

# 118028 - Quantum Transport in Solids

Assa Auerbach

March 27, 2019

## Abstract

## 1 Introduction

The simplest Hamiltonian is, denoting electrons with  $i$  and ions with  $I$ :

$$H = \sum_i \frac{\mathbf{P}_i^2}{2m_e} + \sum_I \frac{\mathbf{P}_I^2}{2m_I} + \sum_{i,I} \frac{e^2 Z}{|\mathbf{r}_i - \mathbf{R}_I|} + \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{I,J} \frac{e^2 Z^2}{|\mathbf{R}_I - \mathbf{R}_J|} \quad (1)$$

The last part of Hamiltonian is many-body interaction, which makes it complex, due to big amount of degrees of freedom.

We neglect here relativistic (spin-orbit) and radioactive corrections. We'll add electromagnetic field interaction later.

We note that  $\frac{m_e}{m_I} \lesssim 10^3$ , and perform Born-Oppenheimer approximation: neglecting ion movement (frozen ions). Yet electron-electron interactions is many-body problem:

$$H^{el} = \sum_i \frac{\mathbf{P}_i^2}{2m_e} + \sum_i V(\mathbf{r}_i) + \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (2)$$

The problem is still pretty complex one. If we have 200 one-particle states and we put 100 particles in the system. In case of fermions there are  $\binom{200}{100}$  possible states and for bosons  $\binom{200+100-1}{100}$ .

There are phenomena that happen only in large scale: spontaneously broken symmetry, critical phenomena, scale invariance.

### organizing principle

1. Symmetry:  $\mathbb{Z}_2, O(2), O(3)$
2. Statistics of particles (Fermi or Bose statistics)
3. Range of interactions.
4. Gauge fields.
5. Thermal and quantum fluctuations.
6. Topological invariants.

### Particles in the box

$$H = \sum_i \frac{\mathbf{P}_i^2}{2m_e} \quad (3)$$

We use periodic boundary conditions (PBC) and then single-particle eigenfunctions are plane waves:

$$\epsilon_{\mathbf{k}} = \frac{\hbar \mathbf{k}^2}{2m} \quad (4)$$

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k} \cdot \mathbf{x}} \quad (5)$$

Wavenumbers are thus quantized as  $k_i = \frac{2\pi}{L_i} n_i$

**Density of states** We define density of states:

$$\mathcal{N}(\epsilon) = \frac{1}{V} \sum_{\mathbf{k}} \tilde{\delta}(\epsilon - \epsilon_{\mathbf{k}}) \quad (6)$$

$\tilde{\delta}$  approximates delta function with some function wider than distance between two allowed energies. Switching to integral:

$$\mathcal{N}^{3D}(\epsilon) = 2 \cdot \int \frac{d^3k}{(2\pi)^3} \delta(\epsilon - \epsilon_{\mathbf{k}}) = \frac{m}{\hbar^3 \pi^2} \sqrt{2m\epsilon} \quad (7)$$

$$\mathcal{N}^{2D}(\epsilon) = \frac{m}{n} \quad (8)$$

$$\mathcal{N}^{1D}(\epsilon) = \frac{1}{\sqrt{\epsilon}} \quad (9)$$

**Theorem 1.1 (Bloch theorem).** Eigenfunction of periodic Hamiltonian are plane waves times periodic function.

*Proof.* Take a look on a single particle Hamiltonian:

$$H = \frac{\mathbf{p}^2}{2m} + V^{eff}(\mathbf{r}) \quad (10)$$

If  $V^{eff}(\mathbf{r}) = V^{eff}(\mathbf{R} + \mathbf{R}_n)$  for  $\mathbf{R}_n$  lattice vector, then Hamiltonian is symmetric under translations:

$$T^\dagger(\mathbf{R}_n) H T(\mathbf{R}_n) = H \quad (11)$$

$T$  defines Abelian group, and thus  $T$  is unitary operator. Since  $T$  commutes with  $H$ , we can diagonalize  $H$  and  $T$  simultaneously:

$$T(\mathbf{R}_n) |\psi_\alpha\rangle = e^{i\phi(\mathbf{R}_n, \alpha)} |\psi_\alpha\rangle \quad (12)$$

$$H |\psi_\alpha\rangle = \epsilon_\alpha |\psi_\alpha\rangle \quad (13)$$

By looking on two consequent translations, we find out  $\phi$  is linear:

$$T(\mathbf{R}_1) T(\mathbf{R}_2) |\psi_\alpha\rangle = e^{i\phi_\alpha(\mathbf{R}_1)} e^{i\phi_\alpha(\mathbf{R}_2)} |\psi_\alpha\rangle \quad (14)$$

$$\phi_\alpha(\mathbf{R}_1 + \mathbf{R}_2) = \phi_\alpha(\mathbf{R}_1) + \phi_\alpha(\mathbf{R}_2) \quad (15)$$

