n|^2 u_n$
- ▷ Ablowitz-Ladik $f_{\text{AL}} = |u_n|^2 (u_{n+1} + u_{n-1})$
- ▷ Salerno $f_{\text{S}} = 2(1 - \alpha)f_{\text{DNLS}} + \alpha f_{\text{AL}}$
- ▷ Cubic-quintic DNLS $f_{\text{cq}} = (|u_n|^2 + \alpha|u_n|^4)u_n$
- ▷ Saturable DNLS $f_{\text{sat}} = \frac{u_n}{1+|u_n|^2}$

- **Standing wave solutions (Discrete Breathers):**

$$u_n(t) = \phi_n e^{-i\omega t}, \quad \phi_n \in \mathbb{R}, \quad \lim_{|n| \rightarrow \infty} \phi_n = 0$$

exist in the DNLS equations outside of the spectral band.

- **Travelling Breathers** have nonlinear resonances with unbounded spectral bands:

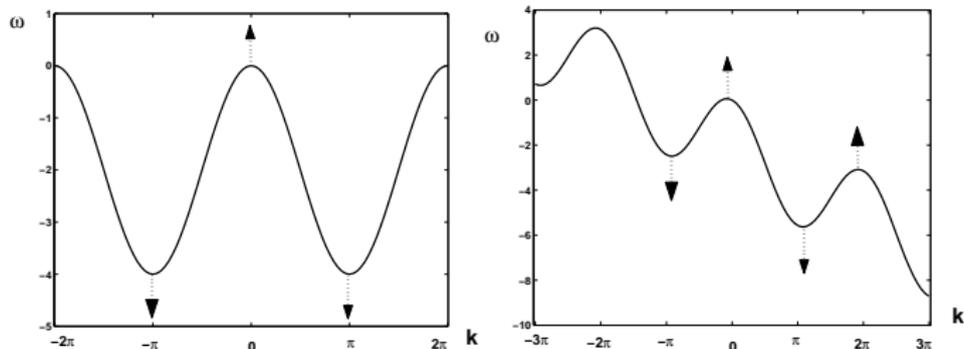
$$u_n(t) = \phi(z) e^{-i\beta n - i\omega t}, \quad z = n - vt, \quad \omega, v \in \mathbb{R},$$

$\phi : \mathbb{R} \rightarrow \mathbb{C}$, $\lim_{|z| \rightarrow \infty} \phi(z) = 0$ **exponential decay** of the travelling wave solution $\phi(z)$:
 $\lim_{|z| \rightarrow \infty} e^{\kappa|z|} \phi(z) = \phi_\infty$, where $\kappa \in \mathbb{R}$ and $\phi_\infty \in \mathbb{C}$. The travelling breather solutions exist only if $(\omega + 2)^2 + v^2 \geq 4$.

Linear properties of the DNLS equations

The ansatz for travelling wave (TW) solutions reduces the DNLS equation to:

$$-iv\phi'(z) = \phi(z+1)e^{-i\beta} + \phi(z-1)e^{i\beta} - (2+\omega)\phi(z) + \epsilon^2 f(\phi(z), \phi(z+1)e^{-i\beta}, \phi(z-1)e^{i\beta}), \quad (8.2)$$



Dispersion curves $\omega = \omega(k) = -vk + 2(\cos(\beta - k) - 1)$ for (a) $v = 0$ and (b) $v = 0.5$, when $\beta = 0$. The vertical arrows show directions of possible bifurcations of travelling wave solutions.

In parameter space (ω, ν) , this could imply bifurcation occurs at the boundary between the linear wave spectrum $\omega = \omega(k) = -\nu k + 2(\cos(\beta - k) - 1)$ and the nonlinear wave spectrum

$$-\omega/2 = 1 - \cos \beta \cosh \kappa, \quad (\nu/2)\kappa = \sin \beta \sinh \kappa, \quad (8.3)$$

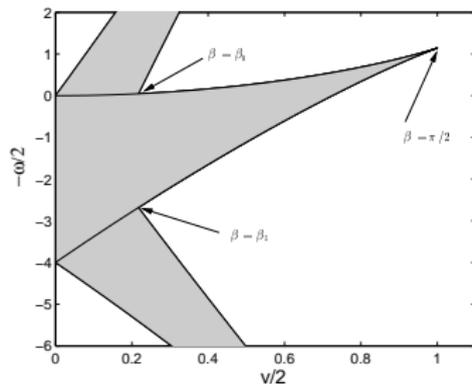


Figure: Bifurcation curve $\kappa = 0$ on the (ω, ν) -plane for $\varepsilon = 1$. Localized solutions of the differential advance-delay equation may bifurcate from the boundary to the white region (with $\kappa \in \mathbb{R}_+$). For $\beta < \beta_0$ and $\beta > \beta_1$, more than one radiation mode exists.

