PERIODIC HOMOGENIZATION AND EFFECTIVE MASS THEOREMS FOR THE SCHRÖDINGER EQUATION

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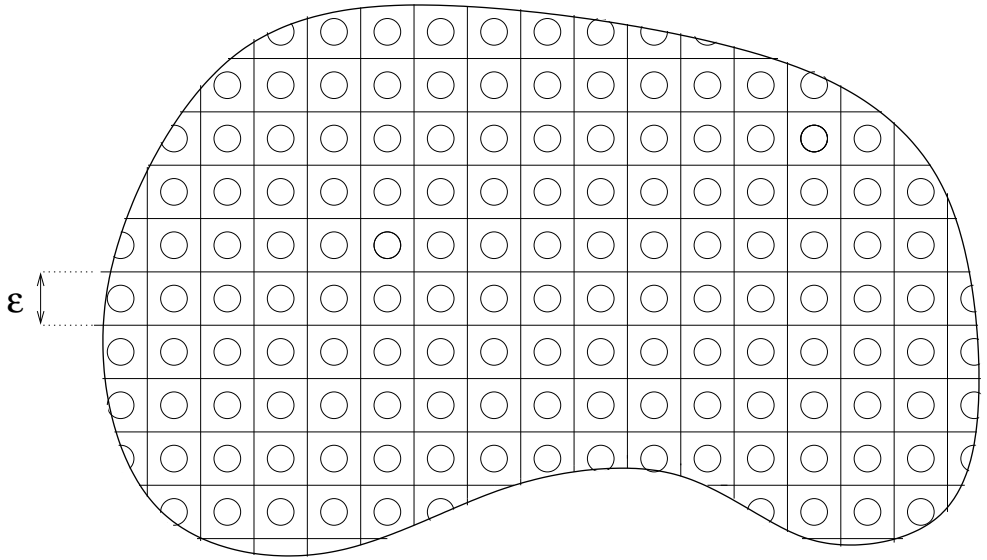
1. **Asymptotic expansions in periodic homogenization**
2. **Two-scale convergence**
3. **Application to homogenization**
4. **Bloch waves**
5. **Schrödinger equation in periodic media**
6. **Homogenization without drift / with drift**
7. **Localization**
8. **Time oscillating potential**

-I- DEFINITION OF HOMOGENIZATION

- Rigorous version of averaging
- Process of asymptotic analysis
- Extract effective or homogenized parameters for heterogeneous media
- Derive simpler macroscopic models from complicated microscopic models
- Different methods :
  - two-scale asymptotic expansions for periodic media
  - two-scale convergence
  - H- or G-convergence for general media
  - stochastic, or variational methods (Γ-convergence)

Periodic homogenization



Periodic domain $\Omega \in \mathbb{R}^N$ with period ϵ. Rescaled unit cell $Y = (0,1)^N$.

$$x \in \Omega, \quad y = \frac{x}{\epsilon} \in Y$$

Example: Composite material with a periodic structure

Model problem

Conductivity or diffusion equation

$$\begin{cases} -\operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases}$$

with a coefficient tensor $A(y)$ which is Y-periodic, uniformly coercive and bounded

$$\alpha|\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(y)\xi_i\xi_j \leq \beta|\xi|^2, \quad \forall\, \xi \in \mathbb{R}^N, \forall\, y \in Y \quad (\beta \geq \alpha > 0).$$

Homogenization and asymptotic analysis

- Direct solution too costly if ϵ is small
- Averaging: replace $A(y)$ by effective homogeneous coefficients
- Asymptotic analysis: limit as $\epsilon \to 0$
  yields a rigorous definition of the homogenized parameters
- Error estimates: compare exact and homogenized solutions
- Similar to Representative Volume Element method (in mechanics)
- Huge literature

Asymptotic analysis

Rather than considering a single heterogeneous medium with a fixed lengthscale ϵ_0, the problem is embedded in a sequence of similar problems parametrized by a lengthscale ϵ.

Homogenization amounts to perform an asymptotic analysis when $\epsilon \to 0$

$$\lim_{\epsilon \to 0} u_\epsilon = u.$$

The limit u is the solution of an homogenized problem, the conductivity tensor of which is called the effective or homogenized conductivity.

This yields a coherent definition of homogenized properties which can be rigorously justified by quantifying the resulting error estimate.

Two-scale asymptotic expansions

Ansatz for the solution

$$u_\epsilon(x) = \sum_{i=0}^{+\infty} \epsilon^i u_i\left(x, \frac{x}{\epsilon}\right),$$

with $u_i(x,y)$ function of both variables x and y, periodic in y

Derivation rule

$$\nabla\left(u_i\left(x, \frac{x}{\epsilon}\right)\right) = \left(\epsilon^{-1}\nabla_y u_i + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right)$$

$$\nabla u_\epsilon(x) = \epsilon^{-1}\nabla_y u_0\left(x, \frac{x}{\epsilon}\right) + \sum_{i=0}^{+\infty} \epsilon^i \left(\nabla_y u_{i+1} + \nabla_x u_i\right)\left(x, \frac{x}{\epsilon}\right)$$

Cascade of equations

$$-\epsilon^{-2}\,[\ \mathrm{div}_y A\nabla_y u_0]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{-1}\,[\ \mathrm{div}_y A(\nabla_x u_0+\nabla_y u_1)+\ \mathrm{div}_x A\nabla_y u_0]\left(x,\frac{x}{\epsilon}\right)$$

$$-\epsilon^{0}\,[\ \mathrm{div}_x A(\nabla_x u_0+\nabla_y u_1)+\ \mathrm{div}_y A(\nabla_x u_1+\nabla_y u_2)]\left(x,\frac{x}{\epsilon}\right)$$

$$-\sum_{i=1}^{+\infty}\epsilon^{i}\,[\ \mathrm{div}_x A(\nabla_x u_i+\nabla_y u_{i+1})+\ \mathrm{div}_y A(\nabla_x u_{i+1}+\nabla_y u_{i+2})]\left(x,\frac{x}{\epsilon}\right)$$

$$=f(x).$$

ϵ^{-2} equation

$$-\operatorname{div}_y\left(A(y)\nabla_y u_0(x,y)\right)=0 \quad \text{in} \quad Y$$

where x is just a parameter.

Its unique solution does not depend on y

$$u_0(x,y)\equiv u(x)$$

Technical lemma on cell problems

Definition.

$$L^2_\#(Y) = \left\{ \phi(y)\ Y\text{-periodic, such that } \int_Y \phi(y)^2 dy < +\infty \right\}$$

$$H^1_\#(Y) = \left\{ \phi \in L^2_\#(Y) \text{ such that } \nabla\phi \in L^2_\#(Y)^N \right\}$$

Lemma. Let $f(y) \in L^2_\#(Y)$ be a periodic function. There exists a solution in $H^1_\#(Y)$ (unique up to an additive constant) of

$$\begin{cases} -\operatorname{div}\left(A(y)\nabla w(y)\right) = f & \text{in } Y \\ y \to w(y) & Y\text{-periodic,} \end{cases}$$

if and only if $\int_Y f(y)dy = 0$ (this is called the Fredholm alternative).

ϵ^{-1} equation

$$-\operatorname{div}_y A(y)\nabla_y u_1(x,y) = \operatorname{div}_y A(y)\nabla_x u(x) \quad \text{in} \quad Y$$

which is an equation for u_1. Introducing the cell problem

$$\begin{cases} -\operatorname{div}_y A(y)\,(e_i + \nabla_y w_i(y)) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic,} \end{cases}$$

by linearity we compute

$$u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(y).$$

ϵ^0 equation

$$-\operatorname{div}_y A(y)\nabla_y u_2(x,y) = \operatorname{div}_y A(y)\nabla_x u_1 + \operatorname{div}_x A(y)\,(\nabla_y u_1 + \nabla_x u) + f(x)$$

which is an equation for u_2. Its compatibility condition (Fredholm alternative) is

$$\int_Y (\operatorname{div}_y A(y)\nabla_x u_1 + \operatorname{div}_x A(y)\,(\nabla_y u_1 + \nabla_x u) + f(x))\,dy = 0.$$

Replacing u_1 by its value yields the homogenized equation

$$\begin{cases} -\operatorname{div}_x A^*\nabla_x u(x) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

with the constant homogenized tensor

$$A^*_{ij} = \int_Y [(A(y)\nabla_y w_i)\cdot e_j + A_{ij}(y)]\,dy = \int_Y A(y)\,(e_i + \nabla_y w_i)\cdot(e_j + \nabla w_j)\,dy.$$

Comments

- The ansatz is not correct after the second term

$$u_\epsilon(x) \approx u(x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i \left(\frac{x}{\epsilon}\right)$$

  (boundary layers should be included for higher order terms)

- Similar ansatz for ∇u_ϵ, $A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon$ and $A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \cdot \nabla u_\epsilon$.
- Explicit formula for the effective parameters (no longer true for non-periodic problems).
- A^* does not depend on ϵ, f, u or the boundary conditions.
- A^* is positive definite (not necessarily isotropic even if $A(y)$ was so).
- Same results for evolution problems.
- Very general method, but heuristic and not rigorous.

Time dependent problems

Schrödinger equation in a periodic medium:

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(x,\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + c\left(x,\dfrac{x}{\epsilon}\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u_\epsilon(t=0,x) = u^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

Complex-valued unknown: $u_\epsilon(t,x) : \mathbb{R}^+ \times \mathbb{R}^N \to \mathbb{C}$

- $y \to A(x,y), c(x,y)$ $(0,1)^N$-periodic, real, measurable and bounded.
- A is a $N \times N$ symmetric, uniformly coercive, tensor.
- c is a scalar function with no specified sign.
- non oscillating initial data $u^0 \in H^1(\mathbb{R}^N)$.

Same results !

$$u_\epsilon(t,x) \approx u(t,x) + \epsilon \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(t,x) w_i(\frac{x}{\epsilon})$$

$$\begin{cases} i\dfrac{\partial u}{\partial t} - \operatorname{div}(A^*\nabla u) + c^* u = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u(t=0,x) = u^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

with $c^*(x) = \int_Y c(x,y)\,dy$ and the homogenized tensor

$$A^*_{ij}(x) = \int_Y A(x,y)\,(e_i + \nabla_y w_i)\cdot(e_j + \nabla w_j)\,dy.$$

$$\begin{cases} -\operatorname{div}_y A(x,y)\,(e_i + \nabla_y w_i) = 0 & \text{in } Y \\ y \to w_i(x,y) & Y\text{-periodic}, \end{cases}$$

Convergence proof

The goal is to mathematically prove the following

Theorem. The sequence $u_\epsilon(x)$ of solutions of the model problem converges weakly in $H_0^1(\Omega)$ and strongly in $L^2(\Omega)$, as ϵ goes to 0, to a limit $u(x)$ which is the unique solution of the homogenized problem.

$$\lim_{\epsilon\to 0}\int_\Omega |u_\epsilon - u|^2 dx = 0, \quad \lim_{\epsilon\to 0}\int_\Omega \nabla(u_\epsilon - u)\cdot\phi\, dx = 0 \quad \forall\,\phi\in L^2(\Omega)^N.$$

Naive idea: pass to the limit in the variational formulation

$$\int_\Omega A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon(x)\cdot\nabla\varphi(x)dx = \int_\Omega f(x)\varphi(x)dx, \quad \forall\,\varphi\in H_0^1(\Omega).$$

impossible because $A\left(\frac{x}{\epsilon}\right)$ and ∇u_ϵ converge only weakly (the limit of the product is not the product of the limits).

-II- TWO-SCALE CONVERGENCE METHOD

This is a simpler method to prove the convergence theorem.

