So Hall coefficient is

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

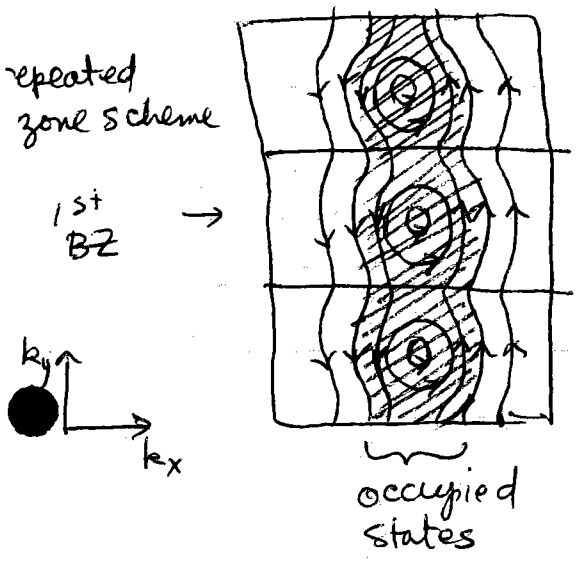
$$= -\frac{\omega_c \tau}{\sigma_0 H} = -\frac{eH}{m^* c}\,\frac{\tau m^*}{n e^2 \tau H} = -\frac{1}{nec} \quad \text{as before.}$$

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 n is n_{eff} if there are several partially filled bands.

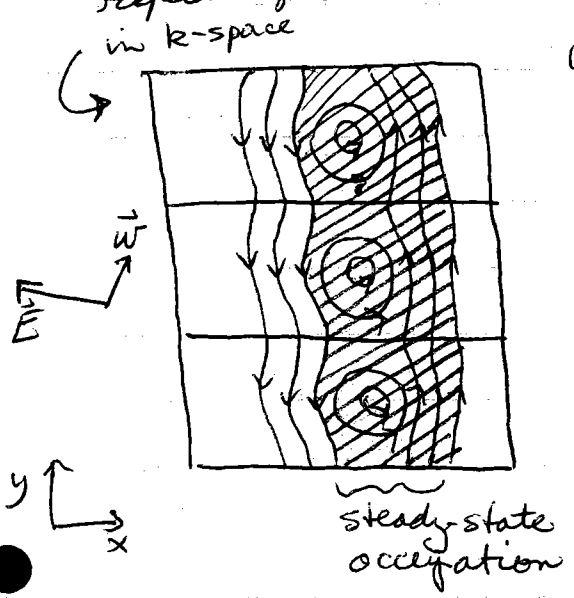
Case (2) Neither all occupied states, nor all unoccupied states have closed orbits $\Rightarrow$ in either electron or hole picture there are open orbits we have to consider

Now we will find that the $\langle \hat{k} \rangle$ 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 - new.



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 current in real space in the $+\hat{x}$ direction (rotate 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 $\Rightarrow v_x = \left\langle \frac{\partial \mathcal{E}}{\hbar \partial k_x} \right\rangle \neq 0 \Rightarrow$ 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 is $-e\vec{E}\cdot\vec{v}\,\tau$ (between collisions).

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

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

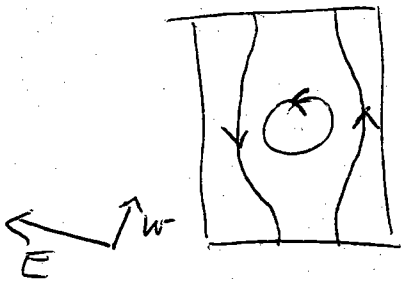
$\Rightarrow$ We assume therefore that the imbalance in occupation of open orbits in steady state gives rise to a net current. If $\hat{n}$ is the direction in real space of the open orbits, then this contribution to the current $\vec{j}$ is in the $\hat{n}$ direction, and proportional to some function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

$\Rightarrow \vec{j}_{\substack{\text{open} \\ \text{orbits}}} \sim \hat{n}\, g(\vec{E}\cdot\hat{n})$ — expand in small $\vec{E}$,

Equivalently, since $\bar{\mathcal{E}} = \mathcal{E} - \hbar \vec{k} \cdot \vec{w}$ is conserved between collisions, if $\Delta\mathcal{E} = -e\vec{E}\cdot\vec{v}\,\tau$ is energy absorbed by electron from E-field then

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

So again we see in our example



that it is the ~~left~~ right hand open orbits moving along $+\hat{k}_y$ that absorb energy, i.e $\vec{w}\cdot\Delta\vec{k} > 0$ 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 ⇒ 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 $(\vec{E}\cdot\hat{n})$.

$$\vec{j}_{\substack{\text{open}\\\text{orbits}}} = \hat{n}\, g(\vec{E}\cdot\hat{n})$$

- expand for small $\vec{E}$, using $j=0$ when $\vec{E}=0$, and $j(E) = -j(-E)$

$$\vec{j}_{\substack{\text{open}\\\text{orbits}}} \sim \hat{n}(\hat{n}\cdot\vec{E})$$

where proportionality constant is independent of magnetic field H

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

$$\vec{j}_{\substack{\text{open}\\\text{orbits}}} = \tilde{\sigma}\cdot\vec{E} \quad \text{where} \quad \tilde{\sigma} = \lambda\sigma_0\,\hat{n}\,\hat{n}$$

