Bloch decomposition based method for quantum dynamics with periodic potentials

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Supported by the NSFC (11071139, 11211120151) and the National Basic Research Program of China (2011CB309705)

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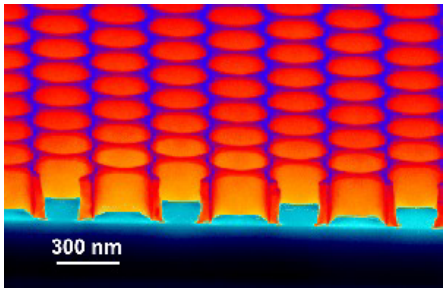
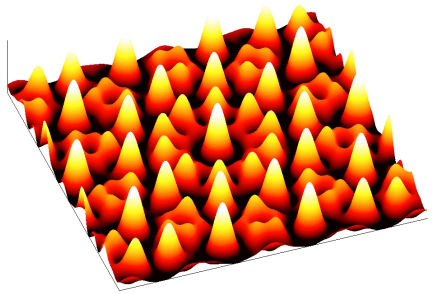
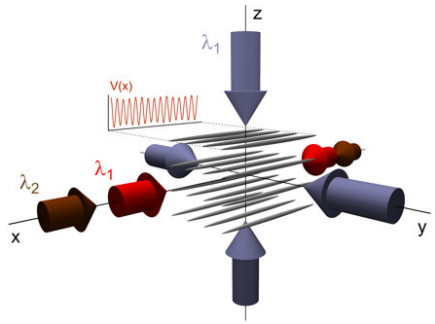
Motivation

In this talk, we consider the propagation of (non)linear *high frequency* waves in heterogeneous media with *periodic microstructures*. Such problems arise, e.g., in the study of

- composite materials,
- photonic crystals,
- laser optics,
- Bose-Einstein condensates in optical lattices,
- . . . . . .

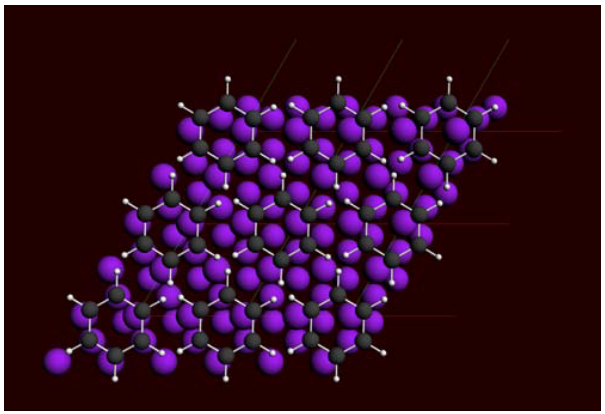






Semiclassical regime

We are interested in the case where the *typical wavelength* is comparable to the *period of the medium*, and both of which are assumed to be *small* on the *length-scale of the considered physical domain*. This consequently leads us to a problem involving *two-scales* where from now on we shall denote by $0 < \varepsilon \ll 1$ the small dimensionless parameter describing the *microscopic / macroscopic scale ratio*.



Typical Methods

- The mathematically precise asymptotic description of these problems has been intensively studied by
  - ⋆ A. Bensoussan, J. L. Lions, and G. Papanicolaou, 1978;
  - ⋆ P. Gérard, P. Markowich, N. Mauser, and F. Poupaud, 1997;
  - ⋆ J. C. Guillot, J. Ralston, and E. Trubowitz, 1998;
  - ⋆ G. Panati, H. Spohn, and S. Teufel, 2003;
  - ⋆ · · · · · ;
- On the other hand, the numerical literature on these issues is not so abundant, *cf.* *L. Gosse, P. A. Markowich, N. Mauser, et al, 2004--2007*.

Numerical Methods and Challenges

- Markowich, Pietra, Pohl, et al, (1999, 2003): Using *finite difference* schemes for linear Schrödinger equation, one needs $\Delta x = o(\varepsilon)$ and $\Delta t = o(\varepsilon)$ to get the correct observables.
- Bao, Jin, Markowich (2002, 2004): Using *Fourier spectral* method for (non)linear Schrödinger equation, to get the correct observables, one needs
  - $\Delta x = O(\varepsilon)$ and $\Delta t = O(\varepsilon)$ for defocusing case,
  - $\Delta x = O(\varepsilon)$ and $\Delta t = o(\varepsilon)$ for strong focusing case.

Therefore, the computational costs are *very expensive* for semiclassical cases ($\varepsilon \ll 1$), especially with highly oscillating potential.

Recently, we developed an efficient numerical approach based on *Bloch-decomposition* method to reduce the computational costs.[1][2][3]

[1] Huang, Jin, Markowich, Sparber, *SISC* 07'/*MMS* 08'/*WM* 09'/*CAM* 10'

[2] Jin, Wu, Yang, Huang, *JCP*, 10'

[3] Wu, Huang, Jin, Yin, *CMS*, 12'

Outline

Outline

Model Problem

Let us first focus on the Schrödinger equation for the electrons in a *semiclassical* asymptotic scaling, *i.e.*

$$\begin{cases} \mathrm{i}\varepsilon\partial_t\psi = -\dfrac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\dfrac{x}{\varepsilon}\right)\psi + U(x)\psi + \beta|\psi|^2\psi, \quad x \in \mathbb{R}^d, \\ \psi\big|_{t=0} = \psi_{\mathrm{in}}(x), \end{cases} \tag{1}$$

where $0 < \varepsilon \ll 1$, denotes the small *semiclassical parameter* describing the microscopic/macroscopic scale ratio.

The equation (1) describes the motion of the electrons on the macroscopic scale induced by the external potentials U and V_Γ.

The highly oscillating *lattice-potential* $V_\Gamma(y)$ is assumed to be *periodic* w.r.t some *regular lattice* Γ.

Conserved Quantities

It is well known that we have two conserved quantities:

Mass

$$M(\psi(t)) = \int_{\mathbb{R}^d} |\psi|^2 dx = M(\psi(0)).$$

Energy

$$E(\psi(t)) = \int_{\mathbb{R}^d} \left[\frac{\varepsilon^2}{2} |\nabla \psi|^2 + (U + V_\Gamma)|\psi|^2 + \frac{\beta}{2}|\psi|^4 \right] dx = E(\psi(0)).$$

- $\beta > 0$ --- defocusing case,
- $\beta < 0$ --- focusing case.

Typical methods for numerical solution

Certainly, one can consider the finite difference method or pseudo-spectral method to solve this problem.

Actually, the time-splitting pseudo-spectral method proposed by Bao, Jin, Markowich (2002, 2004) is almost the optimal method for (non)linear Schrödinger equation *without* lattice potential.

To get the correct observables, one needs

- $\Delta x = O(\varepsilon)$ and $\Delta t = O(\varepsilon)$ for defocusing case,
- $\Delta x = O(\varepsilon)$ and $\Delta t = o(\varepsilon)$ for strong focusing case.

Classical Time-Splitting Spectral Method (TS)

That means, *ignoring* the additional structure provided by the periodic potential V_Γ, one might solve (1) by a classical time-splitting spectral scheme:

Step 1. First, we solve the equation

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi, \tag{2}$$

on a fixed time interval Δt, relying on the *pseudo-spectral* method.

Step 2. Then, we solve the ordinary differential equation

$$\mathrm{i}\varepsilon\partial_t\psi = \left(V_\Gamma\left(\frac{x}{\varepsilon}\right) + U(x) + \beta|\psi|^2\right)\psi, \tag{3}$$

on the same time-interval, where the solution obtained in Step 1 serves as initial condition for Step 2. It is clear that $|\psi|^2$ does not change in Step 2, *i.e.* the exact solution of (3) is

$$\psi(t,x) = \psi(0,x)\,\mathrm{e}^{-\mathrm{i}\left(V_\Gamma(x/\varepsilon)+U(x)+\beta|\psi|^2\right)t/\varepsilon}.$$

Bloch Decomposition Based Algorithm (BD)

Our analysis and numerical simulation show that the former algorithm does not work well for this problem. Another natural time-splitting algorithm is given as follows:

Step 1. First, we solve the equation

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi, \tag{4}$$

on a fixed time-interval Δt. Certainly, we can not use the typical spectral method to solve it. We shall use the *Bloch-decomposition method* in this step.

