Semiclassical asymptotics for nonlinear Schrödinger equation with periodic potential

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1. Basic Setting

We study the asymptotic behavior for $0 < \varepsilon \ll 1$ of the following (weakly) nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = -\frac{\varepsilon^2}{2}\Delta u^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right) u^\varepsilon + U(x)u^\varepsilon + \varepsilon\kappa\,|u^\varepsilon|^2 u^\varepsilon, \tag{1}$$

with $x \in \mathbb{R}^d$, $t \in \mathbb{R}$, and $\kappa \in \mathbb{R}$.

Here $U(x)$ is some given (slowly varying) potential, whereas $V_\Gamma = V_\Gamma(y) \in \mathbb{R}$ is assumed to be periodic with respect to some regular lattice $\Gamma \simeq \mathbb{Z}^d$, *i.e.*

$$V_\Gamma(y+\gamma) = V_\Gamma(y), \quad \forall\, y \in \mathbb{R}^d, \gamma \in \Gamma. \tag{2}$$

where

$$\Gamma \equiv \left\{ \gamma = \sum_{l=1}^{d} \gamma_l \zeta_l \in \mathbb{R}^d : \ \gamma_l \in \mathbb{Z}, \zeta_l \in \mathbb{R}^d \right\}.$$

Equation (1) appears in the description of superfluid dynamics of Bose-Einstein condensates in optical lattices:

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = -\frac{\varepsilon^2}{2}\Delta u^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right) u^\varepsilon + U(x)u^\varepsilon + \varepsilon\kappa\left|u^\varepsilon\right|^2 u^\varepsilon.$$

In this case a particular example of the periodic lattice potential V_Γ is then

$$V_\Gamma(x) = \sum_{l=1}^{3} \frac{\hbar^2\xi_l^2}{2m} \sin^2(\xi_l x_l),$$

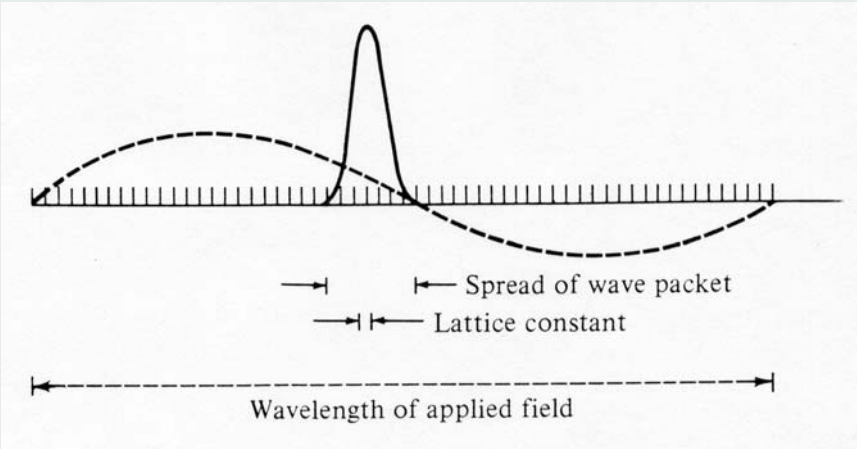
where $\xi = (\xi_1, \xi_2, \xi_3)$ denotes the wave vector of the laser field. Moreover we typically have

$$U(x) = \frac{|x|^2}{2},$$

describing a harmonic trap (needed to obtain a condensate).

Remark. Other applications appear in the modeling of electronic charge transport in crystals or semiconductor superlattices (including Hartree-Nonlinearities).

We are led to a two scale problem:



As $\varepsilon \to 0$, we expect fast oscillations of wavelength $\mathcal{O}(\varepsilon)$ to be induced by the *periodic Hamiltonian operator*

$$H^{\varepsilon}_{\mathrm{per}} := -\frac{\varepsilon^2}{2}\Delta + V_{\Gamma}\left(\frac{x}{\varepsilon}\right), \tag{3}$$

We thus need to understand the spectral properties of $H^{\varepsilon}_{\mathrm{per}}$. To this end recall Bloch's eigenvalue problem (cell problem):

We set $y = x/\varepsilon$ and consider

$$\begin{cases} \left(\frac{1}{2}\left(-\mathrm{i}\nabla_y + k\right)^2 + V_\Gamma(y)\right)\chi_m(y,k) = E_m(k)\chi_m(y,k), & m \in \mathbb{N},\ y \in Y, \\ \chi_m(y+\gamma,k) = \chi_m(y,k), & \text{for } \gamma \in \Gamma. \end{cases}$$

Here, $Y \subset \Gamma$ is the (centered) fundamental domain of the lattice Γ, equipped with periodic boundary conditions. The fundamental domain of the corresponding dual lattice (equipped with periodic b.c.), the so-called Brillouin zone, is denoted by $\mathcal{B} \equiv Y^*$.