Thus

$$\phi_\alpha(\mathbf{R}) = \mathbf{K}_\alpha \cdot \mathbf{R} \quad (16)$$

From PBC we get

$$K_i \cdot L_i = 2\pi n_i \quad (17)$$

Since eigenfunctions of Hamiltonian are eigenfunctions of  $T$ , we conclude that

$$\psi_k(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \mathcal{U}(\mathbf{r}) \quad (18)$$

for  $\mathcal{U}(\mathbf{r}) = \mathcal{U}(\mathbf{r} + \mathbf{R})$ . □

$\mathbf{k}$  are limited in their value by first Brillouin zone. We can rewrite Hamiltonian:

$$H = \sum_{\mathbf{k}, \alpha} \epsilon_{\mathbf{k}, \alpha} |\psi_k^\alpha\rangle \langle \psi_k^\alpha| \quad (19)$$

If  $V$  has additional symmetries, for example, reflection symmetry, energies have same symmetries:

$$R^{-1} V(\mathbf{R}) R = V(\mathbf{r}) \Rightarrow \epsilon_{\mathbf{k}} = \epsilon_{R(\mathbf{k})} \quad (20)$$

While  $\mathcal{U}$  determines short-term behavior of particles,  $e^{i\mathbf{k} \cdot \mathbf{r}}$  governs long-term behavior.

## 2 Tight binding model

We are looking on bands of energies in a single Brillouin zone, especially interested in conductance band (one intersected by Fermi energy).

In tight-binding we rewrite Hamiltonian as nearest neighbor model:

$$H = -\frac{t}{2} \sum_{\mathbf{R}} |\mathbf{R}\rangle \langle \mathbf{R} + \eta| + h.c. \quad (21)$$

, where  $|\mathbf{R}\rangle$  are local states such that  $\langle \mathbf{R} | \mathbf{R}' \rangle = \delta_{\mathbf{R}, \mathbf{R}'}$ .

**Lattice Fourier transform** In 1D,  $\mathbf{R}_j = \mathbf{a} \cdot j$ . Define

$$\mathbf{k} = \underbrace{\frac{1}{\sqrt{N}} \sum_j e^{ika_j} |\mathbf{R}_j\rangle}_{U_{\mathbf{k}}} \quad (22)$$

$U_{\mathbf{k}}$  is unitary matrix:

$$\langle j | U_{\mathbf{k}}^\dagger U_{\mathbf{k}} | j' \rangle = \frac{1}{N} \sum_{j, j'} e^{-ika_j} e^{ika_{j'}} = \frac{1}{N} \sum_{j, j'} e^{-ika(j-j')} = \delta_{jj'} \quad (23)$$

Now

$$\epsilon_{\mathbf{k}} = \langle \mathbf{k} | H | \mathbf{k} \rangle = -\frac{t}{N} \sum_{\mathbf{R}'} \sum_{\mathbf{R}, \eta} e^{i\mathbf{k} \cdot \mathbf{R}} \langle \mathbf{R}' | |\mathbf{R}\rangle \langle \mathbf{R} + \eta| e^{-i\mathbf{k} \cdot \mathbf{R}} = -\frac{1}{N} \sum_{\mathbf{R}, \eta} e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R} + \eta)} = -t \underbrace{\sum_{\eta} e^{i\mathbf{k} \cdot \eta}}_{\gamma_{\mathbf{k}}^{(\eta)}} \quad (24)$$

### Examples

#### 1D

$$\epsilon_{\mathbf{k}} = -2t \cos(ka) \quad (25)$$

#### 2D

$$\epsilon_{\mathbf{k}} = -2t [\cos(k_x a) + \cos(k_y a)] \quad (26)$$

### 2.1 Wannier States

**Reminder** For lattice vectors  $\mathbf{r}_i$ , reciprocal lattice vectors are  $\mathbf{k}_i = \frac{2\pi}{V} \cdot (\mathbf{r}_j \times \mathbf{r}_k)$ .

