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

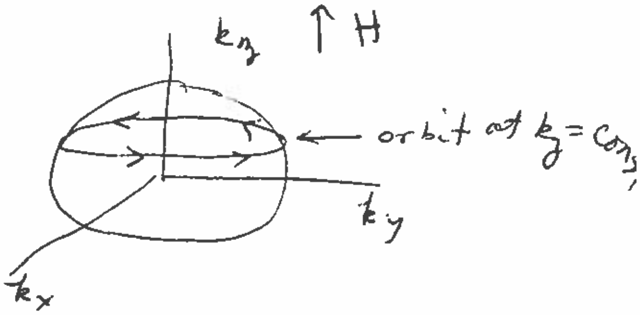
since $\vec{v}\cdot(\vec{v}\times\vec{H}) = 0$

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)~~ $k_{\parallel}$, with surfaces of constant energy.

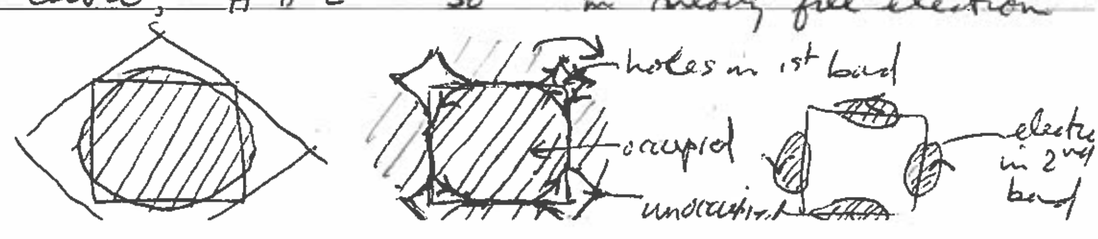
For spherical energy surface



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 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: 2-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

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

so $\vec{r}_\perp(t) - \vec{r}_\perp(0) = -\dfrac{\hbar c}{eH} \hat{H} \times (\vec{k}(t) - \vec{k}(0))$ ~~[illegible]~~

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

in ∥ 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 $\dfrac{\partial}{\partial k_\parallel}\varepsilon(\vec{k})$ 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~~

key for understanding magnetoresistance

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

Hall effect and magnetoresistance

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

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

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

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

To determine orbits in k space note:

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

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

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

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

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

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

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

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

in nearly free electron model

$$\varepsilon(\vec{k}) \simeq \frac{\hbar^2}{2m}\vec{k}^2$$

surface of constant energy ε is sphere of radius $\sqrt{\frac{2m\varepsilon}{\hbar^2}} = k$ in k-space

$$\bar{\varepsilon}(\vec{k}) = \frac{\hbar^2\vec{k}^2}{2m} - \hbar\vec{w}\cdot\vec{k}$$

surface of constant $\bar{\varepsilon}$ is given by

$$\frac{\hbar^2}{2m}\left|\vec{k} - \frac{m\vec{w}}{\hbar}\right|^2 = \bar{\varepsilon} + \tfrac{1}{2}mw^2$$

sphere in k-space of radius

$$k = \sqrt{\frac{2m}{\hbar^2}\left(\bar{\varepsilon} + \tfrac{1}{2}mw^2\right)}$$

centered about $\vec{k}_0 = m\vec{w}/\hbar$

surface of constant $\bar{\varepsilon}$ is shifted by $\vec{w}\cdot\vec{k}$ term in direction $\vec{w}$

<u>Hall effect</u>: $\dot{\vec{r}}_\perp = -\frac{\hbar c}{eH}\,\hat{H}\times\dot{\vec{k}} + \vec{w}$, $\vec{w} = \frac{cE}{H}(\hat{E}\times\hat{H})$

current in plane $\perp$ to H is

$\vec{j} = -ne\langle\dot{\vec{r}}_\perp\rangle$ where $\langle\dot{\vec{r}}_\perp\rangle$ is steady state average over all occupied electron orbits, and over collisions

$$\vec{j} = -ne\vec{w} + \frac{ne\hbar c}{eH}\,\hat{H}\times\langle\dot{\vec{k}}\rangle$$

<u>Case (1)</u> All occupied (or unoccupied) orbits are <u>closed</u>
Then for <u>large enough H</u> so that $\omega_c\tau \gg 1$ (where τ is collision time, and $\omega_c = eH/m^*c$), electron makes many periods of its closed orbits between successive collisions.