Step 2. Second, we solve the ordinary differential equation (ODE)

$$\mathrm{i}\varepsilon\partial_t\psi = \left(U(x) + \beta|\psi|^2\right)\psi, \tag{5}$$

on the same time-interval, where the solution obtained in Step 1 serves as initial condition for Step 2. We easily obtain the exact solution for this linear ODE by

$$\psi(t,x) = \psi(0,x)\,\mathrm{e}^{-\mathrm{i}(U(x)+\beta|\psi|^2)t/\varepsilon}.$$

Outline

Notations and definitions

For the sake of simplicity, first, we let $d = 1$ and assume that $\Gamma = 2\pi\mathbb{Z}$, *i.e.*

$$V_\Gamma(y + 2\pi) = V_\Gamma(y) \quad \forall y \in \mathbb{R}. \tag{6}$$

With V_Γ obeying (6) we have:

- The fundamental domain of our lattice $\Gamma = 2\pi\mathbb{Z}$, is $\mathcal{C} = (0, 2\pi)$.
- The *dual lattice* Γ^* can then be defined as the set of all wave numbers $k \in \mathbb{R}$, for which plane waves of the form $\exp(\mathrm{i}kx)$ have the same periodicity as the potential V_Γ.
- The fundamental domain of the dual lattice, *i.e.* the (first) *Brillouin zone*, $\mathcal{B} = \mathcal{C}^*$ is the set of all $k \in \mathbb{R}$ closer to zero than to any other dual lattice point. In our case, that is $\mathcal{B} = \left(-\frac{1}{2}, \frac{1}{2}\right)$.

Review of Bloch's Decomposition

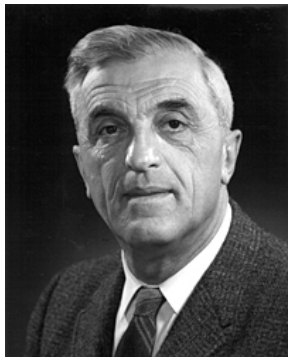
If we want to solve the two-scale problem (4) in Step 1,

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi \equiv H\psi,$$

by a method similar to the pseudo-spectral method in TS algorithm, we need to consider the *Bloch eigenvalue problem* (shifted cell problem),

$$\begin{cases} H(k)\varphi_m(y,k) = E_m(k)\varphi_m(y,k), \\ \varphi_m(y+2\pi,k) = \mathrm{e}^{\mathrm{i}2\pi k}\varphi_m(y,k) \quad \forall\, k \in \mathcal{B}, \end{cases} \tag{7}$$

with $H(k) = \frac{1}{2}(-\mathrm{i}\partial_y + k)^2 + V_\Gamma(y)$.



Felix Bloch

Review of Bloch's Decomposition (cont.)

It is well known that under very mild conditions on V_Γ, the problem (7) has a complete set of *eigenfunctions* $\varphi_m(y,k), m \in \mathbb{N}$, providing, $\forall k \in \overline{\mathcal{B}}$, an orthonormal basis in $L^2(\mathcal{C})$.

Correspondingly, there exists a countable family of *real-valued eigenvalues* which can be ordered according to

$$E_1(k) \leq E_2(k) \leq \cdots \leq E_m(k) \leq \cdots, \ m \in \mathbb{N},$$

including the respective multiplicity.

- The set $\{E_m(k) \,|\, k \in \mathcal{B}\} \subset \mathbb{R}$ is called the mth *energy band* of the operator $H(k)$,
- the eigenfunctions $\varphi_m(\cdot, k)$ are usually called *Bloch functions*. (In the following the index $m \in \mathbb{N}$ will *always* denote the *band index*.)

Review of Bloch's Decomposition (cont.)

According to Bloch's theorem, we can rewrite $\varphi_m(y,k)$ as

$$\varphi_m(y,k) = \mathrm{e}^{\mathrm{i}ky}\chi_m(y,k) \quad \forall\, m \in \mathbb{N}, \tag{8}$$

for some 2π-periodic function $\chi_m(\cdot,k)$. In terms of $\chi_m(y,k)$ the *Bloch eigenvalue problem* reads

$$\begin{cases} H(k)\chi_m(y,k) = E_m(k)\chi_m(y,k), \\ \chi_m(y+2\pi,k) = \chi_m(y,k) \quad \forall\, k \in \mathcal{B}. \end{cases} \tag{9}$$

Solving this eigenvalue problem allows to decompose the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ into a direct sum of, so called, *band spaces*, *i.e.*

$$L^2(\mathbb{R}) = \bigoplus_{m=1}^{\infty} \mathcal{H}_m, \tag{10}$$

$$\mathcal{H}_m := \left\{ \psi_m(y) = \int_{\mathcal{B}} f(k)\,\varphi_m(y,k)\,\mathrm{d}k,\ f \in L^2(\mathcal{B}) \right\}.$$

Review of Bloch's Decomposition (cont.)

This is the well known *Bloch decomposition method*, which allows us to write

$$\forall\, \psi(t,\cdot) \in L^2(\mathbb{R}): \quad \psi(t,y) = \sum_{m\in\mathbb{N}} \psi_m(t,y), \quad \psi_m(t,\cdot) \in \mathcal{H}_m. \tag{11}$$

The corresponding projection of $\psi(t)$ onto the mth band space is thereby given via

$$\begin{aligned} \psi_m(t,y) &\equiv (\mathbb{P}_m\psi)(t,y) \\ &= \int_{\mathcal{B}} \left(\int_{\mathbb{R}} \psi(t,\zeta)\overline{\varphi}_m(\zeta,k)\,\mathrm{d}\zeta \right) \varphi_m(y,k)\,\mathrm{d}k. \end{aligned} \tag{12}$$

In what follows, we denote by

$$C_m(t,k) := \int_{\mathbb{R}} \psi(t,\zeta)\overline{\varphi}_m(\zeta,k)\,\mathrm{d}\zeta \tag{13}$$

the *coefficients of the Bloch decomposition*.

Bloch Transformation

To apply the Bloch decomposition method in our scheme, we need the Bloch transformation applying to C^∞ rapidly decreasing functions on $\mathbb{R}^d$.

From now on, we denote by $\widetilde{\psi}$ the unitary transformation of ψ

$$\widetilde{\psi}(t,y,k) := \sum_{\gamma\in\mathbb{Z}} \psi(t,\varepsilon(y+2\pi\gamma))\,\mathrm{e}^{-\mathrm{i}2\pi k\gamma}, \quad y\in\mathcal{C},\ k\in\mathcal{B}, \tag{14}$$

for any fixed $t\in\mathbb{R}$. We thus get that

$$\widetilde{\psi}(t,y+2\pi,k) = \mathrm{e}^{2\mathrm{i}\pi k}\,\widetilde{\psi}(t,y,k), \quad \widetilde{\psi}(t,y,k+1) = \widetilde{\psi}(t,y,k). \tag{15}$$

The main advantage of $\widetilde{\psi}$ is that we can use the standard *fast Fourier transform (FFT)* in the numerical algorithm.

Furthermore, we have the following inversion formula

$$\psi(t,\varepsilon(y+2\pi\gamma)) = \int_{\mathcal{B}} \widetilde{\psi}(t,y,k)e^{\mathrm{i}2\pi k\gamma}dk. \tag{16}$$

Bloch Transformation (cont.)

From the first step of our BD algorithm, *cf.* (4), if we take the Bloch transformation of ψ, *cf.* (14), we have

$$\mathrm{i}\varepsilon\partial_t\widetilde{\psi} = \left(\frac{1}{2}(-\mathrm{i}\partial_y + k)^2 + V_\Gamma(y)\right)\widetilde{\psi} \equiv H(k)\widetilde{\psi}. \tag{17}$$

Then by the Bloch decomposition method, *cf.* (11)--(13), we obtain

$$\widetilde{\psi}(t,y,k) = \sum_{m\in\mathbb{N}} (\mathbb{P}_m\widetilde{\psi}) = \sum_{m\in\mathbb{N}} C_m(t,k)\varphi_m(y,k), \tag{18}$$

with the coefficients

$$C_m(t,k) := \int_{\mathcal{C}} \widetilde{\psi}(t,\zeta,k)\overline{\varphi}_m(\zeta,k)\,\mathrm{d}\zeta. \tag{19}$$

Therefore, we get the evolution equation for the coefficients

$$\mathrm{i}\varepsilon\partial_t C_m(t,k) = E_m(k)C_m(t,k).$$

Bloch Decomposition algorithm in details

Now we can give the details of our BD algorithm. Let's recall the BD algorithm given before:

Step 1. First, we solve the equation

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi, \tag{20}$$

on a fixed time-interval Δt.

Step 2. Second, we solve the ordinary differential equation (ODE)

$$\mathrm{i}\varepsilon\partial_t\psi = \left(U(x) + \beta|\psi|^2\right)\psi, \tag{21}$$

on the same time-interval.