**Definition 2.1 (Wannier states).** Wannier states are lattice Fourier transform of Bloch wave.

$$W_n^\alpha(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_n} \psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{R}_n} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{R}_n)} \mathcal{U}_{\mathbf{k}}(\mathbf{r} - \mathbf{R}_n) = W^\alpha(\mathbf{r} - \mathbf{R}_n) \quad (27)$$

**Proposition 2.1.**  $W_n^\alpha$  are orthogonal.

*Proof.*

$$\int d\mathbf{r} W_n^\alpha(\mathbf{r}) W_{n'}^\beta(\mathbf{r}) = \frac{1}{N^2} \sum_{\mathbf{k}, \mathbf{k}'} e^{i(\mathbf{k} \cdot \mathbf{R}_n - \mathbf{k}' \cdot \mathbf{R}_{n'})} \int d\mathbf{r} \psi_{\mathbf{k}}^{\alpha*}(\mathbf{r}) \psi_{\mathbf{k}'}^\beta(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_{n'})} = \delta_{nn'} \delta_{\alpha\beta} \quad (28)$$

□

How local are  $W^\alpha$ ?

$$W(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{r}} \mathcal{U}_{\mathbf{k}}(\mathbf{r}) \quad (29)$$

Looking for a maximum of  $\mathcal{U}_{\mathbf{k}}(\mathbf{r})$ , we apply logarithm  $f(\mathbf{r}) = \log(\mathcal{U}_{\mathbf{k}}(\mathbf{r}))$  and Taylor expand it:

$$W(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \mathcal{U}_{\mathbf{k}_0}(\mathbf{r}_0) \exp\left(-\frac{1}{2} \frac{\partial}{\partial \mathbf{k}} f_{\mathbf{k}_0}(\mathbf{r}_0)(\mathbf{k} - \mathbf{k}_0)^2 - \frac{1}{2} \frac{\partial}{\partial \mathbf{r}} f_{\mathbf{k}_0}(\mathbf{r}_0)(\mathbf{r} - \mathbf{r}_0)^2\right) \quad (30)$$

Denote  $\frac{\partial}{\partial \mathbf{k}} f_{\mathbf{k}_0} = a^2$ , taking  $R_n$  large enough and thus neglecting  $\mathbf{r}$  derivative since  $(\mathbf{r} - \mathbf{r}_0)^2$  is small we get:

$$W(\mathbf{R}_n - \mathbf{r}_0) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{R}_n} e^{-\frac{1}{2} a^2 (\mathbf{r}_0)(\mathbf{k} - \mathbf{k}_0)^2} \sim e^{-\frac{\mathbf{R}_n^2}{2a^2}} \quad (31)$$

Thus

$$W(\mathbf{r} - \mathbf{R}_n) \sim e^{-\frac{(\mathbf{r} - \mathbf{R}_n)^2}{a^2}} \quad (32)$$

If  $\mathcal{U}_{\mathbf{k}}(\mathbf{r}_0)$  varies slowly with  $\mathbf{k}$ , Wannier states are localized. In an extreme case of  $\mathcal{U}_{\mathbf{k}}^\alpha = \phi^\alpha(\mathbf{r})$ :

$$W_\alpha(\mathbf{r} - \mathbf{R}_n) = \int d\mathbf{k} e^{i\mathbf{k}(\mathbf{r} - \mathbf{R}_n)} \phi_\alpha(\mathbf{r} - \mathbf{R}_n) = \delta(\mathbf{r} - \mathbf{R}_n) \phi_\alpha(\mathbf{r} - \mathbf{R}_n) \quad (33)$$

If  $\mathcal{U}_{\mathbf{k}}$  is singular function of  $\mathbf{k}$  we get

$$W(\mathbf{r} - \mathbf{R}_n) \sim \frac{1}{(\mathbf{r} - \mathbf{R}_n)^\gamma} \quad (34)$$

## 2.2 Tight-binding

Tight-binding is good when there is a single band and Wannier function is slowly varying (at a momentum scale of Bruilien zone). We can write the Hamiltonian as

$$H = \frac{P^2}{2m_e} + V_{eff}(\mathbf{r}) = \frac{P^2}{2m_e} + \sum_n V_{atom}(\mathbf{r} - \mathbf{R}_n) + \Delta V(\mathbf{r} - \mathbf{R}_n) \quad (35)$$

where  $\Delta V$  is difference between atomic and lattice potentials. If wavefunctions are localized around nuclei the effect of  $\Delta V$  is small.

