LECTURE IV
HOMOGENIZATION OF HYPERBOLIC AND DISPERSIVE EQUATIONS

ENERGY BANDS

- Consider transport of one particle (electron) in a periodic medium, i.e. a crystal.

- This is described by a Schrödinger equation with an additional periodic potential.

- Under the assumption that the lattice period is much smaller than the length scale under consideration, we obtain a homogenization problem for the Schrödinger equation.

- The homogenization problem can be solved in terms of the Bloch transform and the solution of a sequence of eigenvalue problems.

- The result is semi- discrete Schrödinger equation where the quadratic term in the kinetic energy is replaced by the eigenvalue, dependent on a parameter vector, the 'energy band'.

- If the eigenvalue is replaced by a quadratic around its minimum we obtain the so called effective mass approximation.

LATTICE POTENTIALS

Transport of one particle (electron) in a periodic structure (crystal). Structure modeled through periodic interaction potential.

Schrödinger equation:

$$\partial_t \psi = \frac{i\hbar}{2m}\Delta_x \psi - \frac{i}{\hbar}[V + V_L]\psi$$

V_L: rapid periodic oscillations due to interaction with crystal lattice.

$$V_L(x) = V_L(x + \lambda L z), \quad z \in \mathbb{Z}^d, \quad V_L = \frac{1}{\lambda^2} V_L(x/\lambda)$$

L: Lattice matrix, λ: Lattice size, $(det(L) = 1)$

Consider spatial scale much larger than lattice. Homogenization for $\lambda \to 0$.

BLOCH WAVE DECOMPOSITION

Evolution equation with a linear differential operator with highly oscillatory coefficients

$$\partial_t \psi = H(x, \frac{x}{\lambda}, \nabla_x)\psi$$

H lattice periodic in fast variable $\frac{x}{\lambda}$

$$H(x, y + Lz, w) = H(x, y, w), \quad z \in \mathbb{Z}^3,$$

L : lattice matrix, $det(L) = 1$

Bloch decomposition: Slicing and Fourier transform

Step 1: 'slicing'

Decompose x into a fast spatial variable y and a slow, discrete variable r

$$\psi_1(y,r,t) = \psi(r+\lambda y,t), \quad r = \lambda L z, \quad z \in \mathbb{Z}^3,\ y \in L\cdot[0,1]^3$$

Boundary condition:

$$\psi_1(y+Lz',r,t) = \psi_1(y,r+\lambda Lz',t), \quad r \in \lambda L \mathbb{Z}^d$$

Step 2: Fourier transform in z

(discrete FT in the slow variable r)

$$\psi_2(y,\xi,t) = \lambda^3 \sum_z \psi_1(y,\lambda Lz,t)\,\mathrm{exp}(i\lambda\xi^T Lz), \quad \xi \in B = \frac{1}{\lambda}L^{-T}[-\pi,\pi]^3$$

B: Brillouin zone,

Boundary conditions:

$$\psi_2(y+Lz',\xi,t) = \psi_2(y,\xi,t)\,\mathrm{exp}(-i\lambda\xi^T Lz')$$

THE BLOCH TRANSFORM AND ITS INVERSE

$$BT[\psi] = \psi_2(y, \xi, t) = \lambda^3 \sum_z \psi(\lambda y + \lambda L z, t) \exp(i\lambda \xi^T L z),$$

$$\psi(x, t) = BT^{-1}[\psi_2] = (2\pi)^{-3} \int_B \psi_2(y, \xi, t) \exp(-i\lambda \xi^T L z) d\xi,$$

$$x = \lambda y + \lambda L z, \quad y \in L[0, 1]^3, \quad z \in \mathbb{Z}^3, \quad \xi \in \frac{1}{\lambda} L^{-T} [-\pi, \pi]^3$$

