On Nonlinear Dispersive Equations in Periodic Structures: Semiclassical Limits and Numerical Methods

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The linear Schrödinger Equation '26

$$\begin{cases} i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V(x)\psi \quad , \ x \in \mathbb{R}^d \ , \quad t \in \mathbb{R} \\ \psi(x, t=0) = \psi_I^\varepsilon \quad (= \sqrt{\rho_I(x)} \exp\left(\frac{i}{\varepsilon} S(x)\right)) \end{cases}$$

ψ... complex-valued wave function

$\varepsilon > 0$...semiclassical parameter, $\quad << 1$

$V = V(x)$...real-valued potential field

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(averages of) observables are quadratic function(al)s of the wave function, e.g.:

- position density: $\rho = |\psi|^2$,
- current density: $\mathcal{I} = \varepsilon \mathrm{Im}(\overline{\psi}\nabla\psi)$.

Free Schrödinger Equation: $V \equiv 0$

$$\begin{cases} i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi \quad , \ x \in \mathbb{R}^d \, , \quad t \in \mathbb{R} \\ \psi(x, t=0) = \exp\left(\frac{ik\cdot x}{\varepsilon}\right) \quad \text{plane wave, wave-vector } \frac{k}{\varepsilon} \end{cases}$$

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$$\psi(x,t) = \exp\Bigg(i \underbrace{\left(k \cdot \frac{x}{\varepsilon} - \frac{|k|^2}{2}\frac{t}{\varepsilon}\right)}_{\substack{\text{space-time} \\ O(\varepsilon)\text{-wave} \\ \text{length} \\ \text{oscillations}}} \Bigg)$$

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$$E(k) = \frac{|k|^2}{2} \quad \text{...dispersion relation}$$

$V \not\equiv 0 \quad \Rightarrow$ no explicit computation!

W(entzel)-K(ramers)-B(rillouin)-ansatz

$$\psi = \sqrt{\rho}\, e^{i\frac{S}{\varepsilon}}$$

$$\begin{cases} \rho_t + \operatorname{div}(\rho \nabla S) = 0 & \text{transport equation} \\ S_t + \frac{1}{2}|\nabla S|^2 + V(x) = \frac{\varepsilon^2}{2} \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} & \text{phase equation} \end{cases}$$

equivalently, with $v := \nabla S$:

$$\begin{cases} \rho_t + \operatorname{div}(\rho v) = 0 \\ v_t + \nabla\left(\frac{|v|^2}{2} + V(x)\right) = \frac{\varepsilon^2}{2}\nabla\left(\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right) \end{cases}$$

quantum hydrodynamic equations,
dispersively regularized irrotational compressible Euler system, with external pressure $\nabla V(x)$ and internal quantum pressure $-\frac{\varepsilon^2}{2}\nabla\left(\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}\right)$.

Formal semiclassical (zero-dispersion) limit $\varepsilon \to 0$

transport equation

$$\downarrow$$

$$\left.\begin{array}{l} \rho_t^0 + \operatorname{div}(\rho^0 \nabla S^0) = 0 \\ S_t^0 + \frac{1}{2}|\nabla S^0|^2 + V(x) = 0 \end{array}\right\} \quad \text{WKB-system}$$

$$\uparrow$$

Hamilton-Jacobi equation

$$\left.\begin{array}{l} \rho_t^0 + \operatorname{div}(\rho^0 v^0) = 0 \\ v_t^0 + \nabla \left(\frac{|v^0|^2}{2} + V(x) \right) = 0 \end{array}\right\}$$

irrotational compressible Euler-system with external pressure

problem: the solution S^0 of the HJ-equation generally develops finite-time singularities!

Theorem

(J. Keller, P. Lax, ..., '50): Let $T_c > 0$ *be the caustic onset time of the HJ-equation. Then* $\left\| \psi - \sqrt{\rho^0} \exp\left(i \frac{S^0}{\varepsilon} \right) \right\|_{L^\infty((0,T);L^2(\mathbb{R}^d))} = \mathcal{O}(\varepsilon)$ *if* $0 < T < T_c$.

