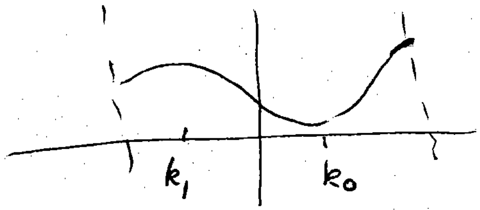
If electron could travel distance in $k$-space larger than BZ size in between collisions, then a DC $\vec{E}$ field would produce oscillating current! However collisions will spoil this effect. electron in general will ~~be~~ have only small changes in $\vec{k}$ before it gets scattered and its $\vec{k}$ 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 $\mathcal{E}''(k_0) \equiv \frac{\hbar^2}{m^*} > 0$

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

Then semiclassical equations are:

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

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

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

$$\cancel{\hbar\dot{k} = -e\left[E + \frac{\hbar k}{cm^*}\times H\right]}$$

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

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

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

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

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

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

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>

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

equation of Motion will be

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

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

$$\dot{\vec{v}} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k}(t))}{\partial \vec{k}}\right) = \frac{1}{\hbar}\frac{\partial \varepsilon(k(t))}{\partial k_i \partial k_j}\frac{dk_j}{dt}$$

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

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

$\pm$ taken depending on whether ~~the~~ the trace $\frac{\partial \varepsilon}{\partial k_i \partial k_j} \gtrless 0$

$M_{ij}$

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

To compute current in a partially full band, note

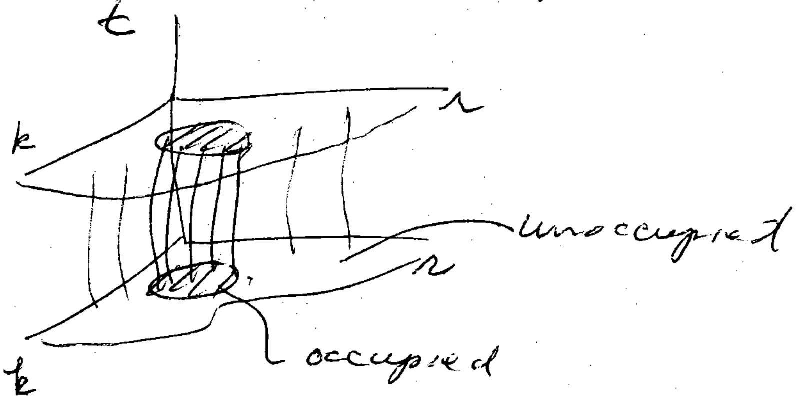
$$\vec{j} = -e\int_{\substack{\text{occupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k}) = -e\left[-\int_{\substack{\text{unoccupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k})\right]$$

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

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

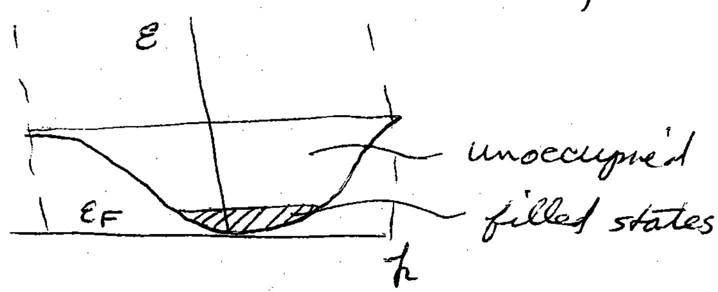
Note: unoccupied states evolve under same equations of motion as occupied states – as if they were filled with electrons of charge $-e$,




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

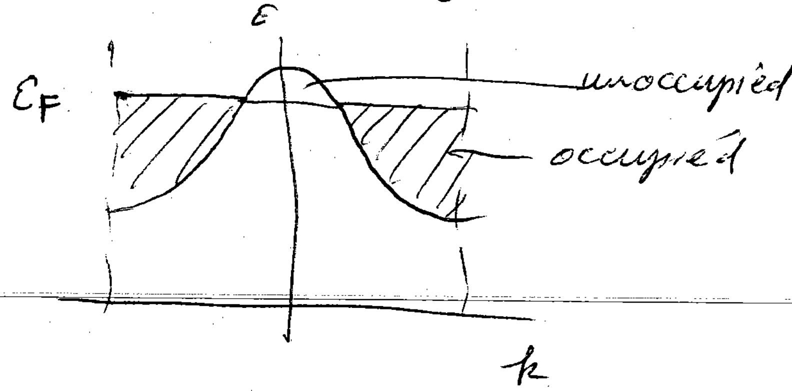
For a given band, we can choose to describe it in *either* the electron or hole picture, *but not both*

For a band mostly *empty*




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

For a band mostly *full*




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

very useful for describing semiconductors.

