# Bloch decomposition based method for wave propagation

Zhongyi Huang

Dept. of Mathematical Sciences
Tsinghua University
Beijing 100084, China

Joint work with: Shi Jin, Peter Markowich, Christof Sparber

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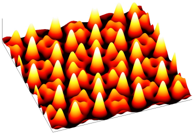
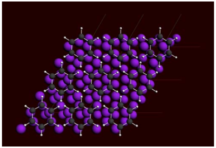
# Motivation

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

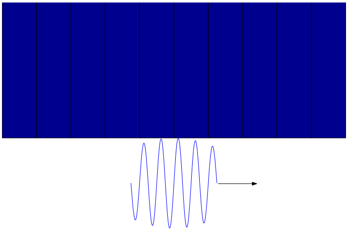
- composite materials,
- photonic crystals,
- laser optics,
- Bose-Einstein condensates in optical lattices,
- ......





# 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;
  - ⋆ $\cdots\cdots$;
- 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, Markowich, Jin (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 ($\varepsilon \ll 1$)!

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

[1] Huang, Jin, Markowich, Sparber, CAM 15, 2010

# Outline

1. Bloch Decomposition Based Algorithm
   - A classical time-splitting spectral method (TS)
   - The Bloch decomposition based algorithm (BD)
   - Review of Bloch's Decomposition
   - Our BD algorithm in details
2. Numerical Implementation and Applications
   - Numerical tests for 1D problems
   - Numerical examples for lattice BEC in 3D
   - Random coefficients: Stability tests and Anderson localization
3. Conclusion

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# Model Problem

In this talk, we shall consider two kinds of problems: the Schrödinger equation and the Klein-Gordon equation.

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

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

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 $V_\Gamma$.

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

# Conserved Quantities

It is well known that we have two conserved quantities:

**Mass**

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

**Energy**

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

- $\beta > 0$ — 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, Markowich, Jin (2002, 2004) was the optimal 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.

# Classical Time-Splitting Spectral Method (TS)

Ignoring the additional structure provided by the periodic potential $V_\Gamma$, 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 $\Delta t$, 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)

Another natural time-splitting algorithm is given as follows:

**Step 1.** First, we solve the equation

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

on a fixed time-interval $\Delta t$. 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)

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

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

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

# 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 $V_\Gamma$ obeying (6) we have:

- The fundamental domain of our lattice $\Gamma = 2\pi\mathbb{Z}$, is $\mathcal{C} = (0, 2\pi)$.
- The *dual lattice* $\Gamma^*$ 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 $V_\Gamma$.
- 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

To solve the two-scale problem (4) in Step 1, we need to consider the *Bloch eigenvalue 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 $H(k) = \left(\frac{1}{2}(-\mathrm{i}\partial_y + k)^2 + V_\Gamma(y)\right)$.

It is well known that under very mild conditions on $V_\Gamma$, 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 $L^2(\mathcal{C})$.

# Review of Bloch's Decomposition (cont.)

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

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

including the respective multiplicity.

- The set $\{E_m(k) \mid k \in \mathcal{B}\} \subset \mathbb{R}$ is called the $m$th *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.)

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 $2\pi$-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.*

$$\begin{aligned} L^2(\mathbb{R}) &= \bigoplus_{m=1}^{\infty} \mathcal{H}_m, \qquad (10)\\ \mathcal{H}_m &:= \left\{ \psi_m(y) = \int_{\mathcal{B}} f(k)\, \varphi_m(y,k)\,\mathrm{d}k,\ f \in L^2(\mathcal{B}) \right\}. \end{aligned}$$

# 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 $m$th 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 to fit the boundary conditions.

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

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

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 $\psi$, *cf.* (14), we have

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

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

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

with the coefficients

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

Therefore, we get the evolution equation for the coefficients

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

# Temporal and spatial discretization

For the convenience of computations, we shall consider the equation (1) on a bounded domain $\mathcal{D} = [0, 2\pi]$ with *periodic boundary conditions*.

In what follows, for some $N \in \mathbb{N}$, $T > 0$, let the time step be

$$\Delta t = T/N, \quad t_n = n\Delta t, \ n = 1, \cdots, N.$$

Suppose that there are $L \in \mathbb{N}$ lattice cells within the computational domain $\mathcal{D}$, and there are $R$ grid points in each lattice cell, which yields the following discretization

$$\begin{cases} k_\ell = -\dfrac{1}{2} + \dfrac{\ell - 1}{L}, & \text{where } \ell = \{1, \cdots, L\} \subset \mathbb{N}, \\ y_r = \dfrac{2\pi(r-1)}{R}, & \text{where } r = \{1, \cdots, R\} \subset \mathbb{N}, \end{cases}$$

and thus finally we evaluate $\psi^n = \psi(t_n)$ at the grid points

$$x_{\ell,r} = \varepsilon(2\pi(\ell - 1) + y_r).$$

# 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 $\Delta t$.

**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

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

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

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

**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

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

**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.

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

First, we consider the 1D linear problem[1]. 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*,

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

[1] 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.)

