

Semi classical approx for dynamics of electrons in periodic potential

Same idea as we used in Sommerfeld model.

Imagine constructing wave packets of Bloch states to localize electrons. \Rightarrow To each electron assign position \vec{r} , crystal momentum \vec{k} , band index n .

Semiclassical equations of motion tell how \vec{r} , \vec{k} , n evolve in time in presence of applied \vec{E} and \vec{H} fields, inbetween collisions.

Then a relaxation approximation will be used to ~~average over effect of collisions~~ modify semiclassical equations to include average effect of collisions.

- *1) Wave packet approx good only when applied fields vary slowly over dimensions of size of primitive cell.
 - ~~*~~ (localize crystal momentum well on scale of 1st BZ \Rightarrow wave packet in \mathcal{R} -space extends over a few primitive cells)
- *2) Quantum effects are handled entirely through the band structure $E_n(\vec{k})$ which we take as given functions. ~~This describes how includes all effects of quantum mechanics or~~ Periodic potential (which varies rapidly on scale of primitive cell) is taken into account in fully quantum mechanical way by use of the Bloch states $E_n(\vec{k})$. External slowly varying fields are treated in semiclassical way

* Collisions can not do with static periodic cons. Their effect already included in $\epsilon_n(\vec{k})$.

(11)

In the absence of collisions, n , \vec{k} , \vec{r} evolve as

i) band index is constant. No interband transitions
Good when field strengths are not too large

see Appendix J) i) $eEa \ll [\epsilon_{\text{gap}}(\vec{k})]^2 / \epsilon_F$ "electric breakdown" when fails

ii) $\hbar\omega_c \ll [\epsilon_{\text{gap}}(\vec{k})]^2 / \epsilon_F$ "magnetic breakthrough" when fails

i) ~~usually~~ always true in metals, can fail in insulators + semiconductors

ii) possible in strong \vec{H} fields

Also need $\begin{cases} \hbar\omega \ll \epsilon_{\text{gap}} & \text{photon cannot excite to higher band} \\ \lambda \gg a & \text{slowly varying fields} \end{cases}$

2) \vec{r} and \vec{k} evolve just like classical particle
if we took $\hbar\vec{k}$ as ordinary momentum (which it is not)

$$\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_n(\vec{k})}{\partial \vec{k}}$$

$$\hbar \dot{\vec{k}} = -e \left[\vec{E}(\vec{r}, t) + \frac{1}{c} \vec{v}_n(\vec{k}) \times \vec{H}(\vec{r}, t) \right]$$

3) States \vec{k} and $\vec{k} + \vec{K}$ are equivalent when \vec{K} is reciprocal lattice vector.

In equilibrium, states occupied with Fermi function
function $f(\epsilon_n(\vec{k})) = \frac{1}{e^{(\epsilon_n(\vec{k}) - \mu) / kT} + 1}$

* $\hbar\vec{k}$ is not total momentum. \vec{p} is given by total force
(... ..) $\hbar\vec{k}$ is analysed force only.

Reasons to believe semi-classical equations: For more see references given in text

$$\vec{v} = \vec{v}_n(\vec{k}) \quad \text{is just definition of velocity}$$

+ we derived earlier that $\vec{v}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial \epsilon_n}{\partial \vec{k}}$

We show that equ for $\dot{\vec{k}}$ is consistent with energy conservation
 For motion in ~~the~~ electric field $\vec{E} = -\vec{\nabla}\phi$ electrostatic potential
 expect $\epsilon_n(\vec{k}(t)) - e\phi(\vec{r}(t))$ to be constant: band energy + electrostatic energy = constant

$$\Rightarrow \frac{d}{dt} [\epsilon_n(\vec{k}(t)) - e\phi(\vec{r}(t))] = 0$$

$$\Rightarrow \frac{d\epsilon_n}{d\vec{k}} \cdot \frac{d\vec{k}}{dt} - e \nabla\phi \cdot \frac{d\vec{r}}{dt} = 0$$

$$\text{or } \hbar \vec{v} \cdot \dot{\vec{k}} = -\vec{v} \cdot e\vec{E} \quad \Rightarrow \text{consistent equation}$$

comes true when $\hbar \dot{\vec{k}} = -e\vec{E}$ although when $\vec{H} = 0$

Could also have piece \perp to \vec{v} ~~to the direction of \vec{v}~~

although we haven't shown that only possible such

$$\text{piece is } -\frac{e}{c} \vec{v}_n \times \vec{H}$$

Consequences: Filled bands do not contribute to transport properties.