Bifurcation of DNLS traveling wave solutions

- The normal form for the bifurcations of TB at the corner point is equivalent to the third-order differential equation for $\Phi = \Phi(z)$:

$$\frac{i}{3\epsilon^2} \Phi''' - iV\Phi' + \Omega\Phi = h(\Phi, \Phi', \Phi'')$$

which corresponds to the continuous NLS eqn with **3rd order** derivative term:

$$iU_t + \frac{i}{3\epsilon^2} U_{xxx} = h(U, U_x, U_{xx})$$

- Existence of single-humped localized solutions in the third order ODE is related to existence of embedded solitons in the third-order derivative NLS equation.

- Ablowitz-Ladik lattice

There is a **continuous two-parameter family of single-humped traveling wave solutions.**

- DNLS lattice on-site interactions There are **no single-humped solutions** BUT there exists an infinite discrete set of one-parameter families of double-humped traveling wave solutions.

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Numerical continuation using pseudospectral methods

Localized solutions to the advance-delay equation (8.2) can easily be sought numerically using a pseudo-spectral method originally proposed by Eilbeck *et al*; see also *Aigner Champneys Rothos '03* for similar results for discrete sine-Gordon lattices.

Taking as our starting point the traveling wave form of the DNLS advance-delay (8.2) with the nonlinearity F , a pseudo-spectral substitution is used to transform the system of algebraic equations. To do this we use a finite Fourier series expansion to approximate the discrete breather by functions $\psi(z)$ on a long finite interval $[-L/2, L/2]$. A particular choice of expansion terms can be made that exploits the underlying symmetry of the localized solutions we seek, namely by choosing even real functions and odd imaginary functions

$$\psi(z) = \sum_{j=1}^N a_j \cos\left(\frac{\pi j z}{L}\right) + i b_j \sin\left(\frac{\pi j z}{L}\right), \quad (8.4)$$

where $a_j, b_j \in \mathbb{R}$ are the coefficient of the Fourier series.

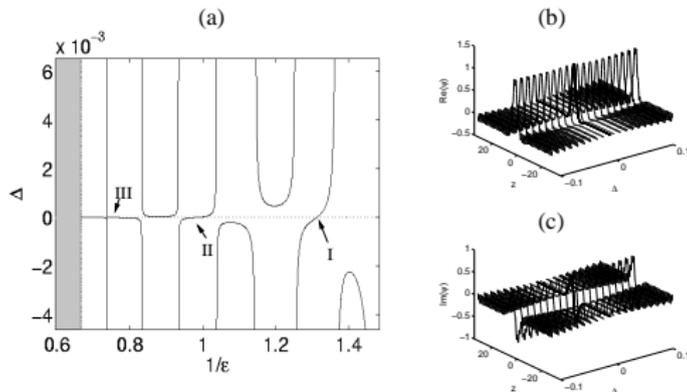
Substituting the expansion (8.4) into advance-delay (8.2) at the series of *collocation* points $z_i = \frac{Li}{2(N+1)}$, $i = 1, \dots, 2N$ gives a system of $2N$ nonlinear algebraic equations for the unknown coefficients a_j, b_j , which can be solved using globally convergent root finding methods. Once a solution is found, this can be continued in a single parameter using a numerical path-followed method built around Newton's method, for example the code AUTO.

To find waves with zero tails we need to add an extra condition and seek zeros of this function. A good choice of such a tail function is

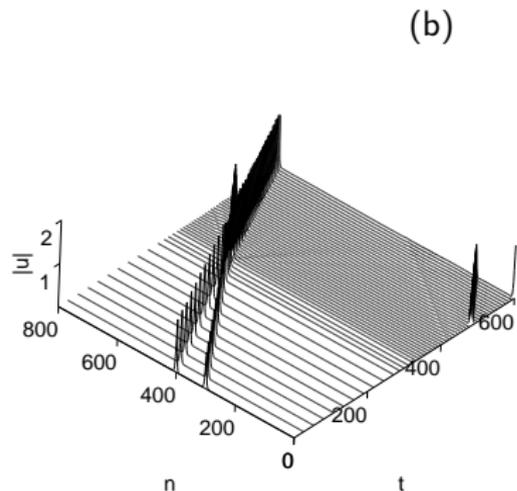
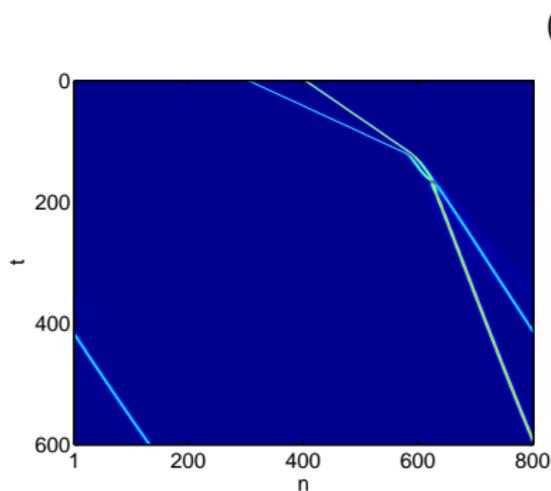
$$\Delta = \text{Im}(\psi(\frac{L}{2})) \quad (8.5)$$

