Justification of the DNLS equation for sign-varying nonlinearities

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The problem

Density waves in Bose–Einstein condensates are modeled by the Gross-Pitaevskii equation

$$iu_t = -u_{xx} + V(x)u + G(x)|u|^2 u, \quad x \in \mathbb{R},$$

where $V(x) = V(x + 2\pi)$ and $G(x) = G(x + 2\pi)$.

The discrete nonlinear Schrödinger (DNLS) equation

$$i\dot{c}_n + \alpha(c_{n+1} + c_{n-1}) + \beta|c_n|^2 c_n = 0, \quad n \in \mathbb{Z},$$

for some nonzero parameters α and β is thought to be the correct approximation in the tight-binding limit of narrow spectral bands.

Main Question: What happens if $\beta = 0$?

The cubic DNLS equation

Derivation and justification of the cubic DNLS equation with the onsite term:

$$i\dot{c}_n + \alpha(c_{n+1} + c_{n-1}) + \beta|c_n|^2 c_n = 0, \quad n \in \mathbb{Z},$$

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The extended cubic DNLS equations

Derivation of the cubic DNLS equation with the intersite terms:

$$\begin{aligned} i\dot{c}_n &= \alpha(c_{n+1}+c_{n-1}) + \gamma(2|c_n|^2(c_{n+1}+c_{n-1}) + c_n^2(\bar{c}_{n+1}+\bar{c}_{n-1})) \\ & \gamma(|c_{n+1}|^2 c_{n+1} + |c_{n-1}|^2 c_{n-1}). \end{aligned}$$

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We will show that the extended cubic DNLS equation is *a wrong model*. The correct model is the quintic DNLS equation:

$$i\dot{c}_n = \alpha(c_{n+1}+c_{n-1}) + \delta|c_n|^4 c_n.$$

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Model example

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Start with the following Gardner equation

$$u_t + \alpha u u_x + u^2 u_x + u_{xxx} = 0, \quad \alpha \in \mathbb{R},$$

and use small-amplitude slowly-varying approximation

$$u(x,t) = \epsilon^{1/2} \left[\left(A(\sqrt{\epsilon}(x - c_0 t), \epsilon t) e^{i(k_0 x - \omega_0 t)} + \text{c.c} \right) + \mathcal{O}(\epsilon) \right],$$

where $\omega_0 = \omega(k_0) = k_0^3$, $c_0 = \omega'(k_0) = 3k_0^2$, and $A(X,T)$ satisfies the cubic NLS equation

$$iA_T + \frac{1}{2}\omega''(k_0) A_{XX} + \beta |A|^2 A = 0,$$

where $\beta = k_0 - \frac{\alpha^2}{6k_0}$.

Model example (cont.)

For $k_0 = \frac{\alpha}{\sqrt{6}}$, we have $\beta = 0$, so that the cubic NLS equation is not applicable.

For $k_0 = \frac{\alpha}{\sqrt{6}}$, the asymptotic expansion can be rescaled as

$$u(x,t) = \epsilon^{1/4}\left[\left(A(\sqrt{\epsilon}(x - c_0 t), \epsilon t)e^{i(k_0 x - \omega_0 t)} + \mathrm{c.c}\right) + \mathcal{O}(\epsilon^{1/2})\right],$$

where $A(X,T)$ satisfies the cubic–quintic NLS equation

$$iA_T + \frac{1}{2}\omega''(k_0)A_{XX} + \gamma|A|^4 A + i\delta A^2 A_X = 0,$$

where $\gamma = \frac{2\alpha^2}{9k_0^2} = \frac{4}{3}$ and $\delta = \frac{2\alpha}{3k_0} = \frac{2\sqrt{2}}{\sqrt{3}}$.

Semi-classical theory

Let $V(x) = \epsilon^{-2} V_0(x)$, where $V_0(x) \in C^\infty(\mathbb{R})$, $V_0(x + 2\pi) = V_0(x)$, and $\epsilon \ll 1$. For instance

$$V_0(x) = 4\sin^2\left(\frac{x}{2}\right) = 2(1 - \cos(x)) = x^2 + \mathcal{O}(x^4).$$

Let $\Psi(x;k)$ be the Bloch function for the lowest energy band function $E(k)$:

$$L\Psi(x;k) = E(k)\Psi(x;k), \quad L = -\partial_x^2 + \epsilon^{-2} V_0(x),$$

where $k \in [0,1)$.

