Families of discrete breathers on 2D lattices

Andrew Hofstrand

2025 Annual Review of Theoretical NLO Basic Research

March 5, 2025

This work was supported by the Air Force Office of Scientific Research with Grant No. FA9550-23-1-0144.

Results

In the pursuit to precisely control energy localization via nonlinearity and dispersion management in two-dimensional spatially discrete and periodic systems, we derive the following:

1. Existence and numerical construction of families exponentially-localized, time-periodic solutions–*discrete breathers* (DBs)–on 2D nonlinear lattices of current physical interest.
2. Exact expressions for gap solitons to leading-order in a long-wave and weakly nonlinear asymptotic description of a honeycomb lattice near a so-called semi-Dirac point in the linear dispersion relation.
3. Construction of dynamically stable and strongly nonlinear gap DBs and exact expressions for *compactly-supported* DBs on a lattice containing a strictly flat phonon band.
4. A powerful connection between opposing asymptotic descriptions of DBs–near the *molecular* and continuum limits–and a route to control localization in gapped lattices.

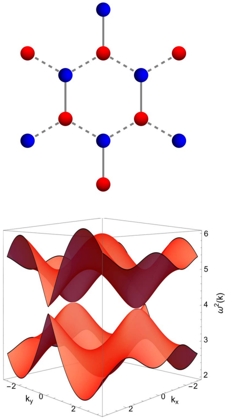
Results

- H. Li, A. Hofstrand, and M. I. Weinstein, *Stability of Traveling Waves in a Nonlinear Hyperbolic System Approximating a Dimer Array of Oscillators*. https://arxiv.org/abs/2402.07567 Accepted to Journal of Nonlinear Science (February 2025).
- A. Hofstrand, *Near Integrable Dynamics of the Fermi-Pasta-Ulam-Tsingou Problem*. Physical Review E, Vol. 109 034204 (March 2024).
- A. Hofstrand, H. Li, and M. I. Weinstein, *Discrete Breathers of Nonlinear Dimer Lattices: Bridging the Anti-Continuous and Continuous Limits*. https://arxiv.org/abs/2210.04387 Journal of Nonlinear Science 33, Article Number: 59 (May 2023).
- A. Hofstrand, *Families of Discrete Breathers on a Nonlinear Kagome Lattice*. https://arxiv.org/abs/2412.06932, under review (December 2024).

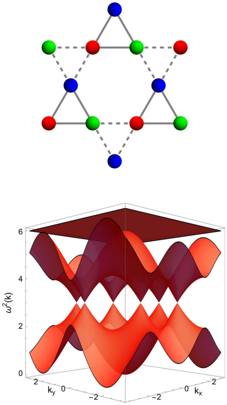
Lattice Geometries and Dispersion Relations

- We consider nonlinear Hamiltonian mechanical lattices with the following 2D geometries:

(i) Honeycomb Lattice



(ii) Kagome Lattice



Universal Behavior of Lattices Near the Continuum Limit

1. Nonlinear Schrödinger (NLS) equation:

$$i\partial_t \Psi + \Delta \Psi + |\Psi|^{2\alpha}\Psi = 0$$

Stationary states:

$$\Psi(t,x) = \psi(x,\omega)e^{-i\omega t}, \quad \omega < 0, \quad \psi(\cdot,\omega) \in H^1(\mathbb{R}^2).$$

The NLS equation is invariant under dilation:

$$\Psi(t,x) \mapsto \lambda^{1/\alpha}\Psi(\lambda^2 t, \lambda x).$$

This implies by uniqueness that

$$\psi(x,\omega) = |\omega|^{1/2\alpha}\psi(|\omega|^{1/2}x, -1)$$

and so

$$\|\psi(\cdot,\omega)\|^2_{L^2(\mathbb{R}^2)} = |\omega|^{(1/\alpha)-1}\|\psi(\cdot,-1)\|^2_{L^2(\mathbb{R}^2)}.$$

Universal Behavior of Lattices Near the Continuum Limit

2. Nonlinear Dirac (ND) equation:

$$i\partial_t \Psi + (i\sigma \cdot \nabla + m\sigma_3)\,\Psi + |\Psi|^{2\alpha}\Psi = 0,$$

where $\sigma = (\sigma_1, \sigma_2)$ and σ_3 are Pauli matrices.

