So Hall coefficient is,

\[ R \equiv \frac{\rho_{xy}}{H} \]

(see Quantum Hall Effect notes)

\[ = -\frac{\mu e c}{\sigma_0 H} = \frac{-eH}{m^* c_0} \frac{m^*}{\hbar e^2 c H} = -\frac{1}{me^2} \text{ as before} \]

magneto resistance

\[ \rho_{xx} = \rho_{xy} = \frac{1}{\sigma_0} \]

saturates to finite value as \( H \to 0 \)

just as was found in Drude model, except now \( n \to n_{\text{eff}} \) 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 \( \langle \hat{\mathbf{k}} \rangle \) contribution to current \( \mathbf{j} \) from these open orbits no longer vanishes in the \( \omega t \to \infty \) limit, and it dominates over the drift contribution to the current \( \mathbf{j} \) now.

When \( \mathbf{E} = 0 \), \( \mathbf{H} = H \hat{z} \) induces motion in orbits on the constant-energy surfaces. An electron moving in an open orbit in \( \mathbf{k} \)-space in the +\( \mathbf{y} \) direction, gives a current in real space in the +\( \mathbf{x} \) direction (rotate by 90° about \( \mathbf{H} \)). However when \( \mathbf{E} = 0 \), 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 $\Rightarrow \langle \frac{\partial E}{\partial k_y} \rangle = 0$ averaged over time. But $k_x(t) \approx$ constant $+$ oscillation $\Rightarrow \langle \frac{\partial E}{\partial k_x} \rangle \neq 0 \Rightarrow$ electron moves in $\hat{x}$ direction.

Repeated zone scheme in $k$-space

When $\mathbf{E} \neq 0$, 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. ($E$ 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 $-e\mathbf{E} \cdot \mathbf{v}$ 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 $\nabla_x > 0 \Rightarrow J_x < 0$

So $J_x \sim E_x$ to lowest order in $E$

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

We assume therefore that the imbalance in occupation of open orbits in steady state gives rise to a 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 $\mathbf{E} \cdot \hat{n}$.

$\vec{J} \sim \hat{n} g(\mathbf{E} \cdot \hat{n}) = \text{expand in small } \mathbf{E}$
Equivalently, since $\Delta E = E - \hbar \kappa \hat{w} \cdot \hat{v}$ is conserved between collisions, if $\Delta E = -e \vec{E} \cdot \hat{v} \geq 0$ energy absorbed by electron from $E$-field then

$$\Delta E = 0 \Rightarrow \Delta E = \hbar \hat{w} \cdot \hat{v} \Delta k$$

So again we see in our example that it is the right hand open orbits moving along $+\hat{k}$ 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 $-\hat{k}$.

So both $\vec{w} \cdot \Delta \vec{k}$ and $-E \cdot \vec{v}$ tell how much energy the electron absorbs from $E$-field.
This imbalance in steady state occupation of open orbits is determined by the quantity $-e\bar{E} \cdot \vec{\omega}_C$, the energy absorbed by electrons along $\vec{E}$-field in between collisions.

If $\hat{n}$ is real space direction of open orbit, $\vec{j}_\text{open} \sim \hat{n}$ in $\hat{n}$ direction, so the current due to open orbits is in the $\hat{n}$ direction, and is some function of $(\vec{E} \cdot \hat{n})$.

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

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

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

where proportionality constant is independent of magnetic field $\vec{H}$.

We can write the contribution to conductivity tensor due to open orbits as

$$\vec{j}_\text{open} = \vec{\Sigma} \cdot \vec{E}$$

where $\vec{\Sigma} = \lambda \sigma_0 \hat{n} \hat{n}$

constant independent of $\vec{H}$.

If we choose $\hat{n} \parallel \vec{\Sigma}$ direction,

$$\vec{\Sigma} = \lambda \sigma_0 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