Bloch and band functions satisfy $E(k) = E(k+1) = E(-k)$ and

$$\Psi(x;k) = \Psi(x;k+1) = e^{-2\pi k i}\Psi(x+2\pi;k) = \bar{\Psi}(x;-k), \quad x \in \mathbb{R}, \quad k \in \mathbb{R}.$$

Wannier functions

Consider Fourier series for $E(k)$ and $\Psi(x;k)$ in $k \in \mathbb{R}$:

$$E(k) = \sum_{n\in\mathbb{Z}} \hat{E}_n e^{i2\pi nk}, \quad \Psi(x;k) = \sum_{n\in\mathbb{Z}} \hat{\psi}_n(x) e^{i2\pi nk}$$

where $\{\hat{\psi}_n(x)\}_{n\in\mathbb{Z}}$ are real-valued functions, which satisfy the reduction

$$\hat{\psi}_n(x) = \hat{\psi}_{n-1}(x-2\pi) = ... = \hat{\psi}_0(x-2\pi n).$$

These functions are referred to as the *Wannier functions*.

If the lowest energy band does not overlap with the other bands, $\hat{\psi}_n(x)$ decays to zero exponentially fast as $|x| \to \infty$, and $\{\psi_n\}_{n\in\mathbb{Z}}$ forms an orthonormal basis for the subspace of $L^2(\mathbb{R})$ associated with the lowest energy band.

Construction of $\hat{\psi}_0(x)$ in tight-binding approximation

The ODE system for Wannier functions

$$\left(L - \hat{E}_0\right) \hat{\psi}_0(x) = \sum_{n\geq 1} \hat{E}_n \left(\hat{\psi}_n(x) + \hat{\psi}_{-n}(x)\right), \quad x \in \mathbb{R},$$

Gaussian approximation near $x = 0$:

$$V(x) \sim \frac{x^2}{\epsilon^2}, \quad \hat{E}_0 \sim \frac{1}{\epsilon}, \quad \hat{\psi}_0(x) \sim \frac{1}{(\pi\epsilon)^{1/4}} e^{-\frac{x^2}{2\epsilon}}.$$

WKB approximation on $(0, 2\pi)$:

$$\hat{\psi}_0(x) \sim A(x) e^{-\frac{1}{\epsilon}\int_0^x S(x')dx'}, \quad x \in (0, 2\pi),$$

where

$$\begin{aligned} S(x) &= \sqrt{V_0(x)}, \\ A(x) &= \frac{1}{(\pi\epsilon)^{1/4}} \exp\left[\int_0^x \frac{1 - S'(x')}{2S(x')} dx'\right], \quad x \in (0, 2\pi). \end{aligned}$$

Note that $\hat{\psi}_0(x)$ diverges as $x \to 2\pi$.

Hierarchy of overlapping integrals

From orthonormality of $\{\hat{\psi}_n\}_{n\in\mathbb{Z}}$, we have

$$\hat{E}_n = \langle L\hat{\psi}_0, \hat{\psi}_n \rangle = \int_{\mathbb{R}} \left[\hat{\psi}_0'(x)\hat{\psi}_n'(x) + \epsilon^{-2} V_0(x)\hat{\psi}_0(x)\hat{\psi}_n(x) \right] dx, \quad n \in \mathbb{N}.$$

Thanks to the small parameter ϵ in the tight-binding limit, we have

$$\ldots \ll |\hat{E}_2| \ll |\hat{E}_1| \ll |\hat{E}_0|,$$

with

$$\hat{E}_1 \sim -\frac{4\sqrt{V_0(\pi)}}{\pi^{1/2}\epsilon^{3/2}} \exp\left(-\frac{2}{\epsilon} \int_0^{\pi} \sqrt{V_0(x)} dx + \int_0^{\pi} \frac{1 - S'(x)}{S(x)} dx \right) \equiv \alpha\mu,$$

where $\mu = \epsilon^{-3/2} e^{-\kappa/\epsilon}$ is a new small parameter.

A. Aftalion, B. Helffer, Rev. Math. Phys. **21** 229-278 (2009)

Reductions to the cubic onsite DNLS equation

Substitute

$$u(x,t) = \epsilon^{1/4}\mu^{1/2}\left(\Psi_0(x,T) + \mu\Psi_1(x,t)\right)e^{-i\hat{E}_0 t},$$

to the Gross–Pitaevskii equation with $T = \mu t$,

$$\Psi_0(x,T) = \sum_{n\in\mathbb{Z}} c_n(T)\hat{\psi}_n(x),$$

for some coefficients $\{c_n(T)\}_{n\in\mathbb{Z}}$. Then,

$$\begin{aligned} i\partial_t\Psi_1 &= (L-\hat{E}_0)\Psi_1 + \sum_{n\in\mathbb{Z}}\left(-i\dot{c}_n + \mu^{-1}\sum_{m\in\mathbb{N}}\hat{E}_m\left(c_{n+m}+c_{n-m}\right)\right)\hat{\psi}_n \\ &\quad + \epsilon^{1/2}G(x)|\Psi_0+\mu\Psi_1|^2(\Psi_0+\mu\Psi_1). \end{aligned}$$

Note that

$$\int_{\mathbb{R}} G(x)\hat{\psi}_0^4(x)dx \sim \frac{1}{\pi\epsilon}\int_{\mathbb{R}} G(x)e^{-\frac{2x^2}{\epsilon}}dx \sim \frac{1}{(2\pi\epsilon)^{1/2}}G(0)$$

whereas overlapping integrals for products of $\{\hat{\psi}_n\}_{n\in\mathbb{Z}}$ are negligibly small.