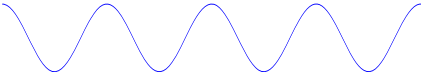
### Example 2 (**Kronig-Penney's model**)

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

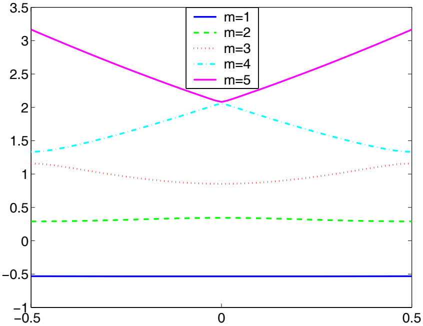
$$V_\Gamma(x) = 1 - \sum_{\gamma \in \mathbb{Z}} \mathbf{1}_{x \in \left[\frac{\pi}{2} + 2\pi\gamma, \frac{3\pi}{2} + 2\pi\gamma\right]}, \tag{30}$$

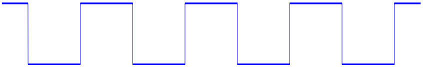
where $\mathbf{1}_\Omega$ denotes the characteristic function of a set $\Omega \subset \mathbb{R}$.

# Mathieu’s model and Kronig-Penney’s model

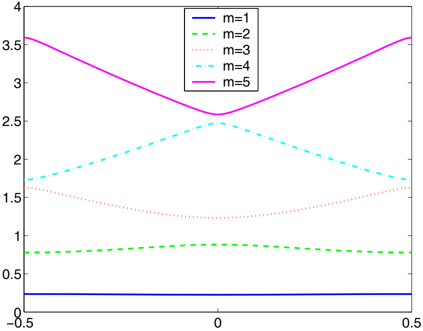


Mathieu’s Model



Kronig-Penney’s Model

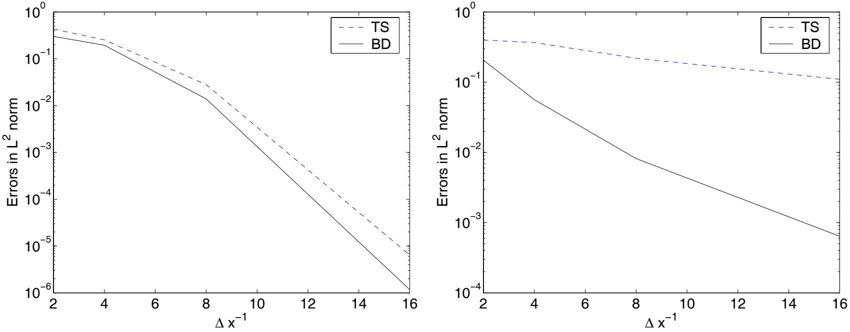



$$E_m(k),\ m = 1, \cdots, 5$$

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

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

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

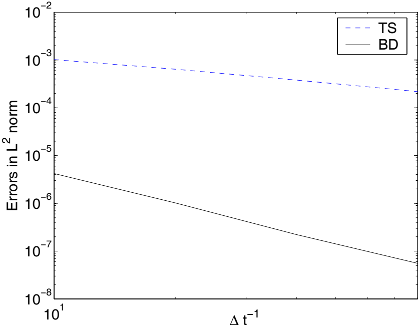


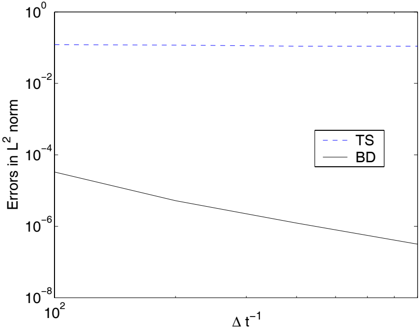
# Temporal discretization error test, $\frac{\triangle x}{\varepsilon} = \frac{1}{128}$

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

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

Right Figure: ($\varepsilon = \frac{1}{1024}$ 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 $\varepsilon$).
  - On the other hand, by using the *time-splitting Fourier spectral method*, one has to refine the time steps (depending on $\varepsilon$) 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 $V_\Gamma$.

# Numerical tests for 1D NLS

Then we consider the NLS [2].