Indeed **Step 1** consists of several intermediate steps by BD:

Step 1.1 We first compute $\widetilde{\psi}$, *cf.* Bloch transform (14), at time t^n by

$$\widetilde{\psi}^n_{\ell,r} = \sum_{j=1}^{L} \psi^n_{j,r}\, \mathrm{e}^{-\mathrm{i}2\pi k_\ell \cdot (j-1)}.$$

Step 1.2 Next, we calculate the coefficients $C_m(t_n, k_\ell)$ via (13),

$$C_m(t_n, k_\ell) \approx C^n_{m,\ell} = \frac{2\pi}{R} \sum_{r=1}^{R} \widetilde{\psi}^n_{\ell,r} \overline{\chi_m}(y_r, k_\ell)\, \mathrm{e}^{-\mathrm{i}k_\ell y_r}.$$

Step 1.3 The obtained Bloch coefficients are then evolved up to t^{n+1},

$$C^{n+1}_{m,\ell} = C^n_{m,\ell}\, \mathrm{e}^{-\mathrm{i}E_m(k_\ell)\Delta t/\varepsilon}.$$

Step 1.4 Then we get $\widetilde{\psi}^{n+1}$ by summing up all band contributions

$$\widetilde{\psi}^{n+1}_{\ell,r} = \sum_{m=1}^{M} (\mathbb{P}_m \widetilde{\psi})^{n+1}_{\ell,r} \approx \sum_{m=1}^{M} C^{n+1}_{m,\ell} \chi_m(y_r, k_\ell)\, \mathrm{e}^{\mathrm{i}k_\ell y_r}.$$

Step 1.5 Finally we perform the inverse transformation (16),

$$\psi^{n+1}_{\ell,r} = \frac{1}{L} \sum_{j=1}^{L} \widetilde{\psi}^{n+1}_{j,r}\, \mathrm{e}^{\mathrm{i}2\pi k_j (\ell-1)}.$$

Numerical Computation of the Bloch Bands

As a preparatory step for our algorithm we shall first calculate Bloch's energy bands numerically as follows. We expand the potential $V_\Gamma \in C^1(\mathbb{R})$ in its *Fourier series*, *i.e.*

$$V_\Gamma(y) = \sum_{\lambda\in\mathbb{Z}} \widehat{V}(\lambda)\,\mathrm{e}^{\mathrm{i}\lambda y}, \quad \widehat{V}(\lambda) = \frac{1}{2\pi}\int_0^{2\pi} V_\Gamma(y)\,\mathrm{e}^{-\mathrm{i}\lambda y}\,\mathrm{d}y. \tag{22}$$

Likewise, we expand any *Bloch eigenfunctions* $\chi_m(\cdot,k)$, in its respective Fourier series

$$\chi_m(y,k) = \sum_{\lambda\in\mathbb{Z}} \widehat{\chi}_m(\lambda,k)\,\mathrm{e}^{\mathrm{i}\lambda y}, \quad \widehat{\chi}_m(\lambda,k) = \frac{1}{2\pi}\int_0^{2\pi} \chi_m(y,k)\,\mathrm{e}^{-\mathrm{i}\lambda y}\,\mathrm{d}y. \tag{23}$$

In general, we only need to take into account a few coefficients.

Numerical computation of the Bloch bands (cont.)

We consequently aim to approximate the Sturm-Liouville problem (9), by the following algebraic eigenvalue problem

$$\mathbf{H}(k)\begin{pmatrix} \widehat{\chi}_m(-\Lambda) \\ \widehat{\chi}_m(1-\Lambda) \\ \vdots \\ \widehat{\chi}_m(\Lambda-1) \end{pmatrix} = E_m(k)\begin{pmatrix} \widehat{\chi}_m(-\Lambda) \\ \widehat{\chi}_m(1-\Lambda) \\ \vdots \\ \widehat{\chi}_m(\Lambda-1) \end{pmatrix} \tag{24}$$

where the $2\Lambda \times 2\Lambda$ matrix $\mathbf{H}(k)$ is given by

$$\mathbf{H}(k) = \begin{pmatrix} \widehat{V}(0) + \frac{(k-\Lambda)^2}{2} & \widehat{V}(-1) & \cdots & \widehat{V}(1-2\Lambda) \\ \widehat{V}(1) & \widehat{V}(0) + \frac{(k-\Lambda+1)^2}{2} & \cdots & \widehat{V}(2-2\Lambda) \\ \vdots & \vdots & \ddots & \vdots \\ \widehat{V}(2\Lambda-1) & \widehat{V}(2\Lambda-2) & \cdots & \widehat{V}(0) + \frac{(k+\Lambda-1)^2}{2} \end{pmatrix} \tag{25}$$

Some Remarks on Our BD Algorithm

- It is easy to check that our BD algorithm conserves the **mass**, and the *total energy* numerically.
- In our BD algorithm, we compute the *dominant effects* from dispersion and periodic lattice potential in one step, and treat the non-periodic potential as a perturbation.
- On the *same spatial grid*, the numerical costs of our Bloch transform based algorithm is of the *same order* as the classical time-splitting spectral method.
- Clearly, if there is *no lattice potential*, *i.e.* $V_\Gamma(y) \equiv 0$, the BD algorithm simplifies to the described time-splitting spectral method.

Outline

Numerical tests for 1D linear problems ($\beta = 0$)

First, we consider the 1D linear problem[4]. We choose the initial data $\psi_{\text{in}} \in \mathcal{S}(\mathbb{R})$ of the following form

$$\psi_{\text{in}}(x) = \left(\frac{2\omega}{\pi}\right)^{1/4} \mathrm{e}^{-\omega(x-\pi)^2}. \tag{26}$$

Concerning slowly varying, external potentials U, we shall choose,

- a *harmonic oscillator* type potential:

$$U(x) = \frac{|x-\pi|^2}{2}, \tag{27}$$

- or an external (non-smooth) *step potential*,

$$U(x) = \begin{cases} 1, & x \in \left[\frac{\pi}{2}, \frac{3\pi}{2}\right] \\ 0, & \text{else.} \end{cases} \tag{28}$$

[4] Huang, Jin, Markowich and Sparber, SIAM Sci. Comput., 07'

Within the setting described above, we shall focus on two particular choices for the lattice potential, namely:

Example 1 (Mathieu's model)

The so-called *Mathieu's model*, *i.e.*

$$V_\Gamma(x) = \cos(x). \tag{29}$$

(For applications in solid state physics this is rather unrealistic, however it fits quite good with experiments on Bose-Einstein condensates in optical lattices.)

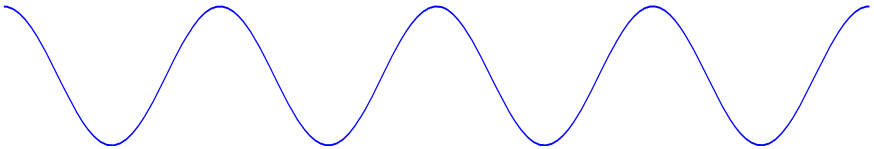
Example 2 (Kronig-Penney's model)

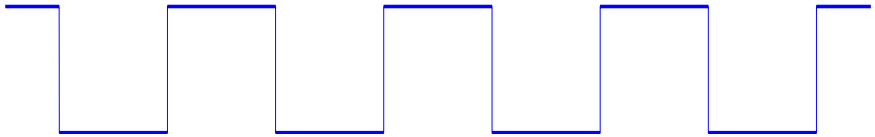
The so-called *Kronig-Penney's model*, *i.e.*

$$V_\Gamma(x) = 1 - \sum_{\gamma\in\mathbb{Z}} \mathbf{1}_{x\in\left[\frac{\pi}{2}+2\pi\gamma,\frac{3\pi}{2}+2\pi\gamma\right]}, \tag{30}$$

where $\mathbf{1}_\Omega$ denotes the characteristic function of a set $\Omega \subset \mathbb{R}$.

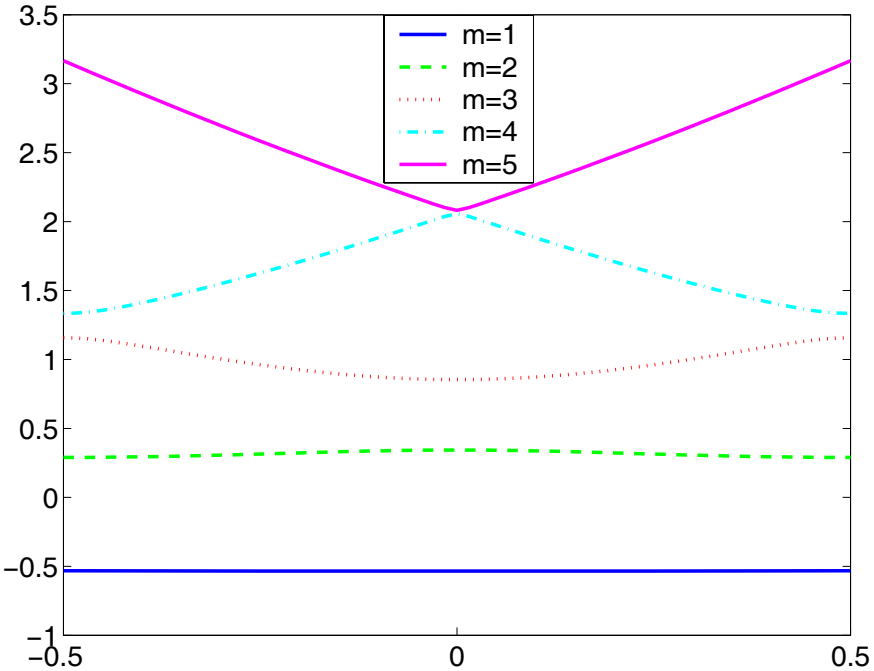
Mathieu's model and Kronig-Penney's model