Justification theorem

If Ψ_1 lies in the orthogonal complement of the lowest energy band, orthogonal projections give at the leading order

$$i\dot{c}_n = \alpha(c_{n+1} + c_{n-1}) + \beta|c_n|^2 c_n,$$

where $\alpha = \hat{E}_1/\mu$ and $\beta = G(0)/(2\pi)^{1/2}$.

Theorem: Let $\mathbf{c}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ be a solution of the cubic DNLS equation, so that initial data $\mathbf{c}(0)$ satisfy the bound

$$\left\| u_0 - \epsilon^{1/4}\mu^{1/2} \sum_{n\in\mathbb{Z}} c_n(0)\hat{\psi}_n \right\|_{H^1} \leq C_0 \mu^{3/2}$$

for some $C_0 > 0$. Then, for any $0 < \mu \ll 1$, there exists a μ-independent constant $C > 0$ such that the Gross–Pitaevskii equation has a solution $u(t) \in C^1([0, T_0/\mu], \mathcal{H}^1)$ satisfying the bound

$$\forall t \in [0, T_0/\mu] : \quad \left\| u(\cdot, t) - \epsilon^{1/4}\mu^{1/2} e^{-i\hat{E}_0 t} \sum_{n\in\mathbb{Z}} c_n(T)\hat{\psi}_n \right\|_{H^1} \leq C\mu^{3/2}.$$

Justification of time-dependent equations

The time-evolution problem can be written in the form

$$i\psi_t = \left(L - \hat{E}_0\right)\psi + \mu R(\mathbf{c}) + \mu N(\mathbf{c}, \psi),$$

where

$$\|R(\mathbf{c})\|_{\mathcal{H}^1} \leq C_R \|\mathbf{c}\|_{l^1(\mathbb{Z})}$$

and

$$\|N(\mathbf{c}, \psi)\|_{\mathcal{H}^1} \leq C_N \left(\|\mathbf{c}\|_{l^1} + \|\psi\|_{\mathcal{H}^1}\right).$$

Remarks:

- The quadratic form norm $\|u\|_{\mathcal{H}^1} := (\langle Lu, u\rangle_{L^2})^{1/2}$ controls the Sobolev space norm $\|u\|_{H^1} \leq \|u\|_{\mathcal{H}^1}$ $H^1(\mathbb{R})$.
- ψ is a remainder term, which occurs after one normal-form transformation to remove the non-resonance cubic terms.

Local well-posedness and energy estimate

- Let $\mathbf{c}(T) \in C^1(\mathbb{R}, l^1(\mathbb{Z}))$ and $\psi_0 \in \mathcal{H}^1(\mathbb{R})$. Then, there exists a $t_0 > 0$ and a unique solution $\psi(t) \in C^0([0,t_0], \mathcal{H}^1(\mathbb{R})) \cap C^1([0,t_0], L^2(\mathbb{R}))$.
- For any $0 < \mu \ll 1$ and every $M > 0$, there exist a μ-independent constant $C_E > 0$ such that

$$\left| \frac{d}{dt} \|\psi(t)\|_{\mathcal{H}^1} \right| \leq \mu C_E \left(\|\mathbf{c}\|_{l^1(\mathbb{Z})} + \|\psi(t)\|_{\mathcal{H}^1} \right) \quad (1)$$

  as long as $\|\psi\|_{\mathcal{H}^1} \leq M$.
- By Gronwall's inequality, we thus have

$$\sup_{t \in [0, T_0/\mu]} \|\psi(t)\|_{\mathcal{H}^1(\mathbb{R})} \leq \left(\|\psi(0)\|_{\mathcal{H}^1(\mathbb{R})} + C_E T_0 \sup_{T \in [0,T_0]} \|\mathbf{c}(T)\|_{l^1(\mathbb{Z})} \right) e^{C_E T_0}$$

D.P., G. Schneider, JDE **248**, 837-849 (2010)

Reductions to the quintic onsite DNLS equation

If $G(0) = 0$, then $\beta = 0$ at the leading order. In particular, let us consider

$$V(-x) = V(x), \quad G(-x) = -G(x), \quad x \in \mathbb{R}.$$

Then,

$$\beta = \epsilon^{1/2} \int_{\mathbb{R}} G(x) \hat{\psi}_0^4(x) dx = 0$$

to all orders of ϵ.