Definition. A sequence of functions u_ϵ in $L^2(\Omega)$ is said to two-scale converge to a limit $u_0(x,y)$ belonging to $L^2(\Omega \times Y)$ if, for any Y-periodic smooth function $\varphi(x,y)$, it satisfies

$$\lim_{\epsilon \to 0} \int_\Omega u_\epsilon(x) \varphi\left(x, \frac{x}{\epsilon}\right) dx = \int_\Omega \int_Y u_0(x,y) \varphi(x,y) dx dy.$$

Theorem 1. From each bounded sequence u_ϵ in $L^2(\Omega)$ one can extract a subsequence, and there exists a limit $u_0(x,y) \in L^2(\Omega \times Y)$ such that this subsequence two-scale converges to u_0.

Theorem 2. Let u_ϵ be a bounded sequence in $H^1(\Omega)$. Then, up to a subsequence, u_ϵ two-scale converges to a limit $u_0(x,y) \equiv u(x) \in H^1(\Omega)$, and ∇u_ϵ two-scale converges to $\nabla_x u(x) + \nabla_y u_1(x,y)$ with $u_1 \in L^2(\Omega; H^1_\#(Y))$.

Lemma 3. For a bounded open set Ω, let $B = C(\bar{\Omega}; C_\#(Y))$ be the space of continuous functions $\varphi(x,y)$ on $\bar{\Omega} \times Y$ which are Y-periodic in y. Then, B is a separable Banach space (i.e. it contains a dense countable family), is dense in $L^2(\Omega \times Y)$, and there exists $C > 0$ such that

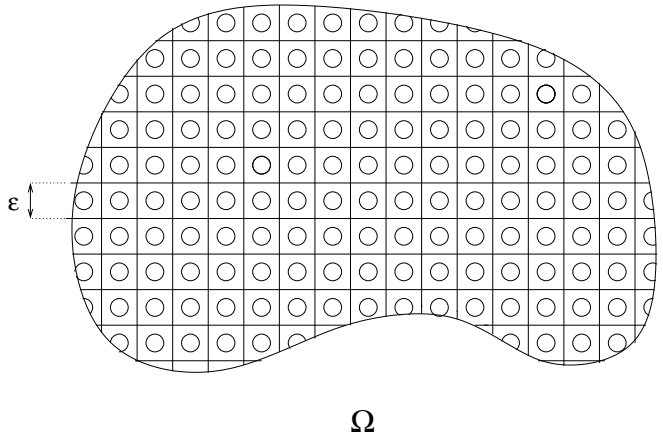
$$\int_\Omega |\varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx \leq C \|\varphi\|_B^2,$$

and

$$\lim_{\epsilon \to 0} \int_\Omega |\varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx = \int_\Omega \int_Y |\varphi(x,y)|^2 dx dy,$$

for any $\varphi(x,y) \in B$.

Remark. The same works with $B = L^2(\Omega; C_\#(Y))$ and Ω not necessarily bounded.



Proof of Lemma 3. We mesh Ω with cubes of the type $(0,\epsilon)^N$

$$\Omega = \cup_{1\le i\le n(\epsilon)} Y_i^\epsilon \quad \text{with } Y_i^\epsilon = x_i^\epsilon + (0,\epsilon)^N.$$

$$\int_\Omega |\varphi\left(x,\frac{x}{\epsilon}\right)|^2 dx = \sum_{i=1}^{n(\epsilon)} \int_{Y_i^\epsilon} |\varphi\left(x,\frac{x}{\epsilon}\right)|^2 dx = \sum_{i=1}^{n(\epsilon)} \int_{Y_i^\epsilon} |\varphi\left(x_i^\epsilon,\frac{x}{\epsilon}\right)|^2 dx + \mathcal{O}(\epsilon)$$

$$= \sum_{i=1}^{n(\epsilon)} \epsilon^N \int_Y |\varphi\left(x_i^\epsilon, y\right)|^2 dy + \mathcal{O}(\epsilon) = \int_\Omega \int_Y |\varphi\left(x,y\right)|^2 dx\, dy + \mathcal{O}(\epsilon)$$

Proof of Theorem 1. By Schwarz inequality, we have

$$\left| \int_\Omega u_\epsilon(x) \varphi\left(x, \frac{x}{\epsilon}\right) dx \right| \leq C \left| \int_\Omega \varphi\left(x, \frac{x}{\epsilon}\right) dx \right|^{\frac{1}{2}} \leq C \|\varphi\|_B .$$

Thus, the l.h.s. is a continuous linear form on B which can be identified to a duality product $\langle \mu_\epsilon, \varphi \rangle_{B',B}$ for some bounded sequence of measures μ_ϵ. Since B is separable, one can extract a subsequence and there exists a limit μ_0 such μ_ϵ converges to μ_0 in the weak * topology of B' (the dual of B). On the other hand, Lemma 3 allows us to pass to the limit in the middle term above. It yields

$$|\langle \mu_0, \varphi \rangle_{B',B}| \leq C \left| \int_\Omega \int_Y |\varphi(x,y)|^2 dx dy \right|^{\frac{1}{2}} .$$

Therefore μ_0 is actually a continuous linear form on $L^2(\Omega \times Y)$, by density of B in this space. Thus, there exists $u_0(x,y) \in L^2(\Omega \times Y)$ such that

$$\langle \mu_0, \varphi \rangle_{B',B} = \int_\Omega \int_Y u_0(x,y) \varphi(x,y) dx dy.$$

Proof of Theorem 2. Since u_ϵ and ∇u_ϵ are bounded in $L^2(\Omega)$, up to a subsequence, they two-scale converge to limits $u_0(x,y) \in L^2(\Omega \times Y)$ and $\xi_0(x,y) \in L^2(\Omega \times Y)^N$. Thus

$$\lim_{\epsilon \to 0} \int_\Omega \nabla u_\epsilon(x) \cdot \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx = \int_\Omega \int_Y \xi_0(x,y) \cdot \vec{\psi}(x,y) dx dy \quad \forall \vec{\psi} \in \mathcal{D}\left(\Omega; C^\infty_\#(Y)^N\right).$$

Integrating by parts the left hand side gives

$$\epsilon \int_\Omega \nabla u_\epsilon(x) \cdot \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx = -\int_\Omega u_\epsilon(x) \left(\operatorname{div}_y \vec{\psi}\left(x, \frac{x}{\epsilon}\right) + \epsilon \operatorname{div}_x \vec{\psi}\left(x, \frac{x}{\epsilon}\right)\right) dx.$$

Passing to the limit yields

$$0 = -\int_\Omega \int_Y u_0(x,y) \operatorname{div}_y \vec{\psi}(x,y) dx dy \quad \Rightarrow \quad u_0(x,y) \equiv u(x) \in L^2(\Omega).$$

Next, we choose $\vec{\psi}$ such that $\operatorname{div}_y \vec{\psi}(x,y) = 0$. We obtain

$$\int_\Omega \nabla u_\epsilon(x) \cdot \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx = -\int_\Omega u_\epsilon(x) \operatorname{div}_x \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx.$$

Passing to the two-scale limit

$$\int_\Omega \int_Y \xi_0(x,y)\cdot\vec{\psi}(x,y)dxdy = -\int_\Omega \int_Y u(x)\ \mathrm{div}_x\vec{\psi}(x,y)dxdy.$$

If $\vec{\psi}$ does not depend on y, it proves that $u(x)\in H^1(\Omega)$. Furthermore,

$$\int_\Omega \int_Y (\xi_0(x,y)-\nabla u(x))\cdot\vec{\psi}(x,y)dxdy = 0 \quad \forall\vec{\psi} \text{ with } \mathrm{div}_y\vec{\psi}=0.$$

The orthogonal of divergence-free functions are exactly the gradients. Thus, there exists a unique function $u_1(x,y)$ in $L^2(\Omega;H^1_\#(Y)/\mathbb{R})$ such that

$$\xi_0(x,y) = \nabla u(x) + \nabla_y u_1(x,y).$$

Theorem 4. Let $u_\epsilon \in L^2(\Omega)$ two-scale converge to $u_0(x,y) \in L^2(\Omega \times Y)$.

1. Then, u_ϵ converges weakly in $L^2(\Omega)$ to $u(x) = \int_Y u_0(x,y)dy$, and we have

$$\lim_{\epsilon \to 0} \|u_\epsilon\|^2_{L^2(\Omega)} \geq \|u_0\|^2_{L^2(\Omega \times Y)} \geq \|u\|^2_{L^2(\Omega)}.$$

2. Assume further that $u_0(x,y)$ is smooth and that

$$\lim_{\epsilon \to 0} \|u_\epsilon\|^2_{L^2(\Omega)} = \|u_0\|^2_{L^2(\Omega \times Y)}.$$

Then, we have

$$\left\| u_\epsilon(x) - u_0\left(x, \frac{x}{\epsilon}\right) \right\|^2_{L^2(\Omega)} \to 0.$$

Remark. In the last case we say that u_ϵ two-scale converges **strongly** to u_0.

Proof of Theorem 4. Take a test function depending only on x

$$\lim_{\epsilon\to 0}\int_\Omega u_\epsilon(x)\varphi\,(x)\,dx=\int_\Omega\int_Y u_0(x,y)\varphi(x)dxdy=\int_\Omega u(x)\,\varphi(x)\,dx.$$

Thus, u_ϵ converges weakly to u in $L^2(\Omega)$. Then, developing the inequality

$$\int_\Omega\left|u_\epsilon(x)-\varphi\left(x,\frac{x}{\epsilon}\right)\right|^2dx\geq 0$$

$$\int_\Omega|u_\epsilon(x)|^2dx-2\int_\Omega u_\epsilon(x)\varphi\left(x,\frac{x}{\epsilon}\right)dx+\int_\Omega|\varphi\left(x,\frac{x}{\epsilon}\right)|^2dx\geq 0$$

$$\liminf_{\epsilon\to 0}\int_\Omega|u_\epsilon(x)|^2dx-2\int_\Omega\int_Y u_0(x,y)\varphi(x,y)dx\,dy+\int_\Omega\int_Y|\varphi\,(x,y)\,|^2dx\,dy\geq 0$$

Take $\varphi=u_0$ to get

$$\lim_{\epsilon\to 0}\|u_\epsilon\|^2_{L^2(\Omega)}\geq\|u_0\|^2_{L^2(\Omega\times Y)}.$$

Proof of Theorem 4 (continued). If we assume

$$\lim_{\epsilon\to 0} \|u_\epsilon\|^2_{L^2(\Omega)} = \|u_0\|^2_{L^2(\Omega\times Y)},$$

the same computation yields

$$\liminf_{\epsilon\to 0} \int_\Omega \left|u_\epsilon(x) - \varphi\left(x, \frac{x}{\epsilon}\right)\right|^2 dx = \int_\Omega \int_Y |u_0(x,y) - \varphi(x,y)|^2 dx\, dy$$

If u_0 is smooth enough to be a test function φ (Carathéodory function), it gives the desired result

$$\left\|u_\epsilon(x) - u_0\left(x, \frac{x}{\epsilon}\right)\right\|^2_{L^2(\Omega)} \to 0.$$

Theorem 5.

1. Let u_ϵ be a bounded sequence in $L^2(\Omega)$ such that $\epsilon\nabla u_\epsilon$ is also bounded in $L^2(\Omega)^N$. Then, there exists a two-scale limit $u_0(x,y) \in L^2(\Omega; H^1_\#(Y)/\mathbb{R})$ such that, up to a subsequence, u_ϵ two-scale converges to $u_0(x,y)$, and $\epsilon\nabla u_\epsilon$ to $\nabla_y u_0(x,y)$.