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

$$\vec{\Sigma} = \frac{\sigma_0}{(\omega_C t)^2} \begin{pmatrix} 1 & -\omega_C \\ -\omega_C & 1 \end{pmatrix} + \lambda \sigma_0 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$= \sigma_0 \begin{pmatrix} \frac{1}{\omega_C t} & -\frac{1}{\omega_C} \\ -\frac{1}{\omega_C} & \frac{1}{(\omega_C t)^2} \end{pmatrix}$$
or resistivity tensor \( \bar{\sigma} = \sigma^{-1} = \frac{1}{\sigma_0 \left[ \lambda \left( \frac{\omega_c}{\gamma} \right)^2 + \frac{1}{\omega_c^2} + \frac{1}{\gamma^2} \right]^2} \left( \begin{array}{cc} \frac{1}{\omega_c^2} & \frac{\omega_c}{\gamma} \\ -\frac{\omega_c}{\gamma} & \lambda + \frac{1}{\omega_c^2} \end{array} \right) \)

\[ \approx \frac{1}{\sigma_0 (1+\lambda)} \left( \begin{array}{cc} 1 & \frac{\omega_c}{\gamma} \\ -\frac{\omega_c}{\gamma} & \lambda (\omega_c)^2 + 1 \end{array} \right) \]

Note \( \sigma_{xy} = \sigma_{-xy} \) as before for closed orbits, and Hall coefficient is \( -\frac{\omega_c}{\gamma} = \frac{1}{n \epsilon (1+\lambda)} \) same as before except for factor \((1+\lambda)\).

But now \( \sigma_{xx} \neq \sigma_{yy} \). We have

\[ \sigma_{xx} \] magnetoresistance for current flowing \( \parallel \) to open orbits in real space \( (\bar{\sigma} \parallel \bar{x}) \)

\[ = \frac{1}{\sigma_0 (1+\lambda)} \] saturates as \( H \to \infty \) as in Drude model \( \sigma_0 (1+\lambda) \to \) width of \( H \)

\[ \sigma_{yy} \] magnetoresistance when current flowing \( \perp \) to direction of open orbits in real space \( (\bar{\sigma} \perp \bar{x}) \)

\[ = \frac{\lambda}{\sigma_0 (1+\lambda)} (\omega_c)^2 \sim H^2 \] 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 $\mathbf{j} = j(\cos \theta, \sin \theta)$, where $\theta$ measures angle from $\hat{x}$, the direction of the open orbits in real space $\mathbf{y}$,

we have

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

and the longitudinal magnetoresistance is

$$\sigma = \frac{\mathbf{E} \cdot \hat{x}}{\mathbf{j} \cdot \hat{x}}$$

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

constant.

Drude-like part from closed orbits

vanishes as $H^2 \sin^2 \theta$ increases without bound as $H^2 \sin^2 \theta$ increases from open orbits.
Real metals

Monovalent metals

(IA) Alkali's (bcc) (IIB) Noble's (fcc)

Li \[1s^22s^1\]
Na \[Ne]3s^1
K \[Ar]4s^1
Rb \[Kr]5s^1
Cs \[Xe]6s^1

Cu \[Ar]3d^{10}4s^1
Ag \[Kr]4d^{10}5s^1
Au \[Xe]4f^{14}5d^{10}6s^1

Rare earth configuration is tightly bound core, electrons here are in very low energy, narrow, well defined 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

\[
\frac{4}{3} \pi \frac{k_F^3}{4\pi^3} = \frac{k_F^3}{3\pi^2} = \pi = \frac{2}{a^3} \quad \text{side of unit cell}
\]

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

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

\[
\Rightarrow k_F = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \left(\frac{2\pi}{a}\right) = 0.42 \cdot \left(\frac{2\pi}{a}\right)
\]

one half of \( \frac{2}{a^3} \) side of unit cell in rect. lattice.

Unit cell of RL has side of length \( \frac{4\pi}{a} \)
$1^{st}$ BZ is Wigner-Seitz cell of fcc lattice of unit cell size $a$.

Nearest neighbor is $\frac{4\pi}{a} \sqrt{\frac{1}{4} + \frac{1}{4}} = \frac{\pi}{2}$ away, so shortest distance to surface of $1^{st}$ BZ is

$$k_0 = \frac{1}{2} \sqrt{\frac{1}{4} + \frac{1}{4}} \left( \frac{4\pi}{a} \right) = 0.707 \left( \frac{2\pi}{a} \right)$$

By bisecting RL, order to get dist to Bragg plane.

So $\frac{k_F}{k_0} = \frac{0.620}{0.707} = 0.877$ for fermi surface.

Goes 0.877 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).

Connections to free electrons are only $\Theta(U^2)$.

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

Li Na K Rb Cs

$-\frac{1}{2}$ 1.8 1.2 1.1 1.0 0.9

$T$ (charge density waves?)

Magnetoresistance also shows to be less field dependent than other materials (Sommerfeld gives indp of $H$).

