Lecture 4:

In lecture 3 we saw how to solve carefully the Hamiltonian of a 1D chain in tight-binding approximation. Now we introduce an "effective" hopping Hamiltonian that can describe the same physics: splitting of many degenerate levels into a band of energies.

First, two levels:

\[ H_0 = E_1 \delta_{1,1} + E_2 \delta_{2,2}. \]

Perturbation that splits the degeneracy will have matrix elements between states 1 and 2:

\[ V = V \delta_{1,2} + V^* \delta_{2,1}. \]

"1 \rightarrow 2" operator takes a particle in state 1 and "pops" it into state 2 — thus called "hopping" Hamiltonian.

We see that the energy level \( E_0 \) gets split into two with energies \( E_0 \pm |V| \).

We can play the same game for many levels, especially effectively if the electrons do not hop too far — hence the name "tight-binding" approximation.
(a) 1D chain:

\[ H_0 = \sum_i \varepsilon_i \langle i \mid i \rangle \] - a bunch of levels with diagonal! maybe different energies \( \varepsilon_i \).

The perturbing “hopping Hamiltonian” is

\[ H_{\text{hop}} = \sum_{\langle i,j \rangle} (-t) \langle i \mid j \rangle 1 \langle j \mid i \rangle \]

\( \langle i,j \rangle \) - \( i \) and \( j \) are nearest neighbors.

\( t \) - hopping matrix element, often positive, can be complex or magnetic field.

In 1D, \( H_{\text{hop}} \) turns into

\[ H_0 = -t \sum_i \left( \langle i \mid i+1 \rangle + \langle i+1 \mid i \rangle \right) \]

\[ \text{from } i \text{ onto } i+1 \]

\[ \text{both terms are needed to keep the Hamiltonian hermitian.} \]

(b) The spectrum: hopping Hamiltonians for regular lattices (without disorder) are diagonal in momentum space.
change of basis (unitary transformation):

\[ | \kappa \rangle = \sum_{k \in \mathbb{Z}} \frac{1}{\sqrt{N}} e^{i \kappa a \hat{n}} | k \rangle, \quad k \in \mathbb{Z} \]

Then

\[ | \kappa + 1 \rangle = \sum_{k \in \mathbb{Z}} \frac{1}{\sqrt{N}} e^{-i \kappa a \hat{n}} | k \rangle \]

and

\[ \sum_{k} | \kappa \rangle < k+1 | \kappa \rangle = \sum_{k} \frac{1}{\sqrt{N}} e^{-i \kappa a \hat{n}} | k \rangle \]

\[ = \sum_{k \in \mathbb{Z}} e^{i \kappa a} | k \rangle < k | \kappa \rangle \text{ --- diagonal in } \kappa \text{-space.} \]

\[ \sum_{k} | \kappa + 1 \rangle < k | \kappa \rangle = \sum_{k \in \mathbb{Z}} e^{-i \kappa a} | k \rangle < k | \kappa \rangle \]

\[ \sum_{k} \sum_{\kappa} | \kappa \rangle < k | \kappa \rangle = \sum_{k \in \mathbb{Z}} \sum_{\kappa} | \kappa \rangle < k | \kappa \rangle \] (all \( \epsilon \) are the same for translational invariance).

Thus, \( H = H_0 + \text{hopp} \) becomes

\[ H = \sum_{k} \epsilon_k | \kappa \rangle < k | \kappa \rangle + 2 + \sum_{k} \epsilon_k a_k^\dagger a_k | k \rangle < k | \kappa \rangle \]

We see that we get the same dispersion as in lecture 3,

\[ \epsilon_\kappa = \epsilon_0 - 2 + \epsilon_k \]

The value of \( t \) should be found from either experiment, or at least calculations.
2D case (or ND case, actually).

\[ \mathbf{R} = n \mathbf{a} + m \mathbf{b} \]

\[ \mathbf{H} = \sum_k E_k | \mathbf{k} \rangle \langle \mathbf{k} | + t \sum \langle \mathbf{k} | \mathbf{S} \cdot \mathbf{k} \rangle \langle \mathbf{k} + \mathbf{q} | \mathbf{k} \rangle \]

Kern. cons. "hop."