(λ: constant indep of H)

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 $\rho_{xy} = \rho_{-xy}$ as before for closed orbits, and Hall coefficient is $\frac{-\omega_c\tau}{\sigma_0(1+\lambda)} = \frac{-1}{nec(1+\lambda)}$ 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 (i.e. $\vec{j} = j\hat{x}$)

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

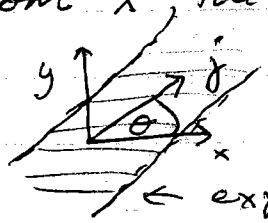
expt'l wire ⊥ to open orbits

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

$\cong \frac{\lambda}{\sigma_0(1+\lambda)} (\omega_c\tau)^2 \sim H^2$ 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

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

and the longitudinal magnetoresistance is

$$\rho \equiv \frac{\vec{E}\cdot\hat{j}}{|\vec{j}|}$$ ← projection of $\vec{E}$ along current $\vec{j}$.

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

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

↑ constant. Drude like part from closed orbits

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

Real metals

Monovalent Metals

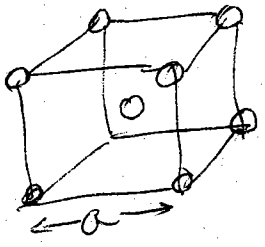
	(1A) Alkali's (bcc)	(1B) Nobel's (fcc)
Li	$[1s^2]2s^1$	—
Na	$[Ne]3s^1$	—
K	$[Ar]4s^1$	Cu $[Ar]3d^{10}4s^1$
Rb	$[Kr]5s^1$	Ag $[Kr]4d^{10}5s^1$
Cs	$[Xe]6s^1$	Au $[Xe]4f^{14}5d^{10}6s^1$

Rare Earth configuration is tightly bound core, electrons here are in very low lying, narrow, filled tight binding bands. Can generally ignore them.

bcc) Alkalis - If we assume the single conduction electron moves completely freely in metal, the fermi surface is a sphere of radius k_F

$$\frac{4}{3}\pi \frac{k_F^3}{4\pi^3} = \frac{k_F^3}{3\pi^2} = n = \frac{2}{a^3}$$ ← side of unit cell

↑ density of ions



$$k_F = (6\pi^2)^{1/3}\frac{1}{a} = \left(\frac{6\pi^2}{(2\pi)^3}\right)\left(\frac{2\pi}{a}\right) = \left(\frac{3}{4\pi}\right)^{1/3}\left(\frac{2\pi}{a}\right)$$

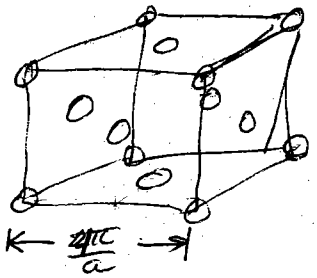
unit cell has 2 atoms $\Rightarrow n = \frac{2}{a^3}$

$$\Rightarrow k_F = \left(\frac{3}{4\pi}\right)^{1/3}\left(\frac{2\pi}{a}\right) = .620\left(\frac{2\pi}{a}\right)$$

← one half of side of unit cell in recip lattice.

unit cell of RL has side of length $\frac{4\pi}{a}$

1st BZ is Wigner Seitz cell of fcc lattice of unit cell size $\frac{4\pi}{a}$



nearest neighbor is $\frac{4\pi}{a}\sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2}$ away, so shortest distance to surface of 1st BZ is

$$k_0 = \frac{1}{2}\sqrt{\frac{1}{4}+\frac{1}{4}}\left(\frac{4\pi}{a}\right) = .707\left(\frac{2\pi}{a}\right)$$

$\vec{l}$ bisect R.L. vector to get dist to Bragg plane

so $\frac{k_F}{k_0} = \frac{.620}{.707} = .877$ fermi surface goes .877 of the way to closest pt on zone boundary

If weak potential, approx good, expect fermi surface to be very spherical - since not near Bragg plane (zone boundary) corrections to free electrons are only $O(U^2)$

This is the case. Sommerfeld model is ~~already~~ good in explaining Alkalis (Li not clear) (charge density wave?)

	Li	Na	K	Rb	Cs
$-1/R_{Hall}$ nec	.8	1.2	1.1	1.0	0.9

(Charge density waves?)

magnetoresistance also ~~shows little~~ is less[17] field dependant than other materials (Sommerfeld gives indep of H)

Low temp specific heat $C_v = \gamma T + O(T^3)$ free elec $\gamma = \frac{\pi^2}{2}\left(\frac{k}{\epsilon_F}\right)^2 n$

$\gamma = \frac{\pi^2}{3} k T g(\epsilon_F)$ in general

γ measures $g(\epsilon_F)$

	γ free electron	γ expt
Li	1.8	4.2
Na	2.6	3.5
K	4.0	4.7
Rb	4.6	5.8
Cs	5.3	7.7

Noble metals (fcc)

as in Alkalis, rare earth core is tightly bound + can be ignored. (also 4f electrons of Au)

Conduction electrons are the 11 $d^{10}s^1$ electrons.
⇒ need 6 bands at least (each band holds 2 elec's per B-Lattice site)

turns out 6 bands are enough. 5 lowest bands completely filled, 6th band half full. Bands look like 5 narrow bands (d-like tight binding) and one (s-band) nearly free electron like. However the nearly free electron s-band is mixed with narrow d-bands.

