On-Site and Off-Site Bound States of the Discrete Nonlinear Schrödinger Equation and the Peierls-Nabarro Barrier

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Nonlinear Schrödinger Equation (NLS) with cubic nonlinearity:

\[ i \partial_t u(x, t) = -\Delta u(x, t) - |u(x, t)|^2 u(x, t), \quad x \in \mathbb{R}, \]

Conserved quantities:

\[ \mathcal{N}[u] = \|u\|_{L^2(\mathbb{R})}^2 = \int_{\mathbb{R}} |u|^2 \, dx, \]

\[ \mathcal{H}[u] = \int_{\mathbb{R}} |\nabla u|^2 \, dx - \frac{1}{2} \int_{\mathbb{R}} |u|^4 \, dx \]

Hamiltonian system:

\[ i \partial_t u = \frac{\delta \mathcal{H}}{\delta u^*} \]

Additional symmetries / invariances:

- Continuous translational
- Galilean  \[ u(x, t) \mapsto \tilde{u}(x, t) = u(x - 2ct, t) \, e^{ic(x-ct)} \]
Several variational approaches on $H^1(\mathbb{R}^d)$ [e.g. Strauss ‘77, Berestycki and Lions ‘83] generate standing wave solutions (bound states), $1 \leq d \leq 3$:

$$u(x, t) = e^{-i\omega t} \psi(x) \implies \omega \psi(x) = -\Delta \psi(x) - \psi(x)^3, \quad \omega < 0$$

Lowest energy state is unique, positive, unimodal ground state [Kwong ‘89; Gidas, Ni, and Nirenberg, ‘81].

*E.g.* Cazenave and Lions, ‘81 for $d = 1$

$$\inf_{u \in H^1(\mathbb{R})} \mathcal{H}[u] \quad \text{subject to} \quad \mathcal{N}[u] = \text{const}$$

attains unique, *orbitally stable* ground state

$$\psi(x) = \sqrt{2\omega} \operatorname{sech}(\sqrt{\omega}x), \quad d = 1$$
Galilean invariance (boost) leads to soliton \( \tilde{u}(x, t) : \)
\[
\tilde{u}(x, t) = \sqrt{2\omega} \text{sech} (x - 2ct) \ e^{ic(x-ct)} e^{-i\omega t}
\]

However - Sobolev embedding and compactness govern

1. Well-posedness (\( \implies \) \( L^2 \) and \( H^1 \) criticality)
2. Existence and stability of bound state solutions of
\[
\omega u = -\Delta u - u^p; \ i.e. \ Pohozaev \ identities, \ 1 \leq d \leq 3 \ when \ p = 3.
\]
Discretize spatial variable:

\[ x \rightarrow nh, \quad u(t) = \{u_n(t)\}_{n \in \mathbb{Z}^d}. \]

Discrete second order difference operator:

\[ \Delta_x u(x, t) \rightarrow \frac{1}{h^2} \left( \delta^2 u \right)_n(t) \equiv \frac{1}{h^2} \sum_{|m-n|=1} u_m - 2du_n \]

NLS becomes the discrete nonlinear Schrödinger equation:

**DNLS**:

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

(Infinite system of coupled discrete nonlinear oscillators)
Discrete Nonlinear Schrödinger Equation

\textbf{DNLS} : \quad i \partial_t u_n(t) = - \frac{1}{\hbar^2} (\delta^2 u)_n(t) - |u_n(t)|^2 u_n(t), \quad n \in \mathbb{Z}^d.

Conserved quantities:

\[ \mathcal{N}[G] = \| G \|_{\ell^2(\mathbb{Z})}^2 = \sum_{n \in \mathbb{Z}^d} |G_n|^2, \]

\[ \mathcal{H}[G] = \sum_{j=1}^{d} \sum_{n \in \mathbb{Z}^d} |G_{n+e(j)} - G_n|^2 - \frac{1}{2} \sum_{n \in \mathbb{Z}^d} |G_n|^4, \]

\[ i \partial_t u = \frac{\delta \mathcal{H}}{\delta u^*}. \]

- No continuous translation invariance.
- No Galilean invariance.

**Question:** What effect does discretization have on dynamics?
Discrete Nonlinear Schrödinger Equation

Global well-posedness for since \( \| f \|_{l^\infty(\mathbb{Z}^d)} \lesssim \| f \|_{l^2(\mathbb{Z}^d)}. \)

\[
\mathcal{N}[G] = \| G \|_{l^2(\mathbb{Z}^d)}^2 = \sum_{n \in \mathbb{Z}^d} |G_n|^2,
\]

\[
\mathcal{H}[G] = \sum_{j=1}^{d} \sum_{n \in \mathbb{Z}^d} |G_{n+e(j)} - G_n|^2 - \frac{1}{2} \sum_{n \in \mathbb{Z}^d} |G_n|^4,
\]

Variational approach [Weinstein ‘99]

\[
\inf \mathcal{H}[u] \quad \text{subject to} \quad \mathcal{N}[u] = \text{const}
\]

generates orbitally stable standing wave solutions (ground states):

\[
u_n(t) = e^{-i\omega t} g_n \quad \Rightarrow \quad \omega g_n = -\frac{1}{\hbar^2} (\delta^2 g)_n - (g_n)^3.
\]

No restriction on dimensionality (criticality).

