A Bloch Band Based Level Set Method for Computing the Semiclassical Limit of Schrödinger Equations

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Kinetic FRG Young Researchers Workshop
March 5, 2009
Joint work with Prof. Hailiang Liu

A general Schrödinger equation

We consider a general 1D Schrödinger equation in the form of

$$i\epsilon\frac{\partial\psi^\epsilon}{\partial t} = -\frac{\epsilon^2}{2}\frac{\partial}{\partial x}\left(b\left(\frac{x}{\epsilon}\right)\frac{\partial\psi^\epsilon}{\partial x}\right) + V\left(\frac{x}{\epsilon}\right)\psi^\epsilon + V_e(x)\psi^\epsilon, \quad (1)$$

$$\psi^\epsilon(0,x) = \exp(\frac{iS_0}{\epsilon})f(x,\frac{x}{\epsilon}), \quad (2)$$

where

$$b(y+2\pi) = b(y) > 0,\ \ V(y+2\pi) = V(y),\ \ f(x,y+2\pi) = f(x,y).$$

Applications and difficulties

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- Fundamental models in solid-state physics
- Models for motion of electrons in small-scale periodic potentials

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Difficulties:

- Solutions become highly oscillatory in semiclassical regime when $\epsilon \ll 1$.
- Direct simulation is unrealistic.
- Approximation models are needed.

Bloch band structure

- The Schrödinger equation

$$\begin{aligned} i\epsilon\partial_t\psi &= -\frac{\epsilon^2}{2}\partial_x\left(b\left(\frac{x}{\epsilon}\right)\partial_x\psi\right)+V\left(\frac{x}{\epsilon}\right)\psi+V_e(x)\psi, \\ \psi(0,x) &= \exp\left(\frac{iS_0}{\epsilon}\right)f\left(x,\frac{x}{\epsilon}\right), \end{aligned}$$

  where the lattice potential V and $b>0$ are $2\pi-$ periodic functions and V_e is a given smooth function.

- A standard WKB $\psi^\epsilon = A^\epsilon(t,x)\exp(iS(t,x)/\epsilon)$ fails:

$$S_t + b\left(\frac{x}{\epsilon}\right)\frac{S_x^2}{2}+V\left(\frac{x}{\epsilon}\right)+V_e(x)=0.$$

Scale separation

- Let $y := x/\epsilon$, the electron coordinate, be independent of space variable x, then the Schrödinger equation becomes

$$i\epsilon\partial_t\psi = \left[-\frac{1}{2}(\partial_y + \epsilon\partial_x)\left(b\left(y\right)\left(\partial_y + \epsilon\partial_x\right)\right) + V\left(y\right) + V_e(x)\right]\psi.$$

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- We now look for approximate solutions of the form

$$\psi(t,x,y;\epsilon) = e^{iS(t,x)/\epsilon}\left[A_0(t,x,y) + \epsilon A_1(t,x,y) + \cdots\right].$$

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- Substitution, and collecting terms which are the same order in ϵ:

$$O(1) \quad 0 = -\left[S_t + H(k(t,x),y) + V_e(x)\right]A_0, \quad k(t,x) = S_x(t,x),$$

$$O(\epsilon) \quad 0 = iLA_0 - \left[S_t + H(k(t,x),y) + V_e(x)\right]A_1,$$

$$H(k,y) = -\frac{1}{2}(\partial_y + ik)[b(y)(\partial_y + ik)] + V(y), \tag{3}$$

$$L = \partial_t - \frac{i}{2}\left[(\partial_y + ik)[b(y)\partial_x] + \partial_x[b(y)(\partial_y + ik)]\right]. \tag{4}$$

Band WKB system and Bloch waves

- (Bloch waves) For smooth $V(y)$ and $b(y) > 0$, $H(k, y)$ admits a complete set of (normalized) eigenfunctions z_n for each fixed k:

$$H(k, y)z_n(k, y) = E_n(k)z_n(k, y), \tag{5}$$

$$z_n(k, y + 2\pi) = z_n(k, y), \quad k \in \mathcal{B}, \quad y \in \mathbb{R}.$$

  Here k is confined to the reciprocal cell $\mathcal{B} = [-0.5, 0.5]$.

