Justification of tight-binding approximation for space-periodic problems

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Conference on Dynamical Systems, Differential Equations and Applications, Arlington Texas USA, May 18 - 21, 2008

Introduction

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

$$iu_t = -\nabla^2 u + V(x)u + \sigma |u|^2 u,$$

where $V(x)$ is a bounded real-valued potential on $\mathbb{R}^N$, $u(x,t)$ is a complex-valued wave function, and $\sigma = \pm 1$.

Examples of $V(x)$ ($N = 1$):

- $V(x) = x^2$ models a parabolic trap
- $V(x + 2\pi) = V(x)$ models an optical lattice

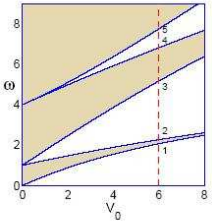
We would like to study dynamics of localized states of the Gross–Pitaevskii equation residing in spectral gaps of the Schrödinger operators with periodic potentials. Such states are often called gap solitons.

Existence of gap solitons

Time-periodic solutions $u(x,t) = \phi(x)e^{-i\omega t}$ with $\omega \in \mathbb{R}$ satisfy a stationary elliptic problem with a periodic potential

$$\omega\phi = -\nabla^2\phi + V(x)\phi + \sigma|\phi|^2\phi$$

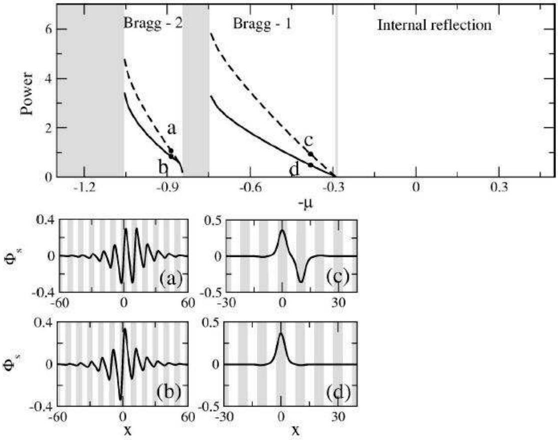
Spectrum of $L = -\nabla^2 + V(x)$ for $V(x) = V_0 \sin^2(x)$ and $N = 1$:



Theorem:[Pankov, 2005] Let V be a real-valued bounded periodic potential. Let ω be in a finite gap of the spectrum of $L = -\nabla^2 + V(x)$. There exists a non-trivial weak solution $U \in H^1(\mathbb{R}^N)$, which is continuous on $x \in \mathbb{R}^N$ and decays exponentially as $|x| \to \infty$.

Numerical approximation of gap solitons

D.P., A. Sukhorukov, Yu. Kivshar, PRE 70, 036618 (2004)
for $V(x) = V_0 \sin^2(x)$ with $V_0 = 1$ and $\sigma = +1$:



Asymptotic reductions of the GP equation

The Gross–Pitaevskii equation in 1D can be reduced asymptotically with a multiple scale expansion method to one of the three models.

- Coupled-mode (Dirac) equations for **small-amplitude** potentials

$$\begin{cases} i(a_t + a_x) + b = \sigma(|a|^2 + 2|b|^2)a \\ i(b_t - b_x) + a = \sigma(2|a|^2 + |b|^2)b \end{cases}$$

- Envelope (NLS) equations for **finite-amplitude** potentials near band edges

$$ia_t + a_{xx} + \sigma|a|^2 a = 0$$

- Lattice (DNLS) equations for **large-amplitude** potentials

$$i\dot{a}_n + \alpha(a_{n+1} + a_{n-1}) + \sigma|a_n|^2 a_n = 0.$$

Formal derivation of the DNLS equation

G. Alfimov, P. Kevrekidis, V. Konotop, M. Salerno, PRE 66, 046608 (2002)

Assume that the l-th spectral band of $L = -\nabla^2 + V(x)$ is isolated from all other bands and fix ω_0 at the central point of the band. Assume that there is a small parameter μ, such that the size of the band is $O(\mu)$. Then, look for solutions of

$$iu_t = -\nabla^2 u + V(x)u + \sigma|u|^2 u,$$

using the asymptotic expansion

$$u(x,t) = \mu^{1/2}\left(u_0(x,T) + \mu U(x,t)\right) e^{-i\omega_0 t},$$

with $T = \mu t$ and $U(x,t)$ is the residual term to the leading-order term

$$u_0(x,T) = \sum_{n\in\mathbb{Z}} \phi_n(T)\hat{u}_{l,n}(x),$$

where $\{\hat{u}_{l,n}\}_{n\in\mathbb{Z}}$ is a complete set of Wannier functions for the l-th spectral band and $\{\phi_n\}_{n\in\mathbb{Z}}$ is a set of complex-valued amplitudes.