$$\text{electric current } \vec{j} = -e \int_{BZ} \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}}$$

$$\text{thermal current } \vec{j}_e = \frac{1}{2} \int_{BZ} \frac{d^3k}{4\pi^3} \frac{e}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}} (\epsilon) = \frac{1}{2} \int_{BZ} \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial \epsilon}{\partial \vec{k}} (\epsilon)^2$$

$$\vec{j} = \vec{j}_e = 0 \quad \text{for filled bands}$$

Proof:

If crystal has inversion symmetry $E(k) = E(-k)$,

$$E^2(k) = E^2(-k) \Rightarrow \frac{d}{dk} E^2(k) = -\frac{d}{dk} E^2(k)$$

$$\frac{d}{dk} E^2(k) = -\frac{d}{dk} E^2(-k) \quad \text{so these are odd functions}$$

so \int over 1st BZ vanishes.

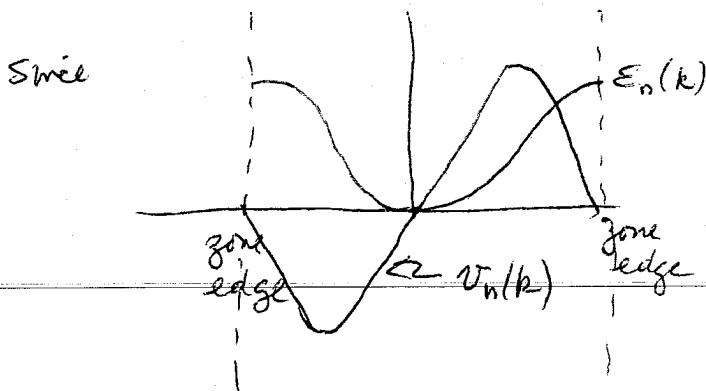
Actually ~~proof~~ this is true more generally, even if no inversion symmetry. Gradient of any periodic function always integrates to zero over unit cell. See text

$E(k)$ is periodic in translation by \vec{K}

Therefore current is carried only by partially full bands.
~~study of~~ Conduction electrons in Drude model should be just electrons in partially full bands.

Motion in DC \vec{E} fields

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}t}{\hbar} \quad \text{in general } \dot{\vec{v}} \neq \dot{\vec{k}}$$



so only when \vec{k} is ~~in center of~~ near band minimum $\dot{\vec{v}} \propto \dot{\vec{k}}$

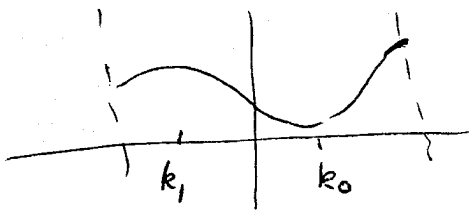
Near band max (near zone edge) $\dot{\vec{v}} \propto -\dot{\vec{k}}$

As electron approaches zone edge, it slows down and ~~also~~ reverses

If electron could travel distance in k -space larger than BZ size in between collisions, then a DC \vec{E} field would produce oscillating current! However collisions will spoil this effect. electron in general will ~~be~~ have only small changes in \vec{k} before it gets scattered and its \vec{k} randomized

However the fact that $\vec{k} \propto -\vec{v}$ near band max, produces the phenomena of holes - metal can behave as if it had positive carriers.

Consider 1-d example. Near band minimum at k_0



we can expand $E(k) \approx E(k_0) + \frac{E''(k_0)}{2}(k-k_0)^2$

where $E''(k_0) \equiv \frac{\hbar^2}{m^*} > 0$

we call m^* the effective mass of electrons at band minimum.

