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

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

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

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

Now we would have

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

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 positive!

Magnetoresistance

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

same for electrons and holes

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

For more than one partially filled band

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

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

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

Hall coefficient is

$$R \equiv -\frac{\rho_{xy}}{H} \quad \text{(see Quantum Hall effect notes)}$$

$$= -\frac{\omega_c \tau}{\sigma_0 H} = -\frac{eH}{m^* c}\,\frac{\tau m^*}{ne^2 \tau H} = -\frac{1}{nec} \quad \text{as before}$$

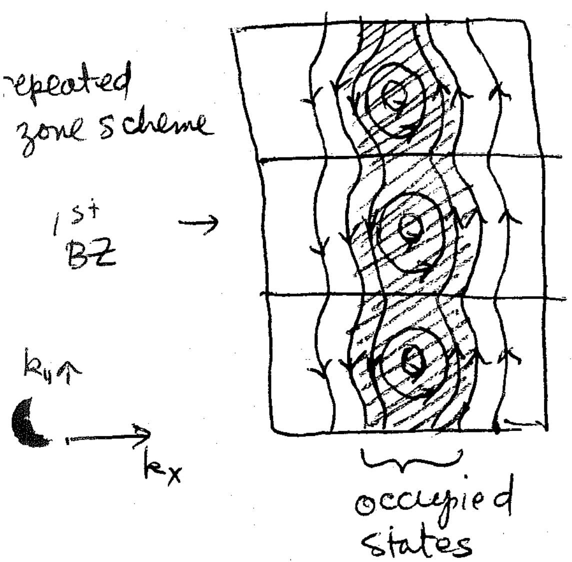
magnetoresistance

$$\rho_{xx} = \rho_{xy} = \frac{1}{\sigma_0}$$

saturates to finite value as $H \to 0$ just as was found in Drude model, except now m is m_{eff} & there are several partially filled bands.

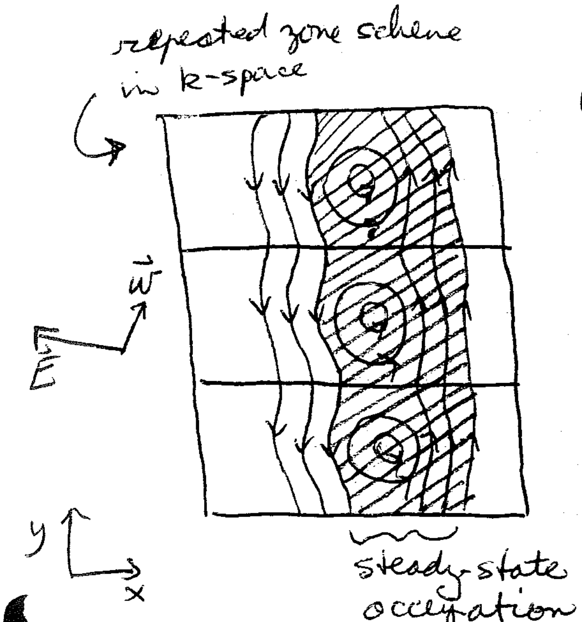
<u>Case (2)</u> Neither all occupied states, nor all unoccupied states have closed orbits $\Rightarrow$ in either electron or hole picture there are open orbits we have to consider

Now we will find that the $\langle \dot{\vec{k}} \rangle$ contribution to current $\vec{j}$ from these open orbits no longer vanishes in the $\omega_c \tau \to \infty$ limit, and it dominates over the drift contribution to the current $-ne\vec{w}$.



when $\vec{E}=0$, $\vec{H} = H\hat{z}$ induces motion in orbits on the constant energy surfaces. An electron moving in an open orbit in $\vec{k}$-space in the $+\hat{k}_y$ direction, gives a particle current in real space in the $+\hat{x}$ direction (rotate clockwise by $90°$ about $\hat{H}$). However when $\vec{E}=0$, each occupied open orbit going in one direction is paired with an occupied open orbit going in the opposite direction, so the net current is zero.

[Note: For an open orbit traveling along $\hat{k}_y$, $k_y(t)$ is periodic in time $\rightarrow$ $v_y = \left\langle \frac{\partial \mathcal{E}}{\hbar \partial k_y} \right\rangle = 0$ averaged over time. But $k_x(t) \approx$ constant + oscillation $\Rightarrow$ $v_x \approx \left\langle \frac{\partial \mathcal{E}}{\hbar \partial k_x} \right\rangle \neq 0$ $\Rightarrow$ electron moves in $\hat{x}$ direction.]



when $\vec{E} \neq 0$, in steady state, there will be an imbalance in occupation of open orbits, so that those orbits which absorb energy from the E-field have a larger population than those which lose energy to the field. ($\vec{E}$ field heats up metal!)