Stationary states:

$$\Psi(t,x) = \psi(x,\omega)e^{-i\omega t}, \quad -m < \omega < m, \quad \psi(\cdot,\omega) \in H^{1/2}(\mathbb{R}^2, \mathbb{C}^2).$$

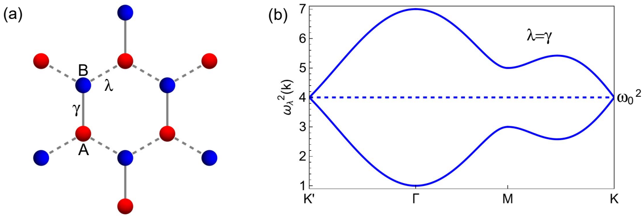
The massless ND equation has the scaling invariance:

$$\Psi(t,x) \mapsto \lambda^{1/2\alpha}\Psi(\lambda t, \lambda x),$$

and so

$$\|\psi(\cdot,\omega)\|^2_{L^2(\mathbb{R}^2,\mathbb{C}^2)} = |\omega|^{(1/2\alpha)-1}\|\psi(\cdot,0)\|^2_{L^2(\mathbb{R}^2,\mathbb{C}^2)}.$$

Nonlinear Honeycomb Lattice With Dimer Couplings



- We consider a honeycomb lattice with an on-site (unit-cell) nonlinearity and dimerized linear couplings with equations of motion:

$$\boxed{\begin{aligned} \ddot{x}^A_{n,m} &= -V'(x^A_{n,m}) + \gamma x^B_{n,m} + \lambda\left[x^B_{n,m-1} + x^B_{n+1,m-1}\right] \\ \ddot{x}^B_{n,m} &= -V'(x^B_{n,m}) + \gamma x^A_{n,m} + \lambda\left[x^A_{n,m+1} + x^A_{n-1,m+1}\right] \end{aligned}}$$

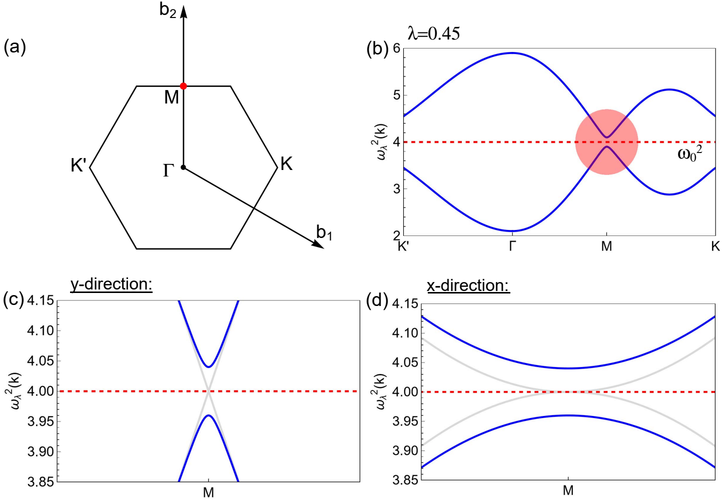
- The potential is given by

$$V(z) = \omega_0^2 z^2/2 + g|z|^{2\alpha} z^2/(2\alpha + 2)$$

where $\alpha \geq 1$ and $g = \pm 1$ for a *hardening* (*softening*) nonlinearity.

Nonlinear Honeycomb Lattice With Dimer Couplings

- One can show that as $\lambda \uparrow \gamma/2$, the phonon band-gap closes about ω_0 at quasi-momentum M. We show the dispersion relation below, setting parameters $\gamma = 1$ and $\omega_0 = 2$:



The Continuum Regime

- Near the continuum limit, centered at the quasi-momenta M, we formally derive the asymptotic solutions to leading-order in $\epsilon := \gamma - 2\lambda$, for $0 < \epsilon \ll 1$ ($\alpha = 1$):

$$\boxed{\begin{pmatrix} x^A_{n,m}(t) \\ x^B_{n.m}(t) \end{pmatrix} \sim 2\epsilon^{1/2}\,(-1)^m \begin{pmatrix} U(\sqrt{\epsilon}n, \epsilon m; \nu) \\ V(\sqrt{\epsilon}n, \epsilon m; \nu) \end{pmatrix} \cos\left(\left[\omega_0 + \frac{\epsilon\nu}{2\omega_0}\right] t\right),}$$

  where the parameter $-1 < \nu < 1$ modulates the frequency inside the bandgap of width $2|\epsilon|$.