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beyond caustics:

- V. Maslov '60: phase shifts
- P. Gerard, P. Markowich, N. Mauser, F. Poupaud, P.L. Lions, T. Paul, C. Sparber '90-'08: semiclassical (Wigner) measures
- S. Jin, S. Osher '02-'08; C. Sparber, P. Markowich, N. Mauser '01: multi-valued solutions of HJ-equations

Semiclassical (Wigner) Measures

Definition

Let $\psi^\varepsilon \in L^2(\mathbb{R}^d)$ be a sequence of wave functions and $(\varepsilon) \to 0$ a scale. Then $w \in \mathcal{M}^+(\mathbb{R}^d_x \times \mathbb{R}^d_\xi)$ is called a semiclassical measure of ψ^ε on the scale (ε) if for all $a \in \mathcal{S}(\mathbb{R}^d_x \times \mathbb{R}^d_\xi)$, along a subsequence:

$$\lim_{\varepsilon \to 0} \int_{\mathbb{R}^d} \psi^\varepsilon(x) a^w(x, \varepsilon D)\psi^\varepsilon \, dx = \int_{\mathbb{R}^d_x \times \mathbb{R}^d_\xi} a(x,\xi) w(dx, d\xi).$$

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Theorem

('80 folklore) The semiclassical measure(s) $w = w(x, \xi, t)$ of the solution $\psi^\varepsilon(t)$ of the IVP-problem for the Schrödinger equation satisfies(y) the Liouville equation

$$\begin{cases} w_t + \xi \cdot \nabla_x w - \nabla_x V \cdot \nabla_\xi w = 0 \quad on \quad \mathbb{R}^d_x \times \mathbb{R}^d_\xi \times \mathbb{R}_t \\ w(t=0) = w_I \quad (a\ semiclassical\ measure\ of\ \psi^\varepsilon_I). \end{cases}$$

Connection to WKB-Asymptotics:

If $\psi_I(x) = \sqrt{\rho_I(x)} \exp\left(\frac{S_I(x)}{\varepsilon}\right)$, then $w_I(x,\xi) = \rho_I(x)\delta(\xi - \nabla S_I(x))$.

The solution of the Liouville equation stays monokinetic

$$w(x,\xi,t) = \rho^0(x,t)\delta(\xi - \nabla S^0(x,t))$$

as long as S^0 is the smooth solution of the HJ-equation

$$\begin{cases} S^0_t + \frac{1}{2}|\nabla S^0|^2 + V(x) = 0 \\ S^0(x,t=0) = S_I(x)\ . \end{cases}$$

After caustic onset: multi-valued solution theory (C. Sparber, P. Markowich, N. Mauser '02; S. Jin, S. Osher '04)!

Nonlinear Schrödinger Equations: $V = f(\rho)$

$$\begin{cases} i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + f(|\psi|^2)\psi \ , \quad x \in \mathbb{R}^d \ , \quad t > 0 \ , \\ \psi(t=0) = \sqrt{\rho_I}\exp\left(i\frac{S_I}{\varepsilon}\right) \ , \quad \rho_I, \ S_I \quad \text{smooth} \end{cases}$$

formal (compressible, isentropic, irrotational) Euler limit as $\varepsilon \longrightarrow 0$:

$$\begin{cases} \rho^0_t + \operatorname{div}(\rho^0 v^0) = 0 \ , \quad \rho^0(t=0) = \rho_I \ , \\ v^0_t + \nabla\left(\frac{1}{2}|v^0|^2 + f(\rho^0)\right) = 0 \ , \quad v^0(t=0) = \nabla S_I \end{cases}$$

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Theorem

(E. Grenier '98; R. Carles '07): $f' > 0$ on $\mathbb{R}^+$. Let $T > 0$ be smaller than the maximal existence time (of smooth solutions) of the irrotational isentropic Euler system. Then

$$\left\| \psi - \sqrt{\rho^0}\exp\left(i\frac{S^0}{\varepsilon}\right) \right\|_{L^\infty((0,T);H^s(\mathbb{R}^d))} \stackrel{\varepsilon \to 0}{\longrightarrow} 0 \quad \textit{for some } s > 0 \ .$$

Proof: Theory of symmetric hyperbolic systems, energy estimates.

Semiclassical Limits in Periodic Structures

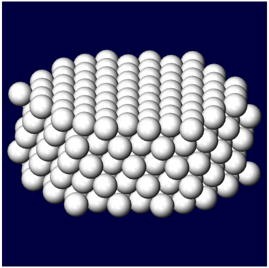

Figure: Periodic crystal lattice, $\delta\Gamma \cong \delta\mathbb{Z}^d$, fundamental domain δC

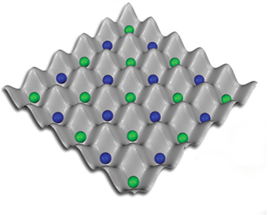

Figure: Electrons moving in a periodic lattice potential, $V_\Gamma = V_\Gamma(x/\delta)$.