We'll use anzatz of sum of local states:

$$\tilde{\psi}_\alpha(\mathbf{r}) = \sum_{\mathbf{R}_n} e^{-i\mathbf{k}\cdot\mathbf{R}_n} \phi^\alpha(\mathbf{r} - \mathbf{R}_n) \quad (36)$$

Those wavefunctions are not eigenstates, but approximate them. We get

$$\langle \tilde{\psi} | \tilde{\psi}' \rangle = \int d\mathbf{r} \sum_{\mathbf{R}_n, \mathbf{R}_{n'}} e^{i\mathbf{k}\cdot\mathbf{R}_n} e^{-i\mathbf{k}'\cdot\mathbf{R}_{n'}} \phi^*(\mathbf{r} - \mathbf{R}_n) \phi(\mathbf{r} - \mathbf{R}_{n'}) \quad (37)$$

Defining  $\alpha(\mathbf{R}_n - \mathbf{R}_{n'}) = \int d\mathbf{r} \phi^{\alpha*}(\mathbf{r} - \mathbf{R}_n) \phi^\alpha(\mathbf{r} - \mathbf{R}_{n'})$  we get

$$\langle \tilde{\psi} | \tilde{\psi}' \rangle = \sum_{\mathbf{R}_n, \mathbf{R}_{n'}} e^{i\mathbf{k}\cdot\mathbf{R}_n} e^{-i\mathbf{k}'\cdot\mathbf{R}_{n'}} \alpha(\mathbf{R}_n - \mathbf{R}_{n'}) = \sum_{\mathbf{R}_n} e^{i(\mathbf{k} - \mathbf{k}')\cdot\mathbf{R}_n} \sum_{\mathbf{R}_{n'}} e^{i(\mathbf{k} - \mathbf{k}')\cdot\mathbf{R}_{n'}} \alpha(\mathbf{R}_n - \mathbf{R}_{n'}) \quad (38)$$

$$\bar{\alpha}(\mathbf{k}) = \sum_{\mathbf{R}_{n'}} e^{i(\mathbf{k} - \mathbf{k}')\cdot\mathbf{R}_{n'}} \alpha(\mathbf{R}_n - \mathbf{R}_{n'}) = 1 + \sum_{\mathbf{R}_{n'} \neq 0} e^{i\mathbf{k}\cdot\mathbf{R}_{n'}} \alpha(\mathbf{R}_{n'}) = 1 + \tilde{\alpha}(\mathbf{k}) \quad (39)$$

And thus

$$\langle \tilde{\psi} | \tilde{\psi}' \rangle = \delta_{\mathbf{k}\mathbf{k}'} \bar{\alpha}(\mathbf{k}) \quad (40)$$

Thus we can normalize and acquire orthonormal states:

$$|\tilde{\psi}_{norm}\rangle = \frac{1}{\sqrt{1 + \tilde{\alpha}(\mathbf{k})}} |\tilde{\psi}\rangle \quad (41)$$

$$\tilde{\epsilon}_{\mathbf{k}} = \langle \tilde{\psi}_{\mathbf{k}} | H | \tilde{\psi}_{\mathbf{k}} \rangle = \frac{1}{1 + \tilde{\alpha}(\mathbf{k})} \sum_{n,n'} \int d\mathbf{r} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_{n'})} \phi_{atom}^*(\mathbf{r} - \mathbf{R}_n) \left[ \underbrace{-\frac{\nabla^2}{2m} + V_{atom}(\mathbf{r})}_{\epsilon_{atom}} + \Delta V(\mathbf{r}) \right] \phi_{atom}(\mathbf{r} - \mathbf{R}_n) = \quad (42)$$