- After some scaling, the stationary states are determined by the PDE system:

$$\begin{cases} 2i\omega_0 \partial_T U + V + \partial_Z V - \partial_Y^2 V - g\left(|U|^2 + |V|^2\right) U = 0 \\ 2i\omega_0 \partial_T V + U - \partial_Z U - \partial_Y^2 U - g\left(|U|^2 + |V|^2\right) V = 0, \end{cases}$$

  where we have assumed the *Manakov-form of nonlinearity*. T, Z, and Y are long independent spatiotemporal variables.

- We refer to the PDEs above as the **semi-Dirac system**.

The Semi-Dirac System in Condensed Matter

- The linear semi-Dirac system was theorized in 2008 and implies a peculiar class of fermions that are massless in one direction and massive in the perpendicular direction.[1]

- The tight-binding model considered in [1], and its resulting disperion relation, is exactly the one we consider here in our toy model of coupled mechanical oscillators on a honeycomb lattice in the linear limit.

- These highly exotic quasiparticles - the semi-Dirac fermions - were experimentally observed in the topological metal ZrSiS this past December.[2]

[1] P. Dietl, F. Piechon, and G. Montambaux, "New magnetic field dependence of landau levels in a graphenelike structure," PRL (2008).

[2] Y. Shao, et. al. "Semi-Dirac fermions in a topological metal," PRX (2024).

Properties of the Semi-Dirac System

- Looking for solutions of the form $\Psi(Z, Y)e^{-i\nu T/2\omega_0}$, we define the linearized operator:

$$\mathcal{L} : \mathcal{D}(\mathcal{L}) := H^1_Z H^2_Y(\mathbb{R}^2, \mathbb{C}^2) \mapsto L^2(\mathbb{R}^2, \mathbb{C}^2),$$

$$\mathcal{L} := i\sigma_2 \partial_Z + \sigma_1(1 - \partial_Y^2).$$

- One can show that $\mathcal{L}$'s spectrum is given by

$$\sigma(\mathcal{L}) = \sigma_e(\mathcal{L}) = (-\infty, -1] \cup [1, \infty),$$

for instance by constructing a Weyl singular sequence of approximate eigenfunctions in $\mathcal{D}(\mathcal{L})$.

- Localized weak solutions to the nonlinear system may be obtained by looking for critical points of the nonlinear functional:

$$I_\nu := \int_{\mathbb{R}^2} \left(\frac{1}{2} \langle \mathcal{L}\Psi, \Psi \rangle + \frac{\nu}{2} |\Psi|^2 + \frac{g}{4} |\Psi|^4 \right) dx.$$

Gap Solitons in the Semi-Dirac System

- Consider the related system of PDEs:

$$\left(\sigma_1 + i\sigma_3\partial_Z + \sigma_0(\nu - \partial_Y^2)\right)\Psi = g|\Psi|^2\Psi \qquad (\star)$$

- Making the ansatz, $\Psi_\nu = \left[U_\nu(Z), U_\nu^*(Z)\right]^\top$, in the above system leads to the scalar equation

$$i\partial_Z U_\nu + \nu U_\nu + U_\nu^* - 2g|U_\nu|^2 U_\nu = 0.$$

- This equation has the explicit exponentially localized "line-soliton" solutions for $\nu \in (-1, 1)$:

$$U_\nu = \frac{\sqrt{(1-\nu^2)}\left[\sqrt{1-\nu}\cosh\left(\sqrt{1-\nu^2}Z\right) - i\sqrt{1+\nu}\sinh\left(\sqrt{1-\nu^2}Z\right)\right]}{\cosh\left(2\sqrt{1-\nu^2}Z\right) - \nu}$$

Gap Solitons in the Semi-Dirac System

- Now consider the general nonlinear system

$$i\partial_T \Psi = \mathcal{H}_{\mathsf{L}}\Psi + \mathcal{H}_{\mathsf{NL}}[\Psi].$$

- For constant unitary transformation, $\mathcal{U} \in \mathsf{SU}(2)$, if we have

$$\mathcal{U}\mathcal{H}_{\mathsf{NL}}[\Psi] = \mathcal{H}_{\mathsf{NL}}[\mathcal{U}\Psi],$$

  then if Ψ is a solution of the above system, $\tilde{\Psi} := \mathcal{U}\Psi$ is a solution to

$$i\partial_T \tilde{\Psi} = \mathcal{U}\mathcal{H}_{\mathsf{L}}\mathcal{U}^\dagger \tilde{\Psi} + \mathcal{H}_{\mathsf{NL}}[\tilde{\Psi}].$$

- Take Ψ_ν to be a solution to $(\star)$, then choosing

$$\mathcal{U}_* = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$$

  gives a line-soliton solution, $\tilde{\Psi}_\nu$, to the semi-Dirac system for every $-1 < \nu < 1$.