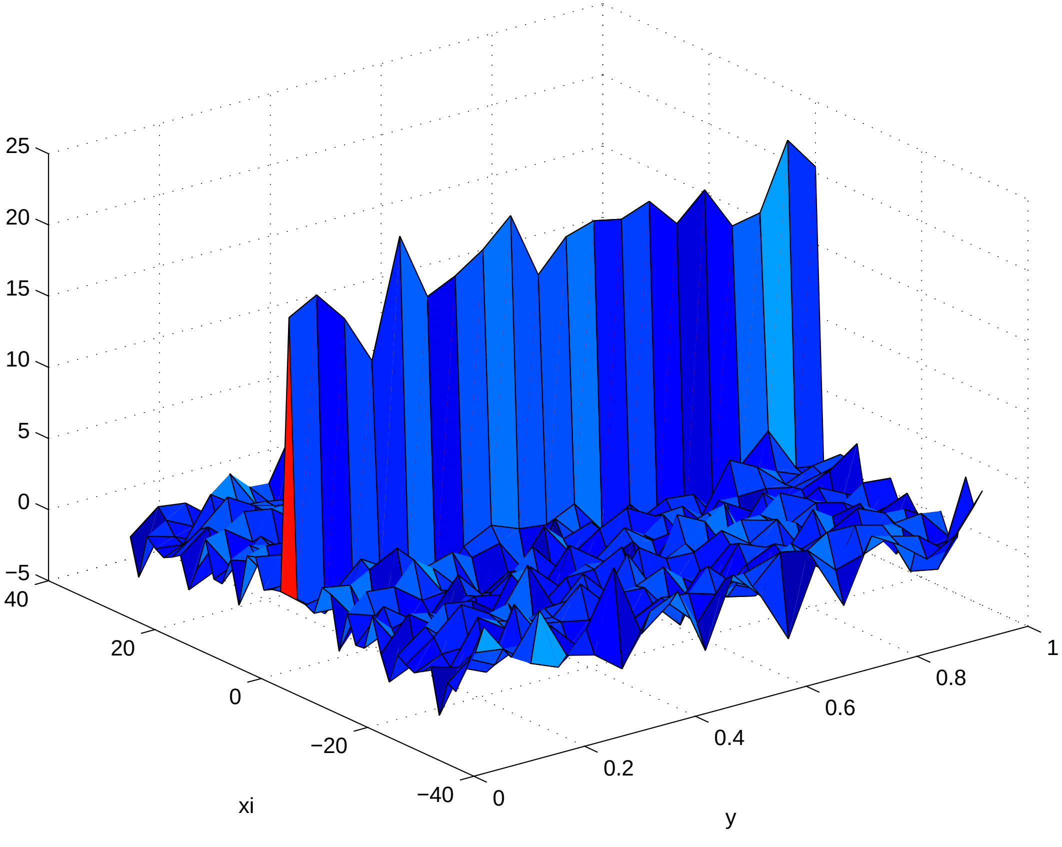
The Bloch transform decomposes a signal into its fast and slow modes by performing a FT in the slow variable only!

Example:

$$\psi(x, t) = \phi(x) f(\frac{x}{\lambda}), \quad f(y + Lz) = f(y)$$

$$BT[\psi](y, \xi) = f(y) \lambda^3 \sum_z \phi(\lambda y + \lambda L z) \exp(i\lambda \xi^T L z) \approx f(y) \widehat{\phi}(\xi)$$

BLOCH TRANSFORM OF A RANDOM VARIABLE



BLOCH TRANSFORM OF LINEAR DIFFERENTIAL OPERATORS

Transformation of $H(x, \frac{x}{\lambda}, \nabla_x)$:

Step 1:

Transformation on 'sliced space': Let derivatives work on the fast variables only.

$$H(x, \frac{x}{\lambda}, \nabla_x)\psi(x) = H_1(y, r, \frac{1}{\lambda}\nabla_y)\psi_1(y, r), \quad r = \lambda L z$$

$$H_1(y, r, \frac{1}{\lambda}\nabla_y) = H(r + \lambda y, y, \frac{1}{\lambda}\nabla_y)$$

Step 2:

$$H_2[\psi_2](y,\xi,t) = (\frac{\lambda}{2\pi})^3 \sum_z \int_B H_1(y,\lambda Lz,\frac{1}{\lambda}\nabla_y)\psi_2(y,\xi',t)\,\text{exp}(i\lambda(\xi-\xi')^T Lz)\ d$$

$$\Rightarrow$$

$$H_2(y,\frac{1}{\lambda}\nabla_y,\nabla_\xi) = H_1(y,\frac{1}{i}\nabla_\xi,\frac{1}{\lambda}\nabla_y) = H(-i\nabla_\xi+\lambda y, y, \frac{1}{\lambda}\nabla_y)$$