$$= \frac{1}{1 + \tilde{\alpha}(\mathbf{k})} \epsilon_{atom} \underbrace{\sum_{n,n'} \int d\mathbf{r} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_{n'})} \phi_{atom}^*(\mathbf{r} - \mathbf{R}_n) \phi_{atom}(\mathbf{r} - \mathbf{R}_n)}_{1 + \tilde{\alpha}(\mathbf{k})} + \quad (43)$$

$$+ \frac{1}{1 + \tilde{\alpha}(\mathbf{k})} \sum_{n,n'} \int d\mathbf{r} e^{i\mathbf{k} \cdot (\mathbf{R}_n - \mathbf{R}_{n'})} \phi_{atom}^*(\mathbf{r} - \mathbf{R}_n) \Delta V(\mathbf{r}) \phi_{atom}(\mathbf{r} - \mathbf{R}_n) \quad (44)$$

We denote

$$t(\mathbf{k}) = - \sum_n \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{R}_n} \phi_{atom}^*(\mathbf{r} - \mathbf{R}_n) \Delta V(\mathbf{r}) \phi_{atom}(\mathbf{r} - \mathbf{R}_n) \quad (45)$$

and thus

$$\tilde{\epsilon}_{\mathbf{k}} = \epsilon_{atom} - \frac{t(\mathbf{k})}{1 + \tilde{\alpha}(\mathbf{k})} \quad (46)$$

In a limit of small characteristic atomic length  $\frac{l_{atom}}{a} \ll 1$ , we get

$$\tilde{\alpha}(\mathbf{k}) \sim \exp\left(-\left(\frac{na}{l_{atom}}\right)^2\right) \quad (47)$$

i.e.,

$$\tilde{\epsilon}_{\mathbf{k}} \sim \epsilon_{atom} - t(\mathbf{k}) \quad (48)$$

For the same reason, due to exponential decay, we can neglect long-distance hopping.

We now take Wannier states of those  $\tilde{\psi}_{norm}$ :

$$W(\mathbf{r} - \mathbf{R}_n) \simeq \phi_{atom}(\mathbf{r} - \mathbf{R}_n) = \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}_n} \tilde{\psi}_{norm}(\mathbf{r}) \quad (49)$$

We denote  $|n\rangle = W_n(\mathbf{r})$ . Those states diagonalize Hamiltonian:

$$H = \sum_n \epsilon_{atom} |n\rangle\langle n| - \sum_{n,n'} t_{nn'} |n\rangle\langle n'| + h.c. \quad (50)$$

The approximation is broken if, for example two bands are touching each other. Then we can describe two bands together as a single tight-bound band.

### 3 Semi-classical dynamics

First we require  $k_B T \sim \hbar\omega \ll \Delta E$ , where  $\Delta E$  is energy difference between two bands.

If we also require long wavelength  $\lambda \gg a$ , we get a wavepacket of width  $\Delta k$  and center in  $\mathbf{k}_0$ :

$$W(\mathbf{r}) = \int d\mathbf{k} e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0)} e^{-\frac{(\mathbf{k} - \mathbf{k}_0)^2}{(\Delta k)^2}} \sim e^{(\Delta k)^2 (\mathbf{r} - \mathbf{r}_0)^2} \quad (51)$$

Thus, using our solution of the Shrödinger equation and expanding to the first order (denoting  $\mathbf{k} - \mathbf{k}_0 = \delta\mathbf{k}$ :

$$W(\mathbf{r}, t) = \int d\mathbf{k} \exp\left(i\epsilon_{\mathbf{k}} t + i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0) - \frac{(\mathbf{k} - \mathbf{k}_0)^2}{(\Delta k)^2}\right) = \quad (52)$$

$$= e^{i\mathbf{k}_0 \cdot \mathbf{r}} \int d\mathbf{k} \exp\left(\left(\epsilon_{\mathbf{k}_0} + \frac{\partial \epsilon}{\partial k} \delta\mathbf{k}\right) t + i\delta\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}_0) - \frac{(\delta\mathbf{k})^2}{(\Delta k)^2}\right) = \quad (53)$$

$$= e^{-(\Delta k)^2 (t(\mathbf{r} - (\mathbf{r}_0 + \frac{\partial \epsilon}{\partial k}))^2)} e^{i\mathbf{k}_0 \cdot \mathbf{r}} \quad (54)$$