The DNLS equation

The function $U(x,t)$ is not growing in t if $\{\phi_n\}_{n\in\mathbb{Z}}$ satisfies the DNLS equation

$$i\dot{\phi}_n = \alpha\left(\phi_{n+1} + \phi_{n-1}\right) + \sigma\beta|\phi_n|^2\phi_n,$$

for some μ-independent constants α and β.

Recent results on justification of lattice equations:

- lattice equations for a nonlinear heat equation with a periodic diffusive term in Scheel–Van Vleck (2007)
- lattice equations for an infinite sequence of interacting pulses in reaction–diffusion equations in Zelik–Mielke (2007)
- interaction of modulated pulses in periodic potentials in Giannoulis, Mielke and Sparber (2008)
- finite-size lattice equations for the Gross–Pitaevskii equation with a multiple-well trapping potential in Bambusi–Sacchetti (2007)

Fourier–Bloch transform for periodic potentials

Operator $L = -\partial_x^2 + V(x)$ is extended to a self-adjoint operator which maps $H^2(\mathbb{R})$ to $L^2(\mathbb{R})$. Spectrum $\sigma(L)$ is purely continuous, real, and consists of the union of spectral bands.

Let $u(x;k) = e^{ikx} w(x;k)$ be the Bloch function, where $k \in [-1/2, 1/2]$ and $w(x;k)$ is a periodic eigenfunction of $L_k w = \omega w$, where

$$L_k = e^{-ikx} L e^{ikx} = -(\partial_x^2 + ik)^2 + V(x).$$

Let (ω_l, u_l) denote the l-th eigenvalue–eigenfunction pair. We normalize the amplitude and phase of the Bloch functions by two conditions:

$$\int_{\mathbb{R}} \bar{u}_{l'}(x,k') u_l(x,k) dx = \delta_{l,l'} \delta(k - k')$$

and

$$u_l(x;-k) = \bar{u}_l(x;k)$$

Wannier functions

The band function $\omega_l(k)$ and the Bloch function $u_l(x;k)$ are periodic with respect to k with period 1. Therefore, we can use the Fourier series

$$\omega_l(k) = \sum_{n\in\mathbb{Z}} \hat{\omega}_{l,n} e^{i2\pi nk}, \quad u_l(x;k) = \sum_{n\in\mathbb{Z}} \hat{u}_{l,n}(x) e^{i2\pi nk}$$

Because of the phase normalization of $u_l(x;k)$, the functions $\{\hat{u}_{l,n}\}$ are real-valued.

Because of the Floquet theorem, we have

$$u_l(x+2\pi;k) = u_l(x;k)e^{i2\pi k} \Rightarrow \hat{u}_{l,n}(x) = \hat{u}_{l,n-1}(x-2\pi) = \hat{u}_{l,0}(x-2\pi n).$$

The functions in the set $\{\hat{u}_{l,n}\}$ are called the Wannier functions.

Properties of Wannier functions

W. Kohn, Phys. Rev. **115**, 809 (1959)

- Orthogonality

$$\langle \hat{u}_{l',n'}, \hat{u}_{l,n} \rangle := \int_{\mathbb{R}} \hat{u}_{l',n'}(x) \hat{u}_{l,n}(x) dx = \delta_{l,l'} \delta_{n,n'}$$

- Basis and unitary transformation in $L^2(\mathbb{R})$

$$\forall u \in L^2(\mathbb{R}) : \quad u(x) = \sum_{l \in \mathbb{N}} \sum_{n \in \mathbb{Z}} c_{l,n} \hat{u}_{l,n}(x), \quad c_{l,n} = \langle \hat{u}_{l,n}, u(x) \rangle.$$

- If the l-th spectral band is disjoint from other bands, then

$$|\hat{u}_{l,n}(x)| \leq C_l e^{-\eta_l |x - 2\pi n|}, \quad \forall n \in \mathbb{Z}, \ \forall x \in \mathbb{R}.$$

New properties of Wannier functions

Fix $l \in \mathbb{N}$ and assume that the l-th spectral band is disjoint from other spectral bands.

