118028 – Quantum Transport in Solids

Assa Auerbach

April 3, 2019

Abstract

1 Introduction

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

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

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:

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

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 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

$$H = \sum_i \frac{\mathbf{P}_i^2}{2m_e} \tag{3}$$

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

$$\epsilon_{\mathbf{k}} = \frac{\hbar \mathbf{k}^2}{2m} \tag{4}$$

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

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

Density of states We define density of states:

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

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

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

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

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

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

Proof. Take a look on a single particle Hamiltonian:

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

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

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

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

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

$$H |\psi_\alpha\rangle = \epsilon_\alpha |\psi_\alpha\rangle \tag{13}$$

By looking on two consequent translations, we find out ϕ is linear:

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

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

Thus

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

From PBC we get

$$K_i \cdot L_i = 2\pi n_i \tag{17}$$

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

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

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:

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

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

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

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:

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

, 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

$$\mathbf{k} = \underbrace{\frac{1}{\sqrt{N}}\sum_j e^{ikaj}}_{U_{\mathbf{k}}} |\mathbf{R}_j\rangle \tag{22}$$

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

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

Now

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

Examples

1D

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

2D

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

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.

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

Proposition 2.1. W_n^{α} are orthogonal.

Proof.

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

□

How local are W^{α}?

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

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:

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

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:

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

Thus

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

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

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

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

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

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

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

where ΔV is difference between atomic and lattice potentials. If wavefunctions are localized around nuclei the effect of ΔV is small.
We'll use anzatz of sum of local states:

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

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

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

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

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

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

And thus

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

Thus we can normalize and acquire orthonormal states:

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

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

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

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

We denote

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

and thus

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

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

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

i.e.,

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

For the same reason, due to exponential decay, we can neglect long-distance hopping.
We now take Wannier states of those $\tilde{\psi}_{norm}$:

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

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

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

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

3 Semi-classical dynamics

First we require $k_B T \sim \hbar\omega \ll \Delta E$, where ΔE is energy difference between two bands.
If we also require long wavelength $\lambda \gg a$, we get a wavepacket of width Δk and center in $\mathbf{k}_0$:

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

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

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

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

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

Group velocity is thus $\boldsymbol{\nabla}_{\mathbf{k}}\epsilon_{\mathbf{k}}$

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

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

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

$$= \langle\psi_n(\alpha)|\frac{\mathrm{d}}{\mathrm{d}\alpha}h_\alpha|\psi_n(\alpha)\rangle + 2\epsilon_\alpha\underbrace{\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle\psi_n(\alpha)|\psi_n(\alpha)\rangle}_{0} = \langle\psi_n(\alpha)|\frac{\mathrm{d}}{\mathrm{d}\alpha}h_\alpha|\psi_n(\alpha)\rangle \tag{57}$$

Proposition 3.2 (Rules of semiclassical approximation)**.**

1. Wave will move keeping same band index.
2. Position obeys

$$\langle\mathbf{r}\rangle \sim \frac{\partial\epsilon}{\partial\mathbf{k}} \tag{58}$$

3.

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

Proof. Lets write Shrödinger equation

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

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

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

$$\epsilon_{\alpha,\mathbf{k}} = \epsilon_{\alpha,\mathbf{k}_0}\boldsymbol{\nabla}_\mathbf{k}\epsilon_{\alpha,\mathbf{k}_0}\delta\mathbf{k} + \frac{1}{2}\sum_{i,j}\delta\mathbf{k}_i\cdot\delta\mathbf{k}_j\frac{\partial^2\epsilon}{\partial\mathbf{k}_i\partial\mathbf{k}_j} \tag{62}$$

$$\epsilon_\mathbf{k} = \langle\psi_k|H|\psi_k\rangle = \langle\mathcal{U}_\mathbf{k}|H_\mathbf{k}|\mathcal{U}_\mathbf{k}\rangle \tag{63}$$

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

Thus

$$\frac{\partial H_\mathbf{k}}{\partial k} = \frac{-i\hbar\boldsymbol{\nabla} - \mathbf{k}}{m} \tag{65}$$

We also define effective mass tensor:

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

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

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

Thus

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\mathbf{E} \tag{68}$$

□

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

$$\mathbf{k} = -\frac{e}{\hbar}\mathbf{E}t \tag{69}$$

What will be the velocity?

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

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

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

This effect was actually observed in cold atoms.