Group velocity is thus  $\nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}$

**Theorem 3.1** (Hellmann-Feynman theorem). Let  $\epsilon_\alpha = \langle \psi_n(\alpha) | h_\alpha | \psi_n(\alpha) \rangle$  for some hermitian  $h_\alpha$ .

$$\frac{d}{d\alpha} \epsilon_\alpha = \left\langle \frac{d}{d\alpha} \psi_n(\alpha) \left| h_\alpha \right| \psi_n(\alpha) \right\rangle + \langle \psi_n(\alpha) | \frac{d}{d\alpha} h_\alpha | \psi_n(\alpha) \rangle + \left\langle \psi_n(\alpha) \left| h_\alpha \right| \frac{d}{d\alpha} \psi_n(\alpha) \right\rangle = \quad (55)$$

$$= \langle \psi_n(\alpha) | \frac{d}{d\alpha} h_\alpha | \psi_n(\alpha) \rangle + \epsilon_\alpha \left[ \left\langle \psi_n(\alpha) \left| \frac{d}{d\alpha} \psi_n(\alpha) \right\rangle + \left\langle \frac{d}{d\alpha} \psi_n(\alpha) \left| \psi_n(\alpha) \right\rangle \right] = \quad (56)$$

$$= \langle \psi_n(\alpha) | \frac{d}{d\alpha} h_\alpha | \psi_n(\alpha) \rangle + 2\epsilon_\alpha \underbrace{\frac{d}{d\alpha} \langle \psi_n(\alpha) | \psi_n(\alpha) \rangle}_0 = \langle \psi_n(\alpha) | \frac{d}{d\alpha} h_\alpha | \psi_n(\alpha) \rangle \quad (57)$$

**Proposition 3.2** (Rules of semiclassical approximation). 1. Wave will move keeping same band index.

2. Position obeys

$$\langle \mathbf{r} \rangle \sim \frac{\partial \epsilon}{\partial \mathbf{k}} \quad (58)$$

3.

$$\hbar \mathbf{k} = e - \mathbf{E} - \frac{e}{c} \dot{\mathbf{r}} \times \mathbf{B} \quad (59)$$

*Proof.* Lets write Shrödinger equation

$$\left( \underbrace{\frac{\hbar^2 \mathbf{k}^2}{2m} - \frac{2i\hbar \mathbf{k} \cdot \nabla}{2m} + \frac{\hbar \nabla^2}{2m}}_{H_{\mathbf{k}}} + V(\mathbf{r}) \right) \mathcal{U}_{\alpha, \mathbf{k}}(\mathbf{r}) = \epsilon_{\alpha, \mathbf{k}} \mathcal{U}_{\alpha, \mathbf{k}}(\mathbf{r}) \quad (60)$$

Since  $\psi_{\alpha, \mathbf{k}}(\mathbf{r})$  is a Bloch wave

$$\left( -\frac{\hbar \nabla^2}{2m} + V(\mathbf{r}) \right) \psi_{\alpha, \mathbf{k}}(\mathbf{r}) = \epsilon_{\alpha, \mathbf{k}} \psi_{\alpha, \mathbf{k}}(\mathbf{r}) \quad (61)$$

$$\epsilon_{\alpha, \mathbf{k}} = \epsilon_{\alpha, \mathbf{k}_0} \nabla_{\mathbf{k}} \epsilon_{\alpha, \mathbf{k}_0} \delta \mathbf{k} + \frac{1}{2} \sum_{i,j} \delta \mathbf{k}_i \cdot \delta \mathbf{k}_j \frac{\partial^2 \epsilon}{\partial \mathbf{k}_i \partial \mathbf{k}_j} \quad (62)$$

$$\epsilon_{\mathbf{k}} = \langle \psi_{\mathbf{k}} | H | \psi_{\mathbf{k}} \rangle = \langle \mathcal{U}_{\mathbf{k}} | H_{\mathbf{k}} | \mathcal{U}_{\mathbf{k}} \rangle \quad (63)$$

