Abstract

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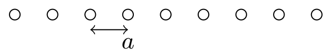
0.1 Electrons in metallic solids

Not really such a thing as a free electron. Mostly, we have atoms in a lattice. Let's start with a 1-d situation



We can write down $|n\rangle$, the state of e^- sitting on an atom n, which gives $\langle n|m\rangle = \delta_{nm}$. We can write down the hamiltonian as H_0, the usual, and some H_1 to account for the dynamics, where the electrons are only allowed to move between neighbors.

$$H_0 = E_0 \sum_N |n\rangle \langle n| \qquad\qquad H_1 = -t \sum_N |n\rangle \langle n+1| + |n+1\rangle \langle n|$$

We just want to find eigenstates of this now, by putting this into Schroedingers equation and solving the eigenvalue equation, which gives us

$$E_0 \sum_M \psi_m |m\rangle - t \sum_m \psi_{m+1} |m\rangle + \psi_m |m+1\rangle = E \sum_m \psi_m |m\rangle$$

Let's inner product on another state n, which gives us a set of equations for another state n, this gives us an equation

$$E_o \psi_n - t(\psi_{n+1} + \psi_{n-1}) = E\psi_n$$

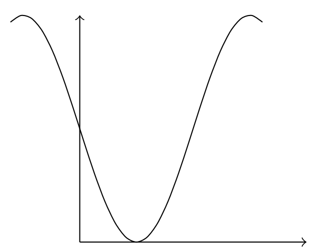
We can solve this to get

$$\psi_n = \frac{e^{ikna}}{\sqrt{N}}$$

If we take the symmetry $k \to k + \frac{2\pi}{a}$, then we only need to look at $k \in \left[\frac{-\pi}{a}, \frac{\pi}{a}\right]$. This is actually just the **Brilloun Zone** of the lattice. k comes in a discrete unit, $\frac{2\pi}{aN}$. This allows the counting of the basis. We can get this out by just enforcing periodic boundary conditions on k. This spits out

$$E = E_0 - 2t \cos ka$$

We can plot this as



Remarks

1. For arbitrary small perturbations, the hopping wavefunction (pos space) completely delocalized.
2. All of original degeneracy has been lifted
3. For small $|k| \ll \frac{\pi}{a}$, we have $E_k \approx \frac{\hbar^2 k^2}{2m^*}$, with $m^* = \frac{\hbar^2}{2a^2 t}$.

This m^* can be tought of as a sort of renormalized mass that comes from the interaction with the lattice, but leaves our wavefunction completelet delocalized, as we expect.

0.1.1 More Realistic Treatment

Assume e^- can move anywhere along $\hat{x}$, but assume there's some weak periodic potential $V(x) = V(x + a)$. The hamiltonian is just

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

Bare energies of the problem can be obtained by taking the fourier transform, and getting

$$E_0(k) = \frac{\hbar^2 k^2}{2m}$$

We probably should do perturbation theory. Naively, it looks as if since for $\pm k$, $E_o(\pm k)$ is the same, we should do degenerate perurbation theory. We can just get a new basis expressed as linear combinations of $|\pm k\rangle$. We should always check, however, that

$$\langle k| V |k'\rangle \neq 0$$

Since we know that V is periodic, we can re-expand our perturbation V in the fourier basis. Let's expand V as

$$V(x) = \sum_n V_n e^{2\pi n x/a}$$

with

$$V_n = \frac{1}{a} \int_0^a dx V(x) e^{-2\pi i n x/a}$$

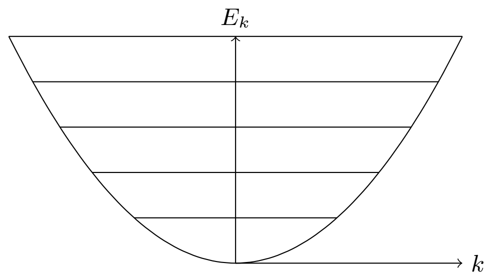
We can combine this all to get

$$\langle k| V |k'\rangle = \int dx \sum_n V_n e^{i\left(k-k'+\frac{2\pi n}{a}\right)x} = \sum_n V_n \delta\left(k' - k + \frac{2\pi n}{a}\right)$$

Momenta k, k' have to match $\frac{2\pi n}{a}$ in order for the V to have an effect. That is to say, that mixing occurs as

$$k = k' + \frac{2\pi n}{a}$$

Now, we apply the condition to our degenerate states



This is another way of thinking about the emergence of the Brillouin Zone. It's just the first place a periodic perturbation mixes a $|\pm k\rangle$ state. We can consider some basic limits of this.

Case 1: Low momenta For low momenta, $|k| \ll \frac{\pi}{2a}$.

$$E(k) = \frac{\hbar^2 k^2}{2m} + \langle k| V |k\rangle + \sum_{k=k'} \frac{|\langle k| V |k'\rangle|^2}{E_0(k) - E_0(k')} + \dots$$

but the perturbation is small, so it should behave like a free particle.

Case 2: At Edge of Brillouin Zone