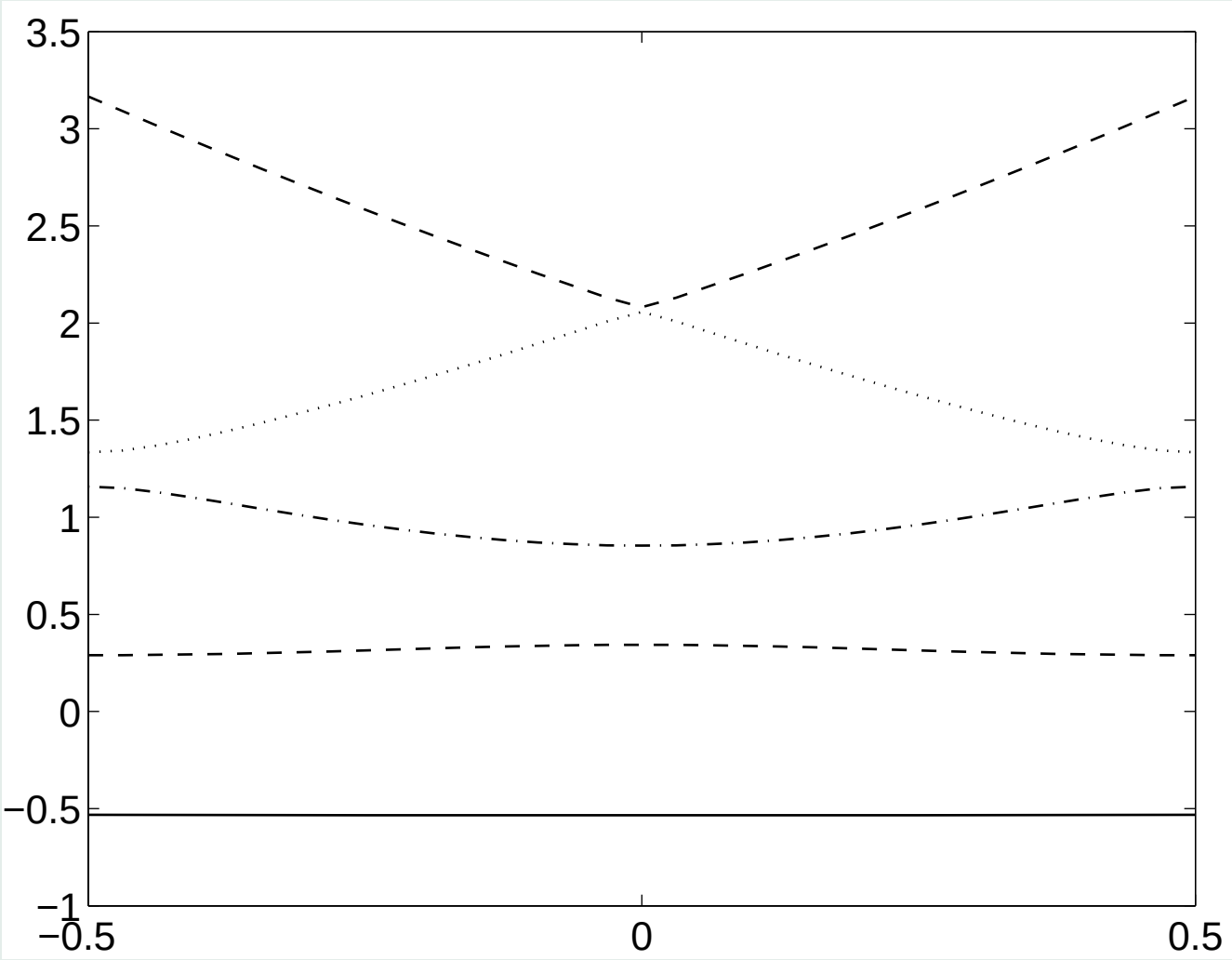
Under very mild conditions on V_Γ, the eigenfunctions $\chi_m(y,k)$ exist and form a complete ONB of $L^2(Y)$. The set

$$\{E_m(k) \in \mathbb{R} : E_m(k) \le E_{m+1}(k),\ k \in Y^*\}$$

is called the m-th energy band, or Bloch band. A band $E_m(k)$ is called isolated if it holds:

$$E_{m-1}(k) < E_m(k) < E_{m+1}(k), \quad \text{for all } k \in \mathcal{B}.$$

The first few Bloch bands for $V_\Gamma = \cos x$, drawn over $\mathcal{B} \equiv Y^*$.



2. Asymptotic results

In [Carles-S.-Markowich, JSP 04] we assumed that the initial data is of WKB type and concentrated in a single (isolated) Bloch band $E_m(k) \in \mathbb{R}$. Then it has been proved (adiabatic decoupling)

$$u^\varepsilon(t,x) \sim a(t,x)\chi_m\left(\frac{x}{\varepsilon}, \nabla_x S(t,x)\right) \mathrm{e}^{\mathrm{i}S(t,x)/\varepsilon} + \mathcal{O}(\varepsilon), \quad m \in \mathbb{N},$$

where $S(t,x) \in \mathbb{R}$ solves the semi-classical Hamilton-Jacobi equation

$$\partial_t S + E_m(\nabla_x S) + U(x) = 0. \tag{4}$$

This fully nonlinear equation determines S only locally in time, since in general caustics will appear in the corresponding rays of geometrical optics.