which measures the amplitude of the imaginary part of the tail of a solution of period L .

$$\text{saturable DNLS } F_{\text{sat}} = \frac{U_n}{1+|U_n|^2}$$

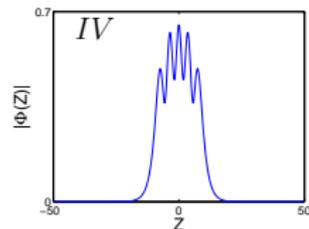
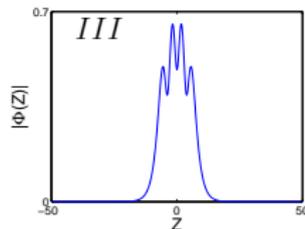
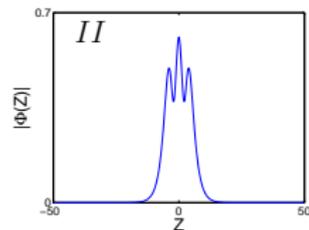
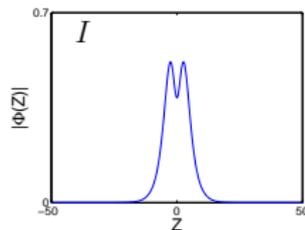
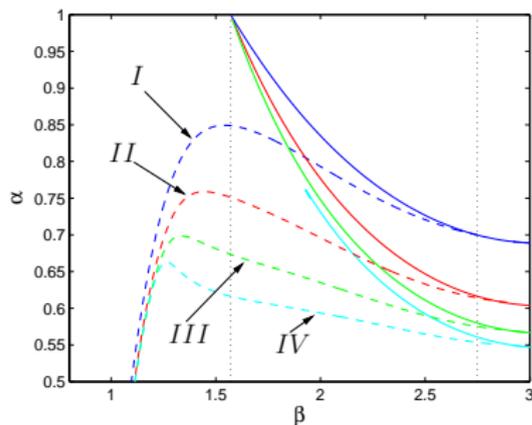


(a) Continuation of weakly localized solutions (with non-zero oscillatory tails) to (8.2) for the saturable nonlinearity F_{sat} solitons for various values of $\epsilon = 1/\sqrt{\epsilon}$ against $\Lambda = -\omega$ for $\nu = 0.7$, $\omega = -0.5$, and $L = 60$ showing three zeros of Δ at $\epsilon \approx 0.76, 1.02, 1.36$. The shaded region represents the spectral band where any embedded solitons would be of co-dimension 2. (b, c) Continuation of branch with second zero of Δ at $\epsilon \approx 1.02$. for $c = 0.7, \Lambda = 0.5, L = 60$. (b) $\text{Re}(\psi)$, (c) $\text{Im}(\psi)$



Melvin, Rothos, Champneys '09, Interaction of two soliton solutions with $\varepsilon = 1$ and $\Lambda = 0.5$. The branch I soliton is initially centered on site $n = 300$ with $v = 1.00926$ and the branch II soliton is centered on site $n = 400$ with $v = 0.67725$.

$$\text{Salerno DNLS } f_S = 2(1 - \alpha)f_{\text{DNLS}} + \alpha f_{\text{AL}}$$



Melvin, Rothos, Champneys '09. Existence of traveling wave solutions in the Salerno model for $\alpha = 0.65$ computed via calculation of the radiation tail amplitude Δ ($\kappa = 0.5$). For $\beta < \pi/2$ the solutions are multi-humped.

Conclusions

- Type of Solutions for nonlinear PDEs
- Evans functions
- We briefly reviewed the solitonic solutions of NLS.
- We studied the existence and bifurcation of quasiperiodic travelling wave solutions of DNLS. We employed dynamical systems method (center manifold reduction, normal form) to analyze the existence of traveling breathers of DNLS.
- We examined the combined effects of cubic and quintic terms of the long range type in the dynamics of a double well potential (optical thermal media) *Nonlocal NLS*

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