- If $\vec{\mathbf{c}} \in l^1(\mathbb{Z})$ and $u(x) = \sum_{n \in \mathbb{Z}} c_n \hat{u}_{l,n}(x)$, then $u \in H^1(\mathbb{R})$, such that the function $u(x)$ is bounded, continuous, and decaying to zero as $|x| \to \infty$.
- If $\hat{u}_{l,n}(x)$ satisfies the exponential decay and $|c_n| \leq C r^{|n|}$ uniformly on $n \in \mathbb{Z}$ for some $C > 0$ and $0 < r < 1$, then $u(x)$ decays to zero exponentially fast as $|x| \to \infty$.

Tight-binding approximation

Let μ be a small parameter of $V(x)$ and consider a small interval $0 < \mu \ll 1$. Fix $l \in \mathbb{N}$ and assume the following properties:

- The l-th spectral band is bounded away from the rest of $\sigma(L)$:

$$\inf_{\forall m \in \mathbb{N} \backslash \{l\}} \inf_{\forall k \in \mathbb{T}} |\omega_m(k) - \hat{\omega}_{l,0}| \geq 1$$

- Center of the l-th band is bounded as $\mu \to 0$:

$$|\hat{\omega}_{l,0}| \lesssim 1$$

- The width of the l-th band is small as $\mu \to 0$:

$$C_1^- \mu \leq |\hat{\omega}_{l,1}| \leq C_1^+ \mu, \qquad |\hat{\omega}_{l,k}| \leq C_2 \mu^2, \quad k \geq 2.$$

- There exists a non-zero $\hat{u}_0$ such that

$$\|\hat{u}_{l,0} - \hat{u}_0\|_{L^\infty(\mathbb{R})} \lesssim \mu$$

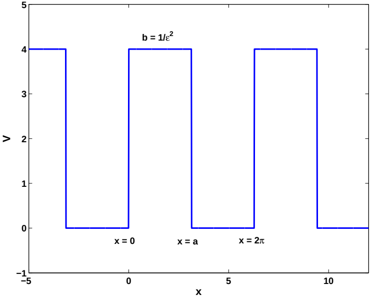
- The Wannier function $\hat{u}_{l,0}$ decays exponentially in the sense

$$\sup_{[-2\pi n, -2\pi(n-1)] \cup [2\pi n, 2\pi(n+1)]} |\hat{u}_{l,0}(x)| \leq C \mu^n, \qquad n \geq 1.$$

Example of V

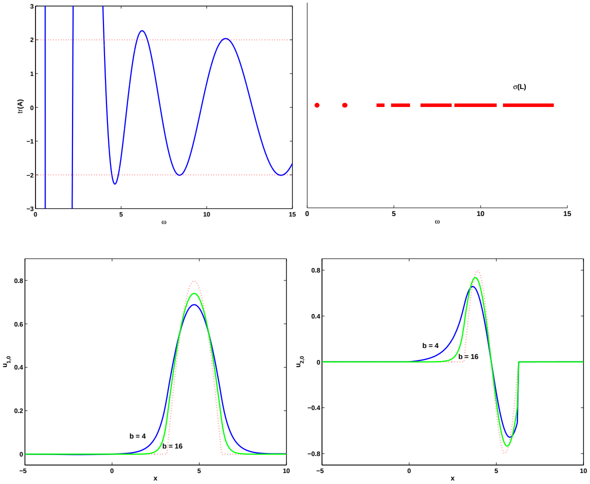
Let us consider V in the form

$$V(x) = \begin{cases} \varepsilon^{-2}, & x \in (0,\pi) \bmod (2\pi) \\ 0, & x \in (\pi, 2\pi) \bmod (2\pi) \end{cases}$$



Explicit computations show that $\mu = \varepsilon e^{-\pi/\varepsilon}$.

