EE236
11/19/04
1

In the last lecture, we found that electrons in a crystal can always be expanded over a set of eigenstates of the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

and the displacement operators

$$D\,\psi(\vec{r}) = D\psi(\vec{r} + (\text{lattice vector}))$$

if the potential V is periodic

$$V(\vec{r}) = V(\vec{r} + (\text{lattice vector}))$$

and consequently that they can always be written in the form

$$\psi_\nu(\vec{r}) = u_{\nu k}(r)\, e^{i\vec{k}\cdot\vec{r}}$$

and that $\vec{k}$ is restricted to a finite set which is determined by the B.C.'s at the edge of the crystal.

for periodic B.C.'s on a crystal of size L_x L_y L_z

$$\vec{K} = \frac{2\pi}{L_x}\hat{x}\, S_x + \frac{2\pi}{L_y}\hat{y}\, S_y + \frac{2\pi}{L_z}\hat{z}\, S_z$$

where S_x, S_y & S_z are integers.

To find the energy eigenvalues, we plug

$$\psi_\nu(\vec{r}) = u_{\nu k}(r)\, e^{i\vec{k}\cdot\vec{r}}$$

into the Shrödinger's equation,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right) u_{\nu k}(r)\, e^{i\vec{k}\cdot\vec{r}}$$
$$= E_{\nu k}\, u_{\nu k}(r)\, e^{i\vec{k}\cdot\vec{r}}$$

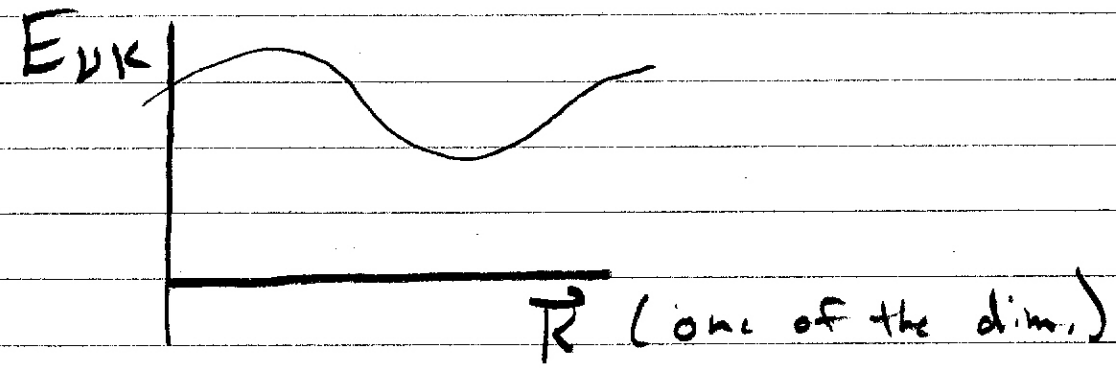
for $K = 0$, we have

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right) u_{\nu k}(r) = E_{\nu k}\, u_{\nu k}(r)$$

so $u_{\nu k}(r)$ is approximately the shape of an orbital around one lattice site.

Of course $E_{\nu K}$ is a function of K as well, and as K changes smoothly, so will $E_{\nu K}$

We can then draw a <u>band diagram</u> of $E_{\nu K} = \hbar \omega_{\nu K}$ vs K



We do not consider values of K outside of the first Brillouin zone, because any factor

$$e^{i\vec{K}\cdot\vec{r}} = \mathcal{U}(\vec{r})\, e^{ik'(r)}$$

where $\mathcal{U}(\vec{r})$ is periodic over the lattice, and we don't want to double count the states.

Distribution functions.

Now that we have built the states, we want to sort of "pour in" the electrons.

This is a little funny, because the potential $V(\vec{r})$ depends on all the other electrons already being there, so we are really just trying to find the statistics for occupancy.

Electrons are fermions, and they are identical, so the joint wavefunction must be antisymmetrical under exchange of any two of them.

$$\Psi(r_1, r_2, r_3 \ldots) = -\Psi(r_2, r_1, r_3 \ldots)$$

where Ψ takes into account both spatial + spin information, and Electron spin $= 1/2$, so electron spin is a two state system.