$H_2(y,\frac{1}{\lambda}\nabla_y,\nabla_\xi)$ is a Pseudo differential operator defined on periodic functions of ξ.

$$\partial_t\psi_2(y,\xi,t) = H_2(y,\frac{1}{\lambda}\nabla_y,\nabla_\xi)\psi_2, \quad \psi_2(y+Lz,\xi,t) = \psi_2(y,\xi,t)\,\text{exp}(-\lambda\xi^T L$$

Split the operator:

$$H_2(y,\frac{1}{\lambda}\nabla_y,\nabla_\xi) = H_2^0(y,\frac{1}{\lambda}\nabla_y) + R(\lambda y,\nabla_\xi)$$

Expand into eigenfunctions of H_2^0:

$$H_2^0(y, \frac{1}{\lambda}\nabla_y)u_m(y,\xi) = \varepsilon_m(\xi)u_m, \quad u_m(y+Lz,\xi) = u_m(y,\xi)\,\mathrm{exp}(-\lambda\xi^T Lz),$$

$$\psi_2(y,\xi,t) = \sum_m \psi_2^m(y,\xi,t) = \sum_m c_m(\xi,t)u_m(y,\xi)$$

$$\partial_t\psi_2^m(y,\xi,t) = \varepsilon_m(\xi)\psi_2^m + \mathbf{R}_m(\nabla_\xi)\Psi_2$$

$$\mathbf{R}_m(\nabla_\xi)\Psi_2 = u_m(y,\xi)\sum_n \int u_m(y',\xi)R(\lambda y',\nabla_\xi)\psi_2^n(y',\xi,t)\ dy'$$

Reverse the Fourier transform in z:

$$\psi_2(y,\xi,t) \to \psi_1(y,r,t), \quad \xi \approx \frac{1}{i}\nabla_r, \quad \nabla_\xi \approx ir, \quad r = Lz, \quad z \in \mathbb{Z}^3$$

$$\partial_t\psi_1^m(y,r,t) = \varepsilon_m(\frac{1}{i}\nabla_r)\psi_2^m + \hat{\mathbf{R}}_m(r)\Psi_1$$

THE SCHRÖDINGER EQUATION WITH A FAST VARYING LATTICE POTENTIAL

$$H(x, \frac{x}{\lambda}, \nabla_x) = -\frac{\hbar^2}{2m}\Delta_x + V(x) + \frac{1}{\lambda^2}V_L(\frac{x}{\lambda})$$

$$i\hbar\partial_t\psi_2(y,\xi,t) = -\frac{\hbar^2}{2m\lambda^2}\Delta_y\psi_2 + \frac{1}{\lambda^2}V_L(y)\psi_2 + V(-i\nabla_\xi + \lambda y)\psi_2$$

Boundary conditions:

$$\psi_2(y + Lz', \xi, t) = \psi_2(y, \xi, t)\,\mathrm{exp}(-i\lambda\xi^T Lz')$$

This is dominated by an operator which is only weakly dependent on λ and ξ (through the boundary conditions), and therefore can be diagonalized asymptotically!

THE EIGENVALUE PROBLEM

$$[-\frac{\hbar^2}{2m}\Delta_y + V_L(y)]u_m(y,\xi) = \varepsilon_m(\xi)u_m(y,\xi)$$

$$u_m(y+Lz',\xi) = u_m(y,\xi)\,\mathrm{exp}(-i\lambda\xi^T Lz')$$

- Self adjoint Sturm - Liouville problem on a bounded domain $\Rightarrow$ complete set of orthonormal eigenfunctions $\forall m, \xi$.

- $\varepsilon_m(\xi)$ are called the energy band functions.

THE SCHRÖDINGER EQUATION IN THE EIGENBASIS

Reverse the Bloch transform

$$\psi_2(y,\xi,t) = \sum_m \psi_2^m(y,\xi,t), \quad \psi_2^m(y,\xi,t) = c_m(\xi,t)u_m(y,\xi),$$

$$i\hbar\partial_t\psi_2^m(y,\xi,t) = \varepsilon_m(\xi)\psi_2^m(y,\xi,t) + u_m \sum_n \int_{B^*} u_m(y',\xi)V(-i\nabla_\xi + \lambda y)\psi_2^n(y',\xi,$$

All band coefficients c_m are (weakly) coupled in general!