\textit{However, at best, we can show positivity and unimodality (i.e. near symmetry)} [\textit{e.g.} Mckenna and Reichel, ‘07]
Seek symmetric, positive, and unimodal standing wave solutions (bound states) to DNLS numerically ($d = 1$):

$$u_n(t) = e^{-i\omega t}g_n \implies \omega g_n = -\frac{1}{\hbar^2} \left(\delta^2 g\right)_n - (g_n)^3.$$
Bound states for $d = 2$: 

- Vertex-centered
- Bond-centered
- Bond-centered
- Cell-centered
Long term goal: understand how on-site and off-site waves participate in general dynamics

What if we attempt to produce a localized traveling wave on the lattice $(d = 1)$?

Consider initial conditions for DNLS which generate a traveling soliton for continuum NLS:

\[(I.C.) \quad u_n(0) = \psi(nh)e^{icnh} = \sqrt{2|\omega|} \text{sech}(|\omega|nh)e^{icnh}\]
Initial condition:

\[ u_n(0) = \psi(nh)e^{icnh} = \sqrt{2|\omega|} \text{sech}(|\omega|nh) e^{icnh} \]
Discrete Pulse Dynamics

Initial condition:

\[ u_n(0) = \psi(nh)e^{icnh} = \sqrt{2|\omega|} \text{sech}(|\omega|nh) \ e^{icnh} \]
Discrete Pulse Dynamics

Initial condition:

\[ u_n(0) = \psi(nh)e^{i cnh} = \sqrt{2|\omega|} \text{sech}(|\omega| nh) e^{i cnh} \]
Initial condition: Gaussian
Large initial condition \((d = 2)\)
Small initial condition \((d = 2)\)
Discrete Pulse Dynamics

- Localization propagates along the lattice and deforms.
- Mass radiates outward in both directions in the form of low amplitude oscillations.
- Pulse slows as it loses mass until stopping at a single lattice point and oscillates as a stable (peaked) standing wave.
Peak Position Dynamics

Plotting $\max_{n \in \mathbb{Z}} |u_n(t)|$:
The two (on-site and off-site) standing wave solutions are “transition states.”

Peierls-Nabarro (PN) Barrier: difference in energy between two states

\[ E_{PN} = E[g^{\text{off}}] - E[g^{\text{on}}] > 0, \]

is energy required to translate wave by one lattice site.

Moving from site \( n \) to site \( n + 1 \):

- loss of energy \( \Delta E \) to lattice vibrations (continuum modes) which radiate to infinity.
- effective dissipation.
- discrete wave relaxes to on-site standing wave (radiation damping).
First, we show...

**DNLS:** \( \omega g_n = -\frac{1}{\hbar^2} (\delta^2 g)_n - |g_n|^2 g_n, \quad n \in \mathbb{Z}^d. \)

**Theorem:** In dimensions \( d = 1, 2, \) and \( 3, \) there exist localized symmetric vertex-, bond-, face-, and cell-centered standing wave solutions to DNLS.

**Theorem:** Bound on Peierls-Nabarro Barrier:

\[
|\mathcal{E}_{PN}| \lesssim (\hbar \sqrt{|\omega|})^{2-d} e^{-c/\hbar \sqrt{|\omega|}}, \quad C > 0.
\]
Physical Example

- Nonlinear optics: arrays of optical waveguides where nonlinearity is a function of intensity (Kerr effect) [Silberberg et. al. ‘98].

\[
i \partial_z \psi = -\partial_x^2 \psi + V(x) \psi - |\psi|^2 \psi \quad \Rightarrow \quad i \partial_z \psi_n = -\frac{1}{\hbar^2} \delta^2 \psi_n - |\psi_n|^2 \psi_n
\]

Nonlinear optics: arrays of optical waveguides where nonlinearity is a function of intensity (Kerr effect) [Silberberg et. al. ‘98].
Existence of breathers:

- Existence in the anti-continuum (very discrete, $h \to \infty$) limit [Aubry-McKay ’94].
- Variational characterization of ground states/excitation thresholds [Weinstein ’99].
- Finite elements / variational construction of on-site and off-site solutions [Bambusi-Penati ’09].
- Variational construction of on-site and off-site waves as limit of periodic solutions [Hermann ’11].
- Construction of on-site and off-site waves near variational approximations in the anti-continuum limit [Chong-Pelinovsky-Schneider ’12].
Connections to PN Barrier and radiation damping:

- Discussion of breathers in the limit of modified Ablowitz-Ladik DNLS [Campbell-Kivshar ’93].
- Dynamical behavior of kinks in discrete sine-Gordon and $\phi^4$ equations [Kevrekidis-Weinstein ’00].
- Evans function calculation of (exponentially small) eigenvalues of linear stability problem in Ablowitz-Ladik limit [Kapitula-Kevrekidis ’01].
- Examination of traveling waves in DNLS for various nonlinearities [Pelinovsky-Rothos ’05, Pelinovsky-Melvin-Champneys ’07].
- Calculation of radiation amplitude for DNLS pulses using asymptotics beyond all orders [Oxtoby-Barashenkov ’07].
- Analogous bifurcation problem for Gross-Pitaevskii equation [Ilan-Weinstein ’10].
- Various results on radiation damping and settling to a ground state [Soffer-Weinstein, Tsai-Yau, Buslaev-Perelman, Buslaev-Sulem, Cuccagna, Cuccagna-Tarulli, etc.].
Approach: construct discrete standing waves as bifurcations from the continuous spectrum of the linear operator (discrete Laplacian)

\[
\omega \ g_n = -\frac{1}{h^2} (\delta^2 g)_n - |g_n|^2 g_n.
\]

Rescale

\[
G_n \equiv h \ g_n, \quad \omega \equiv -\epsilon^2, \quad \alpha \equiv h\epsilon.
\]

\[
- \alpha^2 G_n = - (\delta^2 G)_n - |G_n|^2 G_n,
\]

Two limits contained in one emergent parameter \( \alpha \):

- Physical (homogenized) limit for low amplitude/long wavelength: fix \( h \), take \( \epsilon \to 0 \).
- Continuum limit for small grid spacing (numerical analysis): fix \( \epsilon \), take \( h \to 0 \).
How do we compare function on lattice with function defined on continuous space? \((d = 1)\)

Discrete Fourier Transform (DFT):

\[
\mathcal{F}_D[G](q) = \hat{G}(q) \equiv \sum_{n \in \mathbb{Z}} G_n e^{-i q n}, \quad \mathcal{F}_D^{-1}[\hat{G}]_n = G_n \equiv \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{G}(q) e^{i q n} dq,
\]

Note: \(\hat{G}(q + 2\pi) = \hat{G}(q)\).

Periodic Convolution:

\[
\hat{F} \ast_s \hat{G}(q) \equiv \int_{-\pi/s}^{\pi/s} \hat{F}(q_1) \hat{G}(q - q_1) dq_1.
\]

Continuous Fourier Transform:

\[
\mathcal{F}_C[u](q) = U(q) \equiv \int_{\mathbb{R}} u(x) e^{-i q x}, \quad \mathcal{F}_C^{-1}[U](x) = u(x) \equiv \frac{1}{2\pi} \int_{\mathbb{R}} U(q) e^{i q x} dq,
\]

Standard Convolution:

\[
U \ast V(q) \equiv \int_{\mathbb{R}} U(q_1) V(q - q_1) dq_1.
\]
Heuristic discussion: where is the bifurcation?

We seek small amplitude ($\sim \alpha$) waves of low frequency ($\sim \alpha^2$):

Apply the DFT to DNLS:

$$-\alpha^2 G_n = -(G_{n+1} + G_{n-1} - 2G_n) - (G_n)^3 = 0,$$

to get

$$[\alpha^2 + 4 \sin^2(q/2)] \hat{G}(q) - (2\pi)^{-2} \hat{G} \ast_1 \hat{G} \ast_1 \hat{G}(q) = 0.$$

Expect solution to be concentrated near low frequencies $q \sim 0$. 
Heuristic discussion: where is the bifurcation?

For $|q| \ll 1$, rescale $Q = q/\alpha$ and set $\hat{G}(q) = \hat{\Phi}(q/\alpha) = \hat{\Phi}(Q)$. Then

$$4 \sin^2(q/2) = 4 \sin^2(\alpha Q/2) \sim \alpha^2 |Q|^2,$$

$$\hat{G} \ast_1 \hat{G} \ast_1 \hat{G}(q) = \alpha^2 \hat{\Phi} \ast_\alpha \hat{\Phi} \ast_\alpha \hat{\Phi}(Q) \sim \alpha^2 \hat{\Phi} \ast \hat{\Phi} \ast \hat{\Phi}(Q).$$

giving

$$\left[ 1 + (4/\alpha^2) \sin^2(\alpha Q/2) \right] \hat{\Phi}(Q) - (2\pi)^{-2} \hat{\Phi} \ast_\alpha \hat{\Phi} \ast_\alpha \hat{\Phi}(Q)$$

$$= (1 + |Q|^2) \hat{\Phi}(Q) - (2\pi)^{-2} \hat{\Phi} \ast \hat{\Phi} \ast \hat{\Phi}(Q) + \mathcal{O}(\alpha^2) = 0.$$
Bifurcation of States, $d = 1$

\[
\text{NLS : } \Lambda \psi(x) = -\partial_x^2 \psi(x) - \psi(x)^3,
\]
\[
\text{DNLS : } \Omega \ G_n = - (\delta^2 G)_n - G_n^3
\]