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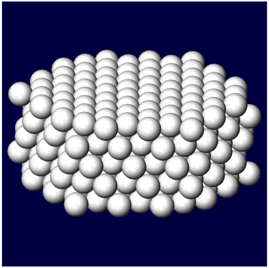

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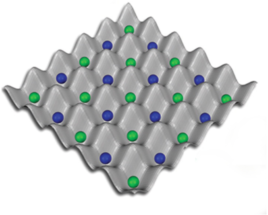

Figure: Electrons moving in a periodic lattice potential, $V_\Gamma = V_\Gamma(x/\delta)$.

Assumption: lattice spacing δ=semiclassical parameter ε

$$\text{NLS:} \quad i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + \underbrace{V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi + V(x)\psi}_{} + \underbrace{\kappa(\varepsilon)|\psi|^2\psi}_{\text{binary interaction}}$$

The Failure of the Standard WKB-Method

Linear case $\kappa = 0$:

$$i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi + V(x)\psi\ , \quad \psi = \sqrt{\rho}\ e^{i\frac{S}{\varepsilon}}$$

$$\begin{cases} \rho_t + \mathrm{div}(\rho\nabla S) = 0 \\ S_t + \frac{1}{2}|\nabla S|^2 + V_\Gamma\left(\frac{x}{\varepsilon}\right) + V(x) = \frac{\varepsilon^2}{2}\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \end{cases}$$

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$\Updownarrow$ drop the $\mathcal{O}(\varepsilon^2)$-pressure term

$$\underbrace{S_t + \frac{1}{2}|\nabla S|^2 + V_\Gamma\left(\frac{x}{\varepsilon}\right) + V(x)}_{H(x,\frac{x}{\varepsilon},\nabla S)} = 0$$

caustic onset time$=\mathcal{O}(\varepsilon^2)$!
H...Hamiltonian Γ-periodic in $y = \frac{x}{\varepsilon}$

Homogenisation theory based on viscosity solutions:

$$S_t^0 + \overline{H}(x, \nabla S^0) = 0$$

- Effective Hamiltonian $\overline{H} = \overline{H}(x, \xi)$: obtained by solving a stationary HJ-equation on a lattice cell.
- References: P.L. Lions, G. Papanicolaou, S. Varadhan '96; D. Gomes, L. Evans, P. Souganidis, P.L Lions '02-'08.
- Problem: viscosity solutions are based on a notion of dissipativity $\Rightarrow$ loss of reversibility! But: the Schrödinger equation *is* time reversible!

Bloch-Spectral Decomposition

$$L^2(\mathbb{R}^d) = \bigoplus_{m=1}^{\infty} S_m \,, \quad S_m \cong L^2(B)$$

B (bounded)...Brillouin zone, fundamental domain of Γ^*

$$\psi(y) = \sum_{m=1}^{\infty} \frac{1}{|B|} \int_B \mathring{\psi}_m(k) \Psi_m(y,k)\, dk$$

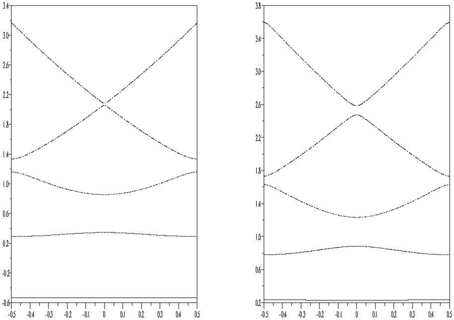
$$\begin{cases} -\frac{1}{2}\Delta_y \Psi_m(y,k) + V_\Gamma(y)\Psi_m(y,k) = E_m(k)\Psi_m(y,k) \\ \Psi_m(y+\gamma,k) = e^{i\gamma\cdot k}\Psi_m(y,k) \quad \forall\, \gamma \in \Gamma \,, \quad y \in \mathbb{R}^d \,, \quad k \in B \end{cases}$$

quasiperiodic Bloch eigenvalue problem

$$E_1(k) \le E_2(k) \le \ldots \le E_m(k) \le E_{m+1}(k) \le \ldots \quad \text{Bloch bands}$$

$$\Psi_m(y,k) = \underset{\uparrow}{e^{ik\cdot y} \chi_m(y,k)} \quad \text{Bloch-eigenfunctions}$$

Γ-periodicity in y, Γ^*-periodicity in k



band gaps!
intersections of
Bloch bands!