We can estimate $\langle\dot{\vec{k}}\rangle$ in this large H case as follows: Averaging over electron motion between two successive collision at $t=0$ and $t=t_0$ we get

$$\langle\dot{\vec{k}}\rangle = \frac{1}{t_0}\int_0^{t_0}\dot{\vec{k}}(t)\,dt = \frac{\vec{k}(t_0)-\vec{k}(0)}{t_0}$$

where $\vec{k}(0)$ is wave vector of electron as it emerges from the first collision at $t=0$, and $\vec{k}(t_0)$ is wave vector of electron just before second collision at $t=t_0$

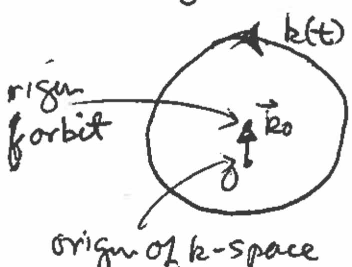
As in the Drude model, we may assume that electrons emerge from a collision with an equilibrium distribution determined by the local temperature + chemical potential. Since the Fermi distribution $f(\varepsilon(k)) = \frac{1}{1+e^{\beta(\varepsilon-}}$
depends on $\vec{k}$ only via energy $\varepsilon(\vec{k})$, and $\varepsilon(\vec{k}) = \varepsilon(-\vec{k})$,

We have, after averaging over the electron energy from the collision at $t=0$, $\langle \vec{k}(0) \rangle = 0$. So $\langle \dot{\vec{k}} \rangle = \vec{k}(t_0)/t_0$.

We now average over the time until the second collision, $\langle t_0 \rangle = \tau$ (this time is distributed randomly with average equal to τ). Since $\omega_c \tau \gg 1$, the electron makes many orbits between collisions, $\Rightarrow \vec{k}(t_0)$ when averaged over collision time t_0, is equally likely to lie anywhere along the closed orbit.

$\Rightarrow \langle \vec{k}(t_0) \rangle =$ (average $\vec{k}$ on orbit). If electric field $\vec{E}=0$, then (average $\vec{k}$ on orbit) $=0$ also. But when $E \neq 0$, (average $\vec{k}$ on orbit) $\sim m^* \vec{w}/\hbar$. To see this, use effective mass approximation, $\varepsilon(k) \simeq \frac{\hbar^2 k^2}{2m^*}$.

Then orbit lies on curve of constant $\bar{\varepsilon}(k) = \varepsilon(k) - \hbar \vec{k} \cdot \vec{w}$, which lies on sphere centered at $\vec{k}_0 = m^* \vec{w}/\hbar$. So (average $\vec{k}$ on orbit) $= \langle \vec{k}(t_0) \rangle = \vec{k}_0$



$$\Rightarrow \langle \dot{\vec{k}} \rangle = \frac{\langle \vec{k}(t_0) \rangle}{\tau} = \frac{\vec{k}_0}{\tau} = \frac{m^* \vec{w}}{\hbar \tau}.$$

So contribution of $\langle \dot{\vec{k}} \rangle$ term to current is

$$\frac{ne\hbar c}{eH} \hat{H} \times \frac{m^* \vec{w}}{\hbar \tau} = \frac{ne}{\omega_c \tau} \hat{H} \times \vec{w}$$

smaller than drift contribution to current $\vec{j} \simeq -ne\vec{w}$ by a factor $\frac{1}{\omega_c \tau} \ll 1$

So $\vec{j} \simeq -ne\vec{w}$ given just by drift velocity $\vec{w}$ in high field limit.

Let us keep the contribution from $\langle \dot{\vec{k}} \rangle$.

~~Then~~ (we will need that term to get magnetoresistance)

$$\vec{j} = -ne\vec{w} + \frac{ne}{\omega_c\tau}\hat{H}\times\vec{w} \qquad \vec{w} = \frac{cE}{H}(\hat{E}\times\hat{H})$$

Take $\hat{H} = \hat{z}$

$$\vec{j} = \frac{nec}{H}\left(\hat{z}\times\vec{E} + \frac{1}{\omega_c\tau}\vec{E}\right)$$

write in terms of a conductivity tensor $\vec{j} = \overleftrightarrow{\sigma}\cdot\vec{E}$

$$\overleftrightarrow{\sigma} = \frac{nec}{H}\begin{pmatrix} \frac{1}{\omega_c\tau} & -1 \\ 1 & \frac{1}{\omega_c\tau} \end{pmatrix}$$

or using $\frac{nec}{H} = \left(\frac{ne^2\tau}{m^*}\right)\Big/\left(\frac{m^*c}{eH\tau}\right) = \frac{\sigma_0}{\omega_c\tau}$

$$\overleftrightarrow{\sigma} = \sigma_0\begin{pmatrix} \frac{1}{(\omega_c\tau)^2} & \frac{-1}{\omega_c\tau} \\ \frac{1}{\omega_c\tau} & \frac{1}{(\omega_c\tau)^2} \end{pmatrix}$$