W.R.T. square of $\| \cdot \|_2$ norm (for $\Omega = -\alpha^2$ and $\Lambda = -\alpha^2$):

- Bifurcations from the zero state $\sim \alpha$.
- Deviation from leading order continuum solution $\sim \alpha^5$.
- Difference in size of bifurcations $\sim \alpha \ e^{-C/\alpha}$.
Theorem 1 (Existence for $d = 1$):

Let $\psi(x)$ be the soliton solution to NLS: $\psi(x) - \partial_x^2 \psi(x) - \psi(x)^3 = 0$. Consider the DNLS equation

$$-\alpha^2 G_n = -\left(\delta^2 G\right)_n - (G_n)^3, \quad n \in \mathbb{Z}$$

Fix $J \geq 0$. There exist mappings $G_j : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, for $j = 0, 1, \ldots, J$ and a positive constant $\alpha_0 = \alpha_0[J] > 0$ such that for all $0 < \alpha < \alpha_0$, there exist two families of real-valued symmetric solutions to DNLS:

**On-site symmetric (vertex-centered):**

$$G_{n}^{\alpha, \text{on}} = \alpha \sum_{j=0}^{J} \alpha^{2j} G_j[\psi](\alpha n) + \mathcal{E}_n^{\alpha, J, \text{on}},$$

where $\|G_j[\psi](\alpha n)\|_{\ell^2(\mathbb{Z}_n)} \sim \alpha^{-1/2}$, $\|\mathcal{E}^{\alpha, J, \text{on}}\|_{\ell^2(\mathbb{Z})} \lesssim \alpha^{2J+5/2}$.

**Off-site symmetric (bond-centered):**

$$G_{n}^{\alpha, \text{off}} = \alpha \sum_{j=0}^{J} \alpha^{2j} G_j[\psi](\alpha[n - 1/2]) + \mathcal{E}_n^{\alpha, J, \text{off}},$$

where $\|G_j[\psi]\left(\alpha[n - \frac{1}{2}]\right)\|_{\ell^2(\mathbb{Z}_n)} \sim \alpha^{-1/2}$, $\|\mathcal{E}^{\alpha, J, \text{off}}\|_{\ell^2(\mathbb{Z})} \lesssim \alpha^{2J+5/2}$. 
Proof Outline (Existence for $d = 1$)

Discrete FT of DNLS:

$$[\alpha^2 + 4 \sin^2(q/2)] \hat{G}(q) - (2\pi)^{-2} \hat{G} \ast_1 \hat{G} \ast_1 \hat{G}(q) = 0,$$

$$\hat{G}(q + 2\pi) = \hat{G}(q).$$

Fix $\sigma = 0, 1/2$. Decompose and project onto Brillouin zone $B = [-\pi, \pi]$:

$$\hat{G}(q) = e^{-iq\sigma} \sum_{m \in \mathbb{Z}} \chi_B(q - 2m\pi) \hat{\phi}(q - 2m\pi).$$

Seek $\hat{\phi}$ even:

$$\left[\alpha^2 + 4 \sin^2(q/2)\right] \hat{\phi}(q) - \frac{\chi_B(q)}{(2\pi)^2} \left(\hat{\phi} \ast \hat{\phi} \ast \hat{\phi}\right)(q) + \mathcal{R}_I[\hat{\phi}](q) = 0.$$

with

$$\mathcal{R}_I[\alpha, \hat{\phi}] \sim e^{\pm 2\pi i\sigma} \chi_B(q) \hat{\phi} \ast \hat{\phi} \ast \hat{\phi}(q \pm 2\pi).$$
Proof Outline (Existence for $d = 1$)

