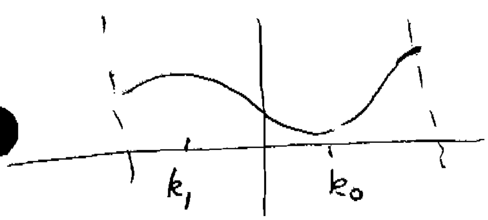
If electron could travel distance in k-space larger than BZ size in between collisions, then a DC $\vec{E}$ field would produce <u>oscillating</u> current! However collisions will spoil this effect. electron in general will ~~be~~ have only small changes in $\vec{k}$ before it gets scattered and its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

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

Consider 1-d example. Near band minimum at k_0



we can expand $\mathcal{E}(k) \sim \mathcal{E}(k_0) + \frac{\mathcal{E}''(k_0)}{2}($

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:

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

$$v = \frac{\hbar(k-k_0)}{m^*}$$ so just like classical parti[cle] of mass m^*, char[ge]

~~momentum~~

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

$$\cancel{\Rightarrow -e\left[E + \frac{\hbar k}{cm^*}\times H\right]} \qquad \cancel{\hbar(k-k_0)} = m^* v$$

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

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

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

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>

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

~~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

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

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

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

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

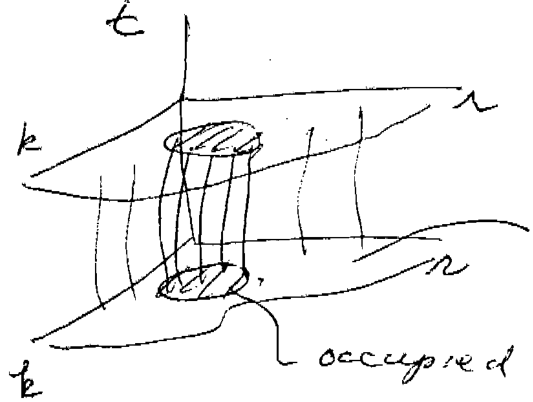
$$\vec{j} = -e\int_{\substack{\text{occupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k}) = -e\left[-\int_{\substack{\text{unoccupied}\\\text{states}}}\frac{d^3k}{4\pi^3}\vec{v}_n(\vec{k})\right]$$

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

~~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 $+e$.

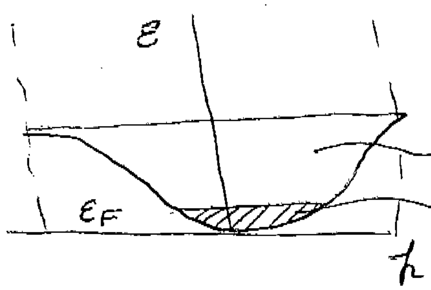
Note: unoccupied states evolve under same equations of motion as occupied states – as if they were filled with electrons of charge $-e$,



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

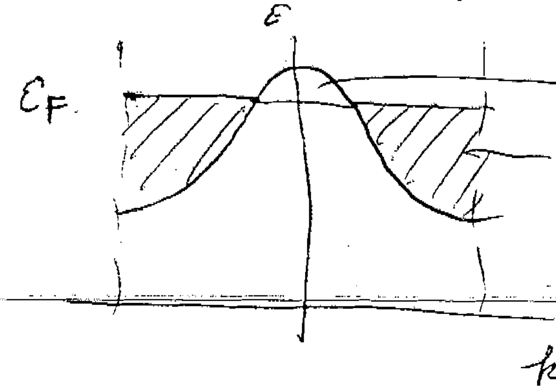
For a given band, we can choose to describe it in either the electron or hole picture, but not both

For a band mostly empty



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

For a band mostly full



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

very useful for describing semiconductors.