- Mathieu-equation: $V_\Gamma(y) = \cos(y)$ (left)
- Kronig-Penney model: $V_\Gamma(y) = 1 - \sum_{j\in\mathbb{Z}} \chi_{[\frac{\pi}{2}+2j\pi,\frac{3\pi}{2}+2j\pi]}$ (right)

(P. Gerard, P. Markowich, N. Mauser, F. Poupaud '96)

$$y = \frac{x}{\varepsilon} \Rightarrow S_m \to S_m^\varepsilon$$

$$\psi = \sum \psi_m \ , \quad \psi_m \in S_m^\varepsilon$$

$$i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi \Leftrightarrow i\varepsilon\frac{\partial}{\partial t}\psi_m = E_m(\varepsilon D)\psi_m \ , \quad m = 1, 2, \ldots$$

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Theorem

(linear case, no slow scale potential) The semiclassical measure $w = w(x, k, t)$ of ψ is given by $w = \sum_{m=1}^{\infty} w_m$, where w_m satisfies the transport equation:

$$\frac{\partial}{\partial_t}w_m + \nabla_k E_m(k) \cdot \nabla_x w_m = 0 \ , \quad w_m(t = 0) = w_{m,I} \geq 0 \ .$$

w_m is Γ^*-periodic in k.

Maxwell Equations in a Periodic Medium

$$\begin{array}{ll} \sigma = \sigma\left(\frac{x}{\varepsilon}\right) \; : \; \varepsilon\Gamma\text{-periodic permittivity} & \text{P.Markowich} \\ \mu = \mu\left(\frac{x}{\varepsilon}\right) \; : \; \varepsilon\Gamma\text{-periodic permeability} & \text{F. Poupaud, '96} \end{array}$$

$$\begin{cases} \sigma\left(\frac{x}{\varepsilon}\right) E_t = \operatorname{curl} H \,, \quad \operatorname{div}\left(\sigma\left(\frac{x}{\varepsilon}\right) E\right) = 0 \quad \text{in } \mathbb{R}^3 \,, \quad t > 0 \,, \\ \mu\left(\frac{x}{\varepsilon}\right) H_t = -\operatorname{curl} E \,, \quad \operatorname{div}\left(\mu\left(\frac{x}{\varepsilon}\right) H\right) = 0 \quad \text{in } \mathbb{R}^3 \,, \quad t > 0 \,. \end{cases}$$

$$\left.\begin{array}{l} E \overset{\varepsilon \to 0}{\rightharpoonup} E^0 \\ H \overset{\varepsilon \to 0}{\rightharpoonup} H^0 \end{array}\right\} \text{solve "homogenised" Maxwell system}$$

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energy density: $e^{\varepsilon} := \sigma\left(\frac{x}{\varepsilon}\right)|E|^2 + \mu\left(\frac{x}{\varepsilon}\right)|H|^2 \rightharpoonup e^0??$

Bloch eigen-value problem
$$\begin{cases} \operatorname{curl}_y\left(\frac{1}{\mu(y)}\operatorname{curl}_y e\right) = \omega(k)^2\sigma(y)e\,, \quad \operatorname{div}_y(\sigma(y)e) = 0 \\ e(y+\gamma,k) = e^{i\gamma\cdot k}e(y,k) \quad \forall\gamma\in\Gamma\,, \quad k\in B\,, \quad y\in\mathbb{R}^3 \end{cases}$$

Slow-Fast Coupling

(P. Bechouche, N. Mauser, F. Poupaud '01; G. Panati, H. Spohn, S. Teufel '02)

$$\begin{cases} i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi + V(x)\psi \\ \psi(t=0) = \psi_I \end{cases}$$

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Theorem

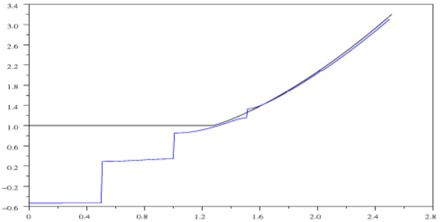
Let ψ_I concentrate in the m-th Bloch band space S_m^ε and assume that the m-th band $E_m = E_m(k)$ is isolated. Then the semiclassical measure of $\psi(t)$ satisfies

$$\begin{cases} w_t + \nabla_k E_m(k)\cdot\nabla_x w - \nabla_x V(x)\cdot\nabla_k w = 0 \\ w(t=0) = w_I \quad (= \text{a semiclassical measure of } \psi_I). \end{cases}$$