$$\frac{d}{d\mathbf{k}} \epsilon_{\alpha, \mathbf{k}} = \frac{d}{d\mathbf{k}} \langle \mathcal{U}_{\mathbf{k}} | H_{\mathbf{k}} | \mathcal{U}_{\mathbf{k}} \rangle = \langle \mathcal{U}_{\mathbf{k}} | \frac{d}{d\mathbf{k}} H_{\mathbf{k}} | \mathcal{U}_{\mathbf{k}} \rangle = \langle \psi_{\mathbf{k}} | \underbrace{e^{i\mathbf{k} \cdot \mathbf{r}} (-i\hbar \nabla - \mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{r}}}_m | \psi_{\mathbf{k}} \rangle = \langle \psi_{\mathbf{k}}^\alpha | \frac{\mathbf{P}}{m} | \psi_{\mathbf{k}}^\alpha \rangle = \mathbf{v}_{\mathbf{k}} \quad (64)$$

Thus

$$\frac{\partial H_{\mathbf{k}}}{\partial \mathbf{k}} = \frac{-i\hbar \nabla - \mathbf{k}}{m} \quad (65)$$

We also define effective mass tensor:

$$\frac{1}{\hbar^2} \frac{\partial^2 \epsilon}{\partial \mathbf{k}_i \partial \mathbf{k}_j} = (M^*)_{ij} = \frac{1}{m} \delta_{ij} - \sum_{\alpha'} \frac{\langle \psi_{\alpha, \mathbf{k}} | P_i | \psi_{\alpha', \mathbf{k}} \rangle \langle \psi_{\alpha', \mathbf{k}} | P_j | \psi_{\alpha, \mathbf{k}} \rangle}{\epsilon_{\alpha, \mathbf{k}} - \epsilon_{\alpha', \mathbf{k}}} \quad (66)$$

Now assume we have a particle in a electric field. We ask what is the power dissipated with electric field:

$$\hbar \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \dot{\mathbf{k}} = \frac{\partial \epsilon_{\mathbf{k}}}{\partial t} = P_{diss} = -e \mathbf{E} \cdot \mathbf{v}_{\mathbf{k}_0} = -e \mathbf{E} \cdot \frac{\partial \epsilon_{\mathbf{k}}}{\partial \mathbf{k}} \quad (67)$$

Thus

$$\dot{\mathbf{k}} = -\frac{e}{\hbar} \mathbf{E} \quad (68)$$

□

**Bloch oscillations** Assume 1D band structure of the form  $\epsilon_{\mathbf{k}} = -2w \cos(k)$ . Since  $\dot{\mathbf{k}} = -\frac{e}{\hbar} \mathbf{E}$ :

$$\mathbf{k} = -\frac{e}{\hbar} \mathbf{E}t \quad (69)$$

What will be the velocity?

$$\mathbf{v}(t) = 2W \sin\left(\frac{e}{\hbar} Et\right) \quad (70)$$

Define characteristic  $\tau = \frac{2\pi\hbar}{eE}$ :

$$\mathbf{v}(t) = 2W \sin\left(\frac{2\pi t}{\tau}\right) \quad (71)$$

This effect was actually observed in cold atoms.

**Alternative derivation** Given PBC in 1D,

$$\psi(x+L) = \psi(x) \quad (72)$$

and Hamiltonian

$$H = \frac{p^2}{2m} + V(x) \quad (73)$$

We can perceive it as a ring. Adding an Aharonov-Bohm magnetic flux  $\Phi$  inside the ring, we create gauge field (vector potential)

$$\mathbf{A} = \frac{\Phi}{L} \hat{\mathbf{x}} \quad (74)$$

The electromotive force, from Lenz's law

$$-\frac{1}{c} \dot{\Phi} = \mathcal{E} = E \cdot L \quad (75)$$

Thus

$$\dot{\mathbf{A}} = -cE \Rightarrow \mathbf{A} = -cEt \quad (76)$$

And we rewrite the Hamiltonian

$$\mathbf{p} \rightarrow \mathbf{p} - \frac{e}{c} \mathbf{A} \quad (77)$$

$$H = \frac{(\mathbf{p} - \frac{e}{c} \mathbf{A})^2}{2m} + V(x) = \frac{(\mathbf{p} - eEt)^2}{2m} + V(x) \quad (78)$$