Gap Solitons in the Semi-Dirac System

Theorem

By explicit construction, the semi-Dirac system admits a family of smooth exponentially localized <u>*line solitons*</u> *for* $-1 < \nu < 1$*. Furthermore, for* $g = \pm 1$ *we have that:*

1. $\lim_{\nu \to -1} \tilde{\Psi}_{\pm\nu} = [0, 0]^\top$
2. $\tilde{\Psi}_0 = \dfrac{1-i}{\sqrt{2}} \operatorname{sech}(2Z) \left[e^{Z}, e^{-Z}\right]^\top$
3. $\lim_{\nu \to +1} \tilde{\Psi}_{\pm\nu} = \dfrac{1-i}{1+4Z^2} [1+2Z, 1-2Z]^\top e^{\mp iT/2\omega_0}$

Existence of DBs Near the Molecular Limit

- Mapping Between Function Spaces: Define the mapping $F(X^\lambda(t), \lambda) : \mathcal{H}^2_{T_b} \times \mathbb{R} \to \mathcal{H}^0_{T_b}$ by

$$F(X, \lambda) = \left\{ \begin{pmatrix} \ddot{x}^A_{n,m} + V'(x^A_{n,m}) - \gamma x^B_{n,m} \\ \ddot{x}^B_{n,m} + V'(x^B_{n,m}) - \gamma x^A_{n,m} \end{pmatrix} + \lambda \left[\mathbf{R} \begin{pmatrix} x^A \\ x^B \end{pmatrix} \right]_{n,m} \right\}_{n,m \in \mathbb{Z}}$$

- For $\lambda = 0$, say we have obtained a T_b- periodic solution, satisfying $F(X_*(t), 0) = 0$

$$X_*(t) = \left\{ \cdots, 0, 0, \begin{pmatrix} x^A_*(t) \\ x^B_*(t) \end{pmatrix}, 0, 0, \cdots \right\}.$$

- Our goal is to construct a mapping $\lambda \mapsto X^\lambda(t)$, defined for all real $\lambda \neq 0$ and sufficiently small in a Banach space of T_b- periodic in time, spatially decaying sequences, such that

$$F(X^\lambda, \lambda) = 0.$$

Existence of DBs Near the Molecular Limit

- Consider the following hypotheses:

  (a) Non-resonance:

  $$(n\omega_b)^2 \neq V''(0) \pm \gamma, \quad \text{for all } n \in \mathbb{Z}.$$

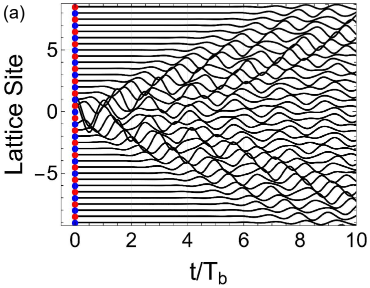
  (b) Non-degeneracy: The nullspace of the linearized operator

  $$L_* = \begin{pmatrix} \frac{d^2}{dt^2} + V''(x_*^A(t)) & 0 \\ 0 & \frac{d^2}{dt^2} + V''(x_*^B(t)) \end{pmatrix} - \gamma \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

  acting in the space $\mathcal{H}^2_{T_b}$ is empty.

- Assuming hypotheses (a) and (b) hold, there exists $\lambda_b > 0$ and C^1 curve $\lambda \in [0, \lambda_b) \mapsto X^\lambda \in \mathcal{H}^2_{T_b}$ such that $X^0 = X_*$ and $F(X^\lambda, \lambda) = 0$ for all $0 \leq \lambda < \lambda_b$.

