Tight-binding approximation and nonlinear Schrödinger lattices

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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 $V(x)$:

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

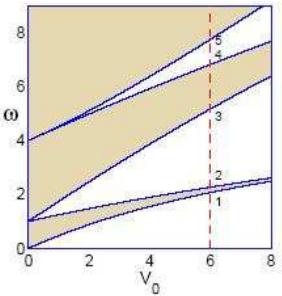
We would like to study localized states of the Gross–Pitaevskii equation residing in spectral gaps of the Schrödinger operators with periodic potentials. Such states are often called gap solitons.

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

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

The associated Schrödinger operator is $L = -\nabla^2 + V(x)$ and an example of its spectrum is computed for $V(x) = V_0 \sin^2(x)$ in one dimension.



Existence of gap solitons

Previous results:

- Construction of multi-humped gap solitons in Alama-Li (1992)
- Bifurcations of gap solitons from band edges in Kupper-Stuart (1990) and Heinz-Stuart (1992)
- Existence of critical points of energy in Stuart (1995) and Pankov (2005)
- Multiplicity of branches of gap solitons in Heinz (1995)
- Existence of critical points of energy with L^2-normalization in Buffoni-Esteban-Sere (2006)

Theorem:[Pankov, 2005] Let $V(x)$ 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 $|x| \to \infty$.

Illustration of solution branches

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

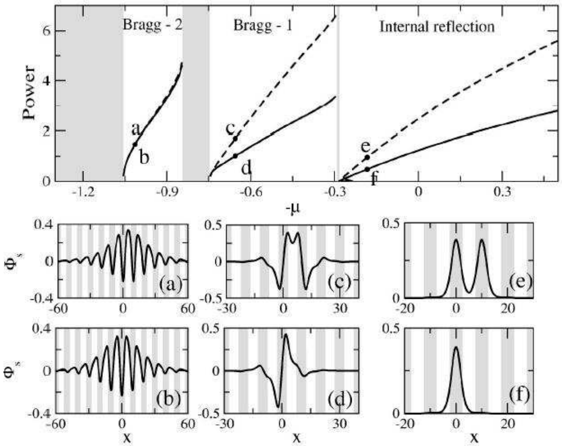
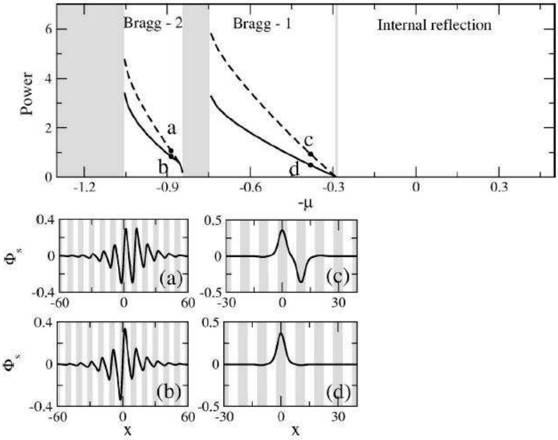


Illustration of solution branches

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

The stationary problem with a periodic potential can be reduced asymptotically to the following problems:

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

$$\left\{ \begin{array}{l} ia'(x) + \Omega a + b = \sigma(|a|^2 + 2|b|^2)a \\ -ib'(x) + \Omega b + a = \sigma(2|a|^2 + |b|^2)b \end{array} \right.$$

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

$$a''(x) + \Omega a + \sigma |a|^2 a = 0$$

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

$$a_{n+1} + a_{n-1} + \Omega a_n + \sigma |a_n|^2 a_n = 0.$$

Localized solutions of reduced equations exist in the analytic form.

Formal derivation of the lattice 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 multi-scale 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. This formal derivation can be extended to the space of any dimension $N \geq 1$.