Rescale

$$Q = \frac{q}{\alpha} \quad \text{and} \quad \hat{\Phi}(Q) = \hat{\Phi}(q/\alpha) = \hat{\phi}(q)$$

to get

$$\left[ 1 + \frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \right] \hat{\Phi}(Q) - \frac{\chi[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}](Q)}{(2\pi)^2} \left( \hat{\Phi} \ast \hat{\Phi} \ast \hat{\Phi} \right)(Q)$$

$$+ \mathcal{R}_2^g[\alpha, \hat{\Phi}](Q) = 0.$$ 

with

$$\mathcal{R}_2^g[\alpha, \hat{\Phi}] \sim e^{\pm 2\pi i \sigma} \chi[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}](Q) \hat{\Phi} \ast \hat{\Phi} \ast \hat{\Phi}(Q \pm 2\pi/\alpha) \sim e^{-C/\alpha},$$

due to exponential decay of solitary wave $\hat{\Phi} \sim e^{-C/\alpha}$

[proof similar to Bona and Li, ‘97; Frank and Lenzmann, ‘10].
Proof Outline (Existence for $d = 1$)

Expand (e.g. to leading order):

$$\hat{\Phi}(Q) \simeq \psi(Q) + \hat{E}^\sigma(Q).$$

Equation for error:

$$\left[ 1 + \frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \right] \hat{E}(Q) - \frac{3}{(2\pi)^2} \chi_{[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}]} \left( \psi \ast \psi \ast \hat{E} \right)(Q) = R^\sigma_3[\alpha, \hat{E}](Q).$$

Solvable via Lyapunov-Schmidt reduction: project onto $|Q| \leq \alpha^{r-1}$ and $|Q| > \alpha^{r-1}$, with $0 < r < 1$:

$$\hat{E}_{lo}(Q) \equiv \chi_{\{ |Q| \leq \alpha^{r-1} \}} \hat{E}(Q), \quad \hat{E}_{hi}(Q) \equiv \chi_{\{ |Q| > \alpha^{r-1} \}} \hat{E}(Q).$$

We obtain weakly coupled system for $\hat{E}_{lo}(Q)$ and $\hat{E}_{hi}(Q)$ (two equations supported on low and high frequencies respectively)
Proof Outline (Existence for \(d = 1\))

Obtain \(\widehat{E}_{hi} = \left[ \alpha, \widehat{E}_{lo} \right] \) via IFT (since \(\frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \geq C \ |Q|^2 \)):

\[
\widehat{E}_{hi} \sim \chi_{\left\{ \alpha^{r-1} < |Q| \leq \frac{\pi}{\alpha} \right\}} \left[ \begin{array}{c} 1 + \frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \end{array} \right]^{-1} \left( \psi * \psi * \widehat{E}_{lo} \right)(Q)
\]

\[
\sim \alpha^{2-2r} \widehat{E}_{lo} \quad \text{in} \quad L^2, \text{a} (\mathbb{R}),
\]

Next, since \(\frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \sim |Q|^2 \) on \(|Q| \leq \alpha^{r-1}\), obtain closed equation for \(\widehat{E}_{lo}\); solution exists via fixed point argument:

\[
\hat{L}_+ \hat{E}_{lo} = \mathcal{R}_4^{\sigma} [\alpha, \hat{E}_{lo}] \sim \alpha^{4r-2} \in L^2, \text{a} (\mathbb{R})
\]

\[
\Rightarrow \quad \hat{E}_{lo} = \left( \hat{L}_+ \right)^{-1} \mathcal{R}_4^{\sigma} [\alpha, \hat{E}_{lo}] \in L^2, \text{a}+2 (\mathbb{R})
\]

Linearized continuum operator:

\[
\hat{L}_+ = 1 + |Q|^2 - \frac{3}{(2\pi)^2} \psi \ast \psi \ast, \quad \ker \hat{L}_+ = \text{span} \ Q\psi
\]
Proof Outline (Existence for $d = 1$)

Remark:

Algebraically small terms:

$$\frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) = |Q|^2 + \sum_{j=1}^{\infty} \alpha^{2j} M_j(Q)$$

Exponentially small terms ($\sigma$ dependent!):

$$\mathcal{R}_2^{\sigma}[\alpha, \hat{\Phi}] \sim e^{\pm 2\pi i \sigma} \chi_{[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}]}(Q) \hat{\Phi} \ast \hat{\Phi} \ast \hat{\Phi} (Q \pm 2\pi/\alpha) \sim e^{-C/\alpha},$$

Note also

$$e^{\pm 2\pi i \sigma} = (-1)^{2\sigma} = \pm 1$$
Theorem 2 (Generalization to $d = 1, 2, 3$):