Numerical Continuation away from the Molecular Limit



- Given $X_*(t) \in \mathcal{H}^2_{T_b}$, and assuming the conditions of non-resonance and non-degeneracy hold, we numerically construct discrete breathers for $\lambda \neq 0$ by iteratively solving for the Fourier coefficients of $X^\lambda(t)$ in $F(X^\lambda, \lambda) = 0$ using a Newton scheme to a prescribed tolerance.

Bifurcation and Stability of Band-Edge Plane Waves

- One expects that the band-edge plane waves, and their nonlinear continuations, play an important role in determining the localization properties of nearby discrete breathers.
- Utilizing a spatial discrete Fourier transform on the honeycomb lattice, we obtain the following system for the nonlinear band-edge plane waves at quasi-momenta M:

$$\ddot{\hat{x}}_{\mathrm{M}}^{A} = -V'\left(\hat{x}_{\mathrm{M}}^{A}\right) + (\gamma - 2\lambda)\,\hat{x}_{\mathrm{M}}^{B}$$
$$\ddot{\hat{x}}_{\mathrm{M}}^{B} = -V'\left(\hat{x}_{\mathrm{M}}^{B}\right) + (\gamma - 2\lambda)\,\hat{x}_{\mathrm{M}}^{A},$$

  where the Fourier components at all other quasi-momenta, k, are zero. We denote the solutions $P^{A,B}(t)$.

- To determine the dynamical stability of these spatially extended states, we linearize about them and obtain

$$\begin{pmatrix} \ddot{y}_k^A \\ \ddot{y}_k^B \end{pmatrix} = \begin{pmatrix} -V''(P^A(t)) & \gamma + \lambda e^{ik\cdot a_2}(1 + e^{-ik\cdot a_1}) \\ \gamma + \lambda e^{-ik\cdot a_2}(1 + e^{ik\cdot a_1}) & -V''(P^B(t)) \end{pmatrix} \begin{pmatrix} y_k^A \\ y_k^B \end{pmatrix}.$$

Bifurcation and Stability of Band-Edge Plane Waves

- For a hardening nonlinearity ($g = 1$), a plane wave bifurcates from the lower band-edge with increasing frequency (and amplitude) into the gap. These periodic states can be solved for analytically at any nonlinearity strength in terms of elliptic functions.

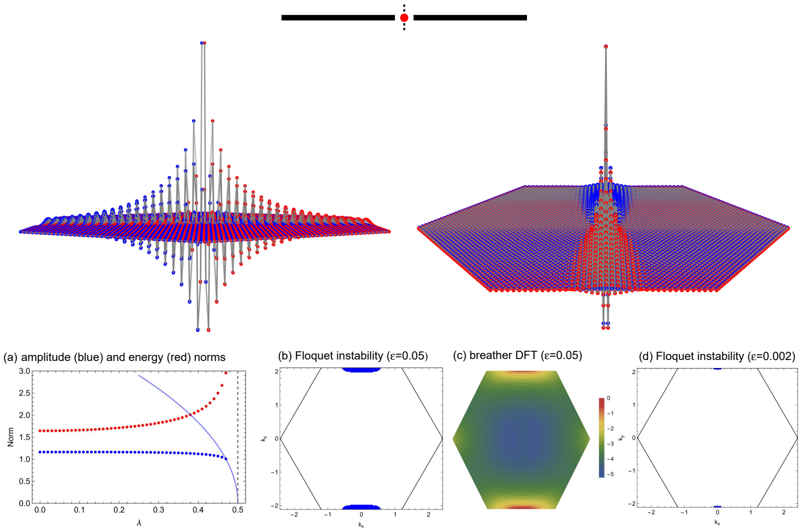
- Writing the above linearization problem as a first-order system:

$$\dot{Y} = A(t; k, \epsilon) Y,$$

  where $A(t; k, \epsilon)$ is T_b-periodic. By Floquet theory, stability is given by the eigenvalues, $\{\mu_j\}$ (Floquet multipliers), of the principal fundamental matrix solution, $\mathcal{Y}(T_b; k, \epsilon)$, to the above system.