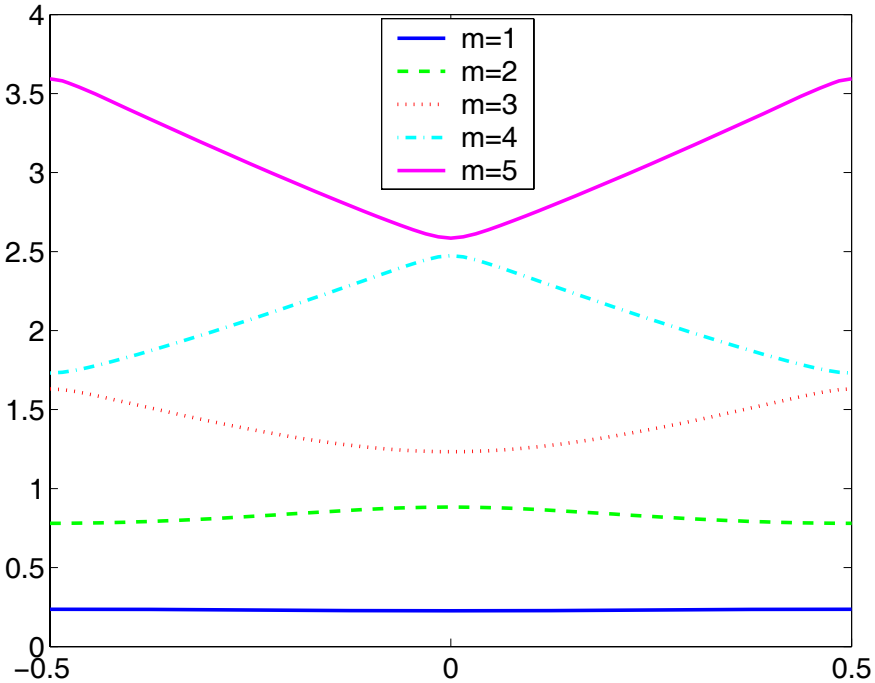




Mathieu's Model

Kronig-Penney's Model



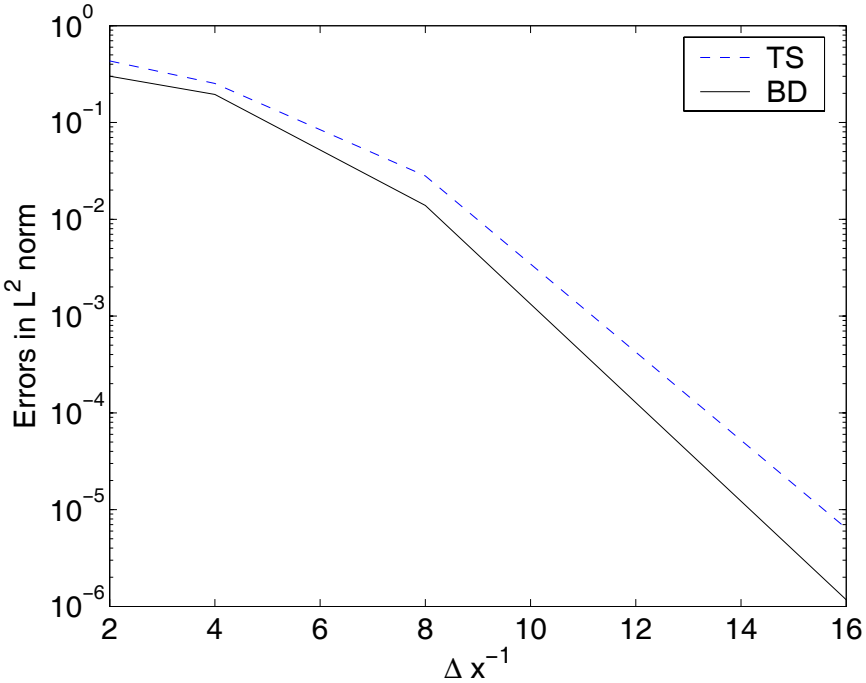


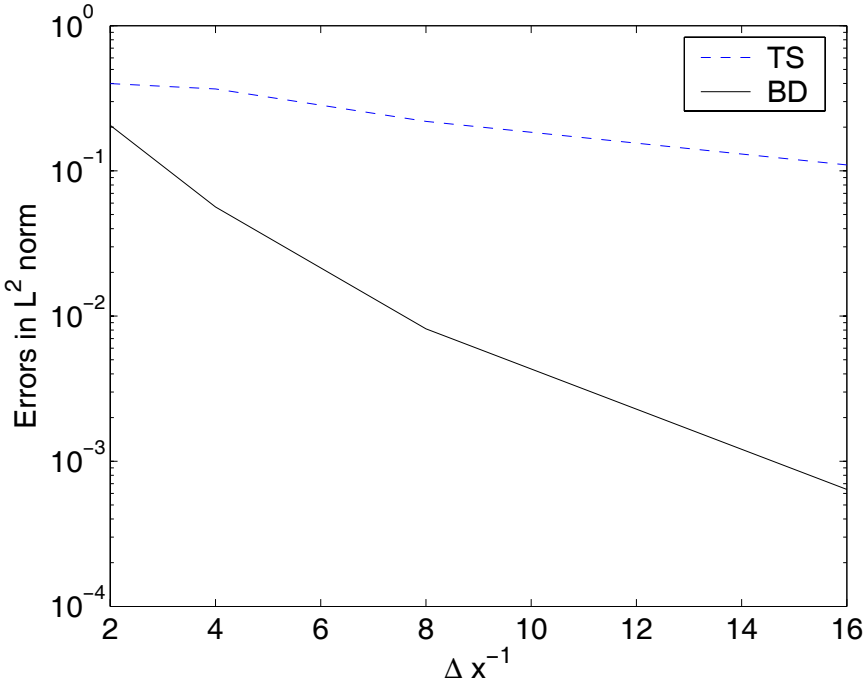
$$E_m(k), m = 1, \cdots, 5$$

Spatial discretization error test, $\varepsilon = \frac{1}{1024}$

Left: Example 1 with $U(x) = 0$. TS: $\triangle t = 10^{-4}$, BD: $\triangle t = 1$.

Right: Example 2 with $U(x) = \frac{|x-\pi|^2}{2}$. TS: $\triangle t = 10^{-6}$, BD: $\triangle t = 10^{-2}$.

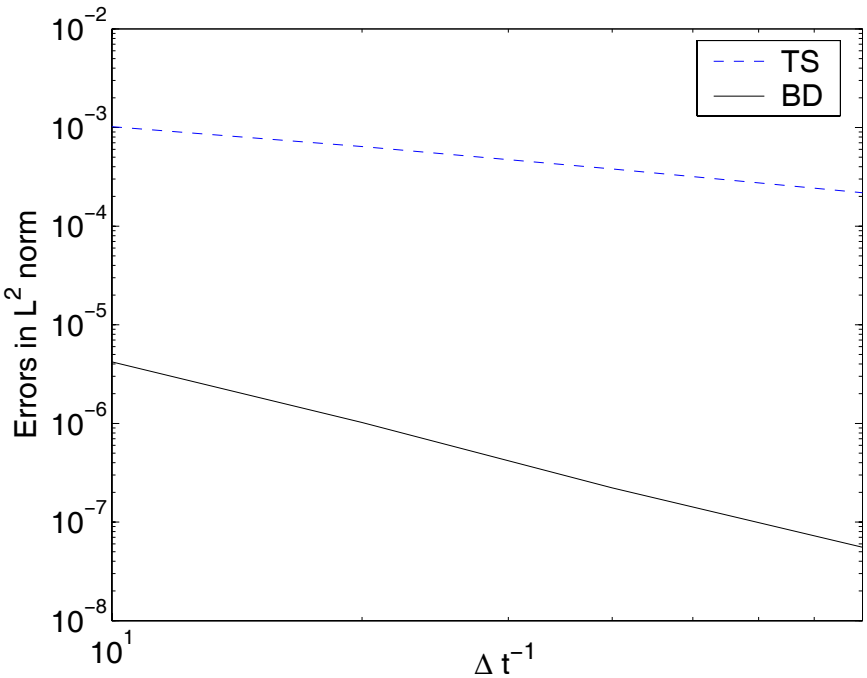




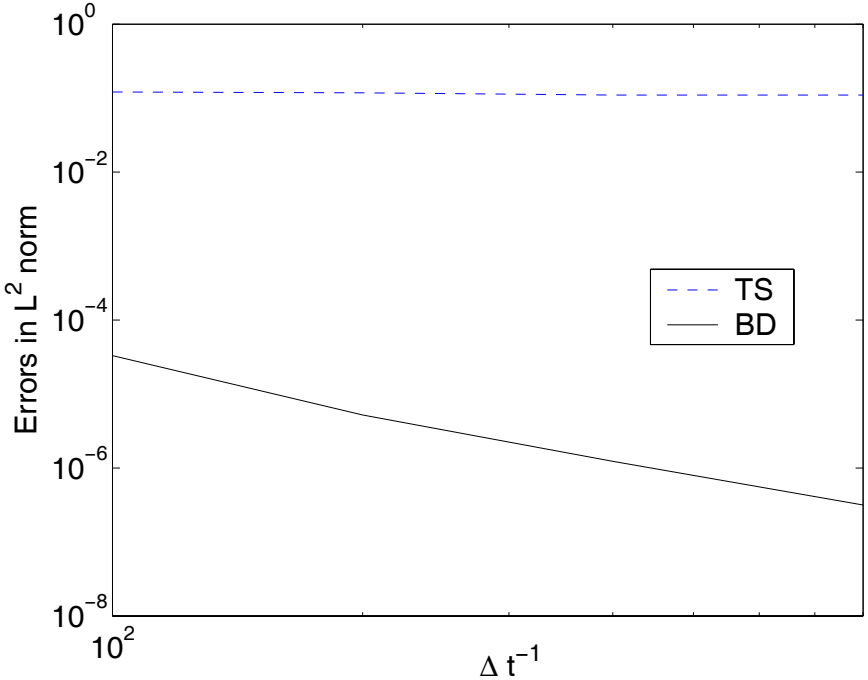
Temporal discretization error test, $\frac{\triangle x}{\varepsilon} = \frac{1}{128}$

Kronig-Penney's Model with $U(x) = \frac{|x-\pi|^2}{2}$

Left: ($\varepsilon = \frac{1}{2}$ at $t = 0.1$).