If $w_I = \rho_I(x)\delta_{\Gamma*}(k - \nabla S_I(x))$, then $w(t) = \rho(x,t)\delta_{\Gamma*}(k - \nabla S(x,t))$ as long as S remains smooth, where

$$\begin{cases} S_t + E_m(\nabla S) + V(x) = 0 \\ S(t=0) = S_I \end{cases}$$

Comparison between $\overline{H}(\xi)$, for $V(x) \equiv 0$ and $V_\Gamma(y) = \cos(y)$ (Mathieu equation), and the Bloch-bands:
$\overline{H}$: black solid line, Bloch bands: blue dotted lines



$$\overline{H}(\xi) = \begin{cases} \xi = \frac{1}{2\pi} \int_0^{2\pi} \sqrt{2(\overline{H}(\xi) - \cos(z))}\, dz, & |\xi| > \frac{\pi}{4} \\ 1 \quad (= \max(\cos(y))!), & |\xi| < \frac{\pi}{4} \end{cases}$$

L. Gosse, P. Markowich '03

Bose-Einstein Condensates in Optical Lattices

BEC: ultracold, dilute quantum gas
below the critical temperature: Gross-Pitaevskii NLS

$$\psi(\underbrace{x_1, x_2, x_3}_{\mathbb{R}^3}, t): \quad \text{condensate wave function}$$

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$$i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + \underbrace{V(x)\psi}_{A} + \underbrace{V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi}_{B} + \underbrace{\kappa\varepsilon|\psi|^2\psi}_{C}$$

A: harmonic laser confinement: $V(x) = \omega_1\frac{x_1^2}{2} + \omega_2\frac{x_2^2}{2} + \omega_3\frac{x_3^2}{2}$
B: periodic lattice
C: two-body interaction, weak nonlinearity

WKB-Asymptotics

Theorem (R. Carles, P. Markowich, C. Sparber '04)
If $\psi(t=0)$ is concentrated in the m-th Bloch band, then

$$\psi^{\varepsilon}(x,t) \sim A(x,t)\chi_m\left(\frac{x}{\varepsilon}, \nabla_x S(x,t)\right)\exp\left(\frac{i}{\varepsilon}S(x,t)\right)$$

where

$$S_t + E_m(\nabla_x S) + V(x) = 0 \quad \text{semiclassical HJ-equation in the m-th band}$$

$$\Uparrow$$

and (P. M., Guillot, E. Trubowitz, I. Ralston, '88; linear case $\kappa \equiv 0$)

$$\Downarrow$$

$$A_t + \nabla_k E_m(\nabla_x S)\cdot\nabla_x A + \frac{1}{2}\operatorname{div}(\nabla_k E_m(\nabla_x S)A) - \beta_m A = -i\kappa_m^*|A|^2 A$$

as long as S is smooth! Here:

$$\beta_m \in i\mathbb{R} : \text{Berry phase}\ , \quad \kappa_m^* = \kappa\int_C |\chi_m(y,\nabla_x S)|^4\, dy$$

Numerics of Lattice SE: Difficulties

$$i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi \quad \Big| \quad \text{Fouriertransform}$$

$$i\varepsilon\tilde{\psi}_t = \frac{\varepsilon^2}{2}|\xi|^2\tilde{\psi}(\xi,t) + \sum_{\alpha\in\Gamma^*}\hat{V}(\omega)\tilde{\psi}\left(\xi - \frac{\alpha}{\varepsilon}, t\right)$$

$$\Uparrow$$

$$\hat{V}(\gamma) = \frac{1}{|C|}\int_C V(y)e^{-iy\cdot\gamma}\,dy$$

Fourier coefficients of the Γ-periodic potential V_Γ.

as $\varepsilon \longrightarrow 0$ higher and higher Fourier modes influence the low modes. $\Rightarrow$ numerical error accumulation!

Bloch-Time splitting Discretisation

(Z. Huang, S. Jin, P. Markowich, C. Sparber '05)

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1. preprocessing: compute the Bloch bands $E_m(k)$ and the Bloch eigenvectors $\chi_m(y,k)$, for $m = 1...M$. This is simple and cheap if $d = 1$, less trivial for $d = 2$ and difficult if $d = 3$.
   For BECs we have, however,

   $$V_\Gamma(y) = V_{\Gamma_1}(y_1) + V_{\Gamma_2}(y_2) + V_{\Gamma_3}(y_3)$$

   which allows to solve only 1-dim. spectral problems combined with a fractional step method.