- The $O(1)$ term vanishes by setting, on each band,

$$A_0(t, x, y) = a(t, x)z(k(t, x), y)$$

  and choosing

$$S_t + E(S_x) + V_e(x) = 0$$

Band dynamics

- Solvability of the $O(\epsilon)$-equation leads to

$$\partial_t a + \frac{1}{2} a \partial_x E'(k(t,x)) + \partial_x a E'(k(t,x)) + \beta a = 0, \quad Re(\beta) = 0$$

- So that the band density $\rho = |a|^2$ satisfies

$$\rho_t + (E'(S_x)\rho)_x = 0.$$

- The classical theory asserts that (before singularity formation) the wave function can be recovered by a superposition of waves on each band

$$\psi^\epsilon(t,x) = \sum_{n=1}^{\infty} a_n(t,x) z_n\left(\partial_x S_n, \frac{x}{\epsilon}\right) e^{iS_n(t,x)/\epsilon} + \mathcal{O}(\epsilon).$$

Ref: [1] Bensoussan, Lions and Papanicolaou (1978)(before caustics)
[3] Gosse and Markowich (2004) (computing multi-valued solutions)
[2] Dimassi, Guillot and Ralston (2006)(Gaussian beam for Bloch electrons)

Band based level set formulation on each band

$$
\begin{aligned}
\partial_t S_n + E_n(\partial_x S_n) + V_e(x) &= 0, \\
\partial_t \rho_n + \partial_x (E_n'(\partial_x S_n)\rho_n) &= 0.
\end{aligned}
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- Let $\{k, \phi(t,x,k) = 0\}$ contains all multi-valued velocity $u_n^j(t,x)$, then ϕ is proven to satisfy

$$\phi_t + E_n'(k)\phi_x - V_e'(x)\phi_k = 0, \tag{6}$$

$$\phi(0,x,k) = k - \partial_x S_0(x), \tag{7}$$

with $E_n'(k)$ is the associated band energy.

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  with $E_n'(k)$ is the associated band energy.
- The corresponding multi-valued density can be evaluated as

$$\rho_n^j \in \left\{ \frac{f}{|\phi_k|} \middle| \quad \phi(t,x,k) = 0 \right\}, \quad \forall (t,x) \in R^+ \times R$$

  where

$$f_t + E_n'(k)f_x - V_e'(x)f_k = 0, \quad f(0,x,p) = \rho_0(x). \tag{8}$$

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- Obtain band velocities/densities
- Evaluate position density over a sample set of bands

Initial band configuration

We now discuss the recovery of the initial band density $\rho_n(0,x)$ from the given data

$$\psi_0^\epsilon\left(x,\frac{x}{\epsilon}\right)=g\left(x,\frac{x}{\epsilon}\right)\exp(iS_0(x)/\epsilon).$$

one needs only to decompose g as follows:

$$g(x,y)=\sum_{n=1}^{\infty}a_n(x)z_n(\partial_x S_0,y),$$

where

$$a_n(x)=\int_0^{2\pi}g(x,y)\bar{z}_n(\partial_x S_0,y)dy.$$

The desired initial band density can be taken as

$$\rho_n=\frac{1}{2\pi}|a_n(x)|^2.$$

Position density in each band

The wave field on each band is calculated as

$$\psi_n^\epsilon(t,x,y) = \int \psi^\epsilon(t,x,y,k)\delta(\phi)\det(\phi_k)dk = \sum_{j=1}^{K_n} \int \psi^\epsilon \delta(k - u_j^n(t,x))dk$$

$$= \sum_{j=1}^{K_n} \psi^\epsilon(t,x,y,u_n^j) = \sum_{j=1}^{K_n} a_n^j z_n\left(u_n^j, y\right) \exp\left(\frac{iS_n^j}{\epsilon}\right).$$

The averaged band density is

$$\bar{\rho}_n^\epsilon(t,x) = \frac{1}{2\pi}\int_0^{2\pi} \left|\psi_n^\epsilon(t,x,y)\right|^2 dy.$$

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Lemma

Away from caustics it holds

$$\bar{\rho}_n^\epsilon(t,x) \rightharpoonup \frac{1}{2\pi}\sum_{j=1}^{K_n} |a_n^j|^2 \quad as \quad \epsilon \to 0.$$

Total density

We now consider all Bloch bands. Since the underlying equation is linear, the wave field over all bands is simply a superposition of wave filed on each band

$$\psi^\epsilon(t,x,y) = \sum_{n=1}^{\infty}\sum_{j=1}^{K_n} a_n^j z_n\left(u_n^j, y\right)\exp\left(\frac{iS_n^j}{\epsilon}\right).$$

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Lemma

Let the total density be defined as

$$\rho^\epsilon(t,x) = \frac{1}{2\pi}\int_0^{2\pi} |\psi^\epsilon(t,x,y)|^2 dy.$$