Right: ($\varepsilon = \frac{1}{1024}$ at $t = 0.01$).



Some remarks on linear problems

- If $U(x) \equiv 0$:
  - As discussed before, we can use only *one step* in time to obtain the numerical solution, because the *Bloch-decomposition method* indeed is ``*exact*'' in this case (independently of ε).
  - On the other hand, by using the *time-splitting Fourier spectral method*, one has to refine the time steps (depending on ε) as well as the mesh size in order to achieve the same accuracy.
- If $U(x) \neq 0$ and $\varepsilon \ll 1$:
  - We can achieve quite good accuracy by using the *Bloch-decomposition method* with $\Delta t = \mathcal{O}(1)$ and $\Delta x = \mathcal{O}(\varepsilon)$.
  - On the other hand, by using the *time-splitting Fourier spectral method*, we have to use $\Delta t = \mathcal{O}(\varepsilon^\alpha)$, $\Delta x = \mathcal{O}(\varepsilon^\alpha)$, for some $\alpha \geq 1$. In particular $\alpha > 1$ is required for the case of a non-smooth lattice potential V_Γ.

Numerical tests for 1D NLS

Then we consider the NLS [5].

Example 3 (Tests for band mixing)

We start with the initial condition likes

$$\psi_{\mathrm{I}}(x) = \mathbb{P}_{m_0}\psi_{\mathrm{in}}(x)e^{\mathrm{i}kx}, \tag{31}$$

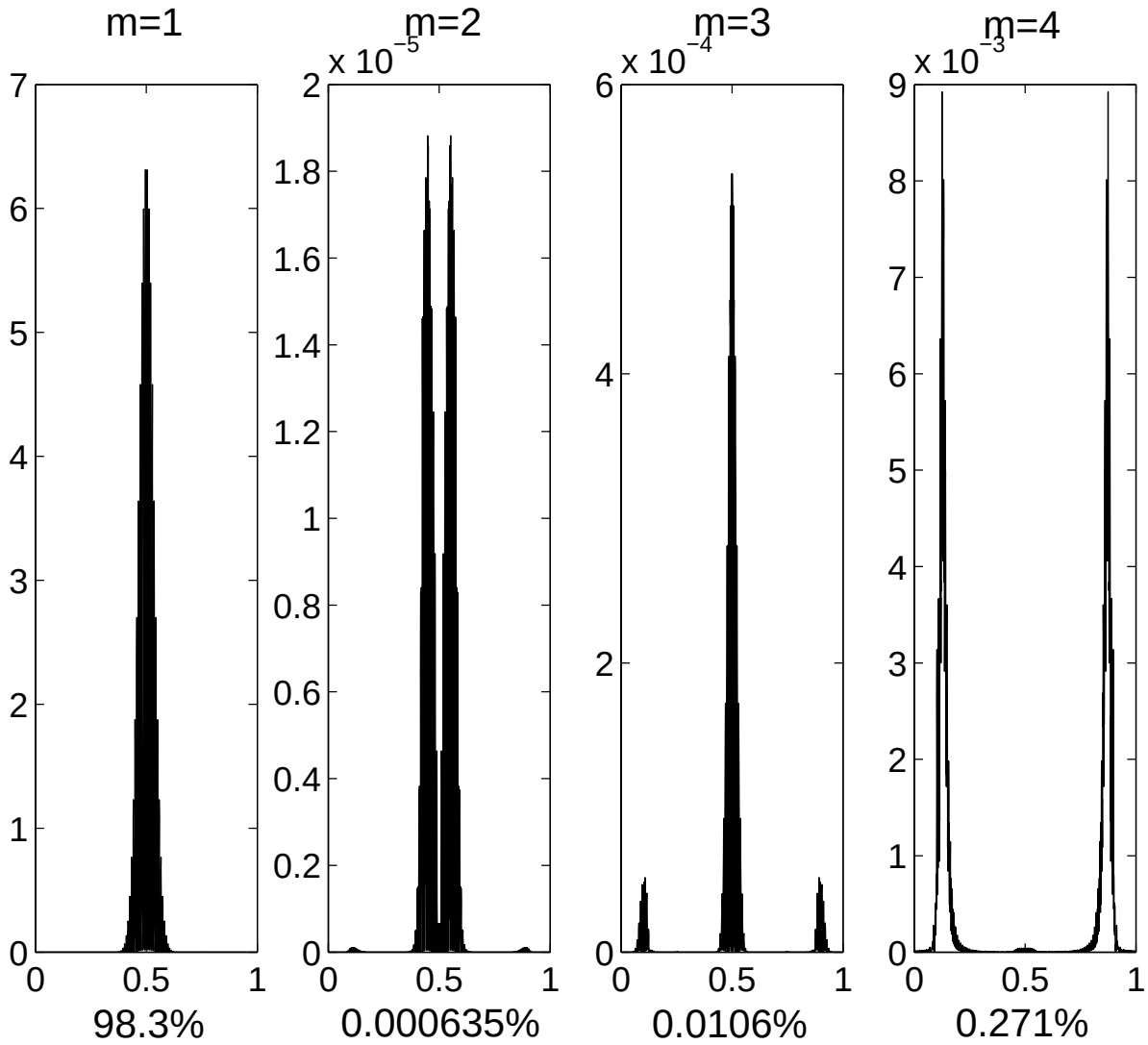
where $\psi_{\mathrm{in}}(x)$ is given in (26). We'll test the mass transition from one band to others.

Here we have the following results,

- The *isolated band* with $m_0 = 1$ is more stable than other bands.
- If m_0 is large, there will be more mass transfers to other bands.
- If E_{m_0} is not isolated, there will be $\mathcal{O}(1)$ mass transfers to other bands.
- If $\beta = \mathcal{O}(1)$, there will be $\mathcal{O}(1)$ Mass density transfers to other bands.