Then semiclassical equations are:

$$\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar} \frac{\partial E_n}{\partial \vec{k}} = \frac{1}{\hbar} \frac{\partial}{\partial \vec{k}} \left(\frac{\hbar^2}{2m^*} (k-k_0)^2 \right)$$

$v = \frac{\hbar(k-k_0)}{m^*}$ so just like classical particle of mass m^* , charge e

$$\hbar \dot{\vec{k}} = -e \left[\vec{E} + \frac{1}{c} \vec{v} \times \vec{H} \right]$$

$$\Rightarrow m^* \dot{\vec{v}} = -e \left[\vec{E} + \frac{1}{c} \vec{v} \times \vec{H} \right]$$

momentum

$$\hbar \dot{(k-k_0)} = m^* \dot{v}$$

So electrons near band minimum behave like classical electron of charge $-e$ and mass $m^* \equiv \hbar^2 / \frac{d^2 E}{dk^2}$

But for an electron near top of band, we expand

$$E(k) \approx E(k_1) + \frac{d^2 E}{dk^2}(k_1) \frac{(k - k_1)^2}{2}$$

where we define $\frac{d^2 E}{dk^2} = -\frac{\hbar^2}{m_h^*}$ where $m_h^* > 0$

Now $v(k) = \frac{-\hbar(k - k_1)}{m^*} \Rightarrow m_h^* \dot{v} = -\hbar \dot{k}$

so $\hbar \dot{k} = -e [E + \frac{v}{c} \times H] \Rightarrow m_h^* \dot{v} = +e [E + \frac{v}{c} \times H]$

electron near top of band behaves like classical particle of mass $m_h^* = -\hbar^2 / (\frac{d^2 E}{dk^2})$ and charge $+e$ - ie like a positive charge.

This is referred to as a hole!

In three dimensions, if max and min of band occur at point of cubic symmetry, we still can expand

$$E(\vec{k}) \approx E(\vec{k}_0) \pm \frac{\hbar^2}{2m^*} (\vec{k} - \vec{k}_0)^2$$

to define effective mass. However if no symmetry, then we need to define effective mass tensor

$$\hbar M_{ij}^{-1} \dot{k}_j = \dot{v}_i \quad m_{ij}^{-1} = \pm \frac{1}{\hbar^2} \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j} \Big|_{\vec{k}=\vec{k}_0}$$

equation of motion will be

$$M \cdot \dot{v} = \mp e (\vec{E} + \frac{\vec{v}}{c} \times \vec{H})$$

in most generality, away from max or min, can write

$$\dot{\vec{r}} = \frac{d}{dt} \left(\frac{1}{\hbar} \frac{\partial \mathcal{E}(\vec{k}(t))}{\partial \vec{k}} \right) = \frac{1}{\hbar} \frac{\partial \mathcal{E}(\vec{k}(t))}{\partial k_i} \frac{dk_i}{dt}$$

$$\text{define } M_{ij}^{-1}(\vec{k}) = \pm \frac{1}{\hbar^2} \frac{\partial \mathcal{E}(\vec{k})}{\partial k_i \partial k_j}$$

$$M^{-1}(\vec{k}) \dot{\vec{r}} = \mp e \left[\vec{E} + \frac{v(\vec{k})}{c} \times \vec{H} \right]$$

\pm taken depending on whether ~~take~~

$$\text{trace } \frac{\partial \mathcal{E}}{\partial k_i \partial k_j} \neq 0$$

\downarrow
 M_{ij}

So states ~~at~~ near top of band behave like (+) particles of mass m_h^*

To compute current in a partially full band, note

$$\vec{j} = -e \int_{\text{occupied states}} \frac{d^3 k}{4\pi^3} \vec{v}_n(\vec{k}) = -e \left[- \int_{\text{unoccupied states}} \frac{d^3 k}{4\pi^3} \vec{v}_n(\vec{k}) \right]$$