Low temp specific heat $C_v = \gamma T + o(T^3)$

\[
\gamma = \frac{\pi^2}{2} \left( \frac{k^3_B}{2\pi^2} \right) n
\]

measures $g(E_F)$ for free electron $\gamma_{exp}$

<table>
<thead>
<tr>
<th></th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
<th>Cs</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma$ free electron</td>
<td>1.8</td>
<td>2.6</td>
<td>4.0</td>
<td>4.6</td>
<td>5.3</td>
</tr>
<tr>
<td>$\gamma$ exp</td>
<td>4.2</td>
<td>3.5</td>
<td>4.7</td>
<td>5.8</td>
<td>7.7</td>
</tr>
</tbody>
</table>

In general $\gamma = \frac{\pi^2}{3} k_B T g(E_F)$.
Noble Metals (fcc)

As in PtRhAl, rare earth core is tightly bound and can be ignored. (also 4f electrons of Au)

Conduction electrons on the 11 d^0 s^1 electrons.

⇒ Need 6 bands at least (each band holds 2 electrons 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 15.9]

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.

As before, add 1 electron per site to 6th band

⇒ \( k_F = \frac{1}{4} \frac{3\pi^2}{a^3} \)

\( = 0.782 \frac{3\pi^2}{a^3} \) (unit cell)

1st BZ in Wigner-Seitz cell of bcc, closest \( k \) on boundary from origin is at \( k_0 = \frac{\sqrt{3}}{4} \frac{2\pi}{a} \) (4 atoms in)

\( k_{\text{max}} = \sqrt{\frac{3}{4}} \frac{2\pi}{a} \) = 0.8660 \( \frac{2\pi}{a} \)
However, in this direction of closest approach (111), Fermi surface distorts from sphere to touch zone boundary and give neck. Fermi surface in repeated zone scheme is multiply connected with open orbits as well as closed orbits.

De Haas van Alphen effects with H in (111) direction have 2 period corresponding to small area neck + wide area sphere.

Magnetic resistance shows dramatic effect on resonance in H dependence with field direction with orientation of current and open orbits

\[
\begin{array}{ccc}
\text{Cu} & \text{Ag} & \text{Au} \\
1.5 & 1.8 & 1.5 \\
0 \text{ free electron} & 1.2 & 1.5 & 1.5 \\
0 \text{ empty} & 1.6 & 1.6 & 1.6
\end{array}
\]

\[ R = \frac{-1}{\text{mec} (1+\lambda)} \] from single model.

\[ \frac{-1}{R_{\text{mec}}} = \frac{\text{mec}(1+\lambda)}{\text{mec}} = 1+\lambda > 1 \] as above.
In all polycrystalline materials, the Fermi level is determined by the combined effect of the individual crystal orientations.

For free electrons with 3 conduction electrons per atom, the Fermi level is close to the free electron Schottky barrier.

Trivalent

Aluminum (FCC)

Aluminum (BCC)

Silver

Absorption of light with a wavelength shorter than the threshold (hv > E_g) causes transitions from the ground state to the conduction band. The photoemission effect is visible when the threshold energy is exceeded.

Silver metal exhibits a yellow color due to the excitation of 4d electrons to higher energy levels.
Since 1st band completely full, need to put \( n \) electrons in 2nd + 3rd bands.

If \( n \) is total conduction electron density

\[
\frac{\text{II}}{2} + \frac{\text{III}}{3} = \frac{n}{3} \quad \text{(2/3 \( n \) in 1st band)}
\]

But also \( \frac{\text{II}}{2} + \frac{\text{II}}{h} = 2 \left( \frac{n}{3} \right) \quad \text{(since 2nd band also holds \( \frac{2}{3} \) \( n \) electrons)}
\]

\[
\Rightarrow \quad \frac{\text{III}}{n} - \frac{\text{II}}{h} = -\frac{n}{3}
\]

Since hole orbits of 2nd band, and electron orbits of 3rd band are closed \( \Rightarrow \) Hall coefficient

\[
R = -\frac{1}{n_{\text{eff}}} \quad \text{with} \quad n_{\text{eff}} = -\frac{n}{3}. \quad \text{Explains anomalous sign of Hall effect}
\]

\[
-\sqrt{\text{rec} \times R_{\text{H, exp}}} = 0.03 \approx -\frac{1}{3} \quad \text{predicted above!}
\]

\( n \approx 4 \) Tetravalent metals - Ti, Sn, Pb

\( n \approx 5 \) Semi metals, Germanium, As, Bi, Sb

Transition metals - Antimony

Rare earth metals - Arsenic