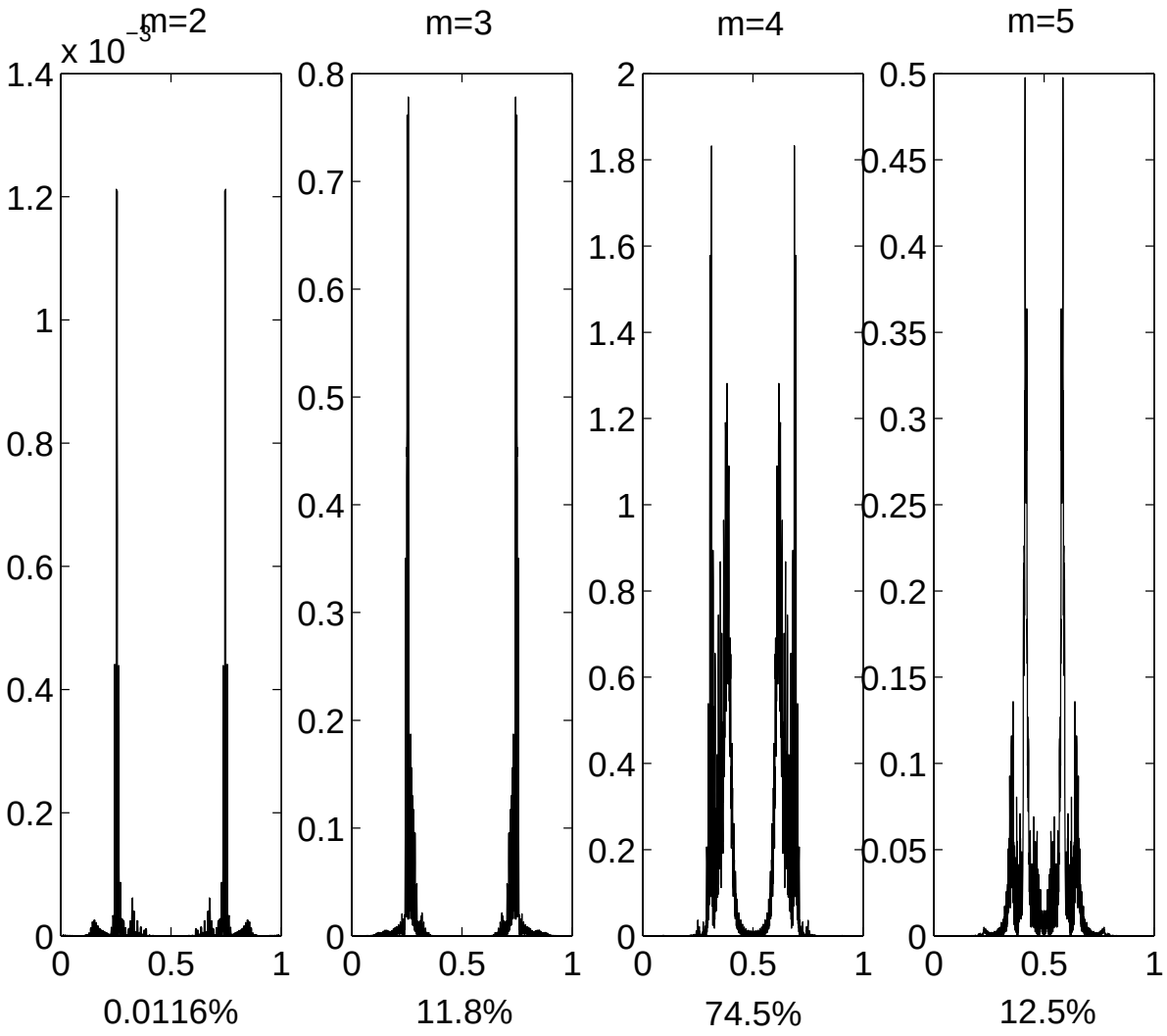
[5] Huang, Jin, Markowich and Sparber, MMS, 08'

Example 3: $U(x) = \frac{|x-\pi|^2}{2}$, $\varepsilon = \frac{1}{128}$, $\beta = \frac{1}{100}$, $m_0 = 1$.



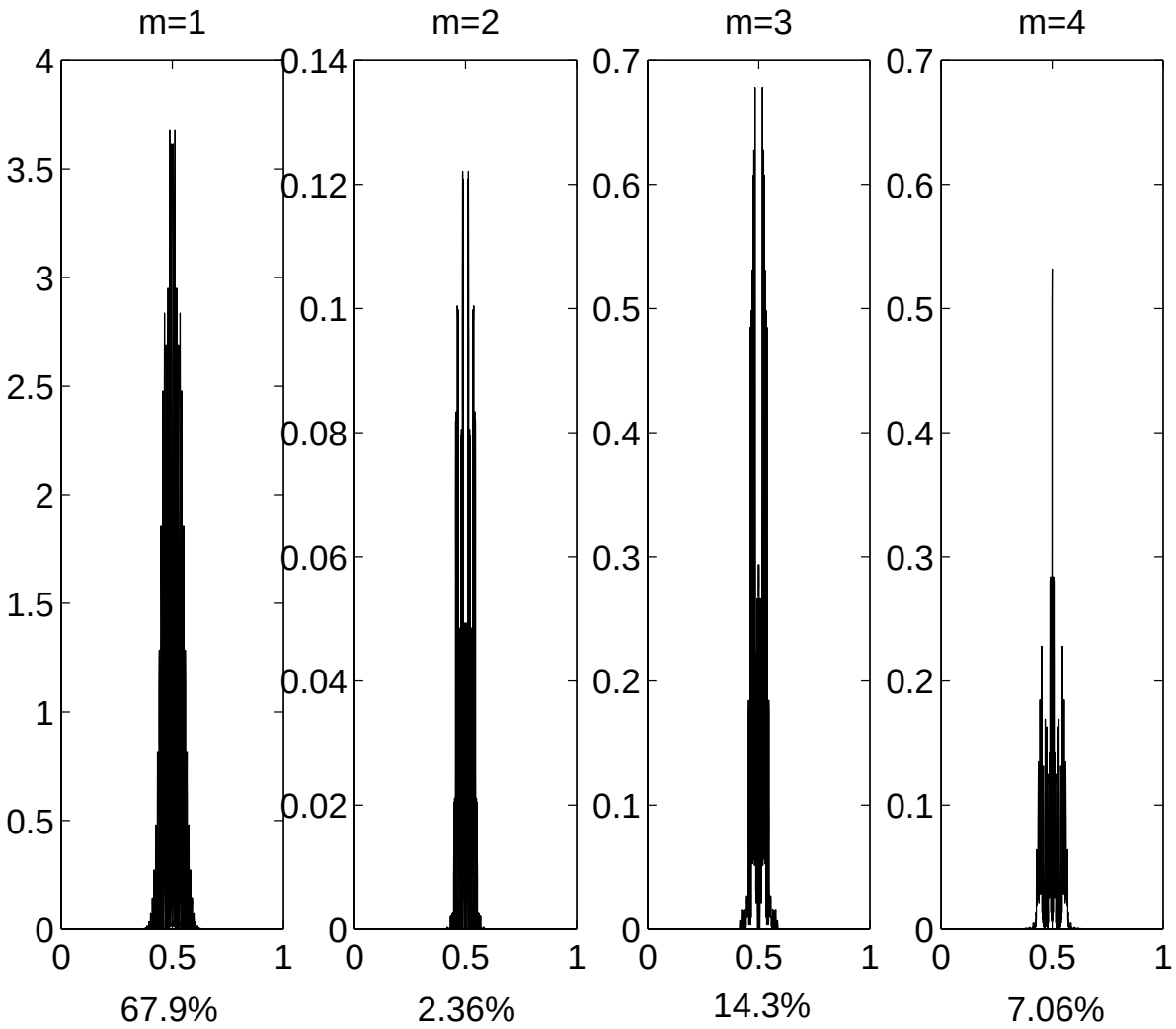
Mass density distribution

Example 3: $U(x) = \frac{|x-\pi|^2}{2}$, $\varepsilon = \frac{1}{128}$, $\beta = \frac{1}{100}$, $m_0 = 4$.



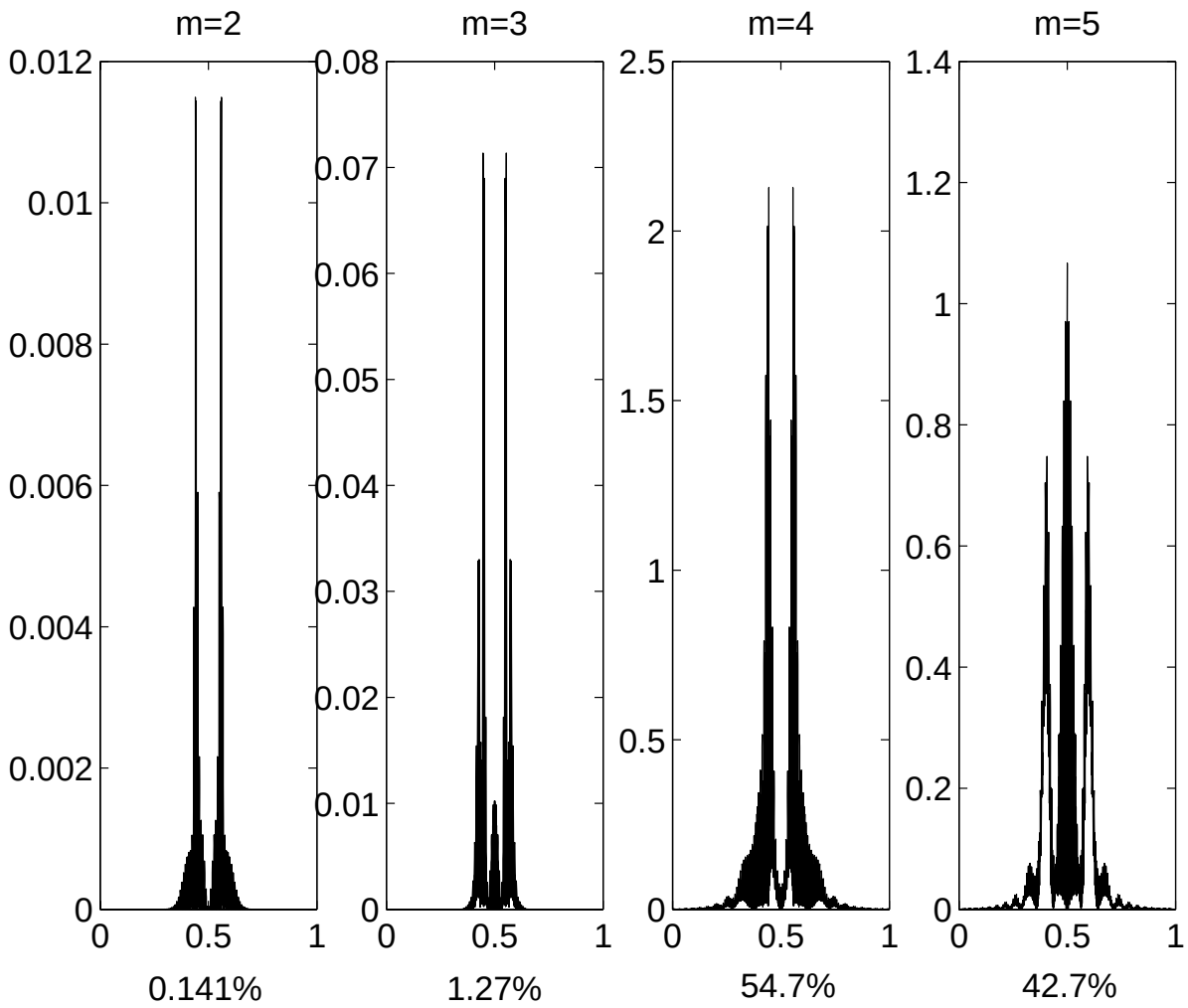
Mass density distribution

Example 3: $U(x) = \frac{|x-\pi|^2}{2}$, $\varepsilon = \frac{1}{128}$, $\beta = 1$, $m_0 = 1$.