If we write the state vector of all the electrons as a composition of the single electron states we have found, we have

$$\Psi(r_1, r_2 \cdots) = \psi_1(r_1)\,\psi_2(r_2) \cdots$$

$$= -\psi_1(r_2)\,\psi_2(r_1) \cdots$$

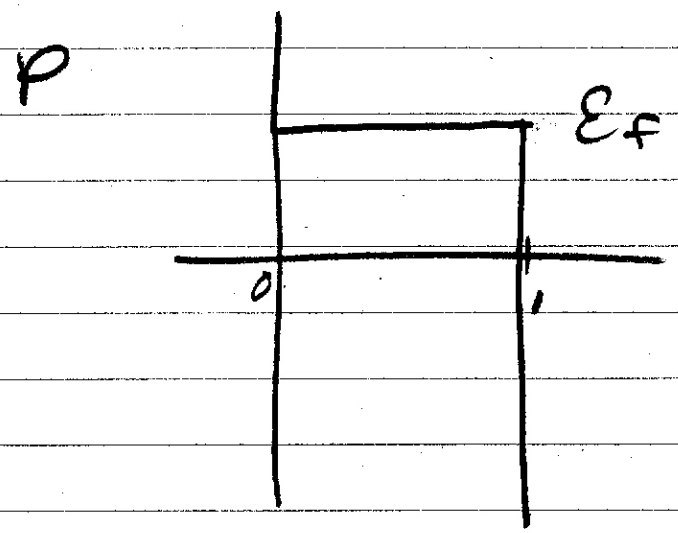
so this is not a possible state for any two electrons. this is expressed as "Fermi Dirac exclusion" which states that only one electron can occupy a specific single electron spin-spatial state.

With this restriction on the statistics, we get the occupancy of any particular state to be