Now we solve the Shrödinger equation:

$$\tilde{\psi}_k(t) = e^{-\frac{ieAx}{\hbar c}} \psi_k(x) \quad (79)$$

The boundary condition is not periodic anymore, and substituting flux quantum ( $\Phi_0 = \frac{\hbar c}{2\pi e}$ ) we get:

$$\tilde{\psi}_k(L) = e^{-\frac{ieAL}{\hbar c}} \tilde{\psi}_k(0) = e^{-\frac{i\Phi}{\hbar c}} \tilde{\psi}_k(0) = e^{-i2\pi\left(\frac{\Phi}{\Phi_0}\right)} \tilde{\psi}_k(0) \quad (80)$$

From Theorem 1.1

$$\tilde{\psi}_k(x) = e^{ikx} \tilde{\mathcal{U}}_k(x) \quad (81)$$

$$e^{ikL} \tilde{\mathcal{U}}_k(0) = \tilde{\psi}_k(L) = e^{-\frac{ieAL}{\hbar c}} \tilde{\psi}_k(0) = e^{ik \cdot 0} \tilde{\mathcal{U}}_k(0) e^{-\frac{ieAL}{\hbar c}} \quad (82)$$

$$e^{ikL} = e^{-\frac{ieAL}{\hbar c}} \quad (83)$$

$$e^{i(kL + \frac{eAL}{c\hbar})} = 1 \quad (84)$$

, i.e., there is a shift in  $k$  values

$$k = \frac{2\pi n}{L} - \underbrace{\frac{eA}{c\hbar}}_{-\delta k} \quad (85)$$

We can verify that

$$H(A)\psi_k(x) = H(A)e^{\frac{ieAx}{c\hbar}}\tilde{\psi}_k(t) = e^{\frac{ieAx}{c\hbar}}H_{A=0}\tilde{\psi} = \epsilon_k e^{\frac{ieAx}{c\hbar}}\tilde{\psi}_k = \epsilon_k \psi_k \quad (86)$$

$$H\tilde{\psi}_k = \left(\frac{p^2}{2m} + V(x)\right)\tilde{\psi}_k \quad (87)$$

If we put, for example, half-quantum flux, we'll get  $\delta k = \frac{1}{2}\frac{2\pi}{L}$  and thus ground state is degenerate. If there is electric field,  $A = -cEt$ ,

$$\hbar\delta\dot{\mathbf{k}} = -e\mathbf{E} \quad (88)$$

If  $\mathbf{E}$  is small enough, such that particles can't change the band, we acquire Bloch oscillation.

**Proposition 3.3** (Semiclassical dynamics in presence of magnetic field).

$$\hbar\dot{\mathbf{k}} = e\mathbf{E} + \frac{e}{c}(\mathbf{v}_{\mathbf{k}} \times \mathbf{B}) \quad (89)$$

### 3.1 Landau-Zener tunneling

$$i\hbar\psi_k^{\alpha'} = \sum_{\alpha} H_{\mathbf{k}}^{\alpha\alpha'}\psi_{\alpha} \quad (90)$$

We look at Hamiltonian which depends on time, and only on two bands near the crossing. We rewrite Hamiltonian as a set of time independent Hamiltonians at  $\bar{t}$ :

$$H_t^{ad}\psi_{\alpha}^{\bar{t}}(x) = \epsilon_{\alpha}(\bar{t})\psi_{\alpha'}^{\bar{t}}(x) \quad (91)$$

**Theorem 3.4** (Adiabatic theorem). A physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenvalue and the rest of the Hamiltonian's spectrum.

#### Model

$$H = \alpha t\sigma_z + \Delta\sigma_x \quad (92)$$

The energies

$$\epsilon^{ad}(\bar{t}) = \pm\sqrt{(\alpha\bar{t})^2 + \Delta^2} \quad (93)$$

Thus the gap is  $2\Delta$  and there is probability to tunnel between bands:

$$P_{\mp}(t \rightarrow \infty) \sim e^{-\frac{\pi}{2}\frac{\Delta^2}{\alpha}} \quad (94)$$

which can be found by solving

$$\begin{pmatrix} \dot{\psi}_{\uparrow} \\ \dot{\psi}_{\downarrow} \end{pmatrix} = H(t) \begin{pmatrix} \psi_{\uparrow} \\ \psi_{\downarrow} \end{pmatrix} \quad (95)$$