Mass density distribution

Example 3: $U(x) = \frac{|x-\pi|^2}{2}$, $\varepsilon = \frac{1}{128}$, $\beta = 1$, $m_0 = 4$.



Mass density distribution

Numerical examples for lattice BEC in 3D [6]

Example 4 (Dynamics of BECs)

Now we want to simulate the dynamics of the BECs. The initial condition is $\psi|_{t=0} = \psi_{\text{in}}(\mathbf{x})$, where $\psi_{\text{in}}(\mathbf{x})$ is the *ground state* of the nonlinear eigenvalue problem (*without the lattice potential term*)

$$\begin{cases} \mu\phi(\mathbf{x}) &= -\frac{1}{2}\Delta\phi + U\phi + \beta|\phi|^2\phi \\ \|\phi\|_{L^2} &= \int_{\mathbb{R}^d} |\phi|^2(x)d\mathbf{x} = 1. \end{cases}$$

For example, in 3D case, with $U(\mathbf{x}) = \frac{|\mathbf{x}|^2}{2}$,

- *weak interaction*: $|\beta| \ll 1$, $\mu_g = \frac{3\varepsilon}{2}$, $\phi_g = \frac{1}{(\pi\varepsilon)^{3/4}} e^{-U(\mathbf{x})/\varepsilon}$;
- *strong interaction*: $\beta = \mathcal{O}(1)$,

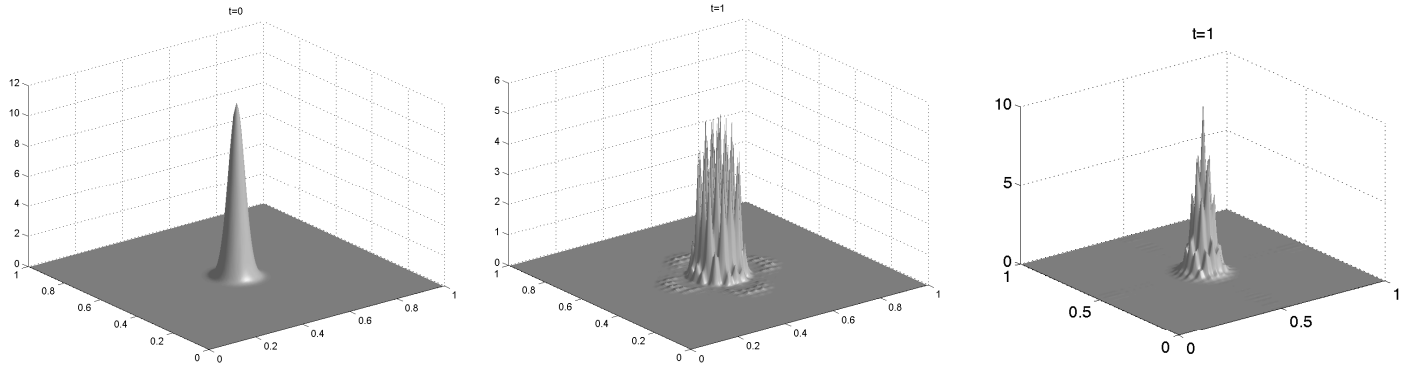
$$\mu_g^s = \frac{1}{2}\left(\frac{15\beta}{4\pi}\right)^{2/5}, \quad \phi_g = \begin{cases} \sqrt{(\mu_g^s - U(x))/\beta}, & U(\mathbf{x}) < \mu_g^s, \\ 0, & otherwise. \end{cases}$$

[6] Huang, Jin, Markowich and Sparber, MMS, 08'

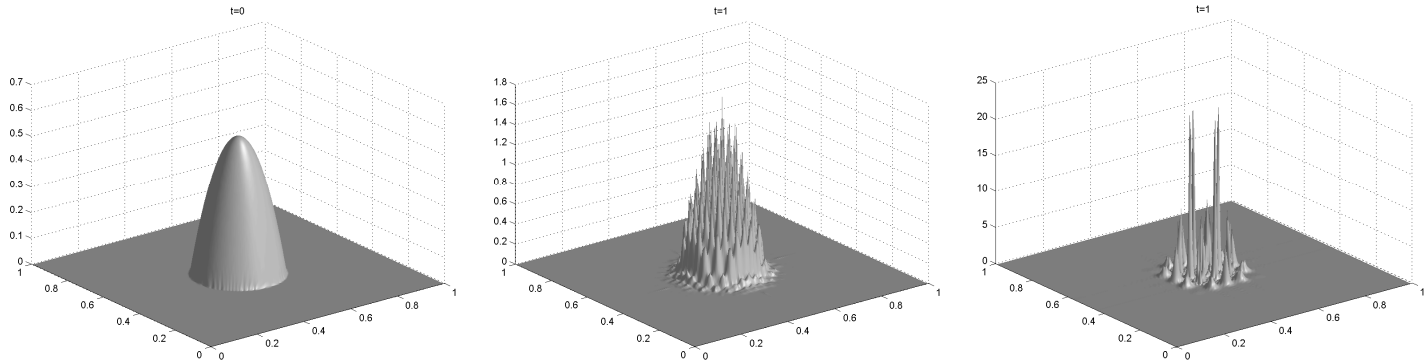
Comparison of the initial and final mass densities, evaluated at $x_3 = 0$.

$$U(\mathbf{x}) = \frac{|\mathbf{x}|^2}{2}, V_\Gamma(\mathbf{x}) = \sum_{l=1}^{3} \sin^2 2\pi x_l.$$

$$|\beta| = \frac{1}{16} \text{ and } \varepsilon = \frac{1}{16}$$



$$|\beta| = 1 \text{ and } \varepsilon = \frac{1}{16}$$



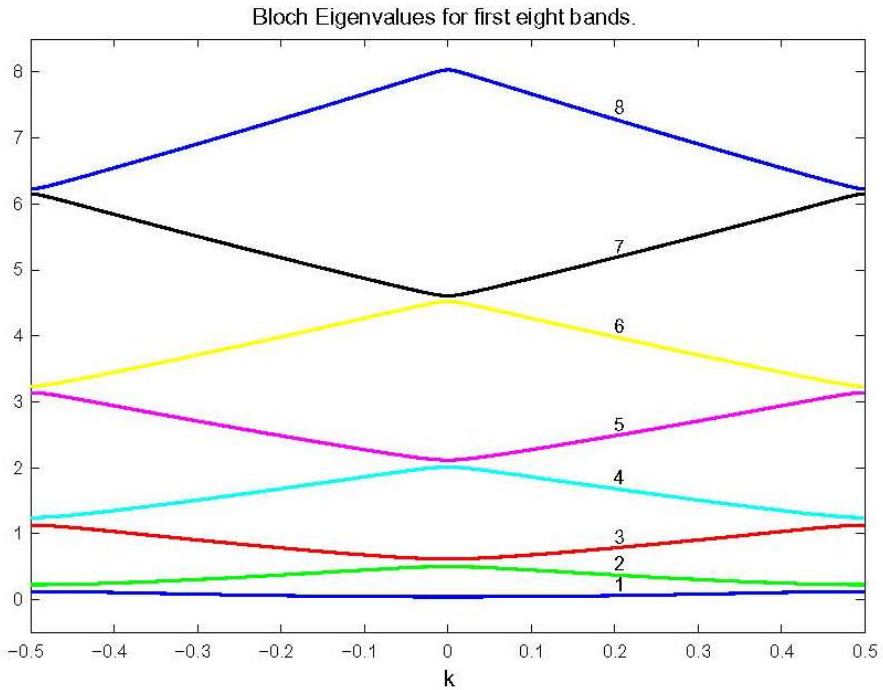
$|\psi(t,\mathbf{x})|^2|_{t=0}$, $|\psi^d(t,\mathbf{x})|^2$(defocusing case) and $|\psi^f(t,\mathbf{x})|^2$(focusing case).