Let $\psi(x), \ x \in \mathbb{R}^d$ be the ground state solution to NLS:

$$-\psi(x) = -\Delta \psi(x) - \psi(x)^3.$$  
Consider the DNLS equation

$$-\alpha^2 G_n = - (\delta^2 G)_n - (G_n)^3, \quad n \in \mathbb{Z}^d$$

Let $\sigma \in \{0, 1/2\}^d$ and $J \geq 0$. There exist mappings $G_j : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$, for $j = 0, 1, \ldots, J$ and a positive constant $\alpha_0 = \alpha_0[J] > 0$ such that for all $0 < \alpha < \alpha_0$, there exist $d + 1$ families of symmetric solutions to DNLS:

$$G_n^{\alpha, \sigma} = \alpha \sum_{j=0}^{J} \alpha^{2j} G_j[\psi](\alpha[n - \sigma]) + \mathcal{E}_n^{\alpha, J, \sigma}, \quad \text{where}$$

$$\|G_j[\psi](n - \sigma)\|_{\ell^2(\mathbb{Z}^d_n)} \sim \alpha^{-d/2}, \quad \|\mathcal{E}_n^{\alpha, J, \sigma}\|_{\ell^2(\mathbb{Z}^d)} \lesssim \alpha^{2J+3-d/2}.$$
Theorem 3 (PN Barrier):

Let $G_n^{\alpha,\sigma_1}$ and $G_n^{\alpha,\sigma_2}$ be two solutions with respective centering $\sigma_1$ and $\sigma_2$ from Theorem 2 of DNLS:

$$-\alpha^2 G_n = -(\delta^2 G)_n - (G_n)^3, \quad n \in \mathbb{Z}^d.$$ 

Then there exists $\alpha_0 > 0$ such that the following holds: for all $0 < \alpha < \alpha_0$, 

$$\left| \mathcal{N}[G^{\alpha,\sigma_1}] - \mathcal{N}[G^{\alpha,\sigma_2}] \right| \lesssim \alpha^{2-d} e^{-C/\alpha},$$

$$\left| \mathcal{H}[G^{\alpha,\sigma_1}] - \mathcal{H}[G^{\alpha,\sigma_2}] \right| \lesssim \alpha^{2-d} e^{-C/\alpha},$$

where 

$$\mathcal{N}[G] = \|G\|_{\ell^2(\mathbb{Z}^d)}^2 = \sum_{n \in \mathbb{Z}^d} |G_n|^2,$$

$$\mathcal{H}[G] = \sum_{j=1}^d \sum_{n \in \mathbb{Z}^d} |G_{n+e(j)} - G_n|^2 - \frac{1}{2} \sum_{n \in \mathbb{Z}^d} |G_n|^4.$$
Main Idea \((d = 1)\)

- Know:

\[
\hat{G}^{on}(q) \simeq \hat{\Phi}^{on} \left( \frac{q}{\alpha} \right),
\]

\[
\hat{G}^{off}(q) \simeq e^{-i q/2} \hat{\Phi}^{off} \left( \frac{q}{\alpha} \right),
\]

- Using Plancherel theorem and an energy identity for bound states, we find

\[
\left| \mathcal{N}[G^{off}] - \mathcal{N}[G^{on}] \right| \lesssim \alpha \| \hat{\Phi}^{off} - \hat{\Phi}^{on} \|_{L^2\left(\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]\right)},
\]

\[
\left| \mathcal{H}[G^{off}] - \mathcal{H}[G^{on}] \right| \lesssim \alpha \| \hat{\Phi}^{off} - \hat{\Phi}^{on} \|_{L^2\left(\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]\right)}.
\]

- Seek equation for \(\hat{\Phi}^{off} - \hat{\Phi}^{on}\) (again even) and find that it’s driven by shifted terms:

\[
\sim \chi_{\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]}(Q) \ \hat{\Phi}^{\sigma} \ast \hat{\Phi}^{\sigma} \ast \hat{\Phi}^{\sigma} (Q \pm 2\pi/\alpha)
\]

\[
\implies \| \hat{\Phi}^{off} - \hat{\Phi}^{on} \|_{L^2\left(\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]\right)} \lesssim e^{-C/\alpha}.
\]
Theorem (Extension to Nonlocal DNLS):

(Motivated by Kirkpatrick-Lenzmann-Staffilani ‘13, Frank-L ’10, F-L-Silvestre ’15)

Let $\psi_p(x)$ be the ground state solution to fractional NLS:

$$-\psi_p(x) = (-\Delta)^p \psi_p(x) - \psi_p(x)^3, \quad 1/4 < p \leq 1.$$ 

Fix $1/4 < s < \infty$, let $p = \min(1, s)$, and consider the DNLS equation

$$-\kappa(\alpha) G_n = -\frac{1}{C_s} \sum_{m \in \mathbb{Z}, m \neq n} \frac{(G_m - G_n)}{|m - n|^{1+2s}} - (G_n)^3, \quad n \in \mathbb{Z},$$

$$\kappa(\alpha) = \begin{cases} \alpha^{2p} & : s \neq 1 \\ (-\log(\alpha)) \alpha^2 & : s = 1 \end{cases}$$