Alternative derivation Given PBC in 1D,

$$\psi(x+L) = \psi(x) \tag{72}$$

and Hamiltonian

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

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

$$\mathbf{A} = \frac{\Phi}{L}\hat{\mathbf{x}} \tag{74}$$

The electromotive force, from Lenz's law

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

Thus

$$\dot{\mathbf{A}} = -cE \Rightarrow \mathbf{A} = -cEt \tag{76}$$

And we rewrite the Hamiltonian

$$\mathbf{p} \to \mathbf{p} - \frac{e}{c}\mathbf{A} \tag{77}$$

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

Now we solve the Shrödinger equation:

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

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

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

From Theorem 1.1

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

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

$$e^{ikL} = e^{-\frac{ieAL}{c\hbar}} \tag{83}$$

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

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

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

We can verify that

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

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

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, $A=-cEt$,

$$\hbar\delta\dot{\mathbf{k}}=-e\mathbf{E} \tag{88}$$

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)**.**

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

3.1 Landau–Zener tunneling

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

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 $\bar{t}$:

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

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

$$H=\alpha t\sigma_z+\Delta\sigma_x \tag{92}$$

The energies

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

Thus the gap is 2Δ and there is probability to tunnel between bands:

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

which can be found by solving

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

Simplest Landau–Zener is

$$H=\alpha t\sigma^z+\Delta\sigma^x \tag{96}$$

We can diagonalize Hamiltonian in each particular moment:

$$H^{ad}(t)=\sqrt{(\alpha t)^2+\Delta t^2}\sigma^z \tag{97}$$

with diagonalizing transformation

$$U^{ad}(t) = e^{\frac{1}{2}\theta(t)\sigma^y} \tag{98}$$

where $\theta(t) = \arctan\left(\frac{\alpha t}{\Delta}\right)$. The evolution operator is

$$U^{\infty} = \mathcal{T}e^{-i\int_{-\infty}^{\infty}\mathrm{d}t' H(t')} = \prod_{t'=-\infty}^{\infty} e^{-iH(t')\mathrm{d}t'} = \prod_{t'=-\infty}^{\infty} U^{ad}(t'){U^{ad}}^{\dagger}(t')e^{-iH(t')\mathrm{d}t'}U^{ad}(t){U^{ad}}^{\dagger}(t') = \tag{99}$$

$$= \prod_{t'=-\infty}^{\infty} U^{ad}(t')e^{-i\Delta E(t')\mathrm{d}t'\sigma^z}{U^{ad}}^{\dagger}(t') \tag{100}$$

But

$${U^{ad}}^{\dagger}(t'+\mathrm{d}t)U^{ad}(t') = \left({U^{ad}}^{\dagger}(t') + \frac{\mathrm{d}U^{\dagger}}{\mathrm{d}t'}\,\mathrm{d}t\right)U^{ad}(t') \approx 1 + \frac{i}{2}\sigma^y\dot{\theta}\,\mathrm{d}t = 1 + \frac{i}{2}\sigma^y\left(\frac{\alpha\Delta}{(\alpha t)^2+\Delta^2}\right)\mathrm{d}t \tag{101}$$

Substituting into the product and taking first order

$$\langle\uparrow|U^{\infty}|\downarrow\rangle = \sum_{t'}\exp\left(-i\int_{t'}^{\infty}\mathrm{d}t''\,\sqrt{(\alpha t'')^2+\Delta t^2}\right)\frac{i}{2}\left(\frac{\alpha\Delta}{(\alpha t')^2+\Delta^2}\right)\exp\left(-i\int_{-\infty}^{t'}\mathrm{d}t''\,\sqrt{(\alpha t'')^2+\Delta t^2}\right) + \mathcal{O}\big(\alpha^2\big) = \tag{102}$$

$$= \exp\left(-i\int_{-\infty}^{\infty}\mathrm{d}t''\,\sqrt{(\alpha t'')^2+\Delta t^2}\right)\int\mathrm{d}t'\,\frac{i}{2}\left(\frac{\alpha\Delta}{(\alpha t')^2+\Delta^2}\right)\exp\left(-2i\int_{-\infty}^{t'}\mathrm{d}t''\,\sqrt{(\alpha t'')^2+\Delta t^2}\right) + \mathcal{O}\big(\alpha^2\big) \tag{103}$$