2. Let u_ϵ be a bounded sequence in $L^2(\Omega)^N$ such that $\mathrm{div} u_\epsilon$ is also bounded in $L^2(\Omega)$. Then, there exists a two-scale limit $u_0(x,y) \in L^2(\Omega \times Y)^N$ with $\mathrm{div}_y u_0 = 0$ and $\mathrm{div}_x u_0 \in L^2(\Omega \times Y)$ such that, up to a subsequence, u_ϵ two-scale converges to $u_0(x,y)$, and $\mathrm{div} u_\epsilon$ to $\mathrm{div}_x u_0(x,y)$.

Proof of Theorem 5 (first part). We have

$$\lim_{\epsilon\to 0}\int_\Omega u_\epsilon(x)\varphi\left(x,\frac{x}{\epsilon}\right)dx=\int_\Omega\int_Y u_0(x,y)\varphi(x,y)dxdy$$

$$\lim_{\epsilon\to 0}\int_\Omega \epsilon\nabla u_\epsilon(x)\cdot\vec{\psi}\left(x,\frac{x}{\epsilon}\right)dx=\int_\Omega\int_Y \xi_0(x,y)\cdot\vec{\psi}(x,y)dxdy$$

By integration by parts

$$\int_\Omega \epsilon\nabla u_\epsilon(x)\cdot\vec{\psi}\left(x,\frac{x}{\epsilon}\right)dx=-\int_\Omega u_\epsilon(x)\left(\operatorname{div}_y\vec{\psi}+\epsilon\operatorname{div}_x\vec{\psi}\right)\left(x,\frac{x}{\epsilon}\right)dx$$

Passing to the two-scale limit

$$\int_\Omega\int_Y \xi_0(x,y)\cdot\vec{\psi}(x,y)dxdy=-\int_\Omega\int_Y u_0(x,y)\operatorname{div}_y\vec{\psi}(x,y)dxdy$$

which implies that $\xi_0(x,y)=\nabla_y u_0(x,y)$.

-III- APPLICATION TO HOMOGENIZATION

Conductivity or diffusion equation

$$\begin{cases} -\operatorname{div}\left(A\left(x,\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega \end{cases}$$

with a coefficient tensor $A(x,y)$ which is Y-periodic, uniformly coercive and bounded

$$\alpha|\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(x,y)\xi_i\xi_j \leq \beta|\xi|^2, \quad \forall\, \xi \in \mathbb{R}^N, \forall\, y \in Y, \forall\, x \in \Omega \quad (\beta \geq \alpha > 0).$$

A priori estimate. If Ω is bounded, then

$$\|u_\epsilon\|_{H^1(\Omega)} \leq C\|f\|_{L^2(\Omega)}.$$

A priori estimate

Variational formulation

$$\int_\Omega A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon(x)\cdot\nabla\varphi(x)dx=\int_\Omega f(x)\varphi(x)dx,\quad\forall\,\varphi\in H_0^1(\Omega).$$

Take $\varphi=u_\epsilon$ and use coercivity

$$\alpha\|\nabla u_\epsilon\|^2_{L^2(\Omega)}\leq\int_\Omega f(x)u_\epsilon(x)dx\leq\|f\|_{L^2(\Omega)}\|u_\epsilon\|_{L^2(\Omega)}$$

Poincaré inequality in Ω

$$\|u_\epsilon\|_{L^2(\Omega)}\leq C(\Omega)\|\nabla u_\epsilon\|_{L^2(\Omega)}$$

Thus

$$\|\nabla u_\epsilon\|_{L^2(\Omega)}\leq\frac{C(\Omega)\|f\|_{L^2(\Omega)}}{\alpha}$$

Two-scale convergence method

First step. We deduce from the a priori estimates the precise form of the two-scale limit of the sequence u_ϵ.

By application of Theorem 2, there exist two functions, $u(x) \in H^1_0(\Omega)$ and $u_1(x,y) \in L^2(\Omega; H^1_\#(Y)/\mathbb{R})$, such that, up to a subsequence, u_ϵ two-scale converges to $u(x)$, and ∇u_ϵ two-scale converges to $\nabla_x u(x) + \nabla_y u_1(x,y)$.

In view of these limits, u_ϵ is expected to behave as $u(x) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right)$.

Two-scale convergence method

Second step. We multiply the p.d.e. by a test function similar to the limit of u_ϵ, namely $\varphi(x) + \epsilon\varphi_1\left(x, \frac{x}{\epsilon}\right)$, where $\varphi(x) \in \mathcal{D}(\Omega)$ and $\varphi_1(x,y) \in \mathcal{D}(\Omega; C^\infty_\#(Y))$. This yields

$$\int_\Omega A\left(x, \frac{x}{\epsilon}\right) \nabla u_\epsilon \cdot \left(\nabla\varphi(x) + \nabla_y\varphi_1\left(x, \frac{x}{\epsilon}\right) + \epsilon\nabla_x\varphi_1\left(x, \frac{x}{\epsilon}\right)\right) dx$$

$$= \int_\Omega f(x)\left(\varphi(x) + \epsilon\varphi_1\left(x, \frac{x}{\epsilon}\right)\right) dx.$$

Regarding $A^t\left(x, \frac{x}{\epsilon}\right)\left(\nabla\varphi(x) + \nabla_y\varphi_1\left(x, \frac{x}{\epsilon}\right)\right)$ as a test function for the two-scale convergence, we pass to the two-scale limit

$$\int_\Omega \int_Y A(x,y)\left(\nabla u(x) + \nabla_y u_1(x,y)\right)\cdot\left(\nabla\varphi(x) + \nabla_y\varphi_1(x,y)\right) dxdy = \int_\Omega f(x)\varphi(x)dx.$$

Two-scale convergence method

Third step. We read off a variational formulation for (u, u_1). Take (φ, φ_1) in the Hilbert space $H^1_0(\Omega) \times L^2\left(\Omega; H^1_\#(Y)/\mathbb{R}\right)$ endowed with the norm

$$\sqrt{(\|\nabla u(x)\|^2_{L^2(\Omega)} + \|\nabla_y u_1(x,y)\|^2_{L^2(\Omega\times Y)})}$$

The assumptions of the Lax-Milgram lemma are easily checked. The main point is the coercivity of the bilinear form defined by the left hand side

$$\int_\Omega \int_Y A(x,y)\,(\nabla\varphi(x) + \nabla_y\varphi_1(x,y)) \cdot (\nabla\varphi(x) + \nabla_y\varphi_1(x,y))\,dxdy \geq$$

$$\alpha \int_\Omega \int_Y |\nabla\varphi(x)+\nabla_y\varphi_1(x,y)|^2 dxdy = \alpha \int_\Omega |\nabla\varphi(x)|^2 dx + \alpha \int_\Omega \int_Y |\nabla_y\varphi_1(x,y)|^2 dxdy.$$

$$\int_\Omega \int_Y A(x,y)\,(\nabla u(x) + \nabla_y u_1(x,y))\cdot(\nabla\varphi(x) + \nabla_y\varphi_1(x,y))\,dxdy = \int_\Omega f(x)\varphi(x)dx.$$

By application of the Lax-Milgram lemma, there exists a unique solution $(u,u_1) \in H^1_0(\Omega) \times L^2\left(\Omega; H^1_\#(Y)/\mathbb{R}\right)$. Consequently, the entire sequences u_ϵ and ∇u_ϵ converge to $u(x)$ and $\nabla u(x) + \nabla_y u_1(x,y)$.

An easy integration by parts shows that the associated p.d.e.'s are the so-called "two-scale homogenized problem",

$$\begin{cases} -\operatorname{div}_y\left(A(x,y)\,(\nabla u(x) + \nabla_y u_1(x,y))\right) = 0 & \text{in } \Omega\times Y \\ -\operatorname{div}_x\left(\int_Y A(x,y)\,(\nabla u(x) + \nabla_y u_1(x,y))\,dy\right) = f(x) & \text{in } \Omega \\ y \to u_1(x,y) & Y\text{-periodic} \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

Two-scale convergence method

Fourth (and optional) step. Eliminate the y variable and the u_1 unknown

$$u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(x,y),$$

where $w_i(x,y)$ are the unique solutions in $H^1_\#(Y)/\mathbb{R}$ of the cell problems

$$\begin{cases} -\operatorname{div}_y \left(A(x,y) \left(\vec{e}_i + \nabla_y w_i(x,y) \right) \right) = 0 & \text{in } Y \\ y \to w_i(x,y) & Y\text{-periodic}, \end{cases}$$

at each point $x \in \Omega$, and

$$\begin{cases} -\operatorname{div}_x \left(A^*(x) \nabla u(x) \right) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

with $A^*_{ij}(x) = \int_Y A(x,y) \left(\vec{e}_i + \nabla_y w_i(x,y) \right) \cdot \left(\vec{e}_j + \nabla_y w_j(x,y) \right) dy$.

-IV- BLOCH WAVES

Theorem 1. For any function $u(y) \in L^2(\mathbb{R}^N)$ there exists a unique function $\hat{u}(y,\theta) \in L^2(Y \times Y)$ such that

$$u(y) = \int_Y \hat{u}(y,\theta) e^{2i\pi\theta\cdot y} d\theta.$$

The function $y \to \hat{u}(y,\theta)$ is Y-periodic while the function $\theta \to e^{2i\pi\theta\cdot y}\hat{u}(y,\theta)$ is Y-periodic. Furthermore, the linear map $\mathcal{B}$, called the Bloch transform and defined by $\mathcal{B}u = \hat{u}$, is an isometry from $L^2(\mathbb{R}^N)$ into $L^2(Y \times Y)$, i.e. Parseval formula holds for any $u, v \in L^2(\mathbb{R}^N)$

$$\int_{\mathbb{R}^N} u(y)\overline{v(y)}\, dy = \int_Y \int_Y \hat{u}(y,\theta)\overline{\hat{v}(y,\theta)}\, dy\, d\theta.$$

Proof. Let $u(y)$ be a smooth compactly supported function in $\mathbb{R}^N$. Define

$$\hat{u}(y,\theta) = \sum_{k\in\mathbb{Z}^N} u(y+k)e^{-2i\pi\theta\cdot(y+k)}.$$

This sum is well defined because it has a finite number of terms since u has compact support. It is also clearly a Y-periodic function of y. On the other hand, for $j \in \mathbb{Z}^N$, we have

$$\hat{u}(y,\theta+j) = e^{-2i\pi j\cdot y}\sum_{k\in\mathbb{Z}^N} u(y+k)e^{-2i\pi\theta\cdot(y+k)} = e^{-2i\pi j\cdot y}\hat{u}(y,\theta).$$

Thus, $\theta \to e^{2i\pi\theta\cdot y}\hat{u}(y,\theta)$ is Y-periodic. Next, we compute

$$\int_{\mathbb{T}^N} \hat{u}(y,\theta)e^{2i\pi\theta\cdot y}d\theta = \sum_{k\in\mathbb{Z}^N} u(y+k)\int_{\mathbb{T}^N} e^{-2i\pi\theta\cdot k}d\theta = u(y)$$

since all integrals vanish except for $k=0$. This proves the result for smooth compactly supported functions.

In particular, it shows that the Bloch transform $\mathcal{B}$ is a linear map, well defined on $C_c^\infty(\mathbb{R}^N)$ and bounded on $L^2(\mathbb{R}^N)$.

Since $C_c^\infty(\mathbb{R}^N)$ is dense in $L^2(\mathbb{R}^N)$, $\mathcal{B}$ can be extended by continuity and the result holds true in $L^2(\mathbb{R}^N)$.

Lemma. Let $a(y) \in L^\infty(\mathbb{T}^N)$ be a periodic function.

For any $u(y) \in L^2(\mathbb{R}^N)$, we have

$$\mathcal{B}(au) = a\mathcal{B}(u) \equiv a(y)\hat{u}(y,\theta).$$

Remark. $\mathbb{T}^N$ is the flat unit torus, i.e. $\mathbb{T}^N \equiv Y+$ periodic B.C.