**Example 3 (Tests for band mixing)**

We start with the initial condition likes

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

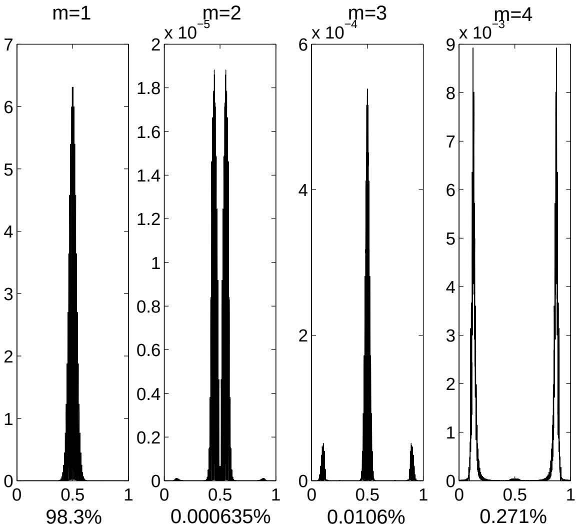
where $\psi_{\mathrm{in}}(x)$ is given in (26). We'll test the mass transition from one band to others.

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 transfers to other bands.

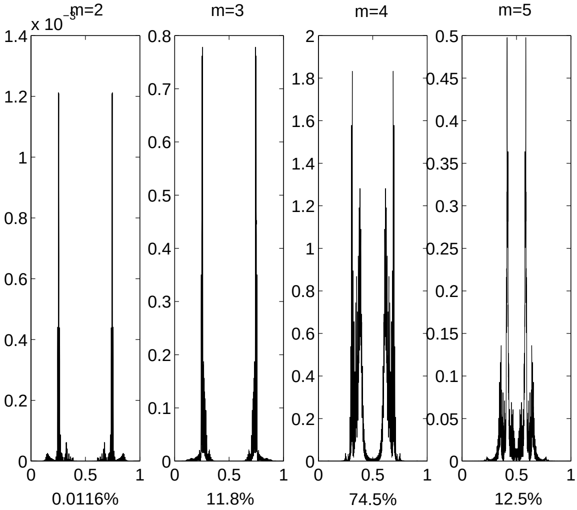
[2] Huang, Jin, Markowich and Sparber, MMS, 08'

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



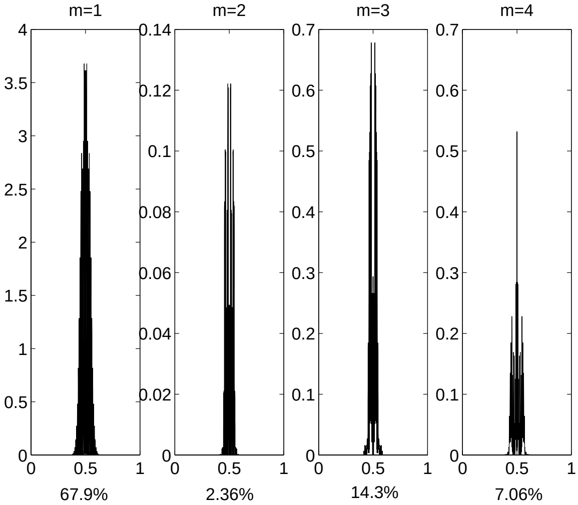

Mass distribution

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



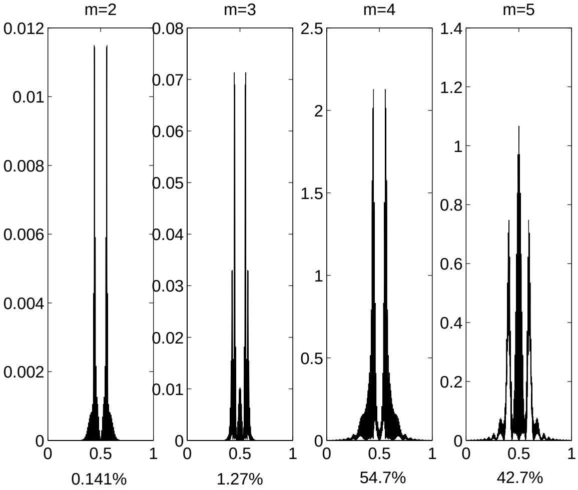

Mass distribution

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




Mass distribution

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




Mass distribution

# Numerical examples for lattice BEC in 3D [2]

## Example 4 (**Dynamics of BECs**)

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

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

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

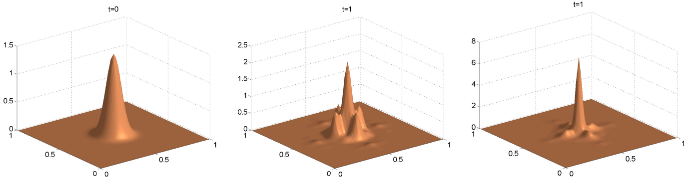
- *weak interaction*: $|\beta| \ll 1, \quad \mu_g = \frac{3\varepsilon}{2}, \quad \phi_g = \frac{1}{(\pi\varepsilon)^{3/4}} e^{-U(x)/\varepsilon}$;
- *strong interaction*: $\beta = \mathcal{O}(1)$,

