<u>Semi classical approx</u> 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, <u>inbetween collisions</u>. 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 1st BZ
    ⇒ wave packet in r-space extends over a few primitive cells)

*) Quantum effects are handled entirely through the band structure $E_n(\vec{k})$ which we take as given functions. ~~This describes this 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 semi classical way.

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

)(<u>In the absence of collisions</u>, n, $\vec{k}$, $\vec{r}$ evolve as

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

A+M
(see Apendix J) i) $eEa \ll [\varepsilon_{gap}(\vec{k})]^2 / \varepsilon_F$ "electric breakdown" when fails

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

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

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

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

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

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

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

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

*) $\hbar \vec{k}$ is not total momentum. $\dot{\vec{p}}$ is given by <u>total force</u>
(includes ion potential) $\hbar \dot{\vec{k}}$ is given by ~~applied force~~ only.

reasons to believe Semi classical equations: For more see references given in text

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

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

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

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

$$\Rightarrow \quad \hbar \vec{v} \cdot \dot{\vec{k}} = -\vec{v} \cdot e\vec{E} \quad \longleftarrow \begin{array}{l} \text{consistent with} \\ \text{semi classical equ} \\ \text{when } \vec{H} = 0 \end{array}$$

~~cross~~ true when $\hbar\dot{\vec{k}} = -e\vec{E}$

Could also have piece $\perp$ to $\vec{v}$

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 $\quad \dot{j}_{\mathcal{E}} = \int_{BZ} \frac{d^3k}{4\pi^3} \frac{\mathcal{E}}{\hbar} \frac{\partial \mathcal{E}}{\partial \vec{k}} \quad = \frac{1}{2} \int \frac{d^3k}{4\pi^3} \frac{1}{\hbar} \frac{\partial}{\partial \vec{k}} (\mathcal{E}^2$

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

Proof:

If crystal has inversion symmetry $\begin{cases} \varepsilon(k) = \varepsilon(-k), \\ \frac{d}{dk}\varepsilon(k) = -\frac{d}{dk}\varepsilon(-k) \end{cases}$

$\begin{cases} \varepsilon^2(k) = \varepsilon^2(-k) \\ \frac{d}{dk}\varepsilon^2(k) = -\frac{d}{dk}\varepsilon^2(-k) \end{cases}$ so $\frac{d\varepsilon}{dk}$ and $\frac{d\varepsilon^2}{dk}$ are odd functions of k

so $\int$ over 1st BZ vanishes.

Actually this is true more generally, even if no inversion symmetry. Gradient of any periodic function always integrates to zero over unit cell. See text $\varepsilon(k)$ is periodic in translation by $\vec{k}$
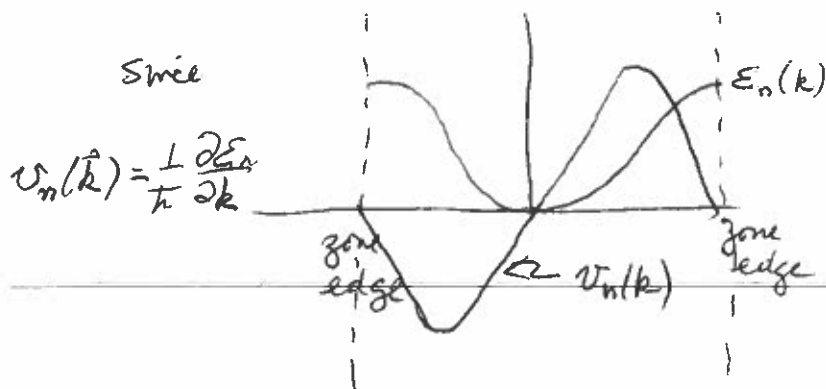
Therefore current is carried only by ~~partially~~ full bands. ~~Conductivity~~ Conduction electrons in Drude model should be just electrons in partially full bands.

Motion in DC $\vec{E}$ field

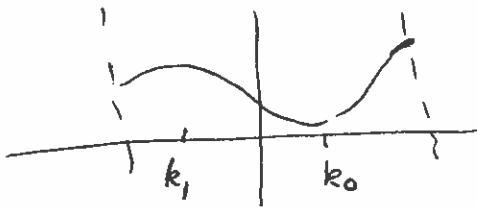$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}t}{\hbar} \qquad \text{in general } \dot{\vec{v}} \not{\propto} \dot{\vec{k}}$$

Since

$$v_n(\vec{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_n}{\partial k}$$

$\varepsilon_n(k)$

zone edge

zone edge

$\leftarrow v_n(k)$

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

If electron could travel distance in k-space larger than BZ size in between collisions, then a DC $\vec{E}$ field would produce <u>oscillating</u> 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.

can see in semiconductor superlattices and cold atoms in optical traps

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

* This effect is called <u>Bloch oscillations</u>

Consider 1-d example. Near band minimum at k_0 we can expand $\varepsilon(k) \sim \varepsilon(k_0) + \frac{\varepsilon''(k_0)(k-k_0)^2}{2}$

