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. ⇒ 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.

*) Wave packet approx good only when applied fields vary slowly over dimensions of size of primitive cell.
(localize crystal momentum well on scale of 1^{st} BZ
⇒ wave packet in r-space extends over a few primitive cells)

*) Quantum effects are handled entirely through the band structure $\mathcal{E}_n(\vec{k})$ which we take as given functions. ~~has describes has 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 $\mathcal{E}_n(\vec{k})$. External slowly varying fields are treated in semi classical way

* Collisions can not be with static periodic ions. Their effect allready included in $\mathcal{E}_n(\vec{k})$.

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

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

see Apendix J) i) $eEa \ll [\mathcal{E}_{gap}(\vec{k})]^2/\mathcal{E}_F$ "electric breakdown" when fails

ii) $\hbar\omega_c \ll [\mathcal{E}_{gap}(\vec{k})]^2/\mathcal{E}_F$ "magnetic breakthrough" when fails

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

ii) possible in strong $\vec{H}$ fields

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

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

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

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

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 $f(\mathcal{E}_n(\vec{k})) = \dfrac{1}{e^{(\mathcal{E}_n(\vec{k})-\mu)/kT}+1}$

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

<u>Reasons to</u> believe Semi classical equations: For more see references given in text

$\dot{\vec{r}} = \vec{v}_n(k)$ is just definition of velocity
+ we derived earlier that $\vec{v}_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n}{\partial \vec{k}}$

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 $\mathcal{E}_n(\vec{k}(t)) - e\phi(\vec{r}(t))$ to be constant: band energy + electrostatic energy = constant

$$\Rightarrow \quad \frac{d}{dt}\left[\mathcal{E}_n(\vec{k}(t)) - e\phi(\vec{r}(t))\right] = 0$$

$$\Rightarrow \quad \frac{d\mathcal{E}_n}{d\vec{k}}\cdot\frac{d\vec{k}}{dt} - e\,\vec{\nabla}\phi\cdot\frac{d\vec{r}}{dt} = 0$$

or $\hbar\vec{v}\cdot\dot{\vec{k}} = -\vec{v}\cdot e\vec{E}$ $\Rightarrow$ consistent — plug in $\hbar\dot{\vec{k}}$ = semi class equation

~~[illegible]~~ true when $\hbar\dot{\vec{k}} = -e\vec{E}$ ~~although~~ when $\vec{H} = 0$
Could also have piece ~~⊥~~ to ~~[illegible]~~ $\vec{v}$
although we havent shown that only possible such piece is $-\frac{e}{c}\vec{v}_n \times \vec{H}$

<u>Consequences</u>: Filled bands do not contribute to transport properties.

electric current $\quad \vec{j} = -e\int_{BZ}\frac{d^3k}{4\pi^3}\,\frac{1}{\hbar}\frac{\partial\mathcal{E}}{\partial\vec{k}}$

thermal current $\quad j_{\mathcal{E}} = \int_{BZ}\frac{d^3k}{4\pi^3}\,\frac{\mathcal{E}}{\hbar}\frac{\partial\mathcal{E}}{\partial\vec{k}} = \frac{1}{2}\int\frac{d^3k}{4\pi^3}\frac{1}{\hbar}\frac{\partial}{\partial\vec{k}}(\mathcal{E}^2)$

$\vec{j} = \vec{j}_\varepsilon = 0$ for filled bands

Proof:

If crystal has inversion symmetry $\varepsilon(k) = \varepsilon(-k)$,
$\varepsilon^2(k) = \varepsilon^2(-k) \Rightarrow \frac{d}{dk}\varepsilon(k) = -\frac{d}{dk}\varepsilon(-k)$
$\frac{d}{dk}\varepsilon^2(k) = -\frac{d}{dk}\varepsilon^2(-k)$ 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 <u>any</u> periodic function always integrates to zero over unit cell. See text
$\varepsilon(k)$ is periodic in translation by $\vec{K}$

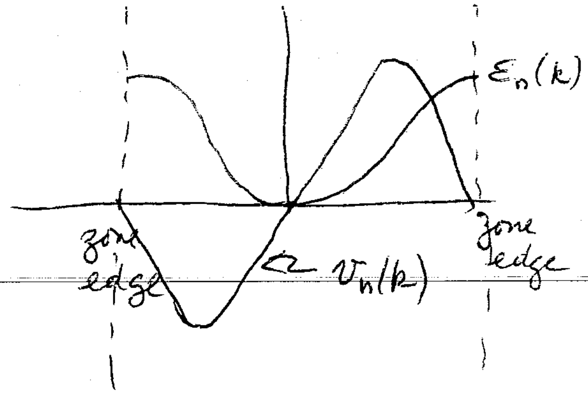
Therefore current is carried only by <u>partially</u> full bands. ~~density of~~ Conduction electrons in Drude model should be just electrons in partially full bands.

<u>Motion in DC $\vec{E}$ field</u>

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}t}{\hbar}$$

in general $\dot{\vec{v}} \not\propto \dot{\vec{k}}$

Since



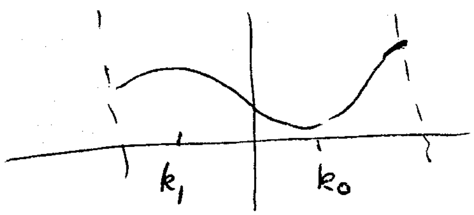
so only when $\vec{k}$ is ~~in center of~~ near band ~~to~~ minimum is $\dot{\vec{v}} \propto \dot{\vec{k}}$. Near band max (near zone edge) $\dot{\vec{v}} \propto -\dot{\vec{k}}$
As electron approaches zone edge, it slows down and ~~slo~~ ... in reverse

due to scattering at Brag...