2. at time $t = 0$ decompose

$$\psi(t=0) \approx \sum_{m=1}^{M} \psi_{I,m} , \quad \psi_{I,m} \in S_m^{\varepsilon} .$$

This is done by adapting FFT $\Rightarrow$ cheap!

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3. first splitting step

$$\left. \begin{array}{l} i\varepsilon\varphi_t = -\frac{\varepsilon^2}{2}\Delta\varphi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\varphi \\ \varphi(t=0) = \psi_{I,m} \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} i\varepsilon\varphi_t = E_m(\varepsilon D)\varphi \\ \varphi(t=0) = \psi_{I,m} \end{array} \right\} i = 1 \ldots M$$

$$\Downarrow$$

$$\tilde{\varphi}(\Delta t) = \tilde{\psi}_{I,m} \exp\left(\tfrac{i}{\varepsilon} E_m(\varepsilon k) t\right)$$

update ψ : $\quad \tilde{\psi}_0(\Delta t) \approx \sum_{m=1}^{M} \tilde{\psi}_{I,m} \exp\left(\tfrac{i}{\varepsilon} E_m(\varepsilon k) t\right)$

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4. second splitting step

$$\left.\begin{array}{l} i\varepsilon\psi_t = V(x)\psi + \sigma|\psi|^2\psi \\ \psi(t=0) = \psi_0(\Delta t) \end{array}\right\} \overset{\text{(explicit)}}{\Rightarrow} \psi(\Delta t)$$

Remarks on the Bloch-time splitting scheme

1. a second order Strang-splitting scheme is straightforward
2. meshsize constraints: $\Delta x = \mathcal{O}(\varepsilon)$, $\Delta t = \mathcal{O}(1)$ in the linear case
3. the computational cost is comparable to the usual spectral time-splitting method
4. mass conservation in each Bloch band
5. BUT: we need good Bloch-spectral information!!!

Band-mixing: mass transfer

$$i\varepsilon\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi + V(x)\psi + \kappa(\varepsilon)|\psi|^2\psi$$

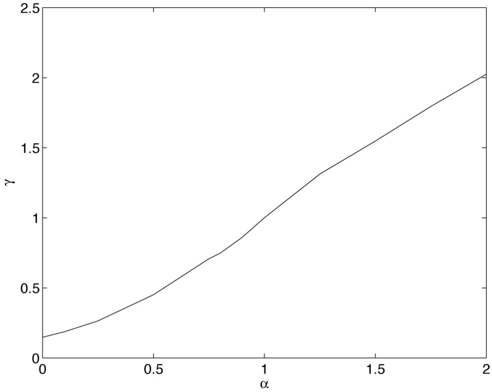
linear case $\kappa \equiv 0$: isolated Bloch bands are adiabatically stable up to small errors; G. Panati, H. Spohn, S. Teufel '03

Theorem

Let $\psi_I = \psi(t=0) = P_m\psi_I$ (concentrated in the m-th Band). Then, if $\kappa = 0$ and the m-th band is isolated: $F_m(t) = \|\psi(t) - P_m\psi(t)\|_{L^2} = \mathcal{O}(\varepsilon)$ on $\mathcal{O}(1)$-time scales.

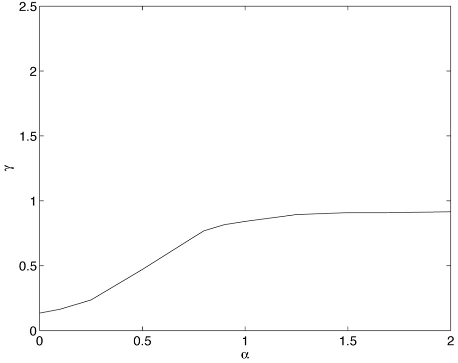
nonlinear case: set $\kappa(\varepsilon) = \varepsilon^{\alpha}$, ansatz: $F_m(t) = O(\varepsilon^{\gamma})$. How are α and γ related? Numerical study!

1. no slow scale potential $V(x) \equiv 0$, $V_\Gamma(y) = \cos(y)$, $m = 1$ (the first Bloch band is isolated), $\varepsilon = \frac{1}{32}$



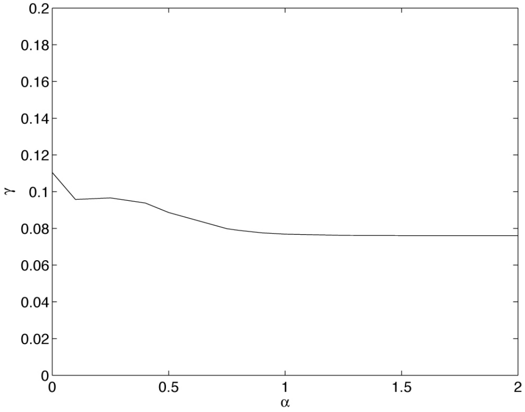
$\alpha \approx \gamma$, the mass transfer rate is of the same order as the nonlinearity.