Lemma. Let $u(y) \in H^1(\mathbb{R}^N)$. The Bloch transform of its gradient is

$$\mathcal{B}(\nabla_y u) = (\nabla_y + 2i\pi\theta)\mathcal{B}(u) \equiv \nabla_y \hat{u}(y,\theta) + 2i\pi\theta\hat{u}(y,\theta)$$

and $y \to \mathcal{B}(u) \equiv \hat{u}(y,\theta)$ belongs to $H^1(\mathbb{T}^N)$.

Application

Find $u \in H^1(\mathbb{R}^N)$ solution of

$$-\operatorname{div}_y\Big(A(y)\nabla_y u\Big) + c(y)u = f \quad \text{in } \mathbb{R}^N,$$

with $f \in L^2(\mathbb{R}^N)$. We assume that $A(y)$ and $c(y)$ belong to $L^\infty(\mathbb{T}^N)$ and $\exists\, \nu > 0$ such that for a.e. $y \in \mathbb{T}^N$

$$A(y)\xi \cdot \xi \geq \nu|\xi|^2 \text{ for any } \xi \in \mathbb{R}^N \text{ and } \quad c(y) \geq c_0 > 0.$$

The variational formulation is to find $u \in H^1(\mathbb{R}^N)$ such that

$$\int_{\mathbb{R}^N} \Big(A(y)\nabla_y u \cdot \overline{\nabla_y \phi} + c(y)u\overline{\phi}\Big)dy = \int_{\mathbb{R}^N} f\overline{\phi}\, dy \quad \forall \phi \in H^1(\mathbb{R}^N).$$

Proposition. The p.d.e. in $\mathbb{R}^N$ is equivalent to the family of p.d.e.'s, indexed by $\theta \in \mathbb{T}^N$,

$$-(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\mathcal{B}u\Big) + c(y)\mathcal{B}u = \mathcal{B}f \quad \text{in } \mathbb{T}^N,$$

which admits a unique solution $y \to (\mathcal{B}u)(y,\theta) \in H^1(\mathbb{T}^N)$ for any $\theta \in \mathbb{T}^N$.

Proof. We apply the previous Lemmas

$$\int_{\mathbb{R}^N} \Big(A(y)\nabla_y u \cdot \overline{\nabla_y \phi} + c(y)u\overline{\phi}\Big)dy = \int_{\mathbb{R}^N} f\overline{\phi}\,dy \quad \forall \phi \in H^1(\mathbb{R}^N)$$

$$\int_{\mathbb{T}^N}\int_Y \Big(A(y)(\nabla_y + 2i\pi\theta)\hat{u} \cdot \overline{(\nabla_y + 2i\pi\theta)\hat{\phi}} + c(y)\hat{u}\overline{\hat{\phi}}\Big)dy\,d\theta = \int_{\mathbb{T}^N}\int_Y \hat{f}\overline{\hat{\phi}}\,dy\,d\theta$$

which is a variational formulation in $y \in \mathbb{T}^N$ integrated with respect to θ which is just a parameter.

For a given $\theta \in Y$, consider the Green operator $\mathcal{G}_\theta$

$$\left\{ \begin{array}{lcl} L^2(\mathbb{T}^N) & \to & L^2(\mathbb{T}^N) \\ g(y) & \to & \mathcal{G}_\theta g(y) = v(y) \end{array} \right.$$

where $v \in H^1(\mathbb{T}^N)$ is the unique solution of

$$-(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)v\Big) + c(y)v = g \quad \text{in } \mathbb{T}^N.$$

One can check that $\mathcal{G}_\theta$ is a self-adjoint compact complex-valued linear operator acting on $L^2(\mathbb{T}^N)$. As such it admits a countable sequence of real increasing eigenvalues $(\lambda_n)_{n\geq 1}$ (repeated with their multiplicity) and normalized eigenfunctions $(\psi_n)_{n\geq 1}$ with $\|\psi_n\|_{L^2(\mathbb{T}^N)} = 1$. The eigenvalues and eigenfunctions depend on the dual parameter or Bloch frequency θ which runs in the dual cell of Y, which is again Y.

In other words, the eigenvalues and eigenfunctions satisfy the so-called Bloch (or shifted) spectral cell equation

$$-(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \quad \text{in } \mathbb{T}^N.$$

$\theta \in Y$ is the Bloch frequency (or quasi momentum).

A Bloch wave is $\phi_n(y) = \psi_n(\theta, y)e^{2i\pi\theta\cdot y}$ which satisfies

$$-\,\mathrm{div}_y\,(A(y)\nabla_y\phi_n) + c(y)\phi_n = \lambda(\theta)\phi_n \quad \text{in } \mathbb{R}^N.$$

Theorem 2. For any $u(y) \in L^2(\mathbb{R}^N)$, $\exists\, \hat{u}_n(\theta) \in L^2(\mathbb{T}^N)$, $n \geq 1$, such that

$$u(y) = \sum_{n\geq 1} \int_{\mathbb{T}^N} \hat{u}_n(\theta)\psi_n(y,\theta)e^{2i\pi\theta\cdot y}d\theta.$$

Furthermore, the linear map $\mathcal{B}$, called the Bloch transform and defined by $\mathcal{B}u = (\hat{u}_n)_{n\geq 1}$, is an isometry from $L^2(\mathbb{R}^N)$ into $\ell_2\left(L^2(\mathbb{T}^N)\right)$, i.e. Parseval formula holds for any $u, v \in L^2(\mathbb{R}^N)$

$$\int_{\mathbb{R}^N} u(y)\overline{v(y)}\,dy = \sum_{n\geq 1} \int_Y \hat{u}_n(\theta)\overline{\hat{v}_n(\theta)}\,d\theta.$$

Proof. We decompose each $\hat{u}(y,\theta)$ on the corresponding eigenbasis

$$\hat{u}(y,\theta) = \sum_{n\geq 1} \hat{u}_n(\theta)\psi_n(y,\theta) \quad \text{with } \hat{u}_n(\theta) = \int_{\mathbb{T}^N} \hat{u}(y,\theta)\overline{\psi_n(y,\theta)}dy.$$

Commuting the sum with respect to n and the integral with respect to θ is a standard Fubini type result.

Application

$$-\operatorname{div}_y\Big(A(y)\nabla_y u\Big) + c(y)u = f \quad \text{in } \mathbb{R}^N,$$

with $f \in L^2(\mathbb{R}^N)$.

We obtain an explicit algebraic formula for the solution

$$\hat{u}_n(\theta) = \frac{\hat{f}_n(\theta)}{\lambda_n(\theta)} \quad \forall n \geq 1, \forall \theta \in Y,$$

which is a generalization of a similar formula, using Fourier transform, for a constant coefficient p.d.e..

Smoothness of the Bloch eigenvalues

Lemma. $\theta \to \lambda_n(\theta)$ is Lipschitz.

Remark: for multiple eigenvalues $\theta \to \lambda_n(\theta)$ is usually not smoother.

Lemma (Kato, Rellich). If an eigenvalue $\lambda_n(\theta)$ is simple at the value $\theta = \theta^n$, then it remains simple in a small neighborhood of θ^n and the n-th eigencouple is analytic in this neighborhood of θ^n.

Assumption: $\lambda_n(\theta^n)$ is a simple eigenvalue.

$$\text{Operator} \quad \mathbb{A}_n(\theta)\psi = -(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(y)\psi - \lambda_n(\theta)\psi,$$

Then, in a neighborhood of θ^n, one can differentiate

$$\mathbb{A}_n(\theta)\frac{\partial\psi_n}{\partial\theta_k} = 2i\pi e_k A(y)(\nabla_y + 2i\pi\theta)\psi_n + (\,\mathrm{div}_y + 2i\pi\theta)\,(A(y)2i\pi e_k\psi_n) + \frac{\partial\lambda_n}{\partial\theta_k}(\theta)\psi_n,$$

and the second derivative is

$$\begin{aligned}
\mathbb{A}_n(\theta)\frac{\partial^2\psi_n}{\partial\theta_k\partial\theta_l} \quad &= 2i\pi e_k A(y)(\nabla_y + 2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_l} + (\,\mathrm{div}_y + 2i\pi\theta)\left(A(y)2i\pi e_k\frac{\partial\psi_n}{\partial\theta_l}\right) \\
&+2i\pi e_l A(y)(\nabla_y + 2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_k} + (\,\mathrm{div}_y + 2i\pi\theta)\left(A(y)2i\pi e_l\frac{\partial\psi_n}{\partial\theta_k}\right) \\
&+\frac{\partial\lambda_n}{\partial\theta_k}(\theta)\frac{\partial\psi_n}{\partial\theta_l} + \frac{\partial\lambda_n}{\partial\theta_l}(\theta)\frac{\partial\psi_n}{\partial\theta_k} \\
&-4\pi^2 e_k A(y)e_l\psi_n - 4\pi^2 e_l A(y)e_k\psi_n + \frac{\partial^2\lambda_n}{\partial\theta_l\partial\theta_k}(\theta)\psi_n
\end{aligned}$$

-V- SCHRÖDINGER EQUATION

Schrödinger equation in a periodic medium:

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right) + d\left(x,\dfrac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

Complex-valued unknown: $u_\epsilon(t,x) : \mathbb{R}^+ \times \mathbb{R}^N \to \mathbb{C}$

- $y \to A(y), c(y), d(x,y)$ $(0,1)^N$-periodic, real, measurable and bounded.
- A is a $N \times N$ symmetric, uniformly coercive, tensor.
- c and d are scalar functions with no sign.
- $d(x,y)$ is a Carathéodory function, $u_\epsilon^0 \in H^1(\mathbb{R}^N)$.

Physical motivation:

☞ Solid state physics: one-electron model in a periodic crystal.

☞ $c(y)$ is the crystal potential and $d(x,y)$ the (small) exterior potential.

Other possible equation:

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - (\,\mathrm{div} + i\epsilon\mathcal{A}_\epsilon)\,(\nabla + i\epsilon\mathcal{A}_\epsilon)\,u_\epsilon + \epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

where $\mathcal{A}_\epsilon = \mathcal{A}\left(t, x, \frac{x}{\epsilon}\right)$ is the electromagnetic vector potential such that the electric field E and magnetic field B are

$$E = -\frac{\partial \mathcal{A}_\epsilon}{\partial t} \quad \text{and} \quad B = \mathrm{curl}\mathcal{A}_\epsilon.$$

✗ Periodic homogenization: $\epsilon \to 0$ is the period.

✗ Singular perturbation: potential of order ϵ^{-2}.

SCALING

✗ This is not the scaling of semi-classical analysis:

$$\frac{i}{\epsilon}\frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\frac{x}{\epsilon}\right) + d\left(x,\frac{x}{\epsilon}\right)\right)u_\epsilon = 0$$

✗ This is a parabolic scaling (for longer times).

✗ Scaling of a long time asymptotic: change of variables $y = x/\epsilon$ and $\tau = t/\epsilon^2$

$\Rightarrow$ cells of size 1, no more oscillations

$$i\frac{\partial u_\epsilon}{\partial \tau} - \operatorname{div}_y\left(A(y)\nabla_y u_\epsilon\right) + \Big(c(y) + \epsilon^2 d(\epsilon y, y)\Big)u_\epsilon = 0$$

$\Rightarrow$ small and slowly varying exterior potential.

Goal: find homogenized models, justify the notion of electron effective mass.

A priori estimates

For any final time $T > 0$, there exists a constant $C > 0$ that does not depend on ϵ such that

$$\begin{aligned} \|u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} &= \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)}, \\ \epsilon\|\nabla u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N)^N)} &\leq C\left(\|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} + \epsilon\|\nabla u_\epsilon^0\|_{L^2(\mathbb{R}^N)^N}\right). \end{aligned}$$

Proof. Multiply the equation by $\overline{u_\epsilon}$ and by $\frac{\partial \overline{u_\epsilon}}{\partial t}$, integrate by parts and take the real part.