Fix $\sigma = 0, 1/2$. Then there exists a positive constant $\alpha_0 = \alpha_0[s] > 0$ such that for all $0 < \alpha < \alpha_0$, there exists a real-valued symmetric solution to nonlocal DNLS:

$$G_n^{\alpha, \sigma} = \kappa_s(\alpha)^{1/2} \psi_p (\alpha[n - \sigma]) + \mathcal{E}_n^{\alpha, \sigma}.$$
Local Stability: Bifurcation in Higher Dimensions

\(d = 1\)

\(d = 2\)

\(d = 3\)
Local Stability Conditions

\[-\alpha^2 \sigma G_n = - (\delta^2 G^\sigma)_n - (G_n^\sigma)^3, \quad \sigma \in \{0, 1/2\}^d.\]

Conditions for the orbital stability of solitary wave:

1. **Morse index:** linearized operator

   \[L^\text{disc}_+ = \alpha^2 - (\delta^2 \cdot)_n - 3 (G_n^\sigma)^2\]

   has only one negative eigenvalue.

2. **Slope condition:**

   \[\frac{d}{d\alpha} \mathcal{N} \left[ G^\sigma[\alpha] \right] = \frac{d}{d\alpha} \| G^\sigma[\alpha] \|_{\ell^2(\mathbb{Z})}^2 = - \frac{1}{\alpha^2} \frac{d}{d\alpha} \mathcal{H} \left[ G^\sigma[\alpha] \right] > 0.\]

   (Vakhitov-Kolokolov ’72: slope $> 0$ implies linear stability; Weinstein ’86, Grillakis-Shatah-Strauss ’87: slope $> 0$ implies stability; Jones ’88, Grillakis ’88: Morse index $\geq 2$ implies instability)
Local Stability \((d = 1)\)

Linearized NLS operator, \(d = 1\):

\[
\hat{L}_+ = 1 + |Q|^2 - \frac{1}{(2\pi)^2} \psi \ast \psi
\]

has one negative eigenvalue and \(\text{ker } \hat{L}_+ = \text{span } Q\psi(Q)\).

Consider rescaled, linearized DNLS operator:

\[
\hat{L}_+^{\text{disc}} \hat{V}(Q)
\]

\[
\equiv \left[1 + \frac{4}{\alpha^2} \sin^2 \left(\frac{Q\alpha}{2}\right)\right] \hat{V}(Q) - \frac{3}{(2\pi)^2} \chi_{\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]}(Q) \left(\hat{\Phi} \ast \hat{\Phi} \ast \hat{V}\right)(Q)
\]

\[
- \frac{3}{(2\pi)^2} \chi_{\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]}(Q) \sum_{m = \pm 1} e^{2m\pi i \sigma} \left(\hat{\Phi} \ast \hat{\Phi} \ast \hat{V}\right)(Q - 2m\pi/\alpha)
\]

as \(O(\alpha^2)\) perturbation of \(\hat{L}_+\).
Local Stability ($d = 1$)

Spectra of $\hat{L}_+$ and $\hat{L}^\text{disc}_+$:

NLS: $0, 1$

DNLS: $\alpha^2, \alpha^2, 0$

Test function $\hat{\Phi}$ gives

$$\left\langle \hat{L}^\text{disc}_+ \hat{\Phi}, \hat{\Phi} \right\rangle = -2 \sum_n \| \Phi_n \|^4 \sim 1 + O(\alpha^2) < 0.$$  

We expect zero eigenvalue of $\hat{L}_+$ to perturb:

1. negatively for off-site state (instability)
2. positively for on-site state (stability)
Local Stability \((d = 1)\)

Key observation: consider “auxiliary equation:"

\[
\left[ 1 + \frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \right] \hat{A} (Q) - \frac{\chi \left[ -\frac{\pi}{\alpha}, \frac{\pi}{\alpha} \right] (Q)}{(2\pi)^2} \left( \hat{A} \ast \hat{A} \ast \hat{A} \right) (Q) = 0.
\]

where

\[
\frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \iff \sum_{k=1}^{\infty} c_k \alpha^{2k-2} \partial_x^{2k}
\]

Linearization:

\[
\hat{L}^A_+ = \left[ 1 + \frac{4}{\alpha^2} \sin^2 \left( \frac{Q\alpha}{2} \right) \right] - \frac{3\chi \left[ -\frac{\pi}{\alpha}, \frac{\pi}{\alpha} \right] (Q)}{(2\pi)^2} \hat{A} \ast \hat{A}^*
\]

Zero eigenstate (translation invariance) is preserved at all polynomial orders:

\[
\hat{L}^A_+ (Q\hat{A}) = 0
\]

\(\implies\) perturbation of \(DNLS\) eigenvalue from zero is ± exponentially small (e.g. Evan’s function calculation of Kapitula & Kevrekidis ‘01)
Local Stability \((d = 1)\)

We seek exponentially small perturbation theory about kernel of \(\hat{L}_A\) for discrete eigenvalue problem.