2. Slow scale potential $V(x) = x$, $m = 1$, $\varepsilon = \frac{1}{32}$



large nonlinearity $0 < \alpha < 1$: $\mathcal{O}(\varepsilon^\alpha)$-mass transfer rate
small nonlinearity $\alpha > 1$: $\mathcal{O}(\varepsilon)$-mass transfer rate

3. Non-isolated band $m = 4$, for $V_\Gamma(y) = \cos(y)$, $V(x) = \frac{1}{2}(\alpha - \pi)^2$, $\varepsilon = \frac{1}{32}$



constant mass transfer rate independent of the nonlinearity.

Simulations of Lattice Bose-Einstein Condensates

$$V_\Gamma(y) = \sum_{i=1}^{3} \sin^2(y_i)\ , \quad V(x) \approx \frac{1}{2}|x|^2\ , \quad \kappa(\varepsilon) = \pm \left\{ \begin{array}{l} \varepsilon \\ 1 \end{array} \right.$$

$\uparrow$

allows to solve only 1-dim. Bloch spectral problems!

Experimental setup: the BEC is formed under the action of the harmonic potential $V(x)$, then the lattice potential $V_\Gamma\left(\frac{x}{\varepsilon}\right)$ is turned on.
Initial datum: ground state (repulsive interaction)

$$\left\{ \begin{array}{l} -\frac{\varepsilon^2}{2}\Delta\psi_g + V(x)\psi_g + |\kappa(\varepsilon)||\psi_g|^2\psi_g = \mu(\varepsilon)\psi_g \\ \|\psi\|_{L^2} = 1\ , \quad \psi_g > 0 \quad \text{(unique!)} \end{array} \right.$$

or its Tomas-Fermi limit (drop the Laplacian...).

Weak Nonlinearity $\kappa = \pm\varepsilon$

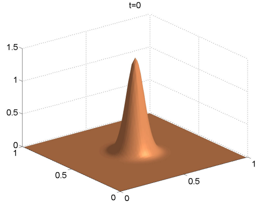


Figure: $\rho(t=0)|_{x_3=0}$
initial density
harmonic oscillator
ground state

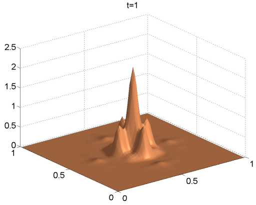


Figure: $\rho(t=1)|_{x_3=1}$
defocusing $\kappa = \varepsilon$

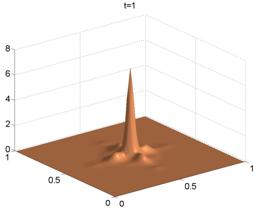


Figure: $\rho(t=1)|_{x_3=1}$
focusing $\kappa = -\varepsilon$

Strong Nonlinearity $\kappa = \pm 1$

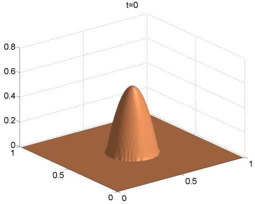


Figure: $\rho(t=0)|_{x_3=0}$
initial density
Tomas-Fermi ground state

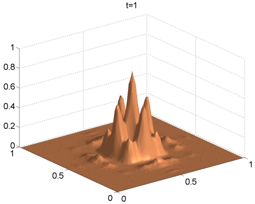


Figure: $\rho(t=1)|_{x_3=1}$
defocusing $\kappa = 1$

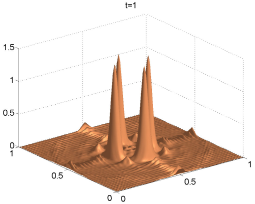


Figure: $\rho(t=1)|_{x_3=1}$
focusing $\kappa = -1$

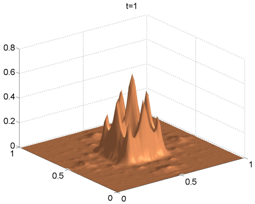


Figure: $\rho(t=2)|_{x_3=0}$
defocusing $\kappa = 1$

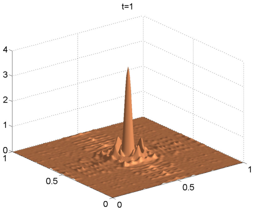


Figure: $\rho(t=2)|_{x_3=1}$
focusing $\kappa = 1$

Wave propagation in Periodic Random Media

Klein-Gordon equation:

$$\frac{\partial^2 u}{\partial t^2} = \operatorname{div}\left(A_\Gamma\left(\frac{x}{\varepsilon};\omega\right)\nabla u\right) - \frac{1}{\varepsilon^2} W_\Gamma\left(\frac{x}{\varepsilon};\omega\right) u\,, \quad x \in \mathbb{R}^d\,, \quad t > 0$$

$$\left.\begin{array}{l} A_\Gamma(y;\omega) \\ W_\Gamma(y;\omega) \end{array}\right\}$$ Γ-periodic functions of y, depending on a mean-zero, uniformly distributed, random variable ω with variance σ

random Bloch-spectral problem:

$$\left\{\begin{array}{l} -\operatorname{div}_y(A_\Gamma(y;\omega)\nabla U_m) + W_\Gamma(y;\omega)U_m = E_m(k;\omega)^2 U_m \\ U_m(y+\gamma,k;\omega) = e^{ik\cdot\gamma}U_m(y,k;\omega)\ \forall\,\gamma\in\Gamma\,, \quad y\in\mathbb{R}^d\,, \quad k\in B \end{array}\right\}$$

A) stability test

1. compute (numerically)

$$\mathbb{E}E_m(k;.)\ ,\quad \mathbb{E}U_m(y,k;.)$$

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2. apply the Bloch-spectral algorithm with the averaged bands and eigenfunctions, for different values of the variance $\sigma \Rightarrow u = u^\sigma(x,t)$
3. apply the algorithm with ω set to $0 \Rightarrow u = u(x,t)$.

Extensive tests show: $\|u^\sigma(t) - u(t)\|_{L^2} \approx \sigma \|u(t)\|_{L^2}$.

Numerical Evidence for Anderson Localisation

When the medium gets "sufficiently" disordered (σ large enough), then waves experience a transition from a dispersive to a localized state (P.W. Anderson '58).

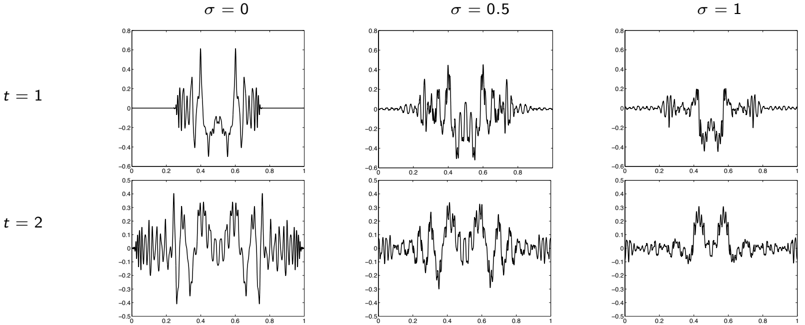
$$e(x,t;\omega) := \frac{1}{2}|u_t(x,t;\omega)|^2 + \nabla u(x,t;\omega)^T A_\Gamma(x,t;\omega)\nabla u(x,t;\omega) + \frac{1}{\varepsilon^2} W_\Gamma(x,t;\omega)|u(x,t;\omega)|^2 \ \ldots \text{ energy density}$$

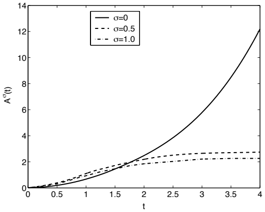
$$E_2(t;\omega) := \int_{\mathbb{R}^d} |x|^2 e(x,t;\omega)\, dx$$

$$A(t) := \mathbb{E}E_2(t;.) \quad \ldots \quad \text{measures the average spread of the wave}$$

(J. Fröhlich, T. Spencer '84)

Test: 1d, Gaussian initial datum, $A_\Gamma(y;\omega) = (\cos(y) + 2.5) + \omega$, $W_\Gamma \equiv 0$, $\varepsilon = \frac{1}{64}$





$\omega = 0$: $A(t)$ grows quadratically in t,
random case: $A(t)$ grows linearly initially (diffusive behaviour), then stabilizes to a constant (localized 'particle').