No strong convergence a priori.

A FIRST SIMPLE RESULT

We use a trick of Vanninathan (81'), Kozlov (84'), A.-Malige (97').

Introduce the spectral cell problem for $\theta = 0$

$$-\operatorname{div}_y\left(A(y)\nabla_y\psi_n\right) + c(y)\psi_n = \lambda_n\psi_n \quad \text{in the unit torus } \mathbb{T}^N.$$

First eigenvalue λ_1 is simple and first eigenfunction $\psi_1(y) > 0$ is positive by Krein-Rutman theorem (maximum principle).

Interpretation of ψ_1: periodic ground state.

Change of unknowns: $v_\epsilon(t,x) = e^{-i\frac{\lambda_1 t}{\epsilon^2}}\,\dfrac{u_\epsilon(t,x)}{\psi_1(\frac{x}{\epsilon})}$

Algebraic trick:

$$\psi_1\,\operatorname{div}\left(A\nabla(\psi_1 v)\right) = \psi_1 v\,\operatorname{div}\left(A\nabla\psi_1\right) + \operatorname{div}\left(\psi_1^2 A\nabla v\right)$$

A simpler equation for v_ϵ:

$$\begin{cases} i|\psi_1|^2\left(\frac{x}{\epsilon}\right)\frac{\partial v_\epsilon}{\partial t} - \operatorname{div}\left((|\psi_1|^2 A)\left(\frac{x}{\epsilon}\right)\nabla v_\epsilon\right) + (|\psi_1|^2 d)\left(x,\frac{x}{\epsilon}\right)v_\epsilon = 0 & \text{in } \mathbb{R}^N\times\mathbb{R}^+ \\ v_\epsilon(t=0,x) = \frac{u_\epsilon^0(x)}{\psi_1\left(\frac{x}{\epsilon}\right)} & \text{in } \mathbb{R}^N. \end{cases}$$

Theorem. (Standard periodic homogenization)

If $u_\epsilon^0(x) = v^0(x)\psi_1\left(\frac{x}{\epsilon}\right)$, then v_ϵ, converges weakly in $L^2\left((0,T);H^1(\mathbb{R}^N)\right)$ to the solution v of the homogenized problem

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A^*\nabla v\right) + d^*(x)\,v = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

where $d^*(x) = \int_{\mathbb{T}^N}|\psi_1|^2(y)d(x,y)\,dy$ and A^* is the "usual" homogenized tensor for $|\psi_1(y)|^2A(y)$.

INTERPRETATION

Convergence result:

$$u_\epsilon(t,x) \approx e^{i\frac{\lambda_1 t}{\epsilon^2}} \psi_1\left(\frac{x}{\epsilon}\right) v(t,x)$$

- It is crucial that $\psi_1(y) > 0$ (maximum principle).
- This trick is called factorization principle.
- Equivalent results for parabolic or hyperbolic equations, transport equation (A.-Bal, A.-Capdeboscq ...).
- Still true if $\psi_1\left(\frac{x}{\epsilon}\right) u_\epsilon^0(x)$ converges weakly to $v^0(x)$ in $L^2(\mathbb{R}^N)$.

What happens if the weak limit is $v^0 \equiv 0$?

WKB METHOD

A different kind of ansatz. Geometric optics or WKB method (Wentzel, Kramers, Brillouin).

$$\begin{cases} \dfrac{i}{\epsilon}\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(x,\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \dfrac{1}{\epsilon^2}c\left(x,\dfrac{x}{\epsilon}\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N\times(0,T), \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N \end{cases}$$

- This is precisely the scaling of semi-classical analysis.
- Short time scaling.
- A is symmetric and uniformly coercive.
- Formal method. For rigorous analysis, see: Buslaev, Guillot-Ralston, Gérard-Martinez-Sjostrand, Gérard-Markowich-Mauser-Poupaud, Panati-Sohn-Teufel...

- Introduce the operator

$$\mathbb{A}(x,\theta)\psi \equiv -(\ \mathrm{div}_y + 2i\pi\theta)\Big(A(x,y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(x,y)\psi$$

- Eigenvalues $\lambda_n(x,\theta)$ and eigenfunctions $\psi_n(x,y,\theta)$.
- Choose an energy level n such that $\lambda_n(x,\theta)$ is simple $\forall\theta \in \mathbb{T}^N, \forall x \in \mathbb{R}^N$.
- Replace θ par ∇S^0 and consider an initial data with oscillating phase

$$u^0_\epsilon(x) = e^{2i\pi\frac{S^0(x)}{\epsilon}} u^0(x)\psi_n\left(x, \frac{x}{\epsilon}, \nabla S^0(x)\right)$$

High frequency asymptotic expansion or WKB ansatz

$$u_\epsilon(t,x) = e^{2i\pi\frac{S(t,x)}{\epsilon}}\left(v\left(t,x,\frac{x}{\epsilon}\right)+\epsilon v_1\left(t,x,\frac{x}{\epsilon}\right)+...\right)$$

The first derivatives are

$$\epsilon\frac{\partial u_\epsilon}{\partial t} = e^{2i\pi\frac{S(t,x)}{\epsilon}}\left(2i\pi(v+\epsilon v_1)\frac{\partial S}{\partial t}+\epsilon\frac{\partial v}{\partial t}+\mathcal{O}(\epsilon^2)\right)$$

$$\epsilon\nabla u_\epsilon = e^{2i\pi\frac{S(t,x)}{\epsilon}}\left(2i\pi(v+\epsilon v_1)\nabla S+\nabla_y v+\epsilon(\nabla_x v+\nabla_y v_1)+\mathcal{O}(\epsilon^2)\right)$$

We compute also the second derivatives, plug the ansatz in the p.d.e. and deduce a cascade of equations.

Cascade of equations

Order ϵ^{-2}:

$$\mathbb{A}(x, \nabla S)v = 2\pi \frac{\partial S}{\partial t} v \quad \text{in} \quad \mathbb{T}^N.$$

This is a spectral problem, y being the space variable and (t, x) being fixed parameters. Thus, we deduce

$$2\pi \frac{\partial S}{\partial t} = \lambda_n(x, \nabla S)$$

and by simplicity of the eigenvalue

$$v(t, x, y) = u(t, x)\psi_n(x, y, \nabla S(t, x)).$$

We have obtained an eikonal equation (Hamilton-Jacobi) to compute the phase with the initial data $S(0, x) = S^0(x)$.

Order ϵ^{-1}:

$$\mathbb{A}(x,\nabla S)v_1 = \lambda_n(x,\nabla S)v_1 + f \quad \text{in} \quad \mathbb{T}^N,$$

with

$$f = -i\frac{\partial v}{\partial t} + \Big(\ \mathrm{div}_y + 2i\pi\nabla S\Big)(A\nabla_x v) + \ \mathrm{div}_x\Big(A(\nabla_y + 2i\pi\nabla S)v\Big).$$

To solve for v_1 the Fredholm alternative requires that

$$\int_{\mathbb{T}^N} f(t,x,y)\overline{\psi_n}(x,y,\nabla S)\,dy = 0.$$

Recall that $v(t,x,y) = u(t,x)\psi_n(x,y,\nabla S)$ and Fredholm alternative for $\nabla_\theta\psi_n$

$$-\nabla_x u\cdot\nabla_\theta\lambda_n = 2i\pi\int_{\mathbb{T}^N}\left[(\ \mathrm{div}_y + 2i\pi\theta)\,(A(y)\nabla_x u\psi_n) + A(y)(\nabla_y + 2i\pi\theta)\psi_n\cdot\nabla_x u\right]dy$$

We deduce an homogenized transport equation

$$\frac{\partial u}{\partial t} - \frac{\nabla_\theta\lambda_n(\nabla S)}{2\pi}\cdot\nabla_x u + b^* u = 0$$

Reminder on Bloch waves

- Bloch eigenvalue $\lambda_n(x,\theta)$ and eigenvector $\psi_n(x,y,\theta)$
- Assumption: $\lambda_n(\theta)$ is a simple eigenvalue.
- Operator

$$\mathbb{A}_n(x,\theta)\psi = -(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(x,y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(x,y)\psi - \lambda_n(x,\theta)\psi,$$

- Bloch spectral problem

$$\mathbb{A}_n(x,\theta)\psi_n = 0$$

- We differentiate with respect to θ

$$\mathbb{A}_n(x,\theta)\frac{\partial\psi_n}{\partial\theta_k} = 2i\pi e_k A(\nabla_y + 2i\pi\theta)\psi_n + (\,\mathrm{div}_y + 2i\pi\theta)\,(A2i\pi e_k\psi_n) + \frac{\partial\lambda_n}{\partial\theta_k}\psi_n,$$

- Fredholm alternative: the r.h.s. is orthogonal to ψ_n.

✘ Group velocity

$$\mathcal{V} = \frac{\nabla_\theta \lambda_n(\nabla S)}{2\pi}$$

✘ If we write $v(t,x,y) = u(t,x,\theta)\psi_n(x,y,\theta)$ with $\theta = \nabla S$, then we deduce an homogenized Liouville equation in the phase space

$$\frac{\partial |u|^2}{\partial t} - \mathcal{V} \cdot \nabla_x |u|^2 + \nabla_x \lambda_n \cdot \nabla_\theta |u|^2 = 0$$

Conclusion

$$u_\epsilon(t,x) \approx e^{2i\pi \frac{S(t,x)}{\epsilon}} \psi_n\left(x, \frac{x}{\epsilon}, \nabla S(t,x)\right) u(t,x,\nabla S(t,x))$$

The semi-classical limit is given by the dynamic of the following Hamiltonian system in the phase space $(x,\theta) \in \mathbb{R}^N \times \mathbb{T}^N$

$$\begin{cases} \dot{x} = \frac{1}{2\pi} \nabla_\theta \lambda_n(x,\theta) \\ \dot{\theta} = -\nabla_x \lambda_n(x,\theta) \end{cases}$$

- Phase S solution of an eikonal equation.
- Amplitude $|u|^2$ solution of a transport equation in the phase space.
- Valid up to caustics.
- Rigorous version by using semi-classical or Wigner measures.
- WKB ansatz are useful for computations too.

Special case

Monochromatic initial data. Periodic coefficients.

Assume $S^0(x) = \theta \cdot x$ and $A(x,y) \equiv A(y)$, $c(x,y) \equiv c(y)$.

Then the explicit solution of the eikonal equation is

$$S(t,x) = \theta \cdot x + 2\pi\lambda_n(\theta)\, t$$

Furthermore $\mathcal{V}$ is constant, $b^* = 0$ and $\nabla_x \lambda_n(\theta) = 0$, thus

$$u(t,x) = u_0(x + \mathcal{V}t)$$

In such a simpler case we can find a better "long time" ansatz of the solution.

-VI- HOMOGENIZATION

We consider a monochromatic wave packet as initial data

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x) \quad \text{with} \quad v^0 \in H^1(\mathbb{R}^N).$$

Assumption: the eigenvalue $\lambda_n(\theta^n)$ is simple.

- ✗ We replace the maximum principle by Bloch wave theory.
- ✗ Simplicity is a generic assumption.
- ✗ Other initial data are possible (up to extracting a weakly two-scale converging subsequence).