System of effective Schrödinger equations in eigenspaces

$$i\hbar\partial_t\psi_1^m(y,r,t) = \varepsilon_m(\frac{1}{i}\nabla_r)\psi_1^m(y,r,t) + \widehat{\mathbf{R}}_m\Psi_1$$

Bloch - Wannier (30's):
Consider only lattice potential ($V = 0 \Rightarrow \mathbf{R} = 0$):

$$i\hbar\partial_t\psi^m(x,t) = \varepsilon_m(\frac{1}{i}\nabla_x)\psi^m$$

Poupaud , CR (1995):
Add slowly varying potential under the assumption $\varepsilon_m(\xi) \neq \varepsilon_n(\xi)$ for $m \neq n$. Let $\lambda \to 0$:

$$i\hbar\partial_t\psi(r) = \varepsilon_0(-i\nabla_r)\psi + V(r)\psi$$

Open problem:
Band crossings $\varepsilon_m(\xi) = \varepsilon_n(\xi)$ (Gerard, wave equation '00)

THE WIGNER PICTURE AND THE (SEMI-) CLASSICAL LIMIT

$$\mathcal{E}(r,\nabla_r) = -\frac{\hbar^2}{2m}\Delta_r + V(r) \to \mathcal{E}_m(r,\nabla_r) = \varepsilon_m(-i\nabla_r) + V(r)$$

$$f(x,\xi,t) = W[\rho]$$

$$\partial_t f + [\mathcal{E}, f]_W = 0$$

$$[\mathcal{E}, f]_w(x,\xi) = \mathcal{E}\circ f - f\circ\mathcal{E} = \frac{i}{\hbar}\sum_{\sigma=\pm1}\sigma[\varepsilon_m(\xi+\frac{\sigma}{i}\nabla_x)+V(x-\frac{\sigma}{i}\nabla_\xi)]f$$

Renaming $p = \hbar\xi$, rescaling ε_m and $\hbar \to 0$ gives the semi-classical Liouville equation in the m-th energy band

$$\partial_t f_m(x,p,t) + \nabla_p\varepsilon_m(p)\cdot\nabla_x f_m - \nabla_x V\cdot\nabla_p f_m = 0$$

EFFECTIVE MASS APPROXIMATIONs

Replace $\varepsilon_m(\xi)$ for small ξ by a quadratic

$$\varepsilon_m(\xi) = \frac{1}{2}\xi^T M^{-1}\xi$$

$$i\hbar\partial_t\psi(r) = -\frac{\hbar^2}{2}\nabla_x^T M^{-1}\nabla_x\psi + V(r)\psi$$

$$\partial_t f_m(x,p,t) + p^T M\nabla_x f_m - \nabla_x V \cdot \nabla_p f_m = 0$$

SUB - BAND APPROXIMATIONS

The Schrödinger equation with directional scaling: Small geometry aspect ratios:

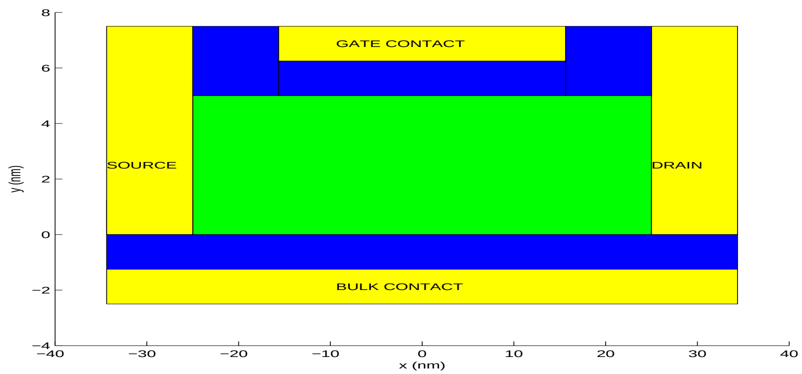
$X = (x, y) \in \Omega = \Omega_x \times \Omega_y$ with $|\Omega_y| << |\Omega_x|$;
x: 'classical' direction, y: 'quantum' direction.