We can use saddle point approximation:

$$\int_{-\infty}^{c}\mathrm{d}t\,e^{iS(t)}p(t) \simeq e^{iS(\bar{t})}p(\bar{t})\int\mathrm{d}\delta t\exp\left(-\frac{\partial^2 S}{\partial t^2} + \mathcal{O}\big((\delta t)^2\big)\right) \tag{104}$$

where $\bar{t}$ is such that

$$\left.\frac{\partial S}{\partial t}\right|_{t=\bar{t}} = 0 \tag{105}$$

However, the solution is complex. We can substitute it since our function is entire on complex plane and continue our function to the saddle point. (In p we substitute $\mathrm{Re}\{\tau\} = 0$ since else it diverges):

$$\langle\uparrow|U^{\infty}|\downarrow\rangle \simeq \exp\left(-i\int_{-\infty}^{\infty}\mathrm{d}t''\,\sqrt{(\alpha t'')^2+\Delta t^2}\right)\frac{\alpha}{\Delta}\exp\left(-2\int_{0}^{\frac{\Delta}{\alpha}}\mathrm{d}\tau'\,\sqrt{\Delta^2-(\alpha\tau')^2}\right) \sim \tag{106}$$

$$\sim \exp\left(-2\left(\frac{\Delta}{\alpha}\right)^2\int_0^1\mathrm{d}u\,\sqrt{1-u^2}\right) = e^{-\frac{\pi}{4}\left(\frac{\Delta}{\alpha}\right)^2} \tag{107}$$

Electric field

$$\mathbf{E} = -\frac{1}{c}\dot{\mathbf{A}} - \boldsymbol{\nabla}\phi \tag{108}$$

If $\dot{\mathbf{A}} = 0$ and $\phi(\mathbf{x}) = -\mathbf{x}\cdot\mathbf{E}$, we have

$$H_E = \frac{p^2}{2m} + e\mathbf{E}\cdot\mathbf{x} + V(x) \tag{109}$$

But this Hamiltonian diverges in $\pm\infty$. Instead we can choose $\Lambda = c\mathbf{E}\cdot\mathbf{x}t$ for gauge transform

$$\mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla}\Lambda(\mathbf{x},t) \tag{110}$$

acquiring

$$\mathbf{A}' = -c\mathbf{E}t \tag{111}$$

4 Boltzmann equation

In equilibrium

$$f_{\mathbf{k},\alpha}^{(0)} = \frac{1}{\exp\left(\frac{\epsilon_{\mathbf{k}}^{\alpha}-\mu}{T}\right)+1} = n_{\mathbf{k}} \tag{112}$$

If we look at phase space, then our states are incompressible liquid in a phase space, i.e., total number of particles doesn't change:

$$\frac{\mathrm{d}f_{\mathbf{k}}}{\mathrm{d}t} = \frac{\partial f_{\mathbf{k}}}{\partial t} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \dot{\mathbf{k}} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{r}} \cdot \dot{\mathbf{r}} = 0 \tag{113}$$

However, in addition, in can get scattered:

$$P_{\mathbf{k},\mathbf{k}'} = 2\pi |\langle \psi_{k'}|V|\psi_k\rangle|^2 \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'} - \omega) \tag{114}$$

Thus

$$\frac{\mathrm{d}f_{\mathbf{k}}}{\mathrm{d}t} = \frac{\partial f_{\mathbf{k}}}{\partial t} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}} \cdot \dot{\mathbf{k}} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{r}} \cdot \dot{\mathbf{r}} = -\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} \tag{115}$$

If we had $f_{\mathbf{k}}(\mathbf{k}, \mathbf{r}, t)$, we could calculate observables, such as charge density, current, heat current, magnetization:

$$\rho(\mathbf{r}, t) = \sum_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{r}, t) \tag{116}$$

$$\mathbf{j}(\mathbf{r}, t) = e\sum_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{r}, t) \cdot \mathbf{v}_{\mathbf{k}} \tag{117}$$

$$\mathbf{j}_Q(\mathbf{r}, t) = \sum_{\mathbf{k}} f_{\mathbf{k}}(\mathbf{r}, t)(E_{\mathbf{k}} - e\mu) \cdot \mathbf{v}_{\mathbf{k}} \tag{118}$$

$$m_z(\mathbf{r}, t) = \sum_{\mathbf{k},s} f_{\mathbf{k}}(\mathbf{r}, t)\left(\frac{\hbar}{2} \cdot s\right) \tag{119}$$

$$\tag{120}$$

Lets evaluate $\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}}$:

$$-\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = \sum_{\mathbf{k}'} P_{\mathbf{k}'\leftarrow\mathbf{k}} f_{\mathbf{k}}(1 - f_{\mathbf{k}'}) - P_{\mathbf{k}\leftarrow\mathbf{k}'} f_{\mathbf{k}'}(1 - f_{\mathbf{k}}) \tag{121}$$