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 $\dot{\vec{k}} \propto -\dot{\vec{v}}$ 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 $\mathcal{E}(k) \sim \mathcal{E}(k_0) + \frac{\mathcal{E}''(k_0)}{2}(k-k_0)^2$
where $\mathcal{E}''(k_0) \equiv \hbar^2/m^* > 0$
we call m^* the effective mass of electrons at band minimum.

Then semiclassical equations are:

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

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

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

~~momentum~~ $\hbar(k-k_0) = m^* v$

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

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

But for an electron near top of band, we expand

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

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

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

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

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

This is refered to as a hole!

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

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

to define effective mass. However if no symmetry, then we need to define effective mass <u>tensor</u>

$\hbar M^{-1}_{ij}\dot{k}_j = \dot{v}_i$ $\qquad M^{-1}_{ij} = \pm\dfrac{1}{\hbar^2}\dfrac{\partial^2\mathcal{E}(\vec{k})}{\partial k_i\,\partial k_j}\Big|_{\vec{k}=\vec{k}_0}$

equation of motion will be

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

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

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

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

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

$\pm$ taken depending on whether ~~both~~ the trace $\underset{M_{ij}}{\frac{\partial \mathcal{E}}{\partial k_i \partial k_j}} \gtrless 0$

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

To compute current in a partially full band, note

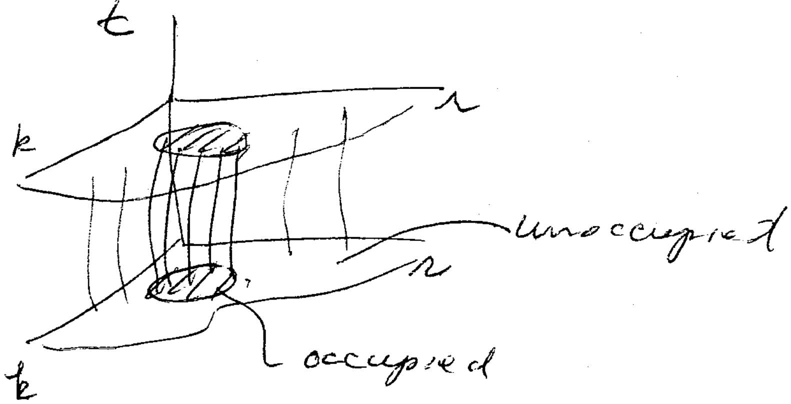
$$\vec{j} = -e\int_{\substack{\text{occupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k}) = -e\left[-\int_{\substack{\text{unoccupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k})\right]$$

$$= +e\int_{\text{unoccupied}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k}) \qquad \text{since } \int_{\text{occupied}}\vec{v} + \int_{\text{unocc}}\vec{v} = 0$$

~~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 ~~we~~ ~~if~~ these levels were~~ empty and the ~~previously~~ unoccupied states were filled with particles of charge $+e$.

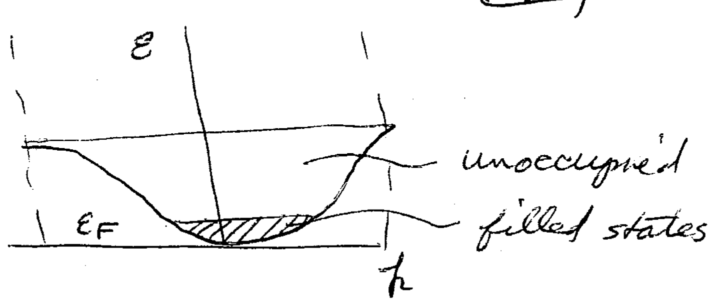
Note: unoccupied states evolve under same equations of motion as occupied states – as if they were filled with electrons of charge $-e$,



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

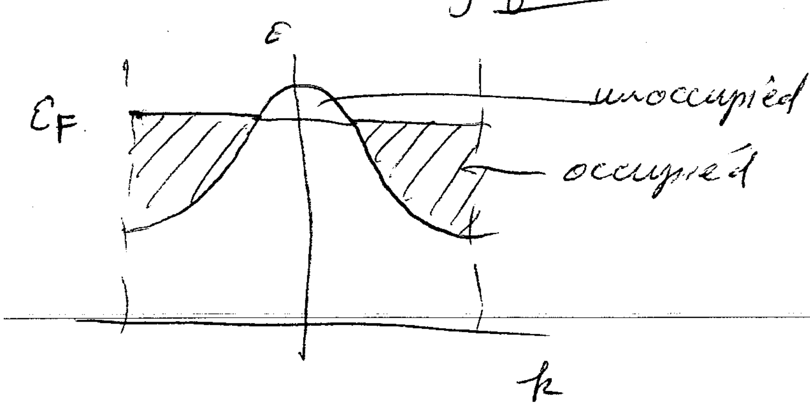
For a given band, we can choose to describe it in <u>either</u> the electron or hole picture, <u>but not both</u>

For a band mostly <u>empty</u>



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

For a band mostly <u>full</u>



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

very useful for describing semiconductors.