For $\theta \in Y$ the Bloch (or shifted) spectral cell equation is

$$-(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \qquad \text{in } \mathbb{T}^N$$

Schrödinger equation in a periodic medium:

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \mathrm{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right) + d\left(x, \dfrac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

Theorem 1. Assume further that the group velocity vanishes

$$\nabla_\theta \lambda_n(\theta^n) = 0.$$

Then $\boxed{u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon},\theta^n\right) v(t,x) + r_\epsilon(t,x)}$ with

$$\lim_{\epsilon\to 0} \sup_{t\in[0,T]} \int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2\, dx = 0,$$

and $v \in C\left((0,T);L^2(\mathbb{R}^N)\right)$ is the unique solution of the homogenized Schrödinger equation

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A_n^*\nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

with $A_n^* = \dfrac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ and $d_n^*(x) = \displaystyle\int_{\mathbb{T}^N} d(x,y)|\psi_n(y)|^2\, dy.$

REMARKS

- The inverse of A_n^* is called the effective mass (a well-known concept in solid state physics).
- The effective mass can be negative or infinite !
- Previous work on effective mass: Bensoussan-Lions-Papanicolaou, Poupaud-Ringhofer.
- The homogenized coefficients do depend on the initial data ! It does not fit in the framework of G- or H-convergence.

Theorem 2. Assume $\lim_{|x|\to+\infty} d(x,y) = d^\infty(y)$ uniformly in $\mathbb{T}^N$. Define the group velocity or drift

$$\mathcal{V} = \frac{1}{2\pi}\nabla_\theta \lambda_n(\theta^n) \in \mathbb{R}^N.$$

Then $\boxed{u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon},\theta^n\right) v\left(t, x+\frac{\mathcal{V}}{\epsilon}t\right) + r_\epsilon(t,x)}$ with $\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2\,dxdt = 0$, where $v \in C\left((0,T);L^2(\mathbb{R}^N)\right)$ is the unique solution of the homogenized Schrödinger equation

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A_n^*\nabla v\right) + d_n^*\, v = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

with $A_n^* = \dfrac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ and $d_n^* = \displaystyle\int_{\mathbb{T}^N} d^\infty(y)|\psi_n(y)|^2\,dy$.

Generalization for a multiple eigenvalue

What happens if $\lambda_n(\theta^n)$ is not simple ? In general, if $\lambda_n(\theta^n)$ is of multiplicity $p > 1$, we expect an homogenized system of p equations.

Assume that $\lambda_n(\theta^n) = \lambda_{n+1}(\theta^n)$ is of multiplicity 2 and that, up to a convenient relabelling, $\lambda_n(\theta)$ and $\lambda_{n+1}(\theta)$ are smooth branches of eigenvalues (and eigenfunctions). (Very strong assumption !)

We can prove that the homogenized system is

$$\begin{cases} i\dfrac{\partial v_1}{\partial t} - \operatorname{div}\left(A_n^* \nabla v_1\right) + d_{11}^*(x)\, v_1 + d_{12}^*(x)\, v_2 = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ i\dfrac{\partial v_2}{\partial t} - \operatorname{div}\left(A_{n+1}^* \nabla v_2\right) + d_{21}^*(x)\, v_1 + d_{22}^*(x)\, v_2 = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ (v_1, v_2)(t=0,x) = (v_1^0, v_2^0)(x) & \text{in } \mathbb{R}^N. \end{cases}$$

Formal proof of Theorem 1

We make an ansatz for the solution

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}}\, e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \sum_{i=0}^{+\infty} \epsilon^i u_i\left(t,x,\frac{x}{\epsilon}\right)$$

where the oscillating phase is deduced from WKB.

We recall the operator

$$\mathbb{A}_n(\theta)\psi \equiv -(\,\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(y)\psi - \lambda_n(\theta)\psi$$

We plug the ansatz in the equation and get a cascade of equations.

Cascade of equations

Order ϵ^{-2}:

$$\mathbb{A}_n(\theta^n)u_0(t,x,y) = 0$$

from which we deduce, by simplicity of $\lambda_n(\theta^n)$, that

$$u_0(t,x,y) \equiv v(t,x)\psi_n(y,\theta^n).$$

Order ϵ^{-1}:

$$\mathbb{A}_n(\theta^n)u_1(t,x,y) = \operatorname{div}_x\left(A(y)(\nabla_y + 2i\pi\theta^n)\psi_n v\right) + \left(\operatorname{div}_y + 2i\pi\theta^n\right)\left(A(y)\nabla_x v\psi_n\right)$$

from which we deduce (up to the addition of a multiple of ψ_n)

$$u_1(t,x,y) \equiv \frac{1}{2i\pi}\sum_{k=1}^{N}\frac{\partial v}{\partial x_k}(t,x)\frac{\partial \psi_n}{\partial \theta_k}(y,\theta^n)$$

Order ϵ^0:

$$\mathbb{A}_n(\theta^n)u_2(t,x,y) = f$$

from which we deduce that

$$u_2(t,x,y) \equiv \frac{-1}{4\pi^2}\sum_{k,l=1}^{N}\frac{\partial^2 v}{\partial x_k \partial x_l}(t,x)\frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l}$$

and, more important, by the Fredholm alternative,

$$\int_{\mathbb{T}^N} f(t,x,y)\overline{\psi_n}(t,x,y)\,dy = 0.$$

This last condition yields the homogenized equation.

Proof of Theorem 1

It is made of 3 steps

1. Deriving the spectral cell problem.
2. Deriving the homogenized equation.
3. Strong convergence.

Main tools: Bloch wave decomposition, two-scale convergence.

STEP 1. SPECTRAL CELL PROBLEM

We apply two-scale convergence to the bounded sequence v_ϵ defined by

$$v_\epsilon(t,x) = u_\epsilon(t,x) e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$

which admits a two-scale limit $v^*(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; H^1(\mathbb{T}^N)\right)$.

We multiply the Schrödinger equation by the complex conjugate of

$$\varphi_\epsilon \equiv \epsilon^2 \phi(t,x,\frac{x}{\epsilon}) e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}$$

Variational formulation

$$\int_0^T \int_{\mathbb{R}^N} \left(i\frac{\partial u_\epsilon}{\partial t}\overline{\varphi_\epsilon} + A^\epsilon \nabla u_\epsilon \cdot \nabla \overline{\varphi_\epsilon} + (\epsilon^{-2} c^\epsilon + d^\epsilon) u_\epsilon \overline{\varphi^\epsilon} \right) dt\, dx = 0.$$

Replace u_ϵ by v_ϵ and φ_ϵ by $\epsilon^2 \phi^\epsilon$

$$\int_0^T \int_{\mathbb{R}^N} \left(A^\epsilon (\epsilon\nabla + 2i\pi\theta^n) v_\epsilon \cdot (\epsilon\nabla - 2i\pi\theta^n)\overline{\phi}^\epsilon + (c^\epsilon - \lambda_n(\theta^n)) v_\epsilon \overline{\phi}^\epsilon \right) dt\, dx = \mathcal{O}(\epsilon^2).$$

Passing to the two-scale limit yields the variational formulation of

$$-(\ \mathrm{div}_y + 2i\pi\theta^n) \Big(A(y)(\nabla_y + 2i\pi\theta^n) v^* \Big) + c(y) v^* = \lambda_n(\theta^n) v^* \quad \text{in } \mathbb{T}^N.$$

Since $\lambda_n(\theta^n)$ is simple, there exists a scalar function $v(t,x) \in L^2((0,T)\times\Omega)$ such that

$$\boxed{v^*(t,x,y) = v(t,x)\psi_n(y,\theta^n).}$$

STEP 2. HOMOGENIZED PROBLEM

We multiply the Schrödinger equation by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon \sum_{k=1}^N \frac{\partial\phi}{\partial x_k}(t,x)\zeta_k(\frac{x}{\epsilon}) \right)$$

where $\zeta_k(y)$ is the solution of

$$\mathbb{A}(\theta^n)\zeta_k = e_k A(y)(\nabla_y + 2i\pi\theta^n)\psi_n + (\ \mathrm{div}_y + 2i\pi\theta^n)\,(A(y)e_k\psi_n) \qquad \text{in } \mathbb{T}^N$$

with the operator $\mathbb{A}(\theta)$ defined on $L^2(\mathbb{T}^N)$ by

$$\mathbb{A}(\theta^n)\psi = -(\ \mathrm{div}_y + 2i\pi\theta^n)\Big(A(y)(\nabla_y + 2i\pi\theta^n)\psi\Big) + c(y)\psi - \lambda_n(\theta^n)\psi$$

The existence of ζ_k is guaranteed because

$$\frac{\partial\psi_n}{\partial\theta_k} = 2i\pi\zeta_k \qquad \text{since} \qquad \nabla_\theta\lambda_n(\theta^n) = 0$$

Everything you always wanted to know about the proof but were afraid to ask

- We integrate by parts and put all derivatives on the test function.
- The ϵ^{-2} terms cancel out because of the equation for ψ_n.
- The ϵ^{-1} terms cancel out because of the equation for ζ_k.
- We pass to the two-scale limit in the ϵ^0 terms.
- We obtain a very weak form of the homogenized equation.
- The homogenized tensor A_n^* is equal to $\frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ because of the compatibility condition (Fredholm alternative) for $\frac{\partial^2\psi_n}{\partial\theta_k\partial\theta_l}$.

$$\int_{\mathbb{R}^N} A^\epsilon \nabla u_\epsilon \cdot \nabla \overline{\Psi}_\epsilon dx = \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\overline{\phi} v_\epsilon) \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon}) \overline{\psi}_n^\epsilon$$

$$+\epsilon \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon) \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon}) \overline{\zeta}_k^\epsilon$$

$$- \int_{\mathbb{R}^N} A^\epsilon e_k \frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon}) \overline{\psi}_n^\epsilon$$

$$+ \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon) \cdot e_k \overline{\psi}_n^\epsilon$$

$$- \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n^\epsilon - \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\epsilon \nabla - 2i\pi \theta^n) \overline{\zeta}_k^\epsilon$$

$$+ \int_{\mathbb{R}^N} A^\epsilon \overline{\zeta}_k^\epsilon (\epsilon \nabla + 2i\pi \theta^n) v_\epsilon \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k}$$

Variational formulation for $\psi_n\left(\frac{x}{\epsilon}\right)$

$$\int_{\mathbb{R}^N} A^\epsilon(\nabla + 2i\pi\frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot (\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}(c^\epsilon - \lambda_n(\theta^n))\psi_n^\epsilon\overline{\Phi} = 0$$

Take $\Phi = \overline{\phi}v_\epsilon \Rightarrow$ cancellation of the ϵ^{-2} terms

Variational formulation for $\zeta_k\left(\frac{x}{\epsilon}\right)$

$$\int_{\mathbb{R}^N} A^\epsilon(\nabla + 2i\pi\frac{\theta^n}{\epsilon})\zeta_k^\epsilon \cdot (\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}(c^\epsilon - \lambda_n(\theta^n))\zeta_k^\epsilon\overline{\Phi} =$$

$$\epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon(\nabla + 2i\pi\frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot e_k\overline{\Phi} - \epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon e_k\psi_n^\epsilon \cdot (\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi}.$$

Take $\Phi = \frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon \Rightarrow$ cancellation of the ϵ^{-1} terms

STEP 3. STRONG CONVERGENCE

This is a consequence of the energy conservation

$$\|v_\epsilon(t)\|_{L^2(\mathbb{R}^N)} = \|u_\epsilon(t)\|_{L^2(\mathbb{R}^N)} = \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} \to \|\psi_n v^0\|_{L^2(\mathbb{R}^N \times \mathbb{T}^N)} = \|v^0\|_{L^2(\mathbb{R}^N)}$$

and of the notion of strong two-scale convergence.

Recall that

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x)$$

Proof of Theorem 2

New ingredient: two-scale convergence with drift.