In equilibrium

$$f = f^0 = \frac{1}{\exp(\beta(\epsilon_{\mathbf{k}} - \mu)) - 1} \tag{122}$$

$$1 - f = 1 - f^0 = \frac{\exp(\beta(\epsilon_{\mathbf{k}} - \mu))}{\exp(\beta(\epsilon_{\mathbf{k}} - \mu)) - 1} = \exp(\beta(\epsilon_{\mathbf{k}} - \mu))f^0 \tag{123}$$

$$\tag{124}$$

Then

$$-\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = \sum_{\mathbf{k}'} P_{\mathbf{k}'\leftarrow\mathbf{k}} \exp(\beta(\epsilon_{\mathbf{k}} - \mu)) f_{\mathbf{k}}^0 f_{\mathbf{k}'}^0 - P_{\mathbf{k}\leftarrow\mathbf{k}'} \exp(\beta(\epsilon_{\mathbf{k}'} - \mu)) f_{\mathbf{k}}^0 f_{\mathbf{k}'}^0 \tag{125}$$

But

$$\frac{P_{\mathbf{k}'\leftarrow\mathbf{k}}}{P_{\mathbf{k}\leftarrow\mathbf{k}'}} = e^{-\beta(\epsilon_{\mathbf{k}'} - \epsilon_{\mathbf{k}})} \tag{126}$$

i.e., everything vanishes. But $P_{\mathbf{k}'\leftarrow\mathbf{k}}$ depends on thing breaking translational symmetry: impurities, phonons, electron-electron interactions.

Relaxation time approximation For phonons we can approximate with

$$-\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = \frac{f(\mathbf{k},\mathbf{r},t) - f^0(\mathbf{k})}{\tau} \tag{127}$$

where τ is relaxation time. The approximation makes sense since we are interested in first order approximation.

Impurities approximation

$$P_{\mathbf{k}',\mathbf{k}} = 2\pi\left|\langle\mathbf{k}|V^{im}|\mathbf{k}'\rangle\right|^2\delta(\epsilon_k - \epsilon_{k'}) \tag{128}$$

$$-\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = \sum_{\mathbf{k}'}\left[f_{\mathbf{k}}(1-f_{\mathbf{k}'}) - f_{\mathbf{k}'}(1-f_{\mathbf{k}})\right]\left|V^{im}_{\mathbf{k},\mathbf{k}'}\right|^2\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) \tag{129}$$

where

$$V^{im} = \sum_i \vartheta(\mathbf{r} - \mathbf{R}_i) \tag{130}$$

$$V_{\mathbf{k},\mathbf{k}'} = \int \psi^* V^{im}\psi\,\mathrm{d}x = \frac{1}{V}\sum_i e^{i\left(\mathbf{k}-\mathbf{k}'\right)\mathbf{R}_i}\vartheta \tag{131}$$

Then

$$\left\langle\left|V^{im}_{\mathbf{k},\mathbf{k}'}\right|^2\right\rangle = \left\langle\sum_{i,j} e^{i(\mathbf{k}-\mathbf{k}')(\mathbf{r}_i\mathbf{R}_j)}\left|V_{\mathbf{k},\mathbf{k}'}\right|^2\right\rangle = \sum_i \delta_{ij}\left|V_{\mathbf{k},\mathbf{k}'}\right|^2 = N\vartheta_{\mathbf{k},\mathbf{k}'} \tag{132}$$

where N is number of impurities.

$$-\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = \sum_{\mathbf{k}'}\left[f_{\mathbf{k}}(1-f_{\mathbf{k}'}) - f_{\mathbf{k}'}(1-f_{\mathbf{k}})\right]\left|V^{im}_{\mathbf{k},\mathbf{k}'}\right|^2\delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}) \tag{133}$$

Thus

$$\frac{\partial f_{\mathbf{k}}}{\partial t} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}}\cdot\dot{\mathbf{k}} + \frac{\partial f_{\mathbf{k}}}{\partial \mathbf{r}}\cdot\dot{\mathbf{r}} = -\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{collisions}} = -\frac{f - f^0}{\tau} \tag{134}$$

We can approximate

$$f = f^0 + \delta f \tag{135}$$

Since

$$\hbar\dot{\mathbf{k}} = e\mathbf{E} \tag{136}$$

we can make scattering approximation

$$\left(\frac{\partial f}{\partial t}\right) = -\frac{\delta f}{\tau} \tag{137}$$

where τ depends on scattering Hamiltonian: impurities (elastic scattering), phonons (inelastic), electron-electron interactions.