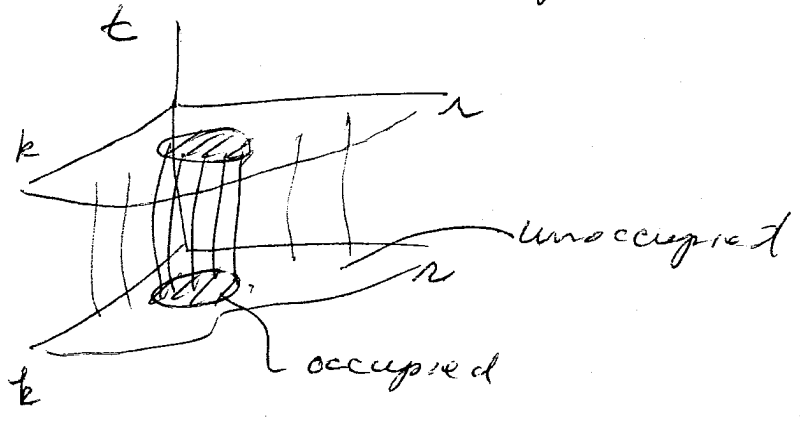
$$= +e \int_{\text{unoccupied}} \frac{d^3 k}{4\pi^3} \vec{v}_n(\vec{k})$$

$$\text{since } \int_{\text{occupied}} \vec{v} + \int_{\text{unocc}} \vec{v} = 0$$

~~So we can regard electric current as due to either the occupied electric states (with~~

So current due to electrons in occupied states is the same as current that would be if ~~no~~ these levels were empty and the ~~previously~~ unoccupied states were filled with particles of charge $+e$.

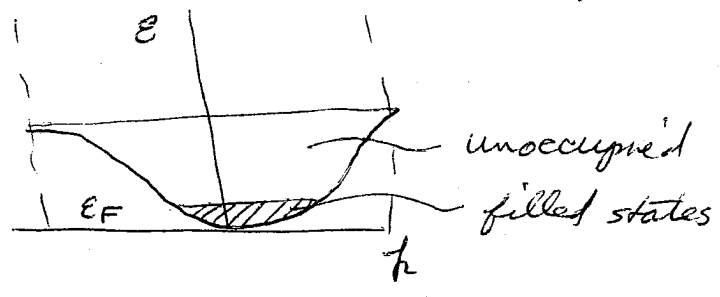
Note: unoccupied states evolve under same equations of motion as occupied states - as if they were filled with electrons of charge $-e$,



But unoccupied states generally lie near top of band, so they evolve in time like classical particles of charge $+e$!

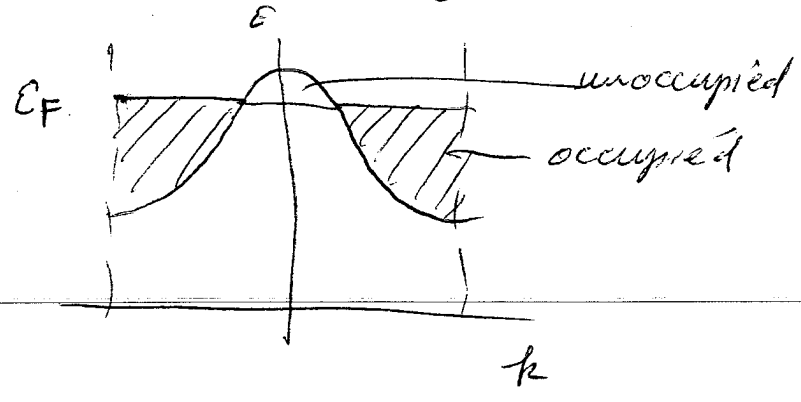
For a given band, we can choose to describe it in either the electron or hole picture, but not both

For a band mostly empty



convenient to describe as classical electrons of charge $-e$ and mass $m^* = \hbar^2 / \left(\frac{d^2E}{dk^2} \right)_{\text{min}}$

For a band mostly full



convenient to describe as classical particles (holes) of charge $+e$ and mass $m^* = -\hbar^2 / \left(\frac{d^2E}{dk^2} \right)_{\text{max}}$

Very unhelpful for describing semiconductors.