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)
- finite-size lattice equations for the Gross–Pitaevskii equation with a multiple-well trapping potential in Bambusi–Sacchetti (2007)
- interaction of modulated pulses in periodic potentials in Giannoulis, Mielke and Sparber (2008)

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 $L^2(\mathbb{R})$. Therefore, $\sigma(L)$ is purely continuous, real, and consists of the union of spectral bands. To define the spectral bands, consider Bloch functions $u(x;k) = e^{ikx} w(x;k)$, 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 Bloch decomposition generalizes the Fourier transform but it is inconvenient for a reduction of a continuous PDE to a lattice equation. Instead, we shall develop the Wannier decomposition.

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 spectral 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

Assume that V is real-valued, piecewise-continuous, and 2π-periodic potential. 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 $|x| \to \infty$.

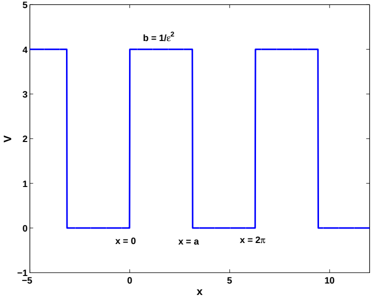
  Proof:
  $$\|u\|_{H^1(\mathbb{R})} \leq \sum_{n \in \mathbb{Z}} |c_n| \|\hat{u}_{l,n}\|_{H^1(\mathbb{R})} = \|\hat{u}_{l,0}\|_{H^1(\mathbb{R})} \|\vec{\mathbf{c}}\|_{l^1(\mathbb{Z})},$$
  where
  $$\|\hat{u}_{l,0}\|^2_{H^1(\mathbb{R})} \leq \int_{\mathbb{R}} \left(\left|\hat{u}'_{l,0}(x)\right|^2 + (1 + V(x)) \left|\hat{u}_{l,0}(x)\right|^2 \right) dx = 1 + \hat{\omega}_{l,0}.$$

- 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 $|x| \to \infty$.

Class of potentials

Let us consider V in the form

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



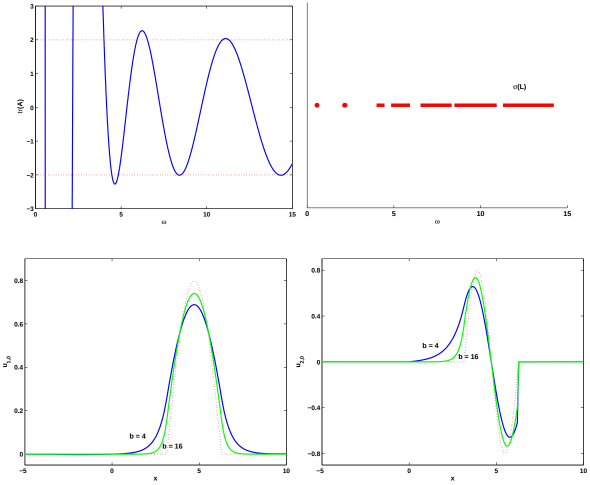
Trace of the monodromy matrix for $0 < \omega < \varepsilon^{-2}$:

$$2\cosh(a\sqrt{b-\omega})\cos\left[(2\pi - a)\sqrt{\omega}\right] + \frac{b-2\omega}{\sqrt{\omega(b-\omega)}}\sinh(a\sqrt{b-\omega})\sin\left[(2\pi-a)\sqrt{\omega}\right]$$

Properties of spectral bands and Wannier functions

- (band separation) $\inf_{\forall m \in \mathbb{N}\backslash\{l\}} \inf_{\forall k \in \mathbb{T}} |\omega_m(k) - \hat{\omega}_{l,0}| \geq 1$
- (band boundness) $|\hat{\omega}_{l,0}| \lesssim 1$
- (tight-binding approximation) $|\hat{\omega}_{l,n}| \leq C_n \varepsilon^n e^{-\frac{na}{\varepsilon}}$
- (boundness of norms) $\|\hat{u}_{l,0}\|_{H^1(\mathbb{R})} \lesssim 1$
- (compact support) $|\hat{u}_{l,0}(x) - \hat{u}_0(x)| \lesssim \varepsilon$, where $\hat{u}_0 = \frac{\sqrt{2}}{\sqrt{2\pi - a}} \sin \frac{\pi l(2\pi - x)}{2\pi - a}$ supported on $[a, 2\pi]$
- (exponential decay) $|\hat{u}_{l,0}(x)| \leq C_n \varepsilon^n e^{-\frac{na}{\varepsilon}}$ on $[-2\pi n, -2\pi(n-1)] \cup [2\pi n, 2\pi(n+1)]$