4.1 Presence of electric field

Let

$$\mathbf{E}_\omega = \mathrm{Re}\left\{e^{i\omega t}\mathbf{E}\right\} \tag{138}$$

we assume homogeneous field, i.e. $\frac{\partial f}{\partial \mathbf{r}} = 0$:

$$\frac{\partial \delta f_{\mathbf{k}}}{\partial t} - \frac{e}{\hbar}\mathbf{E}e^{i\omega t}\left(\frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}}\right) = \frac{\delta f_{\mathbf{k}}}{\tau} \tag{139}$$

Since we are interested in first order part, we can replace $\left(\frac{\partial f_{\mathbf{k}}}{\partial \mathbf{k}}\right)$ with $\left(\frac{\partial f^0}{\partial \mathbf{k}}\right) = \frac{\partial f^0}{\partial E} \cdot \frac{\partial E}{\partial \mathbf{k}}$: The solution is

$$\delta f(t) = e^{i\omega t}\delta f_{\mathbf{k},\omega} \tag{140}$$

$$e\mathbf{v_k} \cdot \mathbf{E}e^{i\omega t}\left(-\frac{\partial f^0}{\partial E}\right) = \delta f_{\mathbf{k},\omega}e^{i\omega t}\left(\frac{1}{\tau} - i\omega\right) \tag{141}$$

i.e.,

$$\delta f_{\mathbf{k},\omega} = \frac{e\mathbf{v_k} \cdot \mathbf{E}\tau}{1 - i\omega t}\left(-\frac{\partial f^0}{\partial E}\right) \tag{142}$$

Then

$$J_x(\omega) = \sigma_{xx}(\omega)E^x_\omega \tag{143}$$

$$J^x_{k,\omega} = e\sum_{\mathbf{k}\in BZ}\delta f_{\mathbf{k},\omega}v^x_k \tag{144}$$

$$J^x_\omega = \underbrace{e^2\sum_{\mathbf{k}\in BZ}\left(-\frac{\partial f^0}{\partial E}\right)_{\mathbf{k}}\frac{{v^x_k}^2\tau}{1 - i\omega\tau}}_{\sigma_{xx}(\omega)} \cdot E^x_\omega \tag{145}$$

$$\tag{146}$$

Note we can approximate pretty well

$$\left(-\frac{\partial f^0}{\partial E}\right) \overset{T\to 0}{\sim} \delta(\epsilon - \mu) \tag{147}$$

4.2 Parabolic bands

We can recove Drude model in a parabolic band (i.e., around extrema).

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m^*} \tag{148}$$

$$\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}}{\mathbf{k}^*}^2 = \frac{1}{3}\sum_{\mathbf{k}}\delta(\epsilon_{\mathbf{k}}|\mathbf{v}|^2 \tag{149}$$

$$\mathbf{v}^2 = \left(v_1^2\right)^2 + \left(v_2^2\right)^2 + \left(v_3^2\right)^2 = \frac{2}{3}\sum_{\mathbf{k}}\frac{\delta(\epsilon_{\mathbf{k}} - \mu)\epsilon_{\mathbf{k}}}{m^*} \tag{150}$$

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m^*} = \frac{{m^*}^2\mathbf{v}^2_{\mathbf{k}}}{2m^*} = \frac{m^*\mathbf{v}^2_{\mathbf{k}}}{2} \tag{151}$$

$$1 = \int \mathrm{d}\epsilon\sum_{\mathbf{k}}\delta(\epsilon - \epsilon_{\mathbf{k}}) = \frac{2}{3}\int \mathrm{d}\epsilon\,\frac{\rho(\epsilon)\delta(\epsilon - \mu)\epsilon}{m^*} = \frac{2}{3m^*}\rho(\epsilon_F)\epsilon_F \tag{152}$$

$$\rho(\epsilon_F) = \frac{\partial N(\epsilon_F)}{\partial \epsilon_F} \tag{153}$$

when

$$N(\epsilon_F) = \left(\frac{1}{2\pi}\right)^3\left(\frac{4\pi}{3}\right)k_F^3 \tag{154}$$

$$k_F = \left(\frac{2m\epsilon_F}{\hbar^2}\right)^{\frac{1}{2}} \tag{155}$$

$$N(\epsilon_F) = \frac{1}{2\pi^2}\left(\frac{2m\epsilon_F}{\hbar^2}\right)^{\frac{3}{2}} \tag{156}$$

$$\rho(\epsilon_F) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\frac{3}{2}\epsilon_F^{\frac{1}{2}} \tag{157}$$

Then

$$\sigma = e^2\tau\left[\frac{2}{3m^*}\frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\epsilon_F^{\frac{3}{2}}\left(\frac{3}{2}\right)\right] = \frac{e^2\tau}{m^*}\left(\frac{1}{2\pi^2}\right)k_F^3 \tag{158}$$