Open orbits in $+\hat{k}_y$ direction have real space direction $+\hat{x}$ $\Rightarrow$ they gain energy from E field if $E_x < 0$ as energy absorbed $\underbrace{\text{is}}_{\text{between collisions}}$ $-e\vec{E}\cdot\vec{v}\,\tau > 0$.

Open orbits in $-\hat{k}_y$ directions have real space direction $-\hat{x}$ $\Rightarrow$ they lose energy if $E_x < 0$.

$E_x < 0 \Rightarrow$ net $v_x > 0 \Rightarrow j_x < 0$

so $j_x \sim E_x$ to lowest order in E

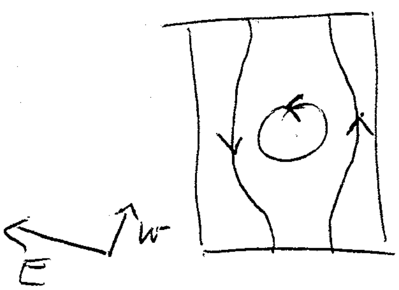
$\vec{j} \sim \hat{x}(\vec{E}\cdot\hat{x})$

~~$\Rightarrow$ We assume therefore that the imbalance in occupation of open orbits in steady state goes like [illegible] gives rise to a net current. If $\hat{n}$ is the direction in real space of the open orbits, then this contribution to current $\vec{j}$ is in the $\hat{n}$ direction, and proportional to some function of $\vec{E}\cdot\hat{n}$.~~

$\Rightarrow \vec{j}_{\text{open orbits}} \sim \hat{n}\, g(\vec{E}\cdot\hat{n})$ — expand in small $\vec{E}$, Equivalently, since $\bar{\varepsilon} = \varepsilon - \hbar \vec{k} \cdot \vec{w}$ is conserved between collisions, if $\Delta \varepsilon = -e\vec{E} \cdot \vec{v}\, \tau$ is energy absorbed by electron from E-field then

$$\Delta \bar{\varepsilon} = 0 \Rightarrow \Delta \varepsilon = \hbar \vec{w} \cdot \Delta \vec{k}$$

So again we see in our example



that ~~it~~ is the ~~left~~ right hand open orbits moving along $+\hat{k}_y$ that absorb energy, ie $\vec{w} \cdot \Delta \vec{k} > 0$ for these orbits, while $\vec{w} \cdot \Delta \vec{k} < 0$ for left hand open orbits moving along $-\hat{k}_y$.

~~right hand open orbits absorb energy from field~~ ~~$\Rightarrow$ right hand orbits~~
~~left hand open orbits lose energy to field~~

So both $\vec{w} \cdot \Delta \vec{k}$ and $-E \cdot v$ tell how much energy the electron absorbs from E-field

This imbalance in steady state occupation of open orbits is determined by the quantity $-e\vec{E}\cdot\vec{v}\tau$, the energy absorbed by electron from $\vec{E}$-field in between collisions.
If $\hat{n}$ is real space direction of open orbit, $\Rightarrow \langle\vec{v}\rangle$ is in $\hat{n}$ direction, so the current due to open orbits is in the $\hat{n}$ direction, and is some function of $(\vec{E}\cdot\hat{n})$.

$\vec{j}_{\text{open orbits}} = \hat{n}\, g(\vec{E}\cdot\hat{n})$ — expand for small $\vec{E}$, using $\begin{cases} j = 0 \text{ when } \vec{E}=0, \text{ and} \\ j(E) = -j(-E) \end{cases}$

$\vec{j}_{\text{open orbits}} \sim \hat{n}(\hat{n}\cdot\vec{E})$ where proportionality constant is independent of magnetic field H

We can write the contribution to conductivity tensor due to <u>open orbits</u> as

$$\vec{j}_{\text{open orbits}} = \tilde{\sigma}\cdot\vec{E} \quad \text{where } \tilde{\sigma} = \underset{\substack{\uparrow \\ \text{constant indep of } H}}{\lambda}\sigma_0\,\hat{n}\,\hat{n}$$

If we choose $\hat{n}$ in $\hat{x}$ direction

$$\tilde{\sigma} = \lambda\sigma_0\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$$

If we treat the contribution to conductivity tensor from <u>closed orbits</u> as before, we get for total conductivity tensor

$$\overleftrightarrow{\sigma} = \frac{\sigma_0}{(\omega_c\tau)^2}\begin{pmatrix}1 & -\omega_c\tau\\ \omega_c\tau & 1\end{pmatrix} + \lambda\sigma_0\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$$