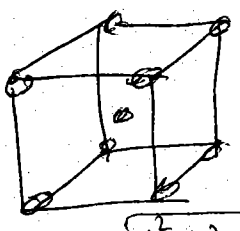
[Show Fig 15.4]

Fermi surface passes through 6th band (s-band) where it looks very free electron like – above narrow d-bands. Try free electron approx for the fermi surface of half filled 6th band.

$$\frac{k_F^3}{3\pi^2} = \frac{4}{a^3}$$

As before, add 1 electron per site to 6th band ↑ (4 atoms in unit cell)

$$\Rightarrow k_F = \left(\frac{2\pi}{a}\right)\left(\frac{6}{4\pi}\right)^{1/3} = .782\left(\frac{2\pi}{a}\right)$$



1st BZ is Wigner Seitz cell of bcc, closest pt on boundary from origin is at $k_0 = \frac{1}{2}\sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2}\left(\frac{4\pi}{a}\right)$

$K_{small} = \sqrt{\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2+\left(\frac{1}{2}\right)^2}\left(\frac{4\pi}{a}\right)$

$$k_0 = \sqrt{\frac{3}{4}}\left(\frac{2\pi}{a}\right) = .866\left(\frac{2\pi}{a}\right)$$

$= .782/.866$

$k_F/k_0 = .903$ ⇒ nearly spherical might be expected

<u>However</u> in this direction of closest approach ⟨111⟩, fermi surface distorts from sphere to touch zone boundry + give neck. Fermi surface in repeated zone scheme is multiply connected with open orbits as well as closed orbits

de Haas von Alphen expts with H ∥ ⟨111⟩ direction have 2 period corresp to small area neck + wide area sphere

[Show Fig 15.6
Fig 15.7]

Magneto resistence shows dramatic effect in H dependence with orientation of current wrt open orbits

	Cu	Ag	Au	
$-1/(R_H)nec$	1.5	1.3	1.5	← open orbits can cause problems!
γ free elect	1.2	1.5	1.5	} not bad
γ expt	1.6	1.6	1.6	

$$R = \frac{-1}{nec(1+\lambda)}$$ from single model

$$\frac{-1}{R\,nec} = \frac{nec(1+\lambda)}{nec} \simeq 1+\lambda > 1$$ as above

For ~~Noble~~ Nobels, d-bands cause complications
threshold occurs for exciting d-band electron
up to conduction s-band unoccupied state. Thus for Cu
occurs at pt where $h\omega \simeq 2$ eV.

[Show Fig 15.11]

Absorption for Cu shows peak at ~2eV, corresponding
to λ in orange part of spectrum - this is why copper is
red! Gold is yellow due to threshold at similar energy.
Silver more complicated - threshold for d-band excitation
+ plasmon excitation merge at about 4 eV

~~Read about Divalent (hcp, fcc, bcc)~~

Trivalent Aluminium (fcc)

Fermi surface close to free electron sphere for fcc B-lattice
with 3 conduction electrons per atom -

For free electrons with 3 conduction electrons,
1st BZ completely full - Fermi surface has branches in
2nd, 3rd, 4th zones. In reduced zone scheme, branch in 2nd zone
is closed surface, contains holes in 3rd zone, connected tubes, in 4th
zone small pockets of electrons

In Al potential causes pockets of electrons in 4th zone
to disappear. Fermi surface just in 2nd + 3rd zones (bands)

"57 per atom

taking 2 of the 3 electrons

Since 1st band completely full, need to put remaining electrons in 2nd + 3rd bands.
If n is total conduction electron density

$$n_e^{II} + n_e^{III} = \frac{n}{3} \qquad \left(\frac{2}{3}n \text{ in } 1^{st} \text{ band}\right)$$

But also $n_e^{II} + n_h^{II} = 2\left(\frac{n}{3}\right)$ (since 2nd band · also holds $\frac{2}{3}n$ electrons)

subtract

$$\Rightarrow \quad n_e^{III} - n_h^{II} = -\frac{n}{3}$$

since hole orbits of 2nd band, and electron orbits of 3rd band are closed $\Rightarrow$ Hall coefficient $R_H = \frac{-1}{n_{eff} ec}$ with $n_{eff} = -\frac{n}{3}$. Explains anomalous sign of Hall effect

$-1/nec R_{H\,exp} \quad -.03 \quad \simeq -1/3$ predicted above!

$z=4$ Tetravalent metals – Tin Lead
$z=5$ Semi metals, Graphite, As, Bi, Sb
Transition metals

Antimony

Arsenic

Rare earth metals