## Motion in Uniform magnetic field

$$\dot{\vec{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \qquad \hbar\dot{\vec{k}} = -e\,\frac{1}{c}\,\vec{v}(\vec{k}) \times \vec{H}$$

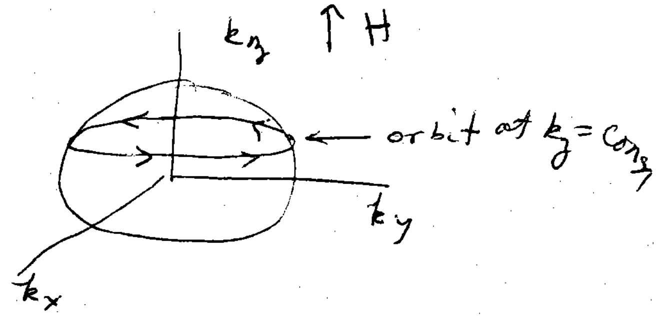
For motion in uniform field, $\dot{\varepsilon}(\vec{k}(t)) = \frac{d\varepsilon}{d\vec{k}} \cdot \frac{d\vec{k}}{dt} = \hbar\vec{v} \cdot \dot{\vec{k}} = 0$

since $\vec{v} \cdot (\vec{v} \times \vec{H}) = 0$

so electron moves on surface of constant energy.
also $\frac{d}{dt}(\vec{k} \cdot \vec{H}) = \dot{\vec{k}} \cdot \vec{H} = 0$ as $\vec{H} \cdot (\vec{v} \times \vec{H}) = 0$

$\Rightarrow$ electrons move on curves formed by intersection of plane of constant ~~$k_z$ (take H in z-dir)~~ $k_{\parallel}$, with surfaces of constant energy.

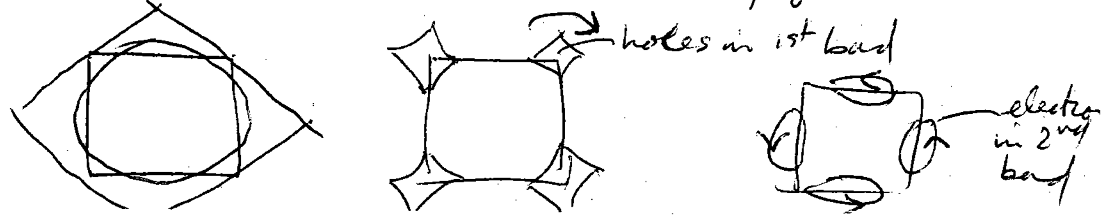
For spherical energy surface




Sence of orbit: since $\vec{v} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial \vec{k}}$ points from low $\varepsilon$ to higher $\varepsilon$
If H is up, one walks in orbit so that higher energy states are on right as $\dot{\vec{k}} \sim \vec{H} \times \vec{v}$

for closed orbits, If surface encloses region of higher energy (hole orbit), direction is oposite than if surface encloses lower energy (electron orbit)

ex: 3-d cubic, $\hat{H} \parallel \hat{z}$ so in nearly free electron approx



$\epsilon_{ijk} \epsilon_{klm} = \delta_{il}\delta_{km} - \delta_{jm}\delta_{lk}$

The real space orbits $(\vec{r}(t))$ can be found:

$$\vec{r}_\perp \equiv \vec{r} - \hat{H}(\hat{H}\cdot\vec{r}) \qquad \text{position in plane} \perp \text{to } H$$

$$\hat{H} \times \hbar\dot{\vec{k}} = -\frac{e\hat{H}}{c} \times (\vec{v} \times \vec{H}) = -\frac{e}{c} H(\dot{\vec{r}} - \hat{H}(\hat{H}\cdot\dot{\vec{r}}))$$

using $\vec{v} = \dot{\vec{r}}$ & vector identity

$$= -\frac{eH}{c}\dot{\vec{r}}_\perp$$

$$\text{so } \vec{r}_\perp(t) - \vec{r}_\perp(0) = -\frac{\hbar c}{eH}\hat{H} \times (\vec{k}(t) - \vec{k}(0))$$

So $\vec{r}_\perp$ orbit is just $\vec{k}$ orbit rotated by $90°$ about $\vec{H}$, and scaled by $\frac{\hbar c}{eH}$

in $\parallel$ direction

$$r_\parallel(t) = r_\parallel(0) + \int_0^t v_\parallel(t)\,dt = r_\parallel(0) + \int_0^t \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial k_\parallel}\,dt$$

need not be uniform in $t$ as $\frac{\partial}{\partial k_\parallel}\varepsilon(\vec{k})$ can vary as $k_\perp$ varies.

For spherical energy surface, we get classical result: electron moves in circular obit $\perp$ to $\vec{H}$.
However energy surfaces need not be spherical - (when they get too near zone boundaries) - need not be <u>closed curves</u>! See figure 12.8 in text

~~When orbits are open, applying H can lead to~~