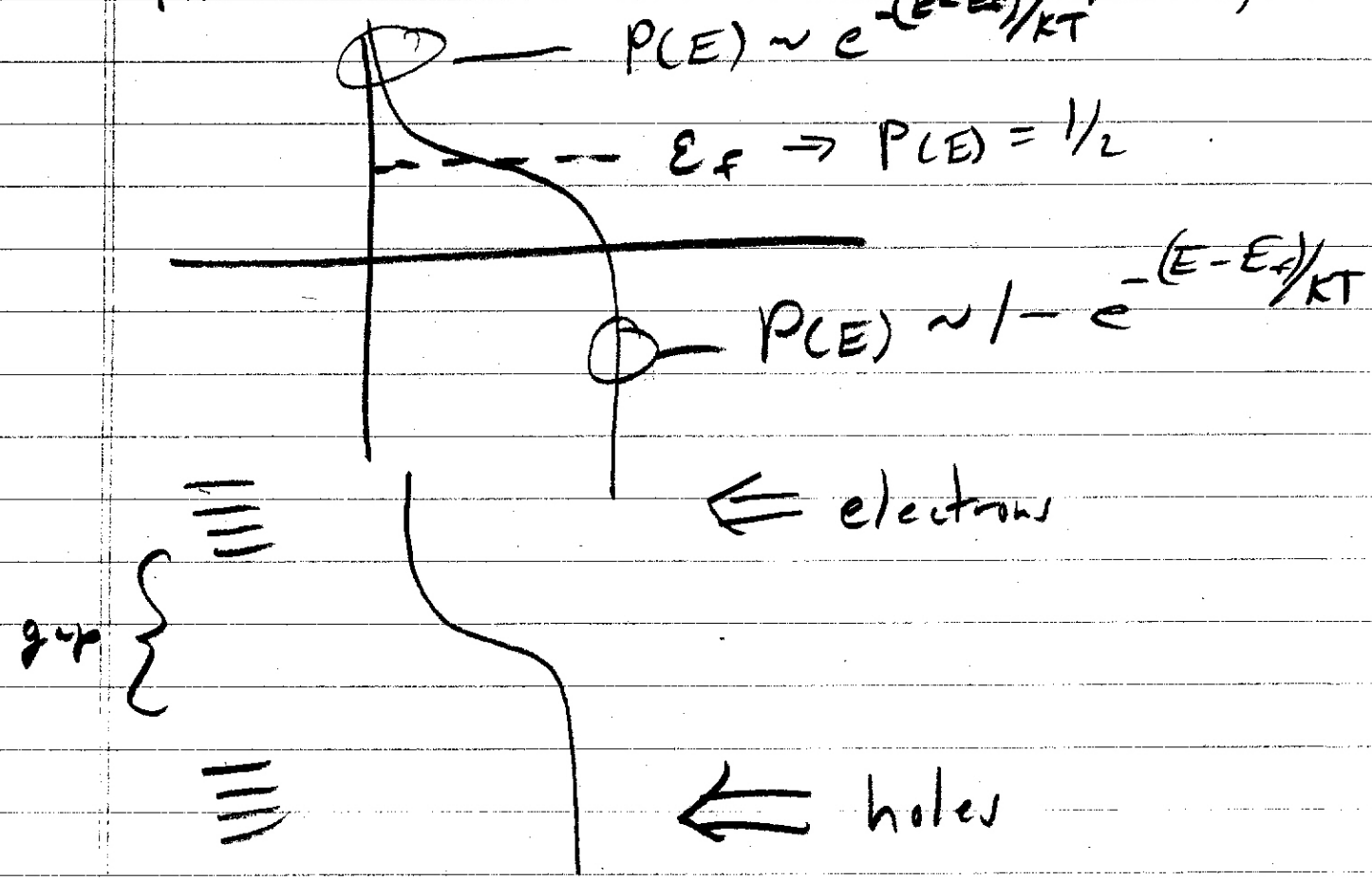
$$f(E = \frac{1}{e^{(E-E_F)/kT} + 1}$$

(See McKelvey Solid state & Semiconductor Physics, for a proof)

If we plot the fermi function for very low t, it comes out to be a step function



if we look at it for higher t,



If the number of electrons which corresponds to neutrality in the crystal just reaches a gap in the bands, the material is called a semiconductor.

Assuming there is a gap, there is a top edge of the band below the gap, and a lower edge to the band just above the gap. Since $E_{\nu k}$ is a smooth function of $\vec{k}$, we are able to fit it to a peribolic surface

$$E(k) = \frac{\hbar^2}{2m_c}|\vec{k}|^2$$

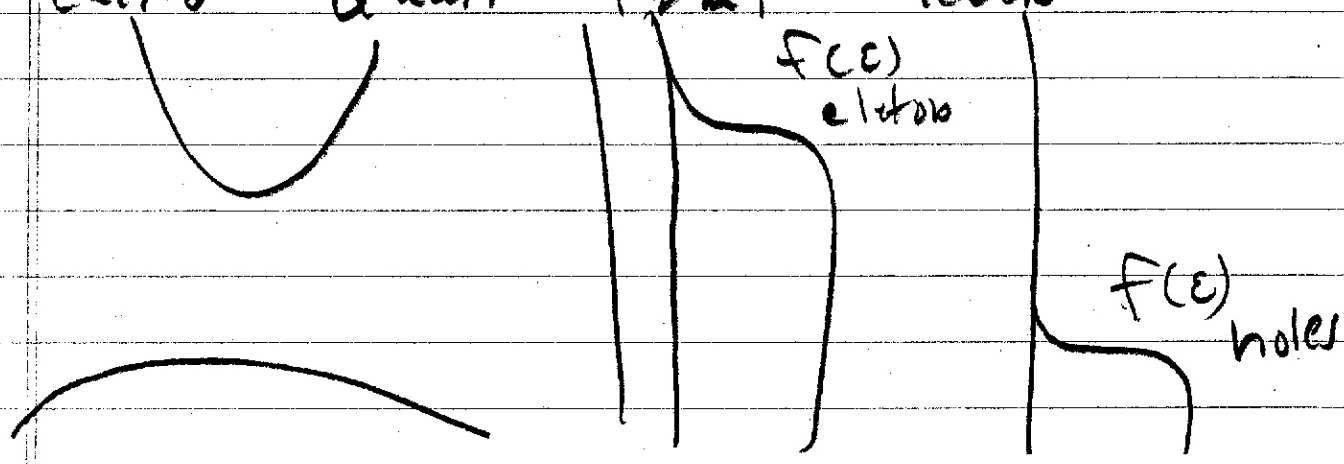
where the value m_c is called the effective mass, but is just a parameter defined by the above relationship

In most cases, these states near the band gap are the only ones we will need to consider,

In electronic devices, the fermi level is so far away from the band edge that we can use the exponential approximations, but for lasers we will have a degenerate population of electrons or holes or both.

This is accomplished by forming a P-N junction, and then biasing it. Since the holes come from the p-side, and the electrons come from the n-side, the fermi level will be different for the electrons in the conduction band and those in the valence band (below the energy gap)

The split Fermi levels are then called Quasi-fermi levels



In this fashion, we can create filled states above empty states, an "inversion" which will give a gain.

The next step is to use Fermi's Golden rule to find the rate of transitions caused by an optical field between pairs of states, and to sum up the total number of transitions per second per unit volume to find the absorbed power & the loss coefficient, in a intrinsic semiconductor

To find gain or loss under bias, we will just need to account for the occupancy of the various pairs of states which interact with the optical field