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

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

Then semiclassical equations are:

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

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

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

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

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

But for an electron near top of band, we expand

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

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

Now

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

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

electron near top of band behaves, like classical particle of mass $m_h^* = -\hbar^2/\left(\frac{d^2\varepsilon}{dk^2}\right)$ 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

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

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

$$\hbar M_{ij}^{-1}\dot{k}_j = \dot{v}_i \quad\bigg\rangle \qquad M_{ij}^{-1} = \pm\frac{1}{\hbar^2}\frac{\partial^2\varepsilon(\vec{k})}{\partial k_i \partial k_j}\bigg|_{\vec{k}=\vec{k}_0} \qquad \begin{array}{l} + \text{ for min} \\ - \text{ for max} \end{array}$$

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

$$\dot{\vec{v}} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial \mathcal{E}(\vec{k}(t))}{\partial \vec{k}}\right) = \frac{1}{\hbar}\frac{\partial \mathcal{E}(k(t))}{\partial k_i \partial k_j}\frac{dk_j}{dt} = M^{-1}_{ij}\hbar\dot{k}_j$$

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

$$\Rightarrow \hbar\dot{k}_\ell = M_{ij}\ddot{\vec{r}}_j$$
$$= M_{ij}\dot{\vec{v}}_j$$

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

$\pm$ taken depending on whether trace $\frac{\partial \mathcal{E}}{\partial k_i \partial k_j} \gtrless 0$

v

M_{ij}

So states near top of band behave like (+) particles of mass $m_h^\times$

To compute current in a partially full band, note

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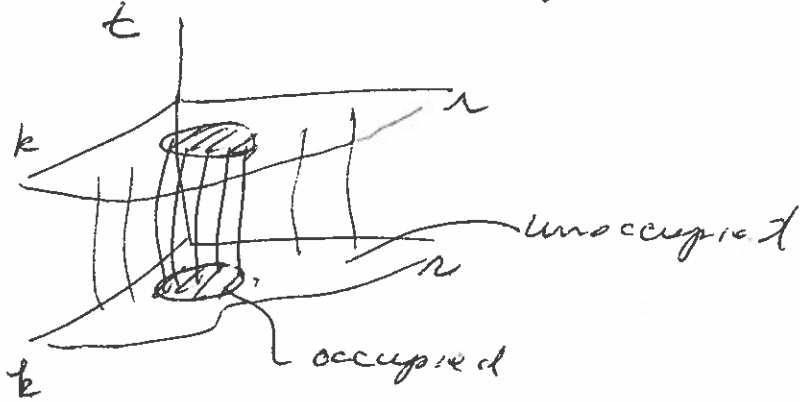
$$= +e\int_{unoccupied}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k})$$

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

~~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 these levels were~~ empty and the ~~previously~~ unoccupied states were filled with particles of charge $+e$.
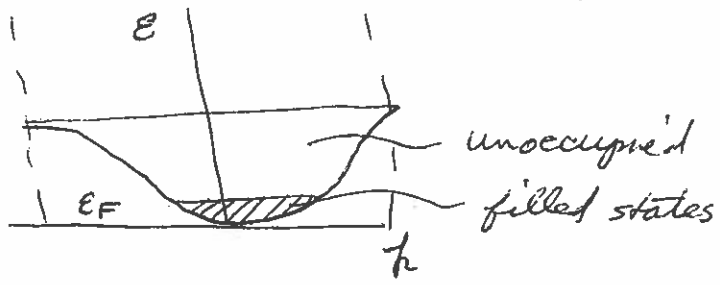
Note: unoccupied states evolve under same equations of motion as occupied states — as if they were filled with electrons of charge $-e$.

— unoccupied

— occupied

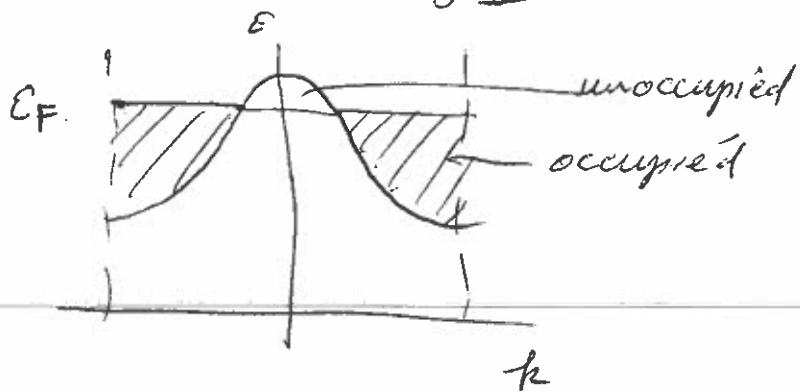But unoccupied states generally lie near top of band, so they evolve in time like _classical_ particles of charge $+e$!

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_

— unoccupied

— filled states

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 _full_

— unoccupied

— occupied

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

very useful for describing semiconductors.