As long as S is smooth, the (complex-valued) amplitude $a(t,x) \in \mathbb{C}$ is determined by the following transport equation:

$$\partial_t a + \nabla_k E_m(\nabla_x S)\cdot\nabla_x a + \frac{1}{2}\,\mathrm{div}_x(\nabla_k E_m(\nabla_x S))a - \beta_m(t,x)a = -i\kappa_m^*|a|^2 a,$$

where

$$\beta_m(t,x) := \langle \chi_m(\cdot,\nabla_x\phi),\, \nabla_k\chi_m(\cdot,\nabla_x\phi)\rangle_{L^2(Y)}\cdot\nabla_x U(x),$$

the so-called Berry phase term $\beta_m(t,x) \in \mathrm{i}\mathbb{R}$ (purely complex) and

$$\kappa^*(t,x) := \kappa \int_Y |\chi_m\,(y,\nabla_x S)|^4\ \mathrm{d}y.$$

the effective self-interaction (for cubic NLS).

Remark. Note that, since the nonlinearity is purely complex, we get the usual conservation law

$$\partial_t n + \mathrm{div}_x(\nabla_k E_n(\nabla_x S)n) = 0.$$

where $n(t,x) := |a(t,x)|^2$.

An extension of the above WKB approach is given in [C.S., SIAM 06] where one looks on even longer time-scales:

To this end, consider the dispersive scaling (semi-classics on longer time-scales)

$$\mathrm{i}\partial_t u^\varepsilon = -\frac{1}{2}\Delta u^\varepsilon + \frac{1}{\varepsilon^2} V_\Gamma\left(\frac{x}{\varepsilon}\right) u^\varepsilon + U(x)u^\varepsilon + \kappa\,|u^\varepsilon|^2 u^\varepsilon, \tag{5}$$

Assuming single-band plane wave initial data of WKB type, we find

$$u^\varepsilon(t,x) \sim f(t,\tilde{x})\chi_m\left(\frac{x}{\varepsilon}, k_0\right) \mathrm{e}^{\mathrm{i}k_0\cdot x/\varepsilon} e^{-\mathrm{i}E_m(k_0)t/\varepsilon^2} + \mathcal{O}(\varepsilon),$$

where we need to take into account a large drift given by

$$\tilde{x} := x - \frac{t}{\varepsilon}\vartheta_m(k_0), \quad \text{with } \vartheta_m(k_0) := \nabla_k E_m(k_0).$$

Moreover f is determined by the (homogenized) effective mass NLS, *i.e.*

$$\mathrm{i}\partial_t f = -\frac{1}{2}\,\mathrm{div}_x(M_m\nabla_x)f + U(x)f + \kappa_m^*\,|f|^2 f,$$

with an effective mass tensor (not necessarily positive definite)

$$M_m(k_0) := \partial_k^2 E_m(k_0) \in \mathbb{R}^{3\times 3},$$

which describes dispersive effects along the rays of geometrical optics.

3. Numerical approach

In [Huang-Jin-Markowich-S., JCP 06] we proposed a new time-splitting algorithm, based on the Bloch decomposition. To this end let $d = 1$, for the moment, and

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

and recall that upon solving Bloch's eigenvalue problem one obtains a decomposition of space $L^2(\mathbb{R})$ into a direct sum of orthogonal band spaces:

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

Thus

$$\forall\, f \in L^2(\mathbb{R}): \quad f(y) = \sum_{m\in\mathbb{N}} f_m(y), \quad f_m \in \mathcal{H}_m.$$

where the correspondingprojection of m-th band space is given by

$$f_m(y) \equiv (\mathbb{P}_m f)(y) = \int_{\mathcal{B}} \left(\int_{\mathbb{R}} f(\zeta)\overline{\varphi}_m(\zeta,k)\,\mathrm{d}\zeta \right) \varphi_m(y,k)\,\mathrm{d}k.$$

In what follows, we will denote by

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

the coefficient of the Bloch decomposition.

The main use of the Bloch decomposition is that it reduces

$$\mathrm{i}\partial_t u = -\frac{1}{2}\partial_{yy}u + V_\Gamma(y)u, \quad u\big|_{t=0} = u_{\mathrm{in}}(y),$$

into countably many, exactly solvable problems on $\mathcal{H}_m$. On each $\mathcal{H}_m$ one finds

$$\mathrm{i}\partial_t u_m = E_m(-\mathrm{i}\partial_y)u_m, \quad u_m\big|_{t=0} = (\mathbb{P}_m u_{\mathrm{in}})(y),$$

where $E_m(-\mathrm{i}\varepsilon\partial_x)$ denotes the Fourier-multiplier corresponding to the symbol $E_m(k)$.