Then away from caustics, we have

$$\rho^\epsilon(t,x) \rightharpoonup \frac{1}{2\pi}\sum_n \sum_{j=1}^{K_n} |a_n^j|^2 \quad \text{as} \quad \epsilon \to 0.$$

Numerical examples 1

$$b(x/\epsilon) \equiv 1, \, V_e \equiv 0 \text{ and } V(x/\epsilon) = \cos(x/\epsilon),$$

$$\psi^{\epsilon}(0, x) = \exp\left(-\frac{(x-\pi)^2}{2}\right) \exp\left(\frac{-0.3i\cos(x)}{\epsilon}\right).$$

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Initial Decomposition

# of bands	4	6	8	10	12
L^1 error	0.017008	0.008111	0.008101	0.008101	0.008101

Table: L^1 error table for initial Bloch decomposition with 101×101 grid points and 101 eigen-matrix.

Comparison with 2^{nd} 2D Strang Splitting (SP2) method

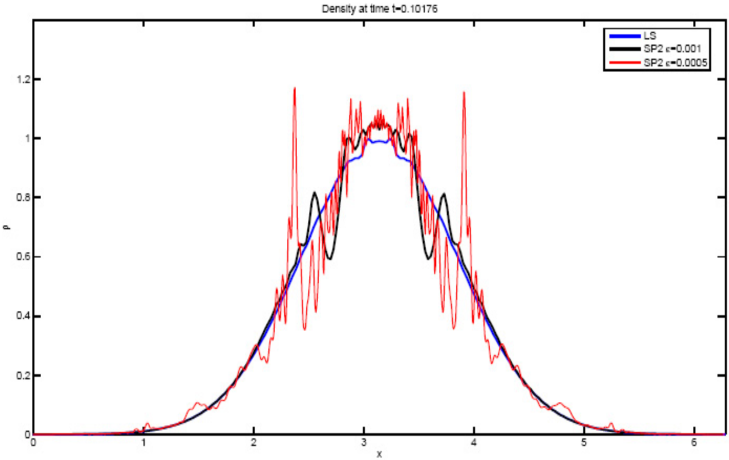


Figure: Total averaged density with 8 bands when $t = 0.1$

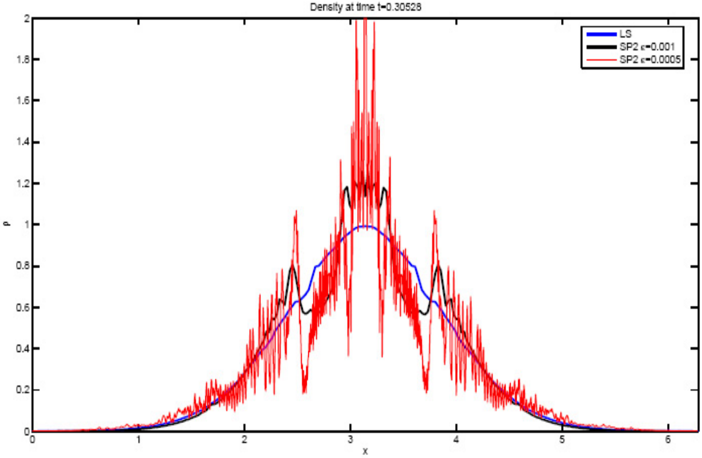


Figure: Total averaged density with 8 bands when $t = 0.3$

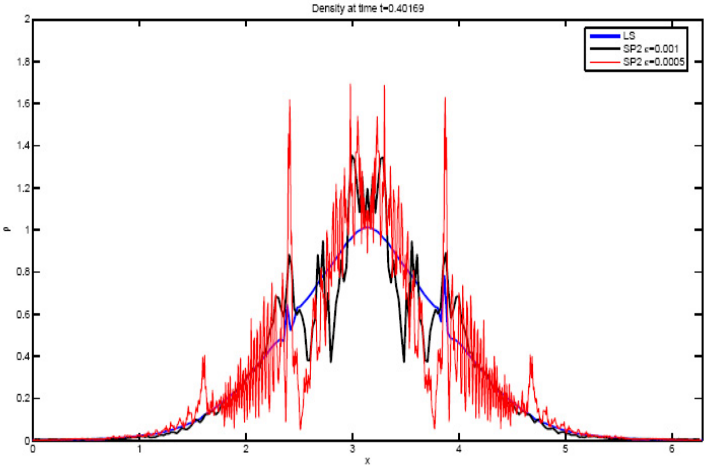


Figure: Total averaged density with 8 bands when $t = 0.4$

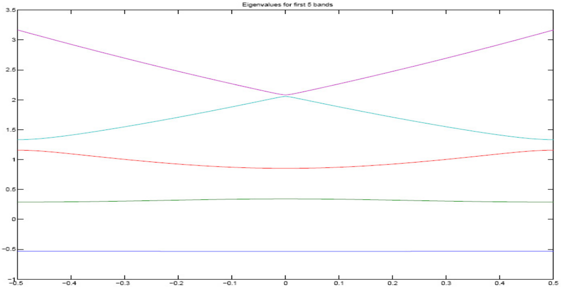
Numerical example 2

$$b(x/\epsilon) \equiv 1,\, V(x/\epsilon) = \cos(x/\epsilon) \text{ and } V_e = 0,$$

$$\psi^\epsilon(0,x) = e^{\frac{-0.3i\cos(x)}{\epsilon}} e^{-(x-\pi)^2} z_n(0.3\sin(x), x/\epsilon), \quad n = 3, 4.$$

In this example, we concentrate the density on a single band to observe the phenomenon:

- n=3: Finite time caustic formation
- n=4: Rarefaction wave



$n = 3, t = 1$

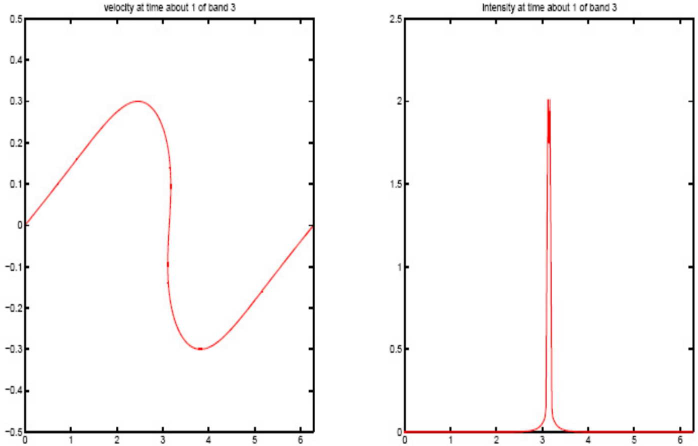


Figure: Multivalued velocity and averaged density on band 3 when $t = 1$

$n = 3, t = 2$

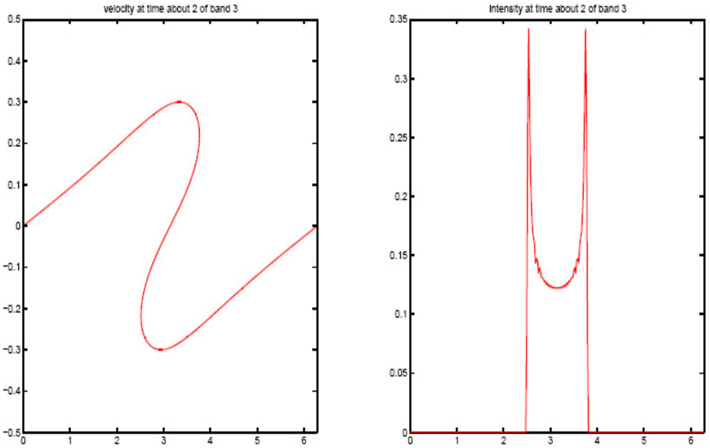


Figure: Multivalued velocity and averaged density on band 3 when $t = 2$

$n = 4, t = 0.1$

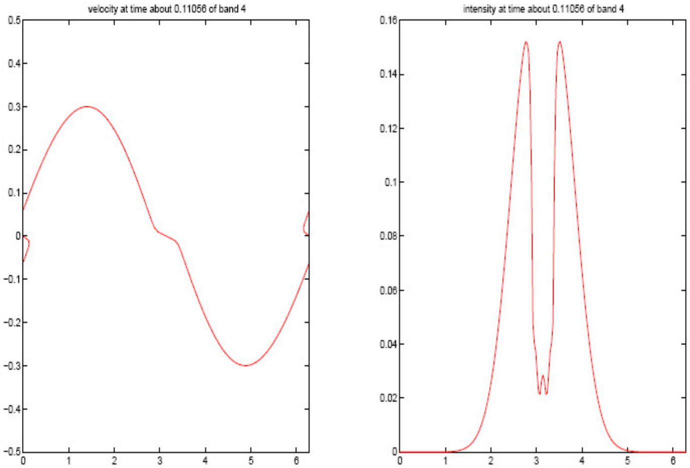


Figure: Multivalued velocity and averaged density on band 4 when $t = 0.1$

$n = 4, t = 0.5$

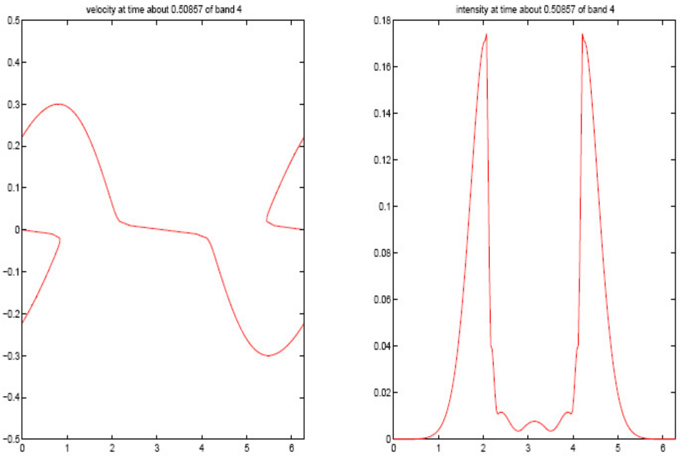


Figure: Multivalued velocity and averaged density on band 4 when $t = 0.5$

Numerical Examples 3: general b

Here we test a general $b(y) = \frac{3}{2} + \sin(y)$, $V(y) = \cos(y)$, $V_e = 0$, and

$$\psi^\epsilon(0, x) = \exp\left(-\frac{(x-\pi)^2}{2}\right)\exp\left(\frac{-0.3i\cos(x)}{\epsilon}\right).$$

Initial Decomposition:

# of bands	4	6	8	10	12
L^1 error	0.015661	0.007301	0.007233	0.007233	0.007233

Table: L^1 error table for initial Bloch decomposition with 101×101 grid points and 101 eigen-matrix.

General coefficient function b

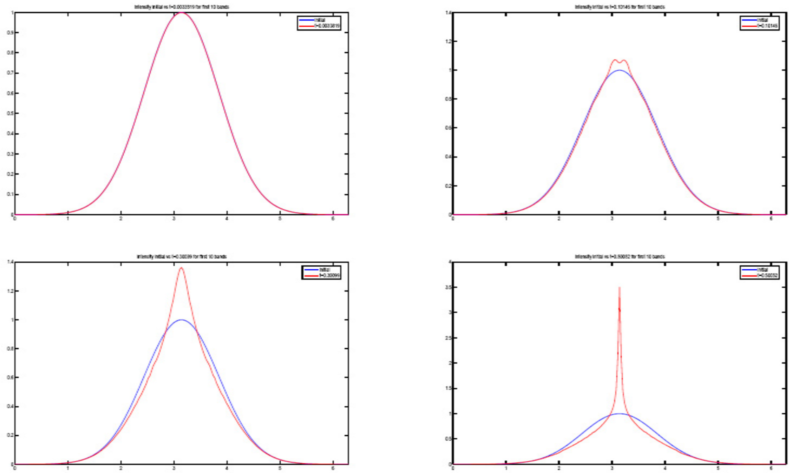


Figure: Total averaged density with 10 bands at different times

Summary and discussions

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- Bloch decomposition is needed in periodic media
- Bloch band based level set method to capture the multi-valued solutions
- Proved superposition in density by weak convergence
- Numerical validation

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Discussion:

- Caustics, e.g., work by Jin *et al.*
- Recovering ψ^{ϵ} with proper phase shift from ϕ and f
- Computational cost, local level set method

Remark 1: WKB higher order terms and multivalued solutions

In the case of $b(x/\epsilon) = 1$ and $V(x/\epsilon) = 0$, WKB approximation leads to

$$S_t + H(x, S_x) = \frac{\epsilon^2}{2}\frac{(A_0)xx}{A_0}, \quad H(x,p) = \frac{1}{2}|p|^2 + V_e(x),$$
$$\rho_t + (\rho S_x)_x = 0.$$

- However, Hamilton-Jacobi equation develops finite time singularity in general and the disispative term on right generates oscillation.
- Conventional viscosity solution is not appropriate, instead multi-valued solutions have to be considered.

Remark 2: Gaussian beam construction for caustics

- Gaussian beam ansatz in Eulerian version (phase space) is no longer an asymptotic solution,
- How to superpose them correctly for the underlying equation?