**Need:**
- For instability / stability: \(\ker\hat{L}_A = \text{span} Q\hat{A}\)

**Proof:** Use Lyapunov-Schmidt reduction argument about \(\hat{L}_A\) to show that

\[
(\hat{L}_A - \lambda I) \hat{f}(Q) = \hat{G}(Q), \quad \mu \in [-C\alpha^2, C\alpha^2]
\]

has unique solution on \(\langle \hat{f}, Q\hat{\psi} \rangle = 0\). Therefore, \(Q\hat{A}\) corresponds to simple zero eigenvalue.

- For stability: \(\hat{L}_A\) has one negative \(O(1)\) eigenvalue

**Proof:** Same argument as above.
Local Stability \((d = 1)\)

Discrete EVP:

\[
\hat{L}_{\text{disc}} \hat{V} = \lambda \hat{V}
\]

Expand:

\[
\begin{align*}
\hat{L}_{\text{disc}} & = \hat{L}^A + \hat{L}^\text{pert} \\
\hat{V}(Q) & = Q\hat{A}(Q) + \hat{E}(Q) + \ldots \\
\lambda & = 0 + \lambda_1 + \ldots
\end{align*}
\]

Here,

\[
\hat{L}^\text{pert}_+ f(Q) \simeq -\frac{3}{\pi} \chi_{\left[-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}\right]}(Q) \left(\sum_{m=\pm1} e^{2m\pi i\sigma} \left(\hat{\Phi} \ast \hat{\Phi} \ast \hat{f}\right)(Q - 2m\pi/\alpha)\right)
\]

We obtain

\[
\hat{L}^A_+ \hat{E} + \hat{L}^\text{pert}_+ Q\hat{A} + \hat{L}^\text{pert}_+ \hat{E} + \ldots = \lambda_1 Q\hat{A} + \lambda_1 \hat{E} + \ldots
\]
Local Stability ($d = 1$): Formal Calculation

"Leading order" terms:

$$\hat{L}_+^A\hat{E} + \hat{L}_+^{\text{pert}}QA + \hat{L}_+^{\text{pert}}\hat{E} + \ldots = \lambda_1 QA + \lambda_1 \hat{E} + \ldots$$

i.e.

$$\hat{L}_+^A\hat{E} = -\hat{L}_+^{\text{pert}}QA + \lambda_1 QA$$

Solvability condition, RHS $\perp \ker \hat{L}_+^A$, gives (after some manipulation)

$$\lambda_1 = \frac{\left\langle \hat{L}_+^{\text{pert}}QA, QA \right\rangle}{\| QA \|_{L^2}^2}$$

$$\sim (-1)^{2\sigma} \tilde{\psi} * \tilde{\psi} * \left[ Q \tilde{\psi} \right] * \left[ Q \tilde{\psi} \right] \left( \frac{2\pi}{\alpha} \right) + \mathcal{O} \left( e^{-2C\pi/\alpha} \right)$$

$$\sim (-1)^{2\sigma} \frac{(1 - \alpha^4)}{\alpha^5} \text{csch} \left( \frac{\pi^2}{\alpha} \right) + \mathcal{O} \left( e^{-2C\pi/\alpha} \right)$$
“Leading order” terms:

\[ \hat{L}_+^A \hat{E} + \hat{L}_+^{\text{pert}} Q \hat{A} + \hat{L}_+^{\text{pert}} \hat{E} + \ldots = \lambda_1 Q \hat{A} + \lambda_1 \hat{E} + \ldots \]

i.e.

\[ \hat{L}_+^A \hat{E} = -\hat{L}_+^{\text{pert}} Q \hat{A} + \lambda_1 Q \hat{A} \]

Solvability condition, RHS \( \perp \ker \hat{L}_+^A \), gives (after some manipulation)

\[ \lambda_1 = \frac{\langle \hat{L}_+^{\text{pert}} Q \hat{A}, Q \hat{A} \rangle}{\|Q \hat{A}\|_{L^2}^2} \]

\[ \sim (-1)^{2\sigma} \hat{\psi} \star \hat{\psi} \star \left[ Q \hat{\psi} \right] \star \left[ Q \hat{\psi} \right] \left( \frac{2\pi}{\alpha} \right) + \mathcal{O} \left( e^{-\pi^2/\alpha} \right) \]

\[ \sim (-1)^{2\sigma} \frac{1 - \alpha^4}{\alpha^5} \text{csch} \left( \frac{\pi^2}{\alpha} \right) + \mathcal{O} \left( e^{-\pi^2/\alpha} \right) \]