In order not avoid the introduction of a numerical Bloch-transform and rely entirely on the use of FFT, we also introduce the following unitary transformation of $f \in L^2(\mathbb{R})$

$$(Tf)(y,k) \equiv \widetilde{f}(y,k) := \sum_{\gamma\in\Gamma} f(\varepsilon(y+2\gamma))\,\mathrm{e}^{-\mathrm{i}k\cdot\gamma}, \quad y \in Y,\ k \in \mathcal{B}.$$

The following inversion formula holds

$$f(\varepsilon(y+\gamma)) = \int_{\mathcal{B}} \widetilde{f}(y,k)\,\mathrm{e}^{\mathrm{i}k\cdot\gamma}\mathrm{d}k.$$

Moreover we can compute $C_m(k)$ via

$$C_m(k) = \int_Y \widetilde{f}(y,k)\overline{\varphi}_m(y,k)\,\mathrm{d}y,$$

which is what we will use in the following.

The splitting-algorithm then works as follows:

Step 0. As a preprocessing one has to compute the Bloch bands $E_m(k)$ and the corresponding $\chi_m(k)$. For smooth V_Γ in $d = 1$ this can be done easily, by expanding

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

and likewise

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

For smooth V_Γ, taking only the first few coefficients suffices and we consequently approximate Bloch's eigenvalue problem by the solution of an algebraic eigenvalue problem.

Note that the number of coefficients is indeed independent of the spatial grid. Thus the numerical costs of this preprocessing are almost negligible compared to those of the evolutionary algorithm.

Step 1. First, we solve the equation

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = -\frac{\varepsilon^2}{2}\,\partial_{xx}u^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right)u^\varepsilon, \quad x\in\mathbb{R},$$

on a fixed time-interval $\triangle t$. To do so we consider for each fixed $t\in\mathbb{R}$, the corresponding transformed solution $(Tu^\varepsilon(t,\cdot))\equiv\widetilde{u}^\varepsilon(t,y,k)$ and decompose it via

$$\widetilde{u}^\varepsilon(t,y,k)=\sum_{m\in\mathbb{N}}(\mathbb{P}_m\widetilde{u}^\varepsilon)=\sum_{m\in\mathbb{N}}C_m^\varepsilon(t,k)\varphi_m(y,k)\,.$$

Of course, we have to truncate this summation at a certain fixed $M\in\mathbb{N}$. Numerical experiments on the band mixing give us enough experience to choose M large enough to guarantee mass conservation up to sufficient high accuracy (typically $M=32$). This yields

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

which implies

$$C_m^\varepsilon(t,k)=C_m^\varepsilon(0,k)\mathrm{e}^{-\mathrm{i}E_m(k)t/\varepsilon}.$$

Step 2. In a second step, we solve the ordinary differential equation

$$\mathrm{i}\varepsilon\partial_t u^\varepsilon = \left(U(x) + \kappa|u^\varepsilon|^2\right) u^\varepsilon,$$

on the same time-interval as before, where the solution obtained in Step 1 serves as initial condition for Step 2. Thus

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

Note that this splitting conserves the particle density $\rho^\varepsilon(t,x) := |u^\varepsilon(t,x)|^2$, also on the fully discrete level.

Remark. Clearly, the algorithm given above is first order in time. But we can easily obtain a second order scheme by the Strang splitting method, i.e. performing Step 1 with time-step $\triangle t/2$, then Step 2 with time-step $\triangle t$, and finally integrate Step 1 again with $\triangle t/2$.

Remarks.

- If $U(x) = 0$ and also $\kappa = 0$ (i.e. no nonlinearity) our algorithm solves the evolutionary problem with periodic potential exact.
- Numerical experiments show that (in the linear case) our algorithm converges with $\triangle x = \mathcal{O}(\varepsilon)$ and $\triangle t = \mathcal{O}(1)$ for quadratic observables in u^ε. The latter is a huge advantage in comparison with a standard time-splitting methods, which require $\Delta t = \mathcal{O}(\varepsilon)$ ($\Rightarrow$ we can compute much longer times).
- The numerical cost of our algorithm is comparable to the one of a usual time-splitting method.
- The algorithm can be easily generalized to higher dimensions $d > 1$, if V_Γ is of the form

$$V_\Gamma(y) = \sum_{j=1}^{d} V_j(x_j), \quad \text{such that } V_j(x_j + \gamma_j) = V_j(x_j),$$

which is the case for our main motivation, namely lattice-BECs. If V_Γ does not separate as above, the solution of Bloch's eigenvalue problem is in itself a highly nontrivial task.

4. Numerical examples

We consider the equation on a bounded domain $\mathcal{D} = [-\lambda, \lambda]$, for some large enough $\lambda > 0$, equipped with periodic boundary conditions.