Numerical illustration of Wannier functions



Main results

Theorem 1: Denote $\mu = \varepsilon e^{-\frac{a}{\varepsilon}}$. Let $\{\phi_n\}_{n\in\mathbb{Z}}$ define a vector solution $\vec{\phi} \in l^1(\mathbb{Z})$ of the lattice equation

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

with $\alpha = \hat{\omega}_{l,1}/\mu$, $\beta = \|\hat{u}_{l,0}\|^4_{L^4(\mathbb{R})}$, and $\Omega = (\omega - \hat{\omega}_{l,0})/\mu$. 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. There exist $\mu_0, C > 0$, such that the stationary elliptic problem

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

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

$$\forall 0 < \mu < \mu_0 : \quad \left\|\phi(x) - \mu^{1/2}\sum_{n\in\mathbb{Z}}\phi_n\hat{u}_{l,n}(x)\right\|_{H^1(\mathbb{R})} \leq C\mu^{3/2}.$$

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

Main results

Theorem 2: Let $\vec{\phi}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ be a solution of the DNLS equation with initial data $\vec{\phi}_0$ satisfying 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 $\mu \in (0, \mu_0)$ with sufficiently small $\mu_0 > 0$, there exists a μ-independent constant $C > 0$ such that the GP equation has a solution $u(t) \in C^1([0, T_0/\mu], \mathcal{H}^1(\mathbb{R}))$ satisfying the bound

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

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

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

and ψ is orthogonal to all $\hat{u}_{l,n}$ in $L^2(\mathbb{R})$. 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

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

where

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

Examples of localized solutions in one dimension

Stationary lattice equation in one dimension:

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

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

$$\lim_{\alpha \to 0} \phi_n = \begin{cases} \pm(\sigma\Omega/\beta)^{1/2}, & n \in U_\pm \\ 0, & n \in U_0 \end{cases}$$

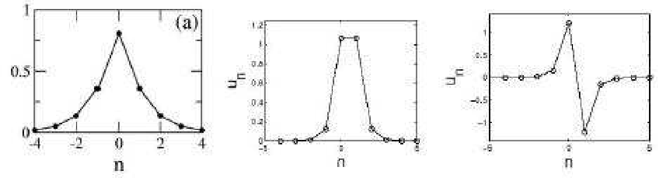
  where $\dim(U_0) = \infty$ and $\dim(U_\pm) < \infty$.
- The linearized lattice equation for real-valued solutions

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

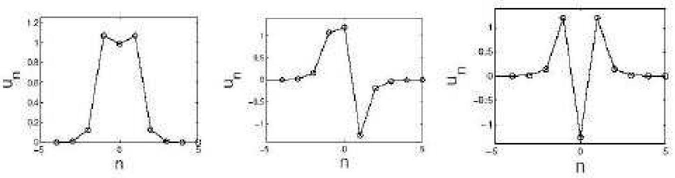
  has no zero eigenvalues for small α.

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

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 $\psi(t) \in C^1([0, t_0], \mathcal{H}^1(\mathbb{R}))$.
- Let $\vec{\phi}_0 \in l^1(\mathbb{Z})$. Then, there exist a $T_0 > 0$ and a unique solution $\vec{\phi}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ of the DNLS equation.
- For any $\mu \in [0, 1]$ and every $M > 0$, there exist a μ-independent constant $C_E > 0$ such that

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

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

- By Gronwall's inequality, we thus have

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

Other extensions

- Results can be extended to the space of two and three dimensions 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 can be extended for piecewise constant potentials of the form

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

in the limit of large L.

- It is more challenging to extend the problem 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 $\hat{\omega}_{l,0}$.