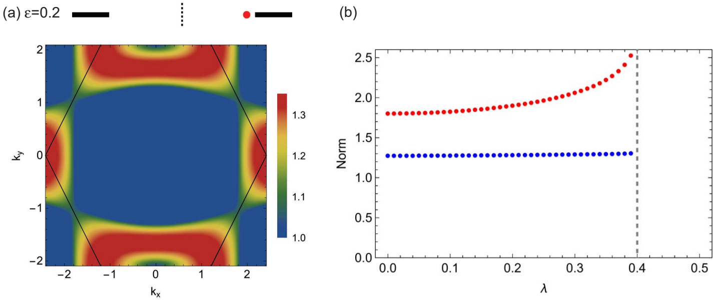
- A tangent bifurcation occurs when two Floquet multipliers collide at $+1$ on the unit circle in the complex plane and generate parameter regions of instability.

Numerical Continuation of Midgap Breather



Band-Edge Stability and Small-Amplitude DBs

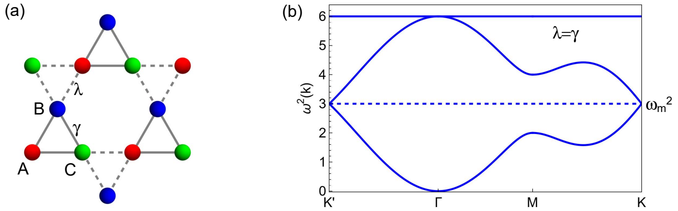
- The occurence of a tangent bifurcation at the quasi-momenta M (or lack thereof) appears to determine the existence (or non-existence) of small-amplitude DBs as $\omega_b \to \omega_{\text{band-edge}}$.
- Here, in the case $g = 1$ and for a fixed $\epsilon > 0$, numerics suggest small-amplitude DBs exist in the lower half of the band-gap, but not in the upper-half.



[3] M. Kastner, "Energy Thresholds for Discrete Breathers," PRL (2004).

[4] M.I. Weinstein "Excitation Thresholds for Nonlinear Localized Modes on Lattices," Nonlinearity (1999).

Nonlinear Breathing Kagome (BK) Lattice



- We consider a breathing Kagome lattice with on-site nonlinearity and equations of motion:

$$\begin{aligned}
\ddot{x}^A_{n,m} &= -V'(x^A_{n,m}) + \gamma\left[x^B_{n,m} + x^C_{n,m}\right] + \lambda\left[x^B_{n,m-1} + x^C_{n-1,m}\right] \\
\ddot{x}^B_{n,m} &= -V'(x^B_{n,m}) + \gamma\left[x^A_{n,m} + x^C_{n,m}\right] + \lambda\left[x^A_{n,m+1} + x^C_{n-1,m+1}\right] \\
\ddot{x}^C_{n,m} &= -V'(x^C_{n,m}) + \gamma\left[x^A_{n,m} + x^B_{n,m}\right] + \lambda\left[x^A_{n+1,m} + x^B_{n+1,m-1}\right]
\end{aligned}$$

- The even potential is given by

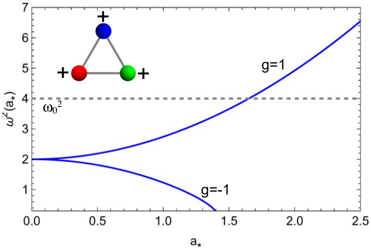
$$V(z) = \omega_0^2 z^2/2 + g|z|^{2\alpha} z^2/(2\alpha+2)$$

where $\alpha \geq 1$ and $g = \pm 1$ for a *hardening* (*softening*) nonlinearity.

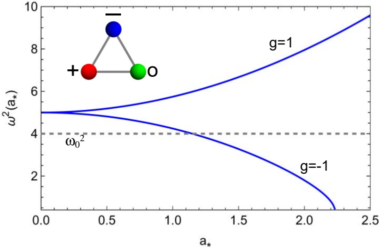
The Molecular Limit of the BK Lattice

- Here, we seed the continuation scheme with either of the following solution types on an isolated unit cell using the initial condtions $|x_{0,0}^{A,B,C}(0)| = a_*$ or 0 and $\dot{x}_{0,0}^{A,B,C}(0) = 0$. In the first case C_3-symmetry is preserved and in the latter it is broken.