For definiteness we also choose V_Γ to be 2π-periodic. For example Mathieu's model

$$V_\Gamma(x) = \cos(x),$$

or the Kronig-Penney model

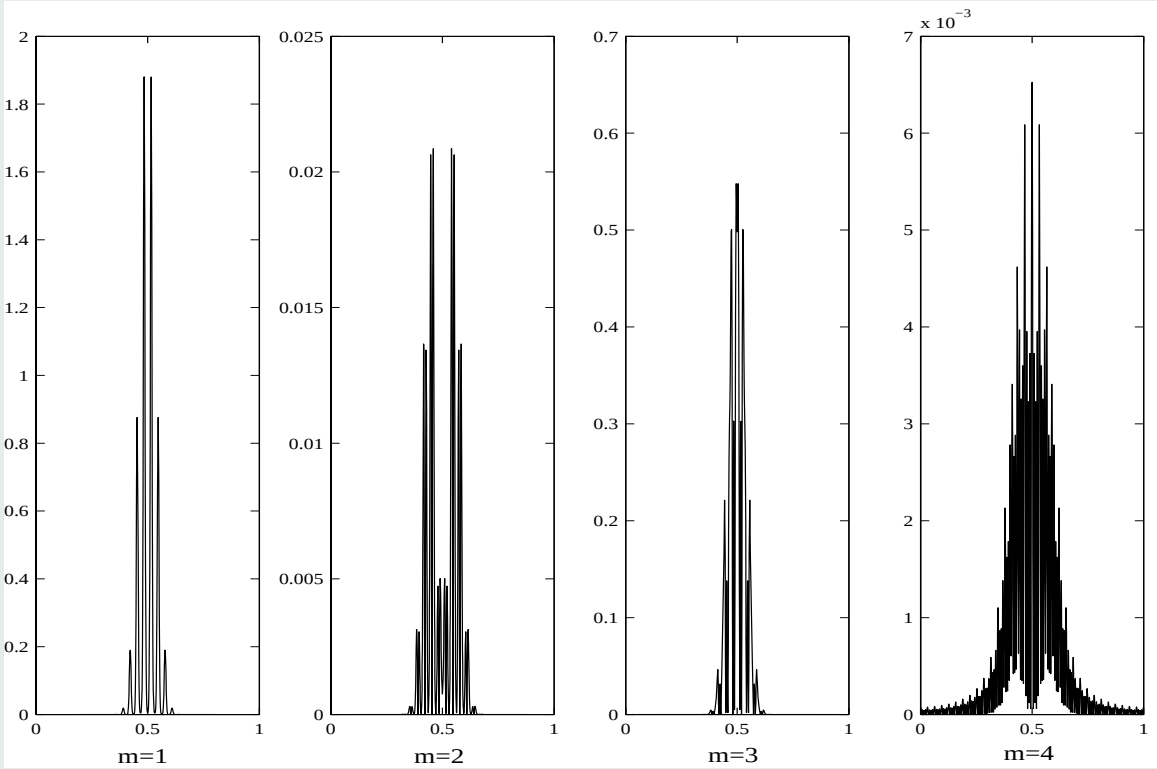
$$V_\Gamma(x) = 1 - \sum_{\gamma \in \mathbb{Z}} \mathbf{1}_{x \in \left[\frac{\pi}{2} + 2\pi\gamma, \frac{3\pi}{2} + 2\pi\gamma\right]},$$