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

or resistivity tensor $\vec{E} = \overleftrightarrow{\rho} \cdot \vec{j}$

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

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

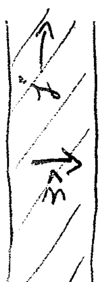
Note $\rho_{xy} = -\rho_{yx}$ as before for closed orbits, and Hall coefficient is $\frac{-\rho_{xy}}{H} = \frac{-\omega_c\tau}{\sigma_0(1+\lambda)H} = \frac{-1}{nec(1+\lambda)}$ same as before except for factor $(1+\lambda)$.

But now $\rho_{xx} \neq \rho_{yy}$. We have

expt'l wire ∥ to open orbits

ρ_{xx} — magnetoresistance for current flowing ∥ to open orbits in real space (ie $\vec{j} = j\hat{x}$)

$= \frac{1}{\sigma_0(1+\lambda)}$ ← indep of H saturates as $H \to \infty$ as in Drude model



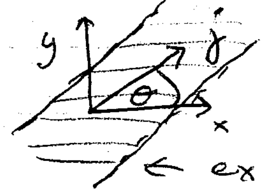
expt'l wire ⊥ to open orbits

ρ_{yy} — magnetoresistance when current flowing ⊥ to direction of open orbits in real space (ie $\vec{j} = j\hat{y}$)

$\cong \frac{\lambda}{\sigma_0(1+\lambda)}(\omega_c\tau)^2 \sim H^2$ does not saturate as $H \to \infty$. grows as H^2!

magnetoresistance which keeps increasing with H is signal for presence of open orbits on Fermi surface.

For a current in a general direction $\vec{j} = j\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$, where θ measures angle from $\hat{x}$, the direction of the open orbits in real space



← expt'l wire at angle θ to open orbits

we have

$$\vec{E} = \overleftrightarrow{\rho} \cdot \vec{j} = \frac{j}{\sigma_0(1+\lambda)} \begin{pmatrix} \cos\theta + (\omega_c\tau)\sin\theta \\ -(\omega_c\tau)\cos\theta + (\lambda(\omega_c\tau)^2+1)\sin\theta \end{pmatrix}$$

and the longitudinal magnetoresistance is

↙ projection of $\vec{E}$ along current $\vec{j}$.

$$\rho \equiv \frac{\vec{E}\cdot\hat{j}}{|\vec{j}|}$$

$$= \frac{1}{\sigma_0(1+\lambda)} \Big[\cos^2\theta + (\omega_c\tau)\sin\theta\cos\theta - (\omega_c\tau)\cos\theta\sin\theta + [\lambda(\omega_c\tau)^2+1]\sin^2\theta \Big]$$

$$\rho = \frac{1}{\sigma_0(1+\lambda)} \Big[1 + \lambda(\omega_c\tau)^2\sin^2\theta \Big]$$

↑ constant. Drude like part from closed orbits

↑ $\sim H^2\sin^2\theta$ increases without bound as H increases – from open orbits

Lattice Vibrations, phonons, and the speed of sound

Assume Hamiltonian of ionic degrees of freedom looks like

$$H = \sum_{R_i} \frac{\vec{P}_i^2}{2M} + \mathcal{U}_{ion}(\{\vec{R}_i\})$$

kinetic — potential due to ion-ion interactions

ions at positions $\vec{R}_i$, momentum $\vec{P}_i$, mass M

Write $\vec{R}_i = \vec{R}_i^0 + \vec{u}_i$

position in periodic BL — small displacement due to elastic distortions

If $\vec{u}_i$ is small, expand $\mathcal{U}_{ion}$ about the BL positions $\vec{R}_i^0$. Since the positions $\vec{R}_i^0$ are assumed to be positions of mechanical equilibrium, the linear term in the expansion must vanish, and the quadratic term is the leading order term.

$$\mathcal{U}_{ion}(\{\vec{u}_i\}) = \mathcal{U}_{ion}^0 + \frac{1}{2}\sum_{\substack{i\alpha \\ j\beta}} u_{i\alpha} \mathbb{D}_{ij}^{\alpha\beta} u_{j\beta}$$

i, j label BL sites

α, β label components x, y, z of the displacement

$$\mathbb{D}_{ij}^{\alpha\beta} = \left.\frac{\partial^2 \mathcal{U}_{ion}}{\partial u_{i\alpha}\, \partial u_{j\beta}}\right|_{\{\vec{R}_i^0\}}$$ is the dynamical matrix