We play the same game:

\[ | \mathbf{w} \rangle = \sum_{k} \frac{1}{\sqrt{N}} e^{i \mathbf{k} \cdot \mathbf{R}} | \mathbf{k} \rangle \]

for \( \mathbf{R} \in \mathbb{Z} \times \mathbb{Z} \times \mathbb{Z} \)

We label NN by \( \mathbf{g} \)-vectors connecting them to the state \( \mathbf{n} \).

\[ \mathbf{H} = \sum_k \mathbf{E}_k | \mathbf{k} \rangle \langle \mathbf{k} | + t \sum_{\mathbf{g}} \left( \sum_{\mathbf{k}} e^{i \mathbf{k} \cdot \mathbf{g}} \right) | \mathbf{k} \rangle \langle \mathbf{k} + \mathbf{g} | \]

For square lattice \( \mathbf{g} = (\pm \mathbf{a}, \pm \mathbf{b}, \pm \mathbf{c}) \)

\[ \mathbf{E}_k = E_0 - 2t \cos k_x a - 2t \cos k_y b \]

The band width is \( 4t \times 2^d \) with number of dimensions:

\[ E_{\text{max}} = E_0 + 4t \]

\[ E_{\text{min}} = E_0 - 4t \]
d) **Effective mass approximation**

1D case

\[ E = E_0 - 2t \cos k \]

One notices that the band near the bottom looks very parabolic:

\[ E(k \ll \frac{E_0}{a}) \approx E_0 - 2t + 2t \cdot \frac{k^2a^2}{2} = E_0 - 2t + a^2k^2. \]

We see that these electrons look like free ones but their mass has nothing to do with bare electron mass \( m \approx 9.10^{-31} \text{kg} \).

Instead, since

\[ E_n = \text{const} + a^2 k^2 = \frac{p^2}{2m} - \frac{a^2}{4} \]

we conclude that \( \text{mass} = \frac{\hbar^2}{2a^2t} \).

Energy \( \left[ \frac{\hbar^2}{2a^2t} \right] \) is mass, indeed.

**NB** here \( k = \pm \frac{\pi}{a} \) (these are the same point), see that \( E = E_0 + 2t - a^2 k \). The mass looks negative!! These are hole states, they move like electrons with a **negative** mass.

**Conclusion:** Effective mass approximation usually works near band extremum (oh!), and the effective mass is generally a tensor, determined by curvature radii near the extremum.
e) Counting electrons: density of states (DOS)

What is the density of Bloch state as a function of energy?

For point masses:

\[ P(x) = \sum_i \delta(x-x_i) \]

Density of mass, \( P(x) \, dx = \text{mass in } dx \text{ interval} \).

For energy we have similarly

\[ N(\epsilon) = \sum \delta(\epsilon - \epsilon_n) \]

For any set of states.

For Bloch states:

\[ N(\epsilon) = \sum \delta(\epsilon - \epsilon_n) = \sqrt{\frac{d^2}{\partial \epsilon} \delta(\epsilon - \epsilon_n)} \]

For 1D band: (\( \epsilon_n \to \infty \))

\[ N(\epsilon) = \int_{-\infty}^{\infty} \frac{d\epsilon}{\partial \epsilon} \delta(\epsilon - 2t \cos k \lambda) = \]

\[ = \int_{-\infty}^{\infty} \Theta(2t-\epsilon) \Theta(\epsilon + 2t) \cdot \sum_n \frac{S(k-k_n)}{\Theta(2t + \cos k \lambda)} = \]

\[ = \Theta(2t-\epsilon) \Theta(\epsilon + 2t) \cdot \frac{\frac{1}{a} \cdot \frac{1}{\sqrt{(2t)^2 - \epsilon^2}}}{\partial \epsilon} \]

Note the divergence at \( \epsilon = \pm 2t \), the band edges.
The Fermi surface: Fermions cannot stay in the same state \( \Rightarrow \) pile up.

Def.: At \( T=0 \), the curve in momentum space that separates occupied Fermi states from the unoccupied ones. Note that this must be an \( \beta \)-scattering curvature.

1D: two points.
2D: line (not necessarily closed).
3D: 2D surface (again not necessarily closed).

Example: 2D tight-binding based on a square lattice
\[
E = -2t \cos k_x a - 2t \cos k_y a
\]

The entire band fits 2N sites electrons.

1) \( N_{el} \ll N_{sites} \): only lowest energies occupied \( \Rightarrow \)
\[
E = -4t + a^2 \left( k_x^2 + k_y^2 \right)
\]
\( \beta_0 - E \) surface is a circle.

2) \( N_{el} = N_{sites} \) - half filling.
Electrons are filled up to \( E=0 \):
\[
\cos k_x a + \cos k_y a = 0 \Rightarrow k_x = k_y = \pm \frac{\pi}{L}, \quad \text{or} \quad k_x = -k_y = \pm \frac{\pi}{L},
\]
hence the curve 2.

3) What happens if the band is almost full, \( 2N_{sites} - N_{el} \ll 2N_{sites} \)? Would the Fermi surface be open or closed?