Motion in Uniform Magnetic field

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

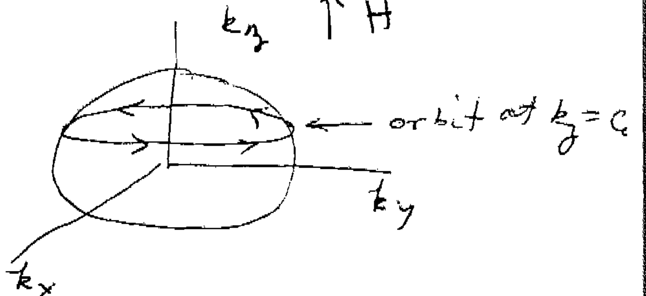
For motion in uniform field, $\dot{\varepsilon}(\vec{k}(t)) = \frac{d\varepsilon}{d\vec{k}}\cdot\frac{d\vec{k}}{dt} = \hbar\vec{v}\cdot\dot{\vec{k}} = 0$ since $\vec{v}\cdot(\vec{v}\times\vec{H}) = 0$

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

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

For spherical energy surface

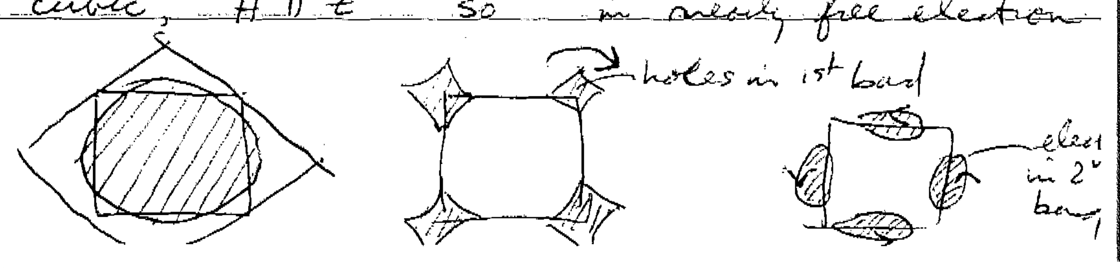


Sence of orbit: since $\vec{v} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}}$ points from low ε to higher ε

If H is up, one walks in orbit so that higher energy state 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



$$\epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$$

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 $\vec{v} = \dot{\vec{r}}$

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

+ vector identity

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

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

<u>in $\parallel$ direction</u>

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

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 orbit $\perp$ to $\hat{H}$.
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~~

Motion in uniform $\perp$ $\vec{E}$ and $\vec{H}$ fields
Hall effect and magnetoresistance

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

$$\Rightarrow \quad \hat{H} \times \hbar \dot{\vec{k}} = -e\,\hat{H} \times \vec{E} - \frac{eH}{c}\dot{\vec{r}}_\perp$$

$$\dot{\vec{r}}_\perp = -\frac{\hbar c}{eH}\hat{H} \times \dot{\vec{k}} + \vec{w} \qquad\qquad \vec{w} = \frac{cE}{H}(\hat{E} \times \hat{H})$$

Motion is as before, but with drift velocity $\vec{w}$ added.

To determine orbits in k space note:

$$\hbar \dot{\vec{k}} = -e\vec{E} - \frac{e}{c}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \vec{k}} \times \vec{H} \qquad\qquad \text{write } \vec{E} = -(\vec{E} \times \hat{H}) \times \hat{H}$$

true when $\vec{E} \perp \vec{H}$

$$= -\frac{e}{c\hbar}\left(\frac{\partial \varepsilon}{\partial \vec{k}} - \frac{c\hbar E}{H}\hat{E} \times \hat{H}\right) \times \vec{H}$$

$$\equiv -\frac{e}{c\hbar}\frac{\partial \bar{\varepsilon}}{\partial \vec{k}} \times \vec{H} \qquad\qquad \bar{\varepsilon} = \varepsilon - \hbar \vec{k} \cdot \vec{w}$$

Same as if $\vec{E}$ was absent and band structure replaced by

$$\bar{\varepsilon}(\vec{k}) = \varepsilon(\vec{k}) - \hbar \vec{k} \cdot \vec{w}$$

Orbits are intersections of surfaces of constant $\bar{\varepsilon}$ with planes $\perp$ to $\vec{H}$

We will assume that $-\hbar \vec{k} \cdot \vec{w}$ small enough so that if the constant $\varepsilon(k)$ surface is closed (open) so is the constant $\bar{\varepsilon}(k)$ surface. Good approx in most cases - see text for estimate of numbers.