Spectrum and Wannier functions



Main results

Theorem 1: Let $\vec{\phi}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ be a solution of the DNLS equation

$$i\dot{\phi}_n + \alpha\left(\phi_{n+1} + \phi_{n-1}\right) + \sigma\beta|\phi_n|^2\phi_n = 0,$$

with $\alpha = \hat{\omega}_{l,1}/\mu$, $\beta = \|\hat{u}_{l,0}\|^4_{L^4(\mathbb{R})}$, and initial data $\vec{\phi}_0$ satisfy the bound

$$\left\| \phi_0 - \mu^{1/2} \sum_{n\in\mathbb{Z}} \phi_n(0)\hat{u}_{l,n}(x) \right\|_{\mathcal{H}^1(\mathbb{R})} \leq C_0 \mu^{3/2}$$

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 $u(t) \in C^1([0, T_0/\mu], \mathcal{H}^1(\mathbb{R}))$ satisfying the bound

$$\forall t \in [0, T_0/\mu] : \quad \left\| \phi(\cdot, t) - \mu^{1/2} \sum_{n\in\mathbb{Z}} \phi_n(T)\hat{u}_{l,n} \right\|_{\mathcal{H}^1(\mathbb{R})} \leq C \mu^{3/2}.$$

Here $\mathcal{H}^1(\mathbb{R})$ is equipped with $\|u\|_{\mathcal{H}^1} = \|(1+L)^{1/2}u\|_{L^2(\mathbb{R})}$.

Main results

Theorem 2: Let $\vec{\phi} \in l^1(\mathbb{Z})$ be a solution of the stationary DNLS equation

$$\alpha\left(\phi_{n+1} + \phi_{n-1}\right) + \sigma\beta|\phi_n|^2\phi_n = \Omega\phi_n$$

with $\Omega = (\omega - \hat{\omega}_{l,0})/\mu$. Assume that the linearized lattice equation at $\vec{\phi}$ has a one-dimensional kernel in $l^2(\mathbb{Z})$ spanned by the eigenmode $\{i\vec{\phi}\}$ and the rest of the spectrum is bounded away from zero. Then, for any $0 < \mu \ll 1$, there exists a μ-independent constant $C > 0$ such that the stationary Gross–Pitaevskii equation

$$-\phi'' + V(x)\phi + \sigma|\phi|^2\phi = \omega\phi$$

has a solution $\phi \in H^1(\mathbb{R})$ with

$$\left\|\phi(x) - \mu^{1/2}\sum_{n\in\mathbb{Z}}\phi_n\hat{u}_{l,n}(x)\right\|_{H^1(\mathbb{R})} \leq C\mu^{3/2}.$$

Moreover, $\phi(x)$ decays to zero exponentially fast as $|x| \to \infty$ if $\{\phi_n\}$ decays to zero exponentially fast as $|n| \to \infty$.

Justification of time-dependent equations

After the substitution

$$u(x,t) = \sqrt{\mu}\left(\varphi(x,T) + \mu\psi(x,t)\right)e^{-i\hat{\omega}_{l,0}t},$$

with

$$\varphi(x,T) = \sum_{n\in\mathbb{Z}} \phi_n(T)\hat{u}_{l,n}(x), \quad T = \mu t,$$

we obtain the time-evolution problem

$$i\psi_t = (L - \hat{\omega}_{l,0})\,\psi + \mu R(\vec{\phi}) + \mu\sigma N(\vec{\phi},\psi),$$

where

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

and

$$\|N(\vec{\phi},\psi)\|_{\mathcal{H}^1(\mathbb{R})} \leq C_N\left(\|\vec{\phi}\|_{l^1(\mathbb{Z})} + \|\psi\|_{\mathcal{H}^1(\mathbb{R})}\right).$$

Local well-posedness and energy estimate

- Let $\vec{\phi}(T) \in C^1(\mathbb{R}, l^1(\mathbb{Z}))$ 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

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

  as long as $\|\psi\|_{\mathcal{H}^1} \leq M$.