In this case,

$$\int_{\mathbb{R}} G(x) \hat{\psi}_0^2(x) \hat{\psi}_0^2(x - 2\pi) dx = 0$$

and the nonzero cubic intersite terms are of the same order as the linear overlapping integrals

$$\int_{\mathbb{R}} G(x) \hat{\psi}_0^3(x) \hat{\psi}_0(x - 2\pi) dx = \mathcal{O}(\epsilon^{1/2} \mu).$$

New asymptotic expansion

Consider a rescaled asymptotic exapansion

$$\Psi(x,t) = \epsilon^{-1/4}\mu^{1/4}\left(\Psi_0 + \mu^{1/2}\Psi_1 + \mu\Psi_2\right) e^{-i\hat{E}_0 t},$$

where

$$\Psi_0 = \sum_{n\in\mathbb{Z}} c_n(T)\hat{\psi}_n(x), \quad \Psi_1 = \sum_{n\in\mathbb{Z}} |c_n(T)|^2 c_n(T)\hat{\varphi}_n(x),$$

and

$$(L - \hat{E}_0)\hat{\varphi}_0(x) = -\epsilon^{-1/2}G(x)\hat{\psi}_0^3(x), \quad x \in \mathbb{R}.$$

If Ψ_2 lies in the orthogonal complement of the lowest energy band, orthogonal projections give at the leading order

$$i\dot{c}_n = \alpha(c_{n+1} + c_{n-1}) + \chi|c_n|^4 c_n,$$

where $\alpha = \hat{E}_1/\mu < 0$ and

$$\chi = 3\epsilon^{-1/2}\int_{\mathbb{R}} G(x)\hat{\psi}_0^3(x)\hat{\varphi}_0(x)dx = -3\langle (L - \hat{E}_0)\hat{\varphi}_0, \hat{\varphi}_0\rangle < 0.$$

Numerical test : existence of gap solitons

Stationary gap solitons of the Gross–Pitaevskii equation

$$-\Phi''(x) + V(x)\Phi(x) + G(x)\Phi^3(x) = \omega\Phi(x), \quad x \in \mathbb{R}$$

for even $V(x)$ and odd $G(x)$ exist in the semi-infinite gap.

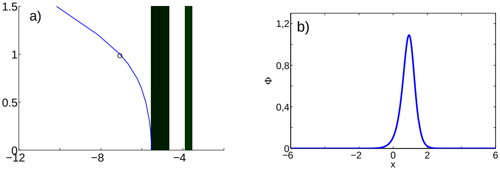

Figure: The solution family of gap solitons for $V(x) = 6(1 - \cos(x))$ and $G(x) = -10\sin(x)$: The L^2-norm N versus ω (left) and the spatial profile of gap soliton corresponding to marked point with a black circle (right).

Another existence test

Stationary quintic DNLS equation

$$\alpha(c_{n+1} + c_{n-1}) + \chi c_n^5 = \Omega c_n, \quad n \in \mathbb{Z},$$

where $\alpha < 0$ and $\chi < 0$ for the lowest energy band. Positive, exponentially decaying solutions $\{\phi_n\}_{n\in\mathbb{Z}}$ exist for $\Omega < 2\alpha$ in the semi-infinite gap.

Stationary cubic intersite DNLS equation

$$\alpha(c_{n+1} + c_{n-1}) + \gamma(3c_n^2(c_{n+1} - c_{n-1}) - c_{n+1}^3 + c_{n-1}^3) = \Omega c_n, \quad n \in \mathbb{Z}.$$

No localized solutions exist for any α, γ, Ω, at least in the slowly varying approximation

$$c_{n\pm1} = c(x_n) \pm hc'(x_n) + \frac{h^2}{2}c''(x_n) + \mathcal{O}(h^3),$$

where

$$\alpha c''(x) - \gamma c'(x)\left[(c')^2 + 3cc''\right] = \Omega c(x), \quad x \in \mathbb{R}.$$

Reduction to the continuous NLS equation

In the continuous limit, the stationary Gross–Pitaevskii equation

$$-\Phi''(x) + V(x)\Phi(x) + G(x)\Phi^3(x) = \omega\Phi(x), \quad x \in \mathbb{R}$$

admits a reduction to the stationary quintic NLS equation

$$\alpha c''(x) + \chi c^5(x) = \Omega c(x), \quad n \in \mathbb{Z},$$

where $\alpha < 0$ and $\chi < 0$ for the lowest energy band.

The quintic NLS equation is critical with respect to L^2 norm of the stationary solution. However, the higher-order terms from the Gross–Pitaevskii equation with $V(x)$ break this criticality and result in orbitally stable stationary gap solitons in the semi-infinite gap.