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

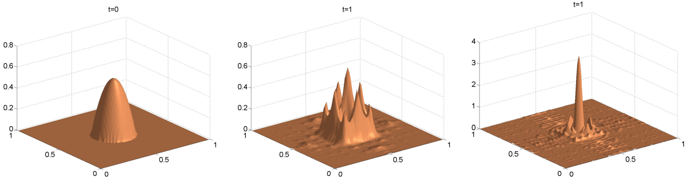
[2] Huang, Jin, Markowich and Sparber, MMS, 08'

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

$|\beta| = \frac{1}{4}$ and $\varepsilon = \frac{1}{4}$




$|\beta| = 1$ and $\varepsilon = \frac{1}{4}$




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

# Anderson localization in disordered media

In this example, we present numerical studies for the Klein-Gordon equation (32) including *random coefficients* [3]. This describes waves propagating in *disordered media*, a topic of intense physical and mathematical research (*cf.* P. A. Robinson, *Phil. Magazine B* **80**, 2000).

The *purely periodic coefficients* $a_\Gamma(y)$ and $W_\Gamma(y)$ describe an idealized situation where *no defects* are present within the material. More realistic descriptions for *disordered media* usually rely on the introduction of *random perturbations* within these coefficients.

Since our numerical method relies on $\{\varphi_m(y,k)\}_{m=1}^M$ as basis functions, the *stability* of our method w.r.t. to *perturbation* of these *Bloch functions* is an important question.

[3] Huang, Jin, Markowich and Sparber, Wave Motion, 09'

# Klein-Gordon equation with random coefficients

We shall study of the following class of (one-dimensional) *Klein-Gordon* type equations

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

with given initial data $u_0(x), v_0(x) \in \mathbb{R}$ and $f(x) \in \mathbb{R}$ describing some slowly varying source term.

The highly oscillatory coefficients $a_\Gamma(y), W_\Gamma(y) \in \mathbb{R}$ are assumed to be *periodic* with respect to some *regular lattice* $\Gamma \simeq \mathbb{Z}$. Equation (32) henceforth describes the propagation of waves on macroscopic length- and time-scales.

# Stability of our BD algorithm

To this end we consider, instead of (7), the *randomly perturbed* eigenvalue problem

$$\left(-\frac{\partial}{\partial_y}\left(a_\Gamma(\omega,y)\frac{\partial}{\partial_y}\right)+W_\Gamma(y)\right)\varphi_m(\omega,y,k) = \lambda_m(\omega,k)\varphi_m(\omega,y,k), \tag{33}$$

subject to the quasi-periodic boundary condition. Here, the coefficient $a_\Gamma = a_\Gamma(\omega,y)$ is assumed to be a function of a *uniformly distributed random variable* $\omega$ with mean zero and variance $\sigma^2 \geq 0$. In the following we shall vary $\sigma$ in such a way that we do not loose the uniform ellipticity.

In our algorithm, we solve the *random eigenvalue problem* (33), for different choices of $\sigma$, to obtain the corresponding eigenvalues $\lambda_m(\omega,k)$ and eigenfunctions $\varphi_m(\omega,y,k)$. We shall then take the *average* of them and use these averaged quantities in our Bloch decomposition based algorithm (as described in Section 7).

## Example 5 **(Stability tests and Anderson localization)**

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

$$u_0(x) = \left(\frac{2}{\pi\varepsilon}\right)^{1/4} \mathrm{e}^{-\frac{(x-\pi)^2}{\varepsilon}}, \quad v_0(x) = 0. \tag{34}$$

The random coefficient $a_\Gamma$ is chosen as

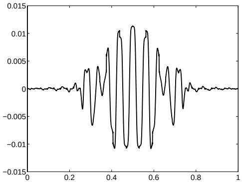
$$a_\Gamma(\omega, y) = a_\Gamma(y) + \omega, \quad a_\Gamma\,(y) = 2.5 + \cos(y), \tag{35}$$

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

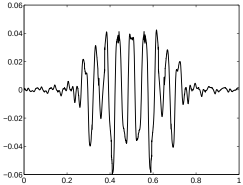
$$E_m(k) := \mathbb{E}\{E_m(\omega, k)\} \approx \frac{1}{N}\sum_{\ell=1}^{N} E_m(\omega_\ell, k), \tag{36}$$

for different values of $\sigma$.