(I) Symmetric Anti-Continuum Solution

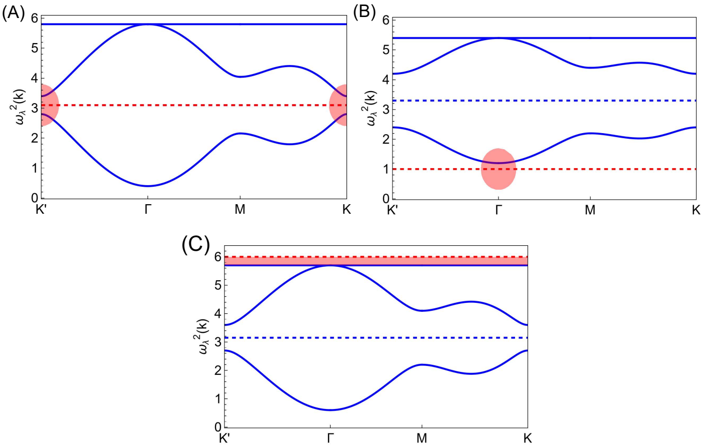


(II) Symmetry-Broken Anti-Continuum Solution

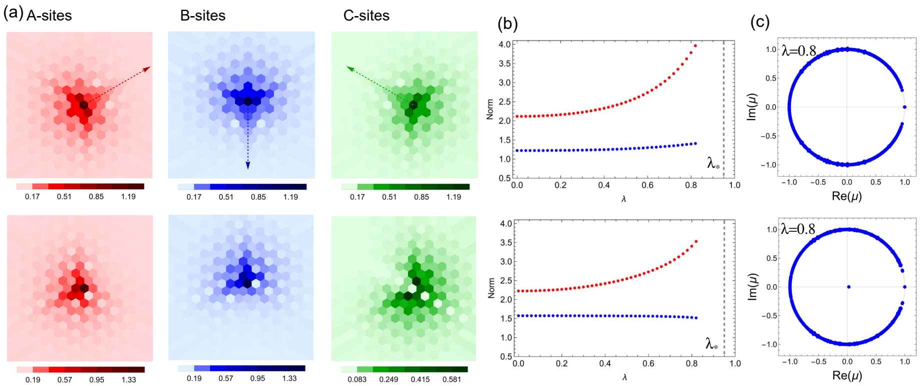


Shaping DBs on the BK Lattice

- We consider DBs having a fixed frequency near three different points relative to the phonon spectrum: (A) *inside the band-gap*; (B) *below the acoustic band*; and (C) *above the optic flat band*.



(A) Symmetric and Symmetry-Broken DBs in the Gap



(B) Leading-Order Asymptotic Description of DBs

- A multiple-scales analysis in $\underline{\epsilon := \gamma/2 - \lambda}$ gives at leading-order:

$$-2i\omega_-\partial_T R - gC_\alpha|R|^{2\alpha}R - 2R + \frac{2}{3}\gamma\Delta R = 0.$$

for the slowly-varying envelope $R(T, Z, H)$.

- We seek solutions of the form

$$R(T, Z, H) = S(Z, H; \nu)e^{i\nu T/2\omega_-}$$

which gives the asymptotic solutions on the BK lattice:

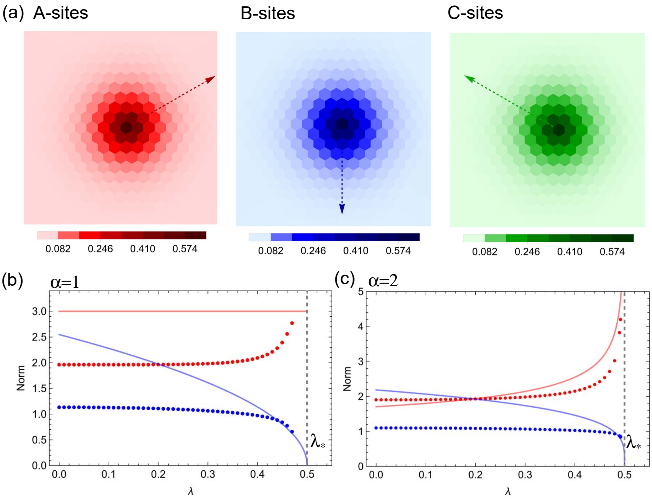
$$\begin{pmatrix} x^A_{n,m}(t) \\ x^B_{n,m}(t) \\ x^C_{n,m}(t) \end{pmatrix} \sim 2\epsilon^{1/2\alpha} S(\sqrt{\epsilon}n, \sqrt{\epsilon}m; \nu) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cos\left(\left[\omega_- + \frac{\nu\epsilon}{2\omega_-}\right] t\right).$$