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

Example. Take $V_\Gamma = \cos x$ and initially

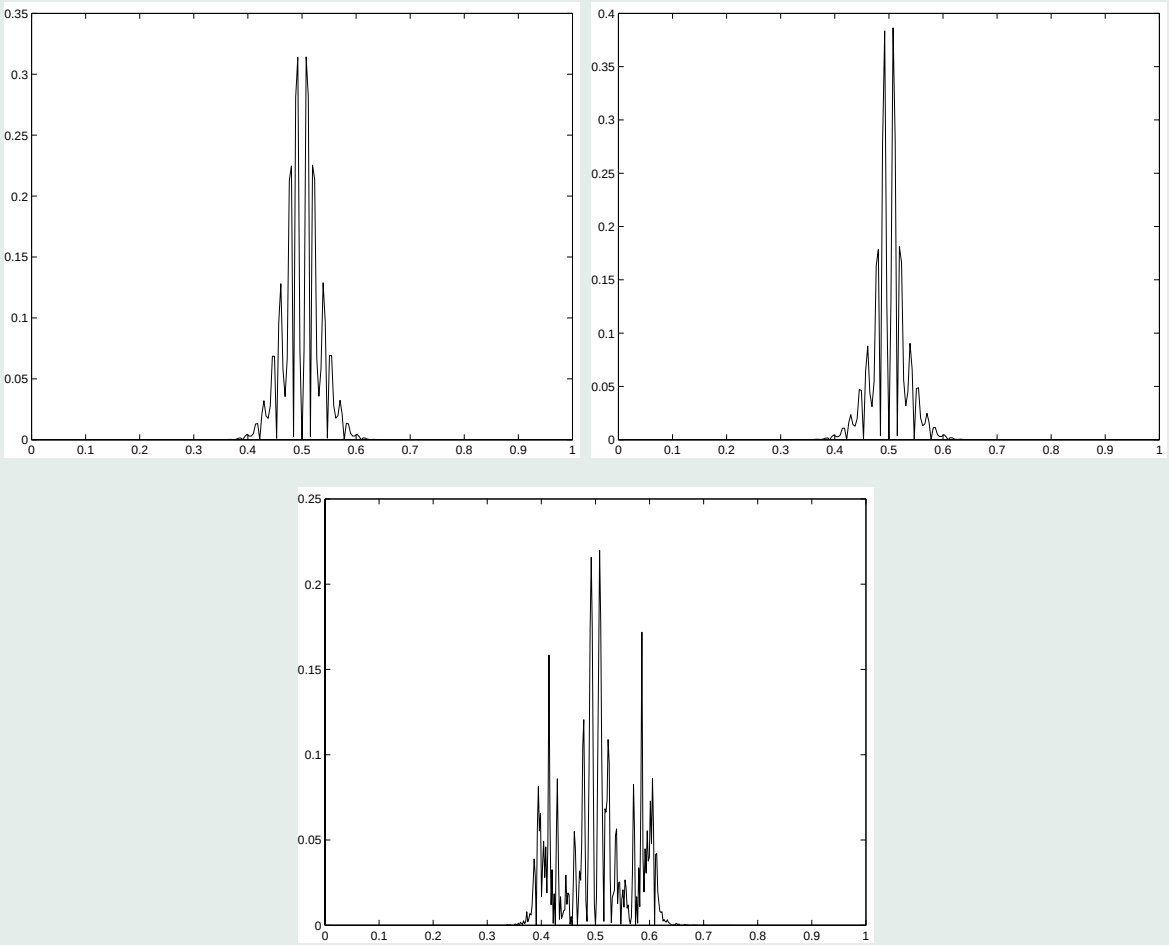
$$u_{\rm in}(x) = (10/\pi)^{1/4}\, {\rm e}^{-5(x-\pi)^2}.$$

The decomposition into the corresponding bands:



$|\mathbb{P}^\varepsilon_m u_{\rm in}|^2$, $m = 1, \cdots, 4$ for $\varepsilon = 1/32$.

In the linear case, for smooth $U(x)$, we only need $M = 8$ bands to guarantee mass conservation up to an error of 10^{-6}.



Time-evolution of $|u^\varepsilon(t,x)|^2$, plotted for $t = 0.1$, $t = 0.25$, and $t = 0.5$.

Example. (band mixing)

In the linear case one also knows that the Bloch bands are adiabatically stable up to small errors. More precisely, let initially $u_{\text{in}}(x) = (\mathbb{P}_{m_0} f(x))$ (i.e. concentrated in a single band), then

$$D_{m_0}(t) := \left\| u^\varepsilon(t,\cdot) - (\mathbb{P}_{m_0} u^\varepsilon(t,\cdot)) \right\|_{L^2(\mathbb{R})} = \mathcal{O}(\varepsilon),$$

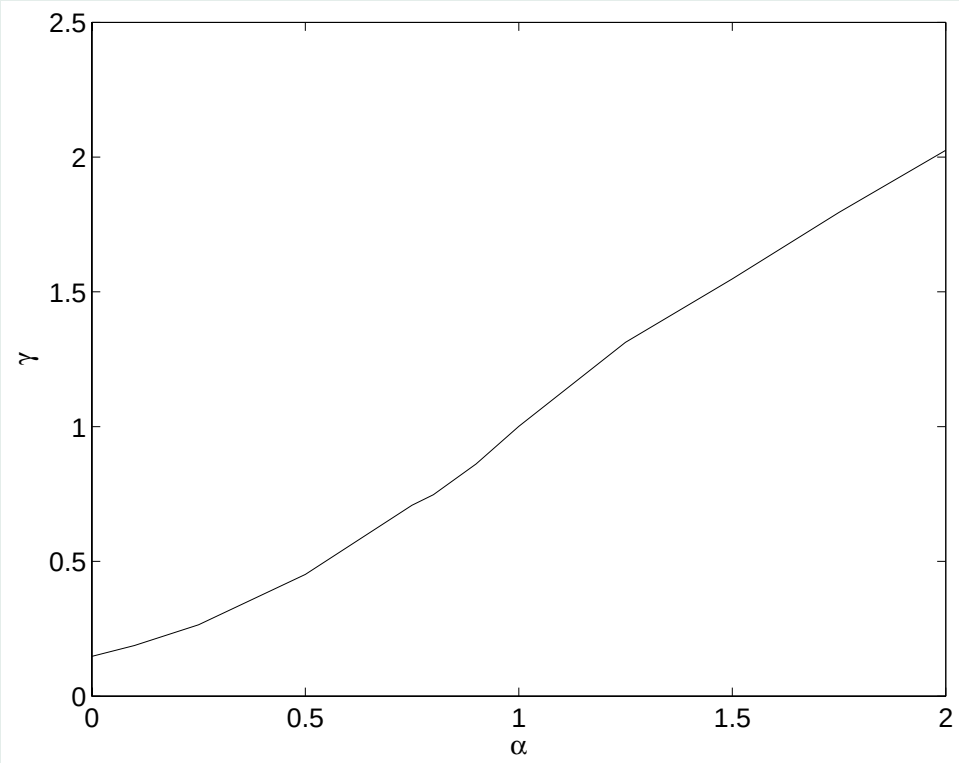
for isolated bands $m_0 \in \mathbb{N}$, on time-scales of order $\mathcal{O}(1)$.