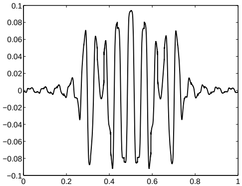
# Graphs of the differences: $u(1, 2\pi x) - u^{\sigma}(1, 2\pi x)$



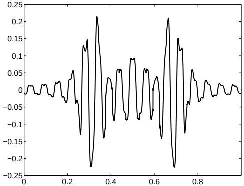

$\sigma = 0.01$




$\sigma = 0.05$




$\sigma = 0.10$




$\sigma = 0.20$

Figure: Comparison between the solution $u^{\sigma}(t, x)$ with noise and the solution $u(t, x)$ without noise. $\varepsilon = \frac{1}{32}$, $\triangle t = \frac{1}{10}$, $\triangle x = \frac{\pi}{512}$.

# Numerical Evidence for the Anderson localization

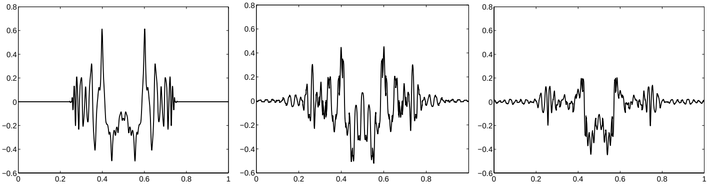
The phenomenon of Anderson localization, also known as the *strong localization*, describes the absence of dispersion for waves in random media with sufficiently *strong random perturbations*. It has been predicted by P. W. Anderson (Philos. Mag. B, **52**, 1985) in the context of (quantum mechanical) 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

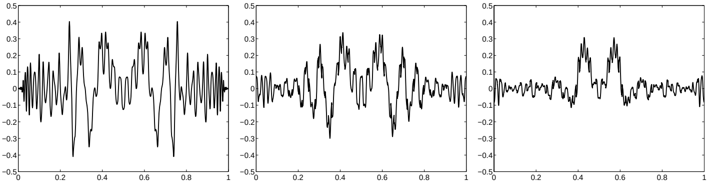
$$\begin{cases} \dfrac{\partial^2 u^\omega}{\partial t^2} = \dfrac{\partial}{\partial x}\left(a_\Gamma\left(\omega, \dfrac{x}{\varepsilon}\right)\dfrac{\partial u^\omega}{\partial x}\right) - \dfrac{1}{\varepsilon^2} W_\Gamma\left(\dfrac{x}{\varepsilon}\right) u^\omega + f(x), \\ u^\omega\big|_{t=0} = u_0(x), \quad \dfrac{\partial u^\omega}{\partial t}\Big|_{t=0} = v_0(x), \end{cases} \tag{37}$$

which describes the propagation of waves in *disordered media*.

# Averaged solutions with random perturbations




$\mathbb{E}\{u^{\omega}(1, 1\pi x)\}$, where, from left to right: $\sigma = 0$, $0.5$, and $1.0$.




$\mathbb{E}\{u^{\omega}(2, 1\pi x)\}$, where, from left to right: $\sigma = 0$, $0.5$, and $1.0$.

Figure: Averaged solutions at different time for different choices of $\sigma$ ($\varepsilon = \frac{1}{64}$).

# 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.

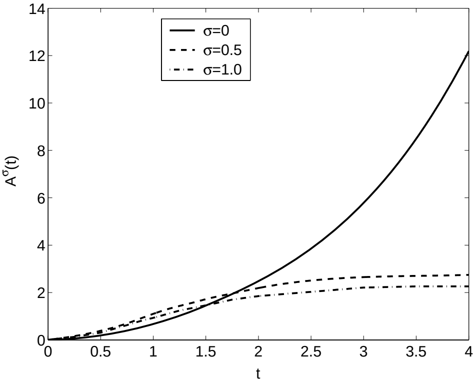
$$E_0^\omega(\omega,t) = \int_{\mathbb{R}} e^\omega(t,x)\mathrm{d}x, \tag{38}$$

and we likewise define

$$E_2^\omega(\omega,t) = \int_{\mathbb{R}} x^2 e^\omega(t,x)\mathrm{d}x, \tag{39}$$

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 $\sigma$ ($\varepsilon = \frac{1}{64}$)




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

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 $\varepsilon \ll 1$.

*Thank you for your attention!*