Proposition (Marusic-Paloka, Piatnitski). Let $\mathcal{V} \in \mathbb{R}^N$ be a given drift velocity. Let u_ϵ be a bounded sequence in $L^2((0,T) \times \mathbb{R}^N)$. Up to a subsequence, there exist a limit $u_0(t,x,y) \in L^2((0,T) \times \mathbb{R}^N \times \mathbb{T}^N)$ such that u_ϵ two-scale converges with drift weakly to u_0 in the sense that

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^N} u_\epsilon(t,x) \phi \left(t, x + \frac{\mathcal{V}}{\epsilon} t, \frac{x}{\epsilon} \right) dt\, dx =$$

$$\int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} u_0(t,x,y) \phi(t,x,y)\, dt\, dx\, dy$$

for all functions $\phi(t,x,y) \in L^2\left((0,T) \times \mathbb{R}^N ; C(\mathbb{T}^N)\right)$.

Lemma (Marusic-Paloka, Piatnitski).

Let $\phi(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; C(\mathbb{T}^N)\right)$. Then

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N}\left|\phi\left(t,x+\frac{\mathcal{V}}{\epsilon}t,\frac{x}{\epsilon}\right)\right|^2 dt\,dx = \int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}|\phi(t,x,y)|^2 dt\,dx\,dy.$$

Proof. Change of variables $x' = x + \frac{\mathcal{V}}{\epsilon}t$

$$\int_0^T\int_{\mathbb{R}^N}\left|\phi\left(t,x+\frac{\mathcal{V}}{\epsilon}t,\frac{x}{\epsilon}\right)\right|^2 dt\,dx = \int_0^T\int_{\mathbb{R}^N}\left|\phi\left(t,x',\frac{x'}{\epsilon}-\frac{\mathcal{V}}{\epsilon^2}t\right)\right|^2 dt\,dx'$$

We mesh $\mathbb{R}^N$ with cubes of size ϵ, $\mathbb{R}^N = \cup_{i\in\mathbb{Z}} Y_i^\epsilon$ with $Y_i^\epsilon = x_i^\epsilon + (0,\epsilon)^N$

$$\int_{\mathbb{R}^N}\left|\phi\left(t,x',\frac{x'}{\epsilon}-\frac{\mathcal{V}}{\epsilon^2}t\right)\right|^2 dx = \sum_i\int_{Y_i^\epsilon}\left|\phi\left(t,x_i^\epsilon,\frac{x'}{\epsilon}-\frac{\mathcal{V}}{\epsilon^2}t\right)\right|^2 dx + \mathcal{O}(\epsilon)$$

$$= \sum_{i\in\mathbb{Z}}\epsilon^N\int_{\mathbb{T}^N}\left|\phi\left(x_i^\epsilon,y\right)\right|^2 dy + \mathcal{O}(\epsilon) = \int_\Omega\int_Y\left|\phi\left(x,y\right)\right|^2 dx\,dy + \mathcal{O}(\epsilon)$$

-VII- LOCALIZATION

We come back to the semi-classical scaling and to locally periodic coefficients

$$\frac{i}{\epsilon}\frac{\partial u_\epsilon}{\partial t} - \text{ div}\left(A\left(x,\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \epsilon^{-2}c\left(x,\frac{x}{\epsilon}\right)u_\epsilon = 0$$

We choose well-prepared initial data, Bloch wave packets.

ASSUMPTIONS

We choose a point $(x^n, \theta^n) \in \mathbb{R}^N \times \mathbb{T}^N$ in the phase space such that

$$\lambda_n(x^n, \theta^n) \text{ is a simple eigenvalue}$$

and

$$\nabla_\theta \lambda_n(x^n, \theta^n) = \nabla_x \lambda_n(x^n, \theta^n) = 0$$

We consider well-prepared initial data

$$u_\epsilon^0(x) = \psi_n\Big(x^n, \frac{x}{\epsilon}, \theta^n\Big) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0\Big(\frac{x - x^n}{\sqrt{\epsilon}}\Big)$$

with $v^0 \in H^1(\mathbb{R}^N)$ (degenerate case for WKB !)

Notations. New scale $z = \frac{x - x^n}{\sqrt{\epsilon}}$

Main result

Theorem (A.-Palombaro).

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(x^n,\theta^n)t}{\epsilon}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\Big(x^n, \frac{x}{\epsilon}, \theta^n\Big) v\Big(t, \frac{x-x^n}{\sqrt{\epsilon}}\Big) + r_\epsilon\Big(t, \frac{x-x^n}{\sqrt{\epsilon}}\Big)$$

with $\lim_{\epsilon\to 0} \int_{\mathbb{R}^N} |r_\epsilon(t,z)|^2\, dz = 0$, uniformly in time, and $v(t,z)$ is the unique solution of the homogenized Schrödinger equation

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}_z\left(A^*\nabla_z v\right) + \operatorname{div}_z(vB^*z) + c^*v + vD^*z\cdot z = 0 & \text{in } \mathbb{R}^N\times\mathbb{R}^+ \\ v(0,z) = v^0(z) & \text{in } \mathbb{R}^N \end{cases}$$

where c^* is a constant coefficient and A^*, B^*, D^* are constant matrices defined by

$$A^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(x^n,\theta^n)\,,\ B^* = \frac{1}{2i\pi}\nabla_\theta\nabla_x\lambda_n(x^n,\theta^n)\,,\ D^* = \frac{1}{2}\nabla_x\nabla_x\lambda_n(x^n,\theta^n)\,.$$

Homogenized problem

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}_z\left(A^*\nabla_z v\right) + \operatorname{div}_z(vB^*z) + c^*v + vD^*z\cdot z = 0 & \text{in } \mathbb{R}^N\times\mathbb{R}^+ \\ v(0,z) = v^0(z) & \text{in } \mathbb{R}^N \end{cases}$$

Lemma. The operator $\mathcal{A}^* : L^2(\mathbb{R}^N) \to L^2(\mathbb{R}^N)$ defined by

$$\mathcal{A}^*\varphi = -\operatorname{div}\left(A^*\nabla\varphi\right) + \operatorname{div}(\varphi B^*z) + c^*\varphi + \varphi D^*z\cdot z$$

is self-adjoint.

Corollary. The homogenized Schrödinger equation is well-posed in $C(\mathbb{R}^+; L^2(\mathbb{R}^N))$ and satisfies the energy conservation

$$||v(t,\cdot)||_{L^2(\mathbb{R}^N)} = ||v^0||_{L^2(\mathbb{R}^N)} \quad \forall\, t\in\mathbb{R}^+ .$$

Proof of the corollary. By self-adjointness

$$\int_{\mathbb{R}^N} \mathcal{A}^* v\overline{v}\, dz = \langle \mathcal{A}^* v, v\rangle = \langle v, \mathcal{A}^* v\rangle = \overline{\langle \mathcal{A}^* v, v\rangle} \in \mathbb{R}.$$

$$i\int_{\mathbb{R}^N} \frac{\partial v}{\partial t}\overline{v}\, dz + \int_{\mathbb{R}^N} \mathcal{A}^* v\overline{v}\, dz = 0$$

Take the imaginary part to get

$$\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^N} |v|^2 dz = 0$$

Proof of the lemma. By integration by parts and since $B^* \in i\mathbb{R}$, $\overline{B^*} = -B^*$

$$\int_{\mathbb{R}^N} \Big(\operatorname{div}(vB^*z)\overline{w} - \frac{1}{2}\operatorname{tr} B^* v\overline{w}\Big)dz = \int_{\mathbb{R}^N} \overline{\Big(\operatorname{div}(wB^*z)\overline{v} - \frac{1}{2}\operatorname{tr} B^* w\overline{v}\Big)dz}$$

Thus

$$\int_{\mathbb{R}^N} \mathcal{A}^* v\overline{w}\, dz = \int_{\mathbb{R}^N} \Big(A^*\nabla v\cdot\nabla\overline{w} + D^*z\cdot z\, v\overline{w} + \operatorname{div}(vB^*z)\overline{w} - \frac{1}{2}\operatorname{tr} B^* v\overline{w}\Big)\, dz + \int_{\mathbb{R}^N} \Big(\frac{1}{2}\operatorname{tr} B^* + c^*\Big) v\overline{w}\, dz$$

which is symmetric (obvious for the blue terms) since

$$\frac{1}{2i}\operatorname{tr} B^* + \operatorname{Im} c^* = 0$$

as a consequence of the Fredholm alternative for $\frac{\partial^2 \psi_n}{\partial z_k \partial \theta_l}$.

Compactness and localization

$$\nabla\nabla\lambda_n = \begin{pmatrix} \nabla_x\nabla_x\lambda_n & \nabla_\theta\nabla_x\lambda_n \\ \nabla_\theta\nabla_x\lambda_n & \nabla_\theta\nabla_\theta\lambda_n \end{pmatrix} (x^n, \theta^n) \, .$$

Lemma. If the matrix $\nabla\nabla\lambda_n$ is positive definite, then there exists an orthonormal basis $\{\varphi_n\}_{n\geq 1}$ in $L^2(\mathbb{R}^N)$ of eigenfunctions of the homogenized problem.

Moreover for each n there exists a real constant $\gamma_n > 0$ such that

$$e^{\gamma_n|z|}\varphi_n \, , \, e^{\gamma_n|z|}\nabla\varphi_n \in L^2(\mathbb{R}^N) \, .$$

This is localization ! (cf. Anderson in a stochastic framework)

Proof. For simplicity assume that $\mathrm{Re}(c^*) = 0$.

$$\langle \mathcal{A}^* v, v\rangle = \int_{\mathbb{R}^N} \mathcal{A}^* v\overline{v}\, dz = \int_{\mathbb{R}^N} \left(A^* \nabla v \cdot \nabla \overline{v} + D^* z \cdot z |v|^2 - iB^* \mathrm{Im}(vz \cdot \nabla \overline{v}) \right) dz$$

Recall that

$$A^* = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n \,, \quad B^* = \frac{1}{2i\pi} \nabla_\theta \nabla_x \lambda_n \,, \quad D^* = \frac{1}{2} \nabla_x \nabla_x \lambda_n \,.$$

Define $\Phi(z) = \Big(2i\pi v(z)\, z \,,\, \nabla v(z) \Big)^t$. Then

$$\langle \mathcal{A}^* v, v\rangle = \int_{\mathbb{R}^N} \frac{1}{8\pi^2} \nabla\nabla\lambda_n \Phi \cdot \overline{\Phi}\, dz \geq C \Big(||\nabla v||^2_{L^2(\mathbb{R}^N)} + ||z\, v||^2_{L^2(\mathbb{R}^N)} \Big)$$

The space $\{v \in H^1(\mathbb{R}^N) \text{ s.t. } (zv) \in L^2(\mathbb{R}^N)\}$ is compactly embedd in $L^2(\mathbb{R}^N)$.

Thus $(\mathcal{A}^*)^{-1}$ is compact and admits an hilbertian basis of eigenfunctions.

It is classical to show that eigenfunctions decay exponentially at infinity.

Proof of the homogenization theorem

Variational proof with an oscillating test function.

1. Change of variables $z = \frac{x - x^n}{\sqrt{\epsilon}}$
2. 2nd order Taylor expansion around $z = 0$ for the macroscopic variable
3. Two-scale convergence at the scale $\sqrt{\epsilon}$
4. Bloch wave decomposition as in the purely periodic case

No need of WKB or semiclassical arguments.

Change of variables:

$$z = \frac{x - x^n}{\sqrt{\epsilon}}\,,$$

Change of unknowns:

$$w_\epsilon(t,z) := e^{2i\pi\frac{\theta^n\cdot z}{\sqrt{\epsilon}}}\, v_\epsilon(t,z) = e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon}}\, u_\epsilon(t,x)\,.$$

New equation:

$$\begin{cases} i\dfrac{\partial w_\epsilon}{\partial t} - \ \mathrm{div}[A\left(\sqrt{\epsilon}z, z/\sqrt{\epsilon}\right)\nabla w_\epsilon] + \dfrac{1}{\epsilon}[c(\sqrt{\epsilon}z, z/\sqrt{\epsilon}) - \lambda_n(\theta^n)]w_\epsilon = 0 \\ \\ w_\epsilon(0,z) = u_\epsilon^0(\sqrt{\epsilon}z) \end{cases}$$

The oscillations are at scale $\sqrt{\epsilon}$: this is the parabolic scaling !