In the nonlinear case band mixing is an open problem: We consider

$$\kappa = \mathcal{O}(\varepsilon^\alpha), \quad D_{m_0}(t) = \mathcal{O}(\varepsilon^\gamma), \quad \alpha, \gamma \geq 0,$$

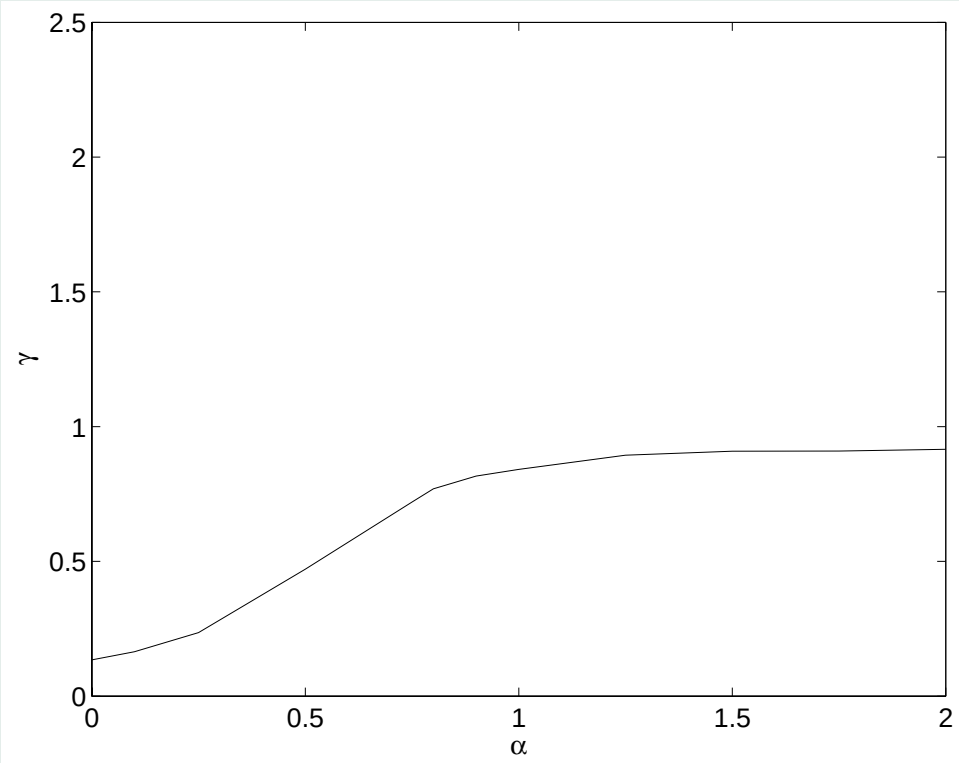
and we aim to numerically quantify the connection between α and γ.

Nonlinear band mixing: $U(x) = 0$ (no external potential).