- We have the general asymptotic scalings of the breather's norms as $\epsilon \to 0$:

$$\boxed{\begin{aligned} &\|\{x^J_{n,m}(0)\}_{\{(n,m)\in\mathbb{Z}^2, J\in(A,B,C)\}}\|_{\ell^\infty} \sim 2\epsilon^{1/2\alpha}\|S\|_{L^\infty(\mathbb{R}^2)} \\ &\|\{x^J_{n,m}(0)\}_{\{(n,m)\in\mathbb{Z}^2, J\in(A,B,C)\}}\|^2_{\ell^2} \sim 2\sqrt{3}\epsilon^{(1-\alpha)/\alpha}\|S\|^2_{L^2(\mathbb{R}^2)}. \end{aligned}}$$

(B) Connecting the Molecular and Continuum Limits

Symmetric breathers just below the parabolic band-edge:



(C) Compactly Localized Discrete Breathers

- The nonlinear BK lattice has the exact *spatially compact*, time-periodic solution:

$$X_c(t,\lambda) := \begin{cases} x^A_{0,0} = x^C_{-1,1} = x^B_{-1,0} = z^{(II)}(t), \\ x^B_{0,0} = x^A_{-1,1} = x^C_{-1,0} = -z^{(II)}(t), \\ x^J_{n,m} \equiv 0 \text{ for all other } (n,m) \in \mathbb{Z}^2, \end{cases}$$

  where $z^{(II)}(t)$ is a T_b-periodic solution to the scalar initial value problem

$$\ddot{z} = -V'(z) - (\gamma+\lambda)z, \quad z(0) = a_*, \quad \dot{z}(0) = 0.$$

- Let $\beta := \omega_0^2 + \lambda + \gamma$, the exact solution is given by the even Jacobi elliptic function

$$z^{(II)}(t) = a_* \mathrm{cn}\left(\sqrt{\beta + g a_*^2}\, t, \sqrt{\frac{g a_*^2}{2(\beta + g a_*^2)}}\right).$$

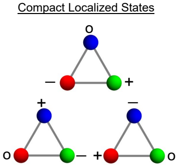
(C) Compactly Localized Discrete Breathers

- The period of the compact solution is

$$T_b = \frac{4}{\sqrt{\beta + g a_*^2}} \mathcal{K}\left(\sqrt{\frac{g a_*^2}{2\left(\beta + g a_*^2\right)}}\right),$$

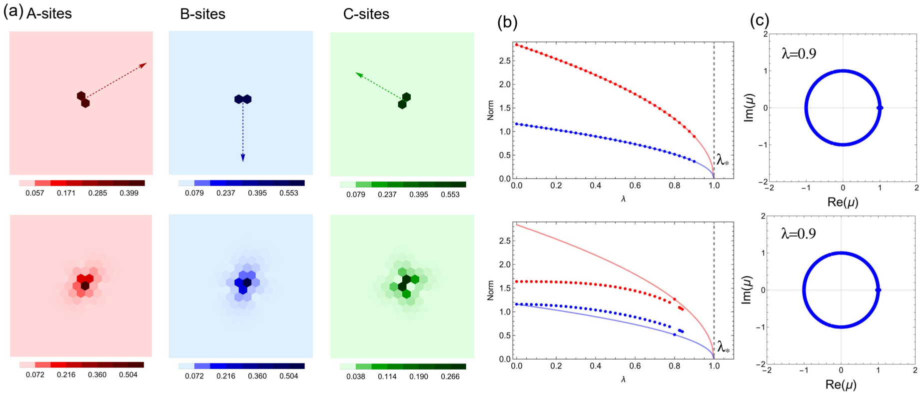
where $\mathcal{K}$ is the complete elliptic integral of the first kind.

- This compact DB is equivalent to three symmetry-broken states in the *molecular limit*, arranged as follows, restoring C_3-symmetry



- These compact DBs exist even with frequencies intersecting the two lower dispersive phonon bands, however in this case they are dynamically unstable.

(C) Symmetric and Symmetry-Broken DBs Above the Flat Band



Conclusion and Future Directions

- We have developed a general method to shape and analyze instrinsically localized modes (asymptotically and numerically) on periodic 2D nonlinear lattices.

  DBs near molecular limit $\Longrightarrow$ gap solitons $\Longrightarrow$ band-edge bifurcations

- A study of DBs in multilayered (twisted) 2D lattices is a path for further research.