Taylor expansion around zero for the macroscopic variable

$$c\left(\sqrt{\epsilon}z,\frac{z}{\sqrt{\epsilon}}\right)=c\left(0,\frac{z}{\sqrt{\epsilon}}\right)+\sqrt{\epsilon}z\cdot\nabla_x c\left(0,\frac{z}{\sqrt{\epsilon}}\right)+\frac{1}{2}\epsilon\nabla_x\nabla_x c\left(0,\frac{z}{\sqrt{\epsilon}}\right)z\cdot z+\mathcal{O}(\sqrt{\epsilon}|z|)^3.$$

We obtain

$$\frac{1}{\epsilon}\Big(c(\sqrt{\epsilon}z,z/\sqrt{\epsilon})-\lambda_n(\theta^n)\Big)=$$

$$\frac{1}{\epsilon}\Big(c(0,z/\sqrt{\epsilon})-\lambda_n(\theta^n)\Big)+\frac{1}{\sqrt{\epsilon}}z\cdot\nabla_x c(0,z/\sqrt{\epsilon})+\frac{1}{2}\nabla_x\nabla_x c\left(0,\frac{z}{\sqrt{\epsilon}}\right)z\cdot z+\mathcal{O}(\sqrt{\epsilon})$$

as usual + new singular term to cancel + bounded harmonic potential

New test function:

$$\Psi_\epsilon(t,z)=e^{2i\pi\theta^n\cdot\frac{z}{\sqrt{\epsilon}}}\left[\psi_n^\epsilon\phi(t,z)+\sqrt{\epsilon}\sum_{k=1}^N\Big(\frac{1}{2i\pi}\frac{\partial\psi_n^\epsilon}{\partial\theta_k}\frac{\partial\phi}{\partial z_k}(t,z)+z_k\frac{\partial\psi_n^\epsilon}{\partial x_k}\phi(t,z)\Big)\right]$$

-VIII- TIME OSCILLATING POTENTIAL

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \Delta u_\epsilon + \left(\epsilon^{-2} c\left(\dfrac{x}{\epsilon}\right) + d_\epsilon(t,x)\right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

Goal: transfer some energy from the initial data to some target final data

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x) \qquad u_\epsilon^T(x) = \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) e^{2i\pi \frac{\theta^m \cdot x}{\epsilon}} v^T(x)$$

For this task, we choose a time oscillating potential

$$d_\epsilon(t,x) = \Re\left(e^{i\frac{(\lambda_m(\theta^m) - \lambda_n(\theta^n))t}{\epsilon^2}} e^{2i\pi \frac{(\theta^m - \theta^n)\cdot x}{\epsilon}}\right) d\left(t, x, \frac{x}{\epsilon}\right),$$

where $d(t,x,y)$ is a real potential defined on $[0,T] \times \mathbb{R}^N \times \mathbb{T}^N$.

Assumptions

We assume

$$\text{for } p = n, m \quad \begin{cases} (i) & \lambda_p(\theta^p) \text{ is a simple eigenvalue,} \\ (ii) & \theta^p \text{ is a critical point of } \lambda_p(\theta) \text{ i.e., } \nabla_\theta \lambda_p(\theta^p) = 0 \end{cases}$$

and a non-resonant assumption

$$(iii) \qquad \text{for any } p \geq 1, \quad \lambda_p(2\theta^n - \theta^m) \neq 2\lambda_n(\theta^n) - \lambda_m(\theta^m).$$

Theorem. For an initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ given by

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x) \quad \text{with } v^0 \in H^1(\mathbb{R}^N),$$

the solution of the Schrödinger equation can be written as

$$\begin{aligned} u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v_n(t,x) \\ + e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi \frac{\theta^m \cdot x}{\epsilon}} \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) v_m(t,x) + r_\epsilon(t,x), \end{aligned}$$

with

$$\lim_{\epsilon \to 0} \int_0^T \int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2 \, dx = 0,$$

and $(v_n, v_m) \in C\left([0,T]; L^2(\mathbb{R}^N)\right)^2$ is the unique solution of the homogenized Schrödinger system

$$\begin{cases} i\dfrac{\partial v_n}{\partial t} - \operatorname{div}\left(A_n^* \nabla v_n\right) + d_{nm}^*(t,x)\, v_m = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_m}{\partial t} - \operatorname{div}\left(A_m^* \nabla v_m\right) + d_{mn}^*(t,x)\, v_n = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v_n(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N \\ v_m(t=0,x) = 0 & \text{in } \mathbb{R}^N, \end{cases}$$

with $A_p^* = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_p(\theta^p)$, for $p = n, m$, and "Fermi golden rule"

$$d_{nm}^*(t,x) = \overline{d}_{mn}^*(t,x) = \frac{1}{2} \int_{\mathbb{T}^N} d(t,x,y) \overline{\psi}_n(y,\theta^n) \psi_m(y,\theta^m)\, dy.$$

Comments

- The exterior potential d^ϵ can be light illuminating the semiconductor.
- The initial data could be a combination of the to states n and m.
- Optical absorption: light excites electrons from the valence band to the conduction band.
- Its converse effect is at the root of lasers, light emitting diodes and photo-detectors.
- The squared modulus of d^*_{nm} is called the transition probability per unit time from state n to m.
- Theorem obtained with M. Vanninathan.

Sketch of the proof

Define two sequences

$$v_\epsilon^n(t,x) = u_\epsilon(t,x) e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$
$$v_\epsilon^m(t,x) = u_\epsilon(t,x) e^{-i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^m\cdot x}{\epsilon}}.$$

They both satisfy the a priori estimate, for $p = n, m$,

$$\|v_\epsilon^p\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} + \epsilon\|\nabla v_\epsilon^p\|_{L^2((0,T)\times\mathbb{R}^N)} \leq C$$

Up to a subsequence they two-scale converge to limits
$w_p(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; H^1(\mathbb{T}^N)\right)$.

Recall that

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \Delta u_\epsilon + \left(\epsilon^{-2} c\left(\dfrac{x}{\epsilon}\right) + d_\epsilon(t,x)\right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases}$$

with the initial data

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x)$$

and a time oscillating potential

$$d_\epsilon(t,x) = \Re\left(e^{i\frac{(\lambda_m(\theta^m) - \lambda_n(\theta^n))t}{\epsilon^2}} e^{2i\pi \frac{(\theta^m - \theta^n)\cdot x}{\epsilon}}\right) d\left(t, x, \frac{x}{\epsilon}\right),$$

where $d(t,x,y)$ is a real potential defined on $[0,T] \times \mathbb{R}^N \times \mathbb{T}^N$.

First step. We multiply the p.d.e. by the complex conjugate of

$$\epsilon^2 \phi(t,x,\frac{x}{\epsilon}) e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}$$

This yields the variational formulation of the cell problem

$$-(\,\mathrm{div}_y + 2i\pi\theta^n)\Big((\nabla_y + 2i\pi\theta^n)w_n\Big) + c(y)w_n = \lambda_n(\theta^n)w_n \quad \text{in } \mathbb{T}^N.$$

By simplicity of $\lambda_n(\theta^n)$, there exists $v_n(t,x) \in L^2\left((0,T)\times\mathbb{R}^N\right)$ such that

$$w_n(t,x,y) = v_n(t,x)\psi_n(y,\theta^n).$$

The same argument works replacing n by m !

$$w_m(t,x,y) = v_m(t,x)\psi_m(y,\theta^m).$$

Second step. We multiply the p.d.e. by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon \sum_{k=1}^N \frac{\partial\phi}{\partial x_k}(t,x)\zeta_n^k(\frac{x}{\epsilon}) \right)$$

We perform the same algebra as before except for the new term

$$\int_0^T \int_{\mathbb{R}^N} d\left(t,x,\frac{x}{\epsilon}\right) \frac{1}{2} \left(e^{i\frac{(\lambda_m(\theta^m)-2\lambda_n(\theta^n))t}{\epsilon^2}} e^{2i\pi\frac{(\theta^m-2\theta^n)\cdot x}{\epsilon}} + e^{-i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^m\cdot x}{\epsilon}} \right)$$
$$u_\epsilon \left(\overline{\psi}_n(\frac{x}{\epsilon},\theta^n)\overline{\phi}(t,x) + \mathcal{O}(\epsilon) \right) dt\,dx$$
$$= \int_0^T \int_{\mathbb{R}^N} d\left(t,x,\frac{x}{\epsilon}\right) \frac{1}{2} \left(v_\epsilon^{2n-m} + v_\epsilon^m \right) \left(\overline{\psi}_n(\frac{x}{\epsilon},\theta^n)\overline{\phi}(t,x) + \mathcal{O}(\epsilon) \right) dt\,dx$$

where we introduced a new sequence v_ϵ^{2n-m} defined by

$$v_\epsilon^{2n-m}(t,x) = u_\epsilon(t,x) e^{-i\frac{(2\lambda_n(\theta^n)-\lambda_m(\theta^m))t}{\epsilon^2}} e^{-2i\pi\frac{(2\theta^n-\theta^m)\cdot x}{\epsilon}}.$$

Applying the same arguments as in the first step, this sequence v_ϵ^{2n-m} two-scale converges to $w_{2n-m}(t,x,y)$ which satisfies

$$-(\,\mathrm{div}_y + 2i\pi(2\theta^n - \theta^m))\Big((\nabla_y + 2i\pi(2\theta^n - \theta^m))w_{2n-m}\Big) + c(y)w_{2n-m}$$
$$= (2\lambda_n(\theta^n) - \lambda_m(\theta^m))w_{2n-m} \quad \text{in } \mathbb{T}^N.$$

Because of the non-resonance assumption

$$2\lambda_n(\theta^n) - \lambda_m(\theta^m) \neq \lambda_p(2\theta^n - \theta^m) \quad \forall p$$

the above spectral problem has no solution other than 0

$$w_{2n-m}(t,x,y) \equiv 0.$$

Finally the two-scale limit is

$$-i\int_{\mathbb{R}^N} v^0\overline{\phi}(t=0)\,dx - i\int_0^T\int_{\mathbb{R}^N} v_n\frac{\partial\overline{\phi}}{\partial t}dt\,dx - \int_0^T\int_{\mathbb{R}^N} A_n^* v_n\cdot\nabla\nabla\overline{\phi}dt\,dx$$
$$+\int_0^T\int_{\mathbb{R}^N} d_{nm}^*(t,x)v_m\overline{\phi}\,dt\,dx = 0.$$

with

$$d_{nm}^*(t,x) = \frac{1}{2}\int_{\mathbb{T}^N} d(t,x,y)\overline{\psi}_n(y,\theta^n)\psi_m(y,\theta^m)\,dy.$$

A symmetric argument works for v_m (changing n in m in the test function Ψ_ϵ).

-IX- CONCLUSION AND GENERALIZATIONS

✗ Asymptotic of wave packets:

$$u_\epsilon(t,x) \approx e^{i\frac{\lambda_1(\theta^n)t}{\epsilon^2}}\, e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}\, \psi_n\left(\frac{x}{\epsilon}\right) v\left(t, x+\frac{\mathcal{V}}{\epsilon}t\right)$$

✗ Justification of the notion of effective mass.

✗ This is not G- or H-convergence.

✗ WKB ansatz for periodic coefficients.

Other generalizations:

☞ Parabolic equation (A., Capdeboscq, Piatnistki, Siess, Vanninathan, ARMA **174**, 2004).

☞ Wave equation. (work in progress)

☞ Nonlinear Schrödinger equation (Ch. Sparber, 2006).