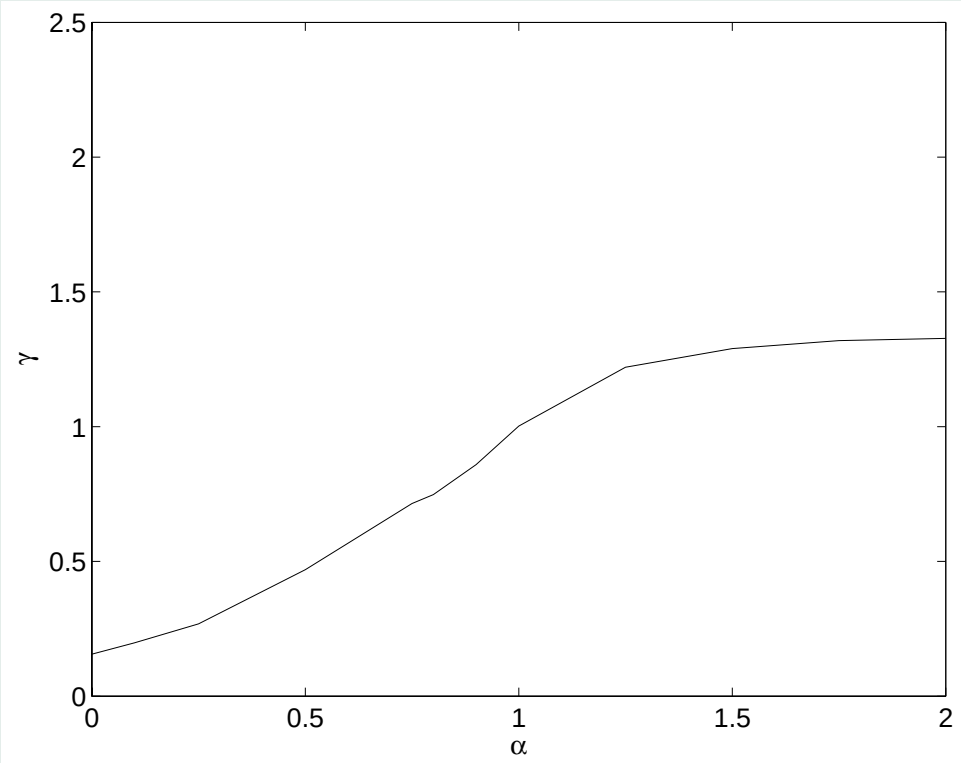
$m_0 = 1, \varepsilon = 1/32.$

Nonlinear band mixing: $U(x) = x$.



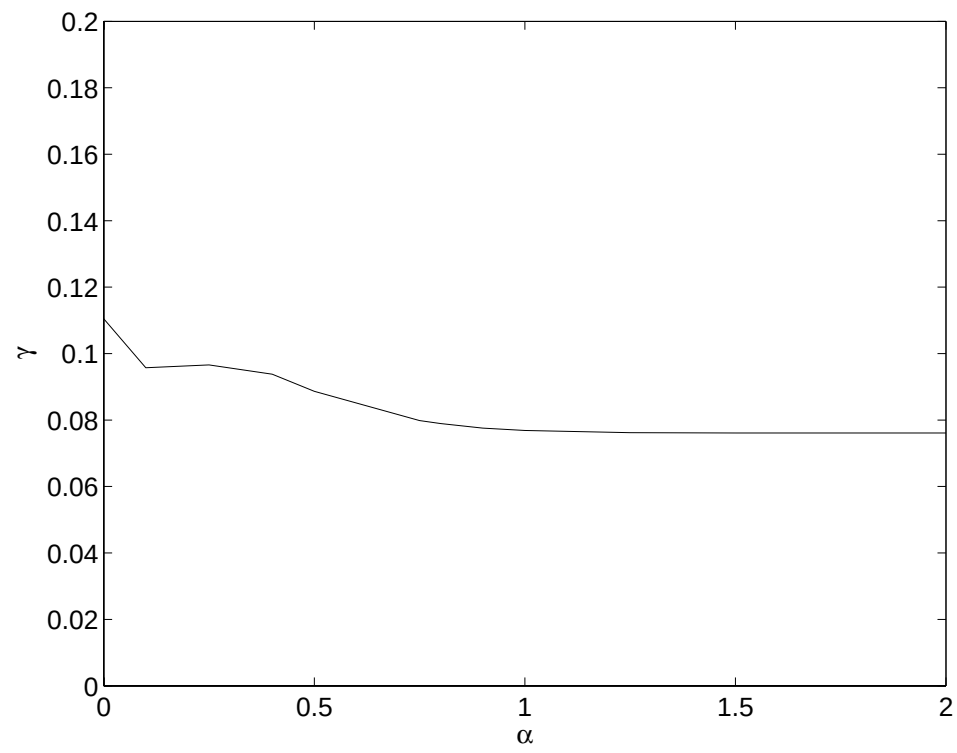
$m_0 = 1, \varepsilon = 1/32$.

Nonlinear band mixing: $U(x) = \frac{1}{2}|x - \pi|^2$.



$m_0 = 2, \varepsilon = 1/32.$

Nonlinear band mixing: $U(x) = \frac{1}{2}|x - \pi|^2$.



$m_0 = 4$ (non-isolated), $\varepsilon = 1/32$.

Example. (3D lattice BEC)

Finally we aim to perform a three dimensional simulation of a lattice BEC, having in mind the following experimental set-up:

First, the BEC is formed only under the influence of a confining $U(x)$ (harmonic oscillator) and then the periodic potential V_Γ is turned on.
The physical relevant initial data is thus given by the ground state of

$$-\frac{\varepsilon^2}{2}\,\Delta\phi^\varepsilon + U\phi + \kappa|\phi^\varepsilon|^2\phi^\varepsilon = \mu^\varepsilon\,\phi^\varepsilon, \quad \|\phi^\varepsilon\|_{L^2(\mathbb{R}^3)} = 1,$$

where $|\kappa| > 0$ (repulsive interaction). In our scaling ϕ^ε can be well approximated by the so-called Thomas-Fermi limit, i.e. discarding the dispersion term $\propto \varepsilon^2$. Thus we take as initial data

$$\phi_g(x) = \sqrt{\frac{1}{\lambda}\big(\mu_g - U(x)\big)_+},$$

where $\mu_g = \frac{1}{2}\left(\frac{15\lambda}{4\pi}\right)^{2/5}$.

Surface plot of $|u^\varepsilon(t,x)| = 0.25$ at different times, with $\kappa = 1$ and $\varepsilon = \frac{1}{4}$.