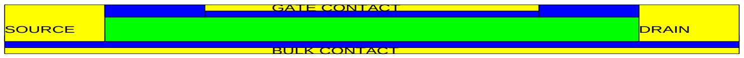
$$i h_x \partial_t \psi(x, y, t) = -\frac{h_x{}^2}{2} \Delta_x \psi - \frac{h_y{}^2}{2} \Delta_y \psi + V(x, y)\psi, \;\; x \in \Omega_x, \;\; y \in \Omega_y$$

$h_x, \; h_y$: Planck constant related to $x-$ and $y-$ length scales.

Close to classical transport in x: $h_x << 1$, quantum transport in y: $h_y = O(1)$.

Example: SOI (Silicon-Oxide-onInsulator) technology

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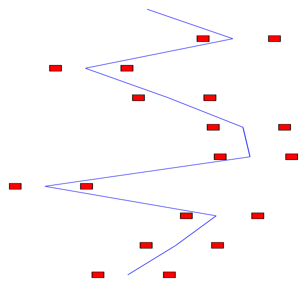
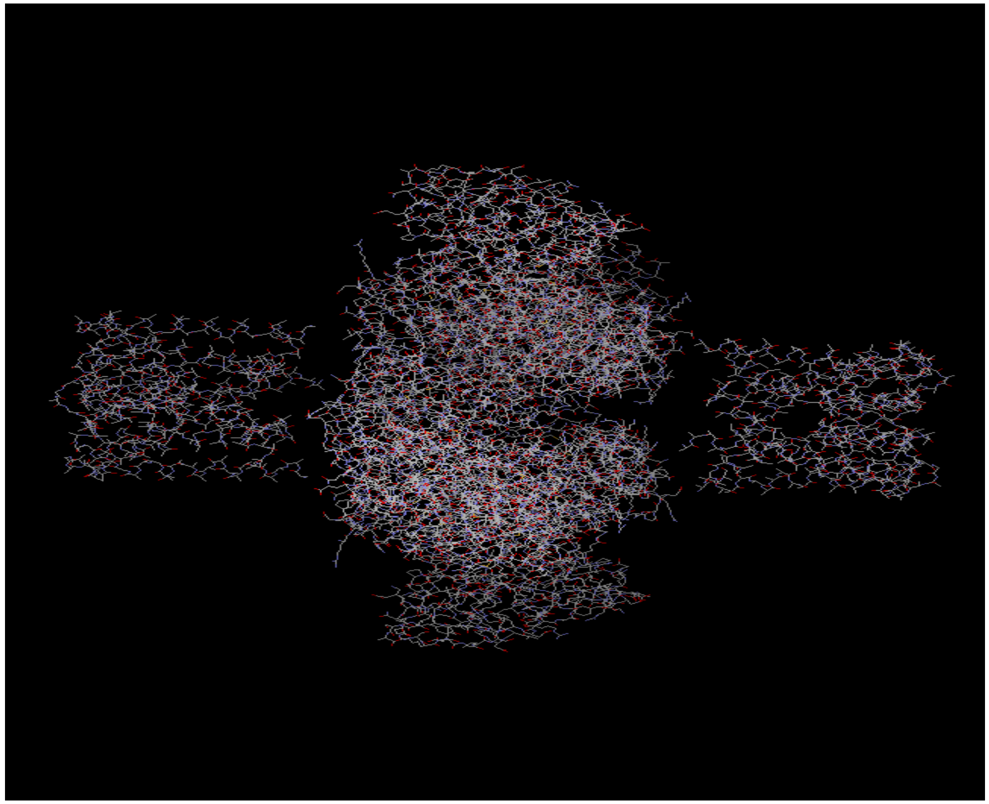
Example: Ion channels, Transport of ions through a protein, confined by charges on protein surface $\Rightarrow$ confinement potential V.