Resistivity tensor is then

$$\overleftrightarrow{\rho} = \overleftrightarrow{\sigma}^{-1} = \frac{1/\sigma_0}{\frac{1}{(\omega_c\tau)^4} + \frac{1}{(\omega_c\tau)^2}}\begin{pmatrix} \frac{1}{(\omega_c\tau)^2} & \frac{1}{\omega_c\tau} \\ \frac{-1}{\omega_c\tau} & \frac{1}{(\omega_c\tau)^2} \end{pmatrix}$$

$$= \frac{1/\sigma_0}{1 + \frac{1}{(\omega_c\tau)^2}}\begin{pmatrix} 1 & \omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix}$$

At large H fields so that $\omega_c\tau \gg 1$ we then have

$$\overleftrightarrow{\rho} \simeq \frac{1}{\sigma_0}\begin{pmatrix} 1 & \omega_c\tau \\ -\omega_c\tau & 1 \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix}$$

$$\rho_{yx} = -\rho_{xy}$$

$$\vec{E} = \overleftrightarrow{\rho} \cdot \vec{j}$$

For $\vec{j} = j\hat{x}$ then $E_y = \rho_{yx} j = -\rho_{xy} j$

Hall coefficient $R = \dfrac{E_y}{jH} = \dfrac{-\rho_{xy}}{H} = \dfrac{-\omega_c\tau}{\sigma_0 H}$

$$R = \frac{-eH}{m^*c}\,\frac{\tau m^*}{ne^2\tau}\,\frac{1}{H} = \frac{-1}{nec}$$ Drude value!

So we regain the Drude prediction, but only in the limit of large H, ie $\omega_c\tau \gg 1$

The above was for <u>closed occupied orbits</u>
If we had <u>closed unoccupied orbits</u>
we would use instead the hole picture

Now we would have

$$\vec{j} = +n_h e\vec{w} - \frac{n_h e\vec{H}^* \times \vec{w}}{\omega_c\tau}$$

where n_h is density of holes, and holes act like particles of charge $+e$

All results follow through just taking $-e \to +e$, ~~and we get~~ $n \to n_h$, $m^* \to m^*_h$, and we get

$$R_H = \frac{+1}{n_h e c}$$

now the Hall coefficient is <u>positive</u>!

<u>Magnetoresistance</u>

$$\rho(H) = \frac{E_x}{j} = \rho_{xx} = \frac{1}{\sigma_0}$$

same for electrons and holes

$$\sigma_0 = \frac{ne^2\tau}{m^*} \text{ electrons}, \quad \sigma_0 = \frac{n_h e^2 \tau}{m^*_h} \text{ for holes}$$

<u>For more than one partially filled band</u>

$$\overleftrightarrow{\sigma} = \overleftrightarrow{\sigma}_1 + \overleftrightarrow{\sigma}_2 = \frac{\sigma_{01}}{\omega_{c1}\tau_1}\begin{pmatrix} \frac{1}{\omega_{c1}\tau_1} & -1 \\ 1 & \frac{1}{\omega_{c1}\tau_1} \end{pmatrix}$$

$$+ \frac{\sigma_{02}}{\omega_{c2}\tau_2}\begin{pmatrix} \frac{1}{\omega_{c2}\tau_2} & -1 \\ 1 & \frac{1}{\omega_{c2}\tau_2} \end{pmatrix}$$

For the Hall coefficient in $\omega_c\tau \gg 1$ limit, we can ignore the diagonal terms to write

$$\overleftrightarrow{\sigma} = \left(\frac{\sigma_{01}}{\omega_{c1}\tau_1} + \frac{\sigma_{02}}{\omega_{c2}\tau_2}\right)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$= \left(\frac{n_1 e_1 c}{H} + \frac{n_2 e_2 c}{H}\right)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

where $e_{1,2} = \begin{cases} e & \text{if electron} \\ -e & \text{if hole} \end{cases}$

$$\overleftrightarrow{\sigma} = \frac{n_{eff}\, e c}{H} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

where $n_{eff} = n_1 + n_2$ if both bands are electrons

$= n_1 - n_2$ if band 1 is electrons, band 2 is holes

etc.

Hall coefficient

$$\Rightarrow R = \frac{-1}{n_{eff}\, e c}$$

n_{eff} explains why R can have non Drude values and even the opposite sign!

To get magnetoresistance we would need to keep the diagonal terms in $\overleftrightarrow{\sigma}_1$ and $\overleftrightarrow{\sigma}_2$. It is then messier to invert $\overleftrightarrow{\sigma}$ and get $\overleftrightarrow{\rho}$. See HW#1

For $n_{eff} = 0$, see text. This is the case for an undoped semiconductor