Coupling with Gaussian Beam method

Example 5 (an application to the insulator)

If ε is very small (for example, about $10^{-4} \sim 10^{-2}$), we will couple with Gaussian Beam method. Here we study an insulator case with

$$V_\Gamma(\mathbf{x}) = e^{-20|\mathbf{x}|^2}.$$



$$E_m(k), m = 1, \cdots, 8$$

Coupling with Gaussian Beam method (cont.)

We adopt the Gaussian beam approximation to the dynamics in m-th band. For more details, please refer to our paper on JCP [7].

Here we consider the external harmonic potential and the initial condition

$$\psi_{\text{in}}(\mathbf{x}) = e^{-50|\mathbf{x}|^2 \frac{0.3(1-\sin|\mathbf{x}|)}{\varepsilon}} \cos\frac{|\mathbf{x}|}{\varepsilon}.$$

We take the number of Bloch bands $M = 8$ and the number of Gaussian beams $N \sim 1/\sqrt{\varepsilon}$. The l^2 errors between the exact solution and the Bloch decomposition-Gaussian beam solution are given in Table 1. The convergence rate is of order 1.17 as $\varepsilon \to 0$ in l^2 norm.

Table 1 : l^2 errors between the exact solution ψ and the Bloch decomposition - Gaussian beam solution ψ_{GB}^{BD}

ε	$1/128$	$1/256$	$1/512$	$1/1024$
$\|\psi - \psi_{GB}^{BD}\|_2$	$8.34\text{E}-2$	$4.27\text{E}-2$	$1.71\text{E}-2$	$7.25\text{E}-3$

[7] Jin, Wu, Yang, Huang, JCP, 2010

Numerical Evidence for the Anderson localization [8]

The phenomenon of Anderson localization, also known as the *strong localization*, describes the absence of dispersion for waves in random media with sufficiently *strong random perturbations*. It has been predicted by P. W. Anderson (Philos. Mag. B, **52**, 1985) in the context of (quantum mechanical) electron dynamics but is now regarded as a general wave phenomenon that applies to the transport of electromagnetic or acoustic waves as well.

We then study the random Klein-Gordon equation

$$\begin{cases} \dfrac{\partial^2 u^\omega}{\partial t^2} = \dfrac{\partial}{\partial x}\left(a_\Gamma\left(\omega, \dfrac{x}{\varepsilon}\right)\dfrac{\partial u^\omega}{\partial x}\right) - \dfrac{1}{\varepsilon^2} W_\Gamma\left(\dfrac{x}{\varepsilon}\right) u^\omega + f(x), \\ u^\omega\big|_{t=0} = u_0(x), \quad \dfrac{\partial u^\omega}{\partial t}\Big|_{t=0} = v_0(x), \end{cases} \tag{32}$$

which describes the propagation of waves in *disordered media*. Here, the coefficient $a_\Gamma = a_\Gamma(\omega, y)$ is assumed to be a function of a *uniformly distributed random variable* ω with mean zero and variance $\sigma^2 \geq 0$.

[8] Huang, Jin, Markowich, Sparber, Wave Motion, 09'

Example 6 (Stability tests and Anderson localization)

Consider (32) with $f(x) \equiv 0$ and initial data

$$u_0(x) = \left(\frac{2}{\pi\varepsilon}\right)^{1/4} \mathrm{e}^{-\frac{(x-\pi)^2}{\varepsilon}}, \quad v_0(x) = 0. \tag{33}$$

The random coefficient a_Γ is chosen as

$$a_\Gamma(\omega, y) = a_\Gamma(y) + \omega, \quad a_\Gamma(y) = 2.5 + \cos(y), \tag{34}$$

i.e. including an *additive noise*. For a given choice of σ we numerically generate $N \in \mathbb{N}$ realizations of ω and consequently take the ensemble average. In our examples we usually choose $N \geq 100$, i.e.

$$E_m(k) := \mathbb{E}\{E_m(\omega, k)\} \approx \frac{1}{N} \sum_{\ell=1}^{N} E_m(\omega_\ell, k), \tag{35}$$

for different values of σ.

Definition of Energy Density

In order to realize the emergence of this localization phenomena we consider the *local energy density* $e^\omega(t,x)$ of the solution $u^\omega(t,x)$:

$$e^\omega(t,x) := \frac{1}{2}\left(\left|\frac{\partial u^\omega}{\partial t}\right|^2 + a_\Gamma\left(\omega,\frac{x}{\varepsilon}\right)\left|\frac{\partial u^\omega}{\partial x}\right|^2 + \frac{1}{\varepsilon^2}W_\Gamma\left(\frac{x}{\varepsilon}\right)|u^\omega|^2\right).$$

The *total energy* $E_0^\omega(t)$ of $u^\omega(t,x)$ is then given by the zeroth spatial moment of $e^\omega(t,x)$, i.e.

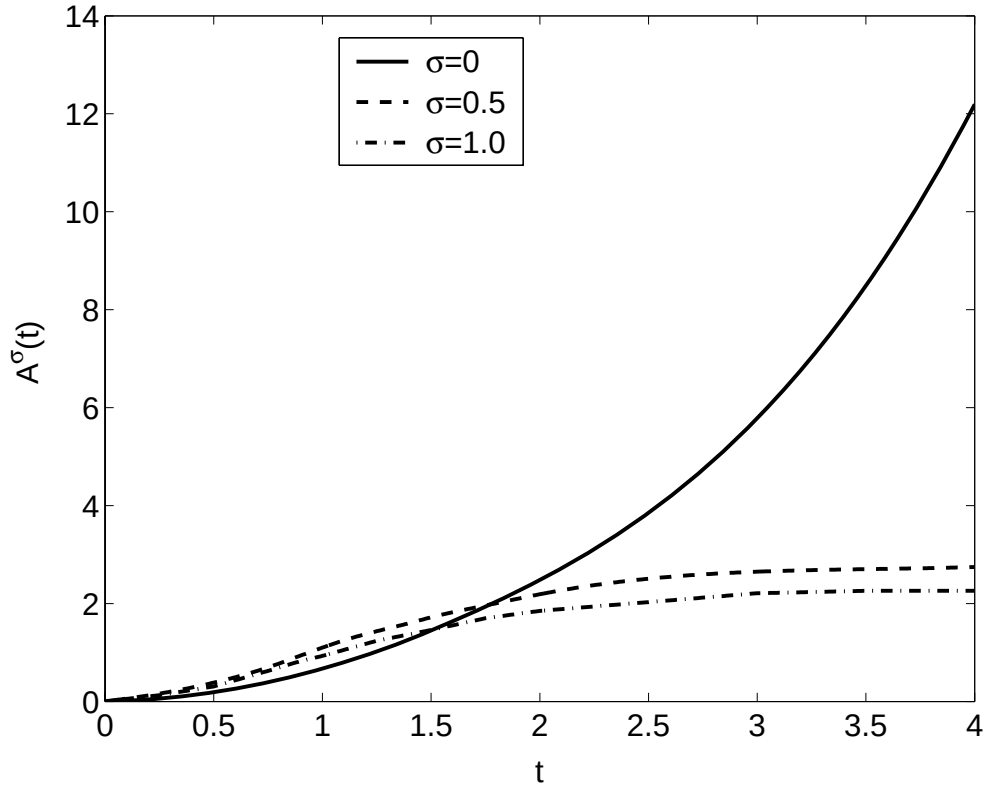
$$E_0^\omega(\omega,t) = \int_{\mathbb{R}} e^\omega(t,x)\mathrm{d}x, \tag{36}$$

and we likewise define

$$E_2^\omega(\omega,t) = \int_{\mathbb{R}} x^2 e^\omega(t,x)\mathrm{d}x, \tag{37}$$

which measures the *spread of the wave*. It represents the mean square of the distance of the wave from the origin at time t.

The graph of $A^\sigma(t)$ for different σ $(\varepsilon = \frac{1}{64})$



$$A^\sigma(t) := \mathbb{E}\{E_2^\omega(t)\}/\mathbb{E}\{E_0^\omega(t)\}$$

The quantity $A^\sigma(t)$ has been introduced as a measure for the presence of *Anderson localization*. As we see it first grows almost linearly in t, a typical diffusive behavior, and then, around $t = 2$ it flattens. The latter is a strong indication of *Anderson localization*.

Outline

Conclusion

We present a new numerical method for accurate computations of solutions to (non)linear dispersive wave equations with periodic coefficients.

- Our approach is based on the classical *Bloch decomposition method*.
- It is shown by the given numerical examples, that our method is *unconditionally stable, highly efficient*, and also conserves the important physical quantities.
- Our new method allows for *much larger time-steps* and usually a *coarser spatial grid*, to achieve the same accuracy as for the usual time-splitting spectral method. This is particularly visible in cases, where the lattice potential is *non longer smooth* and $\varepsilon \ll 1$.

Ongoing projects:

We are trying to couple our BD algorithm with other methods to the simulation of other multiscale problems.

Thank you for your attention!