Sub - Band Approximations

To retain the quantum nature of the transport in $y-$ direction, while using classical approximations in x, we expand the wave function in $x-$ dependent eigenfunctions of the Schrödinger operator in $y-$ direction.

$$\boxed{\psi(x,y,t) = \sum_\alpha \phi_\alpha(x,t) w_\alpha(x,y)}$$

$w_\alpha(x,y),\ E_\alpha(x)$: eigenfunctions and eigenvalues in $y-$ direction.
$\phi_\alpha(x,t)$: expansion coefficients.

$$\boxed{-\frac{h_y^2}{2}\Delta_y w_\alpha(x,y) + V(x,y)w_\alpha = E_\alpha(x)w_\alpha,\ \ \alpha = 1,2,...}$$

- This gives a Schrödinger type equation for the expansion coefficients $\phi_\alpha(x,t)$.

$$ih_x\partial_t\phi_\alpha(x,t) = -\frac{h_x^2}{2}\Delta_x\phi_\alpha + E_\alpha(x)\phi_\alpha + \sum_\alpha C_{\alpha\beta}[\phi_\beta]$$

- Since $h_x << 1$, this is amenable to some form of classical limit asymptotics for $h_x \to 0$.

- Large body of work (Feynmann, Fischetti, BenAbdallah, Mehats, Schmeiser...)

- Advantages: 1) Reduces the dimensionality. 2) Allows for a classical coupling to the outside world for open systems in $x-$ direction. 3) Simulation on larger time scales.

- The coupling operators $C_{\alpha\beta}$ are usually neglected. In this case the structure is the same as in the S.E. with the potential V replaced by E_α.

RESULT

For a given potential and 'strong forces' (∇V), the transport picture can be asymptotically described in the semiclassical limit ($h_x \to 0$ and $h_y > 0$ fixed) by a sub - band Liouville equation

$$\partial_t f_\alpha + p \cdot \nabla_x f_\alpha - \nabla_x (V_\alpha + E_\alpha) \cdot \nabla_p f_\alpha = 0$$

- $E_\alpha(x)$ is the eigenvalue (the sub-band energy)

Adding a (phenomenological) collision operator, dissipating the quantum Von Neumann entropy and computing the large time limit via Chapman - Enskog one obtains a sub - band drift diffusion system

$$\boxed{\partial_t n_\alpha + \nabla_x \cdot J_\alpha = Q[n]_\alpha, \;\; J_\alpha = -\nabla_x n_\alpha - n_\alpha \nabla_x E_\alpha}$$

where

- $n_\alpha(x)$ is the particle density of a mixed state in sub-band α

$$n_\alpha(x,t) = \sum_m c_m |\phi_\alpha^{(m)}(x,t)|^2, \;\; \alpha = 1, 2, ..$$

$$\boxed{\partial_t n_\alpha + \nabla_x \cdot J_\alpha = Q[n]_\alpha, \;\; J_\alpha = -\nabla_x n_\alpha - n_\alpha \nabla_x E_\alpha}$$

- $Q[n]$ is the inter - band collision operator expressing the transfer of mass between the eigenspaces due to the strong forces in $y-$ direction.

$$\boxed{Q[n]_\alpha = \sum_\beta |A_{\alpha\beta}|^2 (n_\beta - n_\alpha)(1 + \frac{E_\beta - E_\alpha}{\ln(n_\beta) - \ln(n_\alpha)})}$$

Theorem:

- Q conserves locally the total mass $\sum_{\alpha=1}^{N} Q[n]_\alpha = 0$ for any finite number of expansion terms.
- The kernel is given by $n_\alpha = c(x)e^{-E_\alpha(x)}$, i.e. $Q[ce^{-E_\alpha}] = 0$.
- Q dissipates the sub - band entropy $\mathcal{E}[n] = \sum_\alpha n_\alpha(\ln(n_\alpha) + E_\alpha - 1)$ locally in x, i.e. $\sum_\alpha(\ln(n_\alpha) + E_\alpha)Q[n]_\alpha \leq 0$ holds.

Summary:

- Strong cross - directional forces introduce scattering between the sub-band eigenspaces.
- The resulting collision mechanism relaxes the system towards a global equilibrium $n_\alpha = const \cdot e^{-E_\alpha}$ independently of the boundary conditions.
  transport: $n_\alpha(x) = c_\alpha e^{-E_\alpha(x)}, \ \forall c_\alpha$;
  collisions: $c_\alpha = c, \ \forall\alpha$