- By Gronwall's inequality, we thus have

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

Justification of stationary equations

Let $\omega = \hat{\omega}_{l,0} + \mu\Omega$ and consider a decomposition

$$\phi(x) = \mu^{1/2} \left(\varphi(x) + \mu\psi(x) \right),$$

where $\varphi \in \mathcal{E}_l$ and $\psi \in \mathcal{E}_l^{\perp}$. Then, ψ solves

$$-\psi'' + V(x)\psi - \hat{\omega}_{l,0}\psi = \mu\Omega\psi - \sigma\mu Q|\varphi + \mu\psi|^2 (\varphi + \mu\psi)$$

while $\vec{\phi}$ satisfies

$$\frac{1}{\mu}\sum_{m\in\mathbb{N}} \hat{\omega}_{l,m} \left(\phi_{n+m} + \phi_{n-m}\right) + \sigma \sum_{(n_1,n_2,n_3)} K_{n,n_1,n_2,n_3}\phi_{n_1}\bar{\phi}_{n_2}\phi_{n_3} = \Omega\phi_n - \sigma\mu P_n(\varphi + \mu\psi)$$

where

$$K_{n,n_1,n_2,n_3} = \int_{\mathbb{R}} \hat{u}_{l,n}(x)\hat{u}_{l,n_1}(x)\hat{u}_{l,n_2}(x)\hat{u}_{l,n_3}(x)dx$$

Stationary localized solutions

Solutions of the stationary DNLS equation

$$\left(\Omega - \sigma\beta\phi_n^2\right)\phi_n = \alpha\left(\phi_{n+1} + \phi_{n-1}\right)$$

have the following properties (MacKay, Aubry, 1994):

- All solutions in $l^1(\mathbb{Z})$ are real-valued.
- Solutions can be classified by the number of non-zero nodes in the limiting compact solutions at $\alpha = 0$:

$$\lim_{\alpha\to 0}\phi_n = \left\{ \begin{array}{c} \pm(\sigma\Omega/\beta)^{1/2}, \quad n \in U_\pm \\ 0, \quad n \in U_0 \end{array} \right.$$

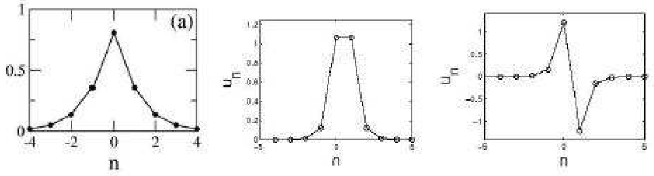
  where $\dim(U_0) = \infty$ and $\dim(U_\pm) < \infty$.
- The linearized lattice equation for real-valued solutions

$$\left(L_\alpha\vec{\psi}\right)_n = \left(\Omega - 3\sigma\phi_n^2\right)\psi_n - \alpha\left(\psi_{n+1} + \psi_{n-1}\right)$$

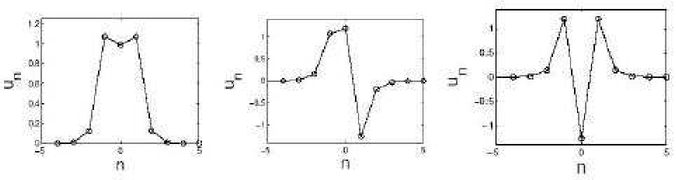
  has no zero eigenvalues for small α.

Examples of localized solutions

D.P., P. Kevrekidis, D. Franzeskakis, Physica D **212**, 1-19 (2005)



Left: $U_+ = \{0\}$; Middle: $U_+ = \{0, 1\}$; Right: $U_+ = \{1\}$, $U_- = \{0\}$



Left: $U_+ = \{-1, 0, 1\}$; Right: $U_+ = \{-1, 1\}$, $U_- = \{0\}$

Other extensions

- Results remain valid in $N = \{2, 3\}$ for a class of separable potentials

$$V(x_1, x_2, x_3) = V_1(x_1) + V_2(x_2) + V_3(x_3).$$

  Assumption of non-degeneracy for linearized lattice equations is satisfied for many localized solutions such as 2D and 3D discrete vortices.

- Results remain valid for piecewise constant potentials of the form

$$V(x + L) = V(x)$$

  in the limit of large L.

- It is more challenging to extend results to non-separable and non-constant potentials, for instance to the potential

$$V(x) = \epsilon^{-2} \sin^2(x)$$

  The distance between spectral bands diverge as $\epsilon \to 0$ but so are the values of $\hat{\omega}_{l,0}$.