118028 - Quantum Transport in Solids

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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:

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

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

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

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

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

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

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

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:

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

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 $k_BT \sim \hbar\omega \ll \Delta E$, 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

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

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

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

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

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

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

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.