Hall coefficient is

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

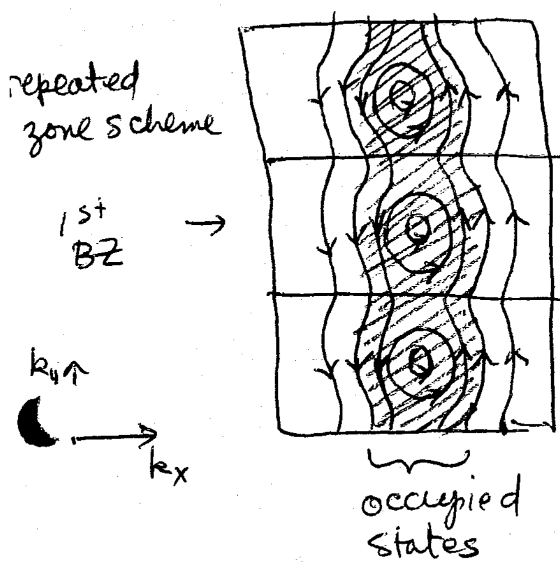
$$= -\frac{\omega_c \tau}{\sigma_0 H} = -\frac{eH}{m^* c}\frac{\tau m^*}{ne^2 \tau H} = -\frac{1}{nec} \quad \text{as before.}$$

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

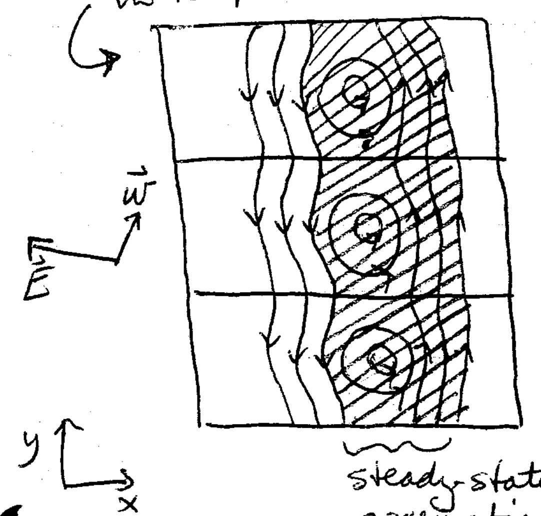
Now we will find that the $\langle \dot{\vec{k}} \rangle$ contribution to current $\vec{j}$ from these open orbits no longer vanishes in the $\omega_c \tau \to \infty$ limit, and it dominates over the drift contribution to the current $-ne\vec{w}$.



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 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 $\Rightarrow$ $v_x = \left\langle \frac{\partial \mathcal{E}}{\hbar \partial k_x} \right\rangle \neq 0$ $\Rightarrow$ electron moves in $\hat{x}$ direction.]

repeated zone scheme in k-space



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 $\underbrace{-e\vec{E}\cdot\vec{v}\,\tau}_{\text{between collisions}}$.

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

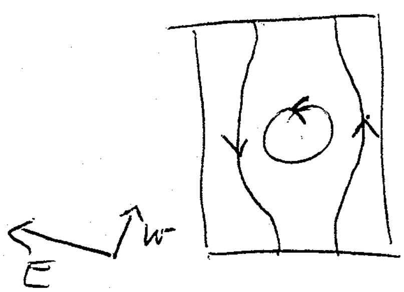
$\vec{j} \sim \hat{x}(\vec{E}\cdot\hat{x})$

~~$\Rightarrow$ 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 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~~
~~left hand open orbits lose energy to field~~ ~~$\Rightarrow$ right hand side ...~~

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

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

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

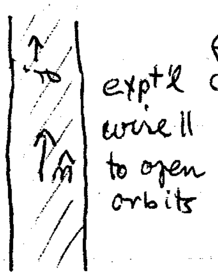
$$\overleftrightarrow{\rho} = \sigma^{-1} = \frac{1}{\sigma_0} \frac{1}{\left[\frac{\lambda}{(\omega_c\tau)^2} + \frac{1}{(\omega_c\tau)^2} + \frac{1}{(\omega_c\tau)^4}\right]} \begin{pmatrix} \frac{1}{(\omega_c\tau)^2} & \frac{1}{\omega_c\tau} \\ \frac{-1}{\omega_c\tau} & \lambda + \frac{1}{(\omega_c\tau)^2}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

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

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 $(1+\lambda)$.

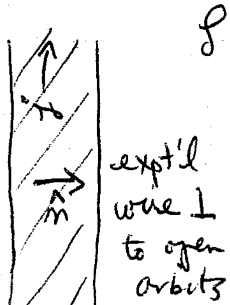
But now $\rho_{xx} \neq \rho_{yy}$. We have



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



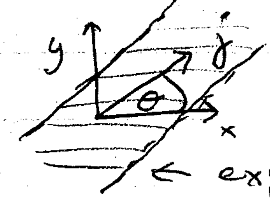
ρ_{yy} – magnetoresistance when current flowing ⊥ to direction of open orbits in real space (ie $\vec{j} = j\hat{y}$)

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

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 $\vec{j}$.

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

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

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

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

The classical equations of motion for the ions are then

$$M\ddot{\vec{u}}_i = -\frac{\partial U_{ion}}{\partial \vec{u}_i} \Rightarrow M\ddot{u}_{i\alpha} = -\sum_{j\beta} D_{ij}^{\alpha\beta} u_{j\beta}$$

Now by translational invariance of the Bravais Lattice $D_{ij}^{\alpha\beta}$ depends only on $\vec{R}_i^0 - \vec{R}_j^0$.

We can define the Fourier transforms

$$\vec{u}_i(t) = \int_{q\in 1^{st}BZ} d^3q \int_{-\infty}^{\infty} d\omega \; e^{i\vec{q}\cdot\vec{R}_i^0} e^{-i\omega t} \vec{u}(\vec{q},\omega)$$

$$D_{ij}^{\alpha\beta} = \int_{q\in 1^{st}BZ} d^3q \; e^{i\vec{q}\cdot(\vec{R}_i^0-\vec{R}_j^0)} D^{\alpha\beta}(\vec{q})$$

Note: in defining Fourier transform of a function that exists only on the discrete sites of a B.L., the only wave vectors we need to consider are those $\vec{q}$ in the 1^{st} BZ. This is because any wavevector $\vec{k}$ can always be written as $\vec{k} = \vec{q} + \vec{K}$ with $\vec{K}$ a unique R.L. vector and $\vec{q}$ in the 1^{st} BZ. Then the plane wave factor would be

$$e^{i\vec{k}\cdot\vec{R}_i^0} = e^{i(\vec{q}+\vec{K})\cdot\vec{R}_i^0} = e^{i\vec{q}\cdot\vec{R}_i^0} \quad \text{since } e^{i\vec{K}\cdot\vec{R}_i^0} = 1$$

so we still only get oscillations at $\vec{q}$ in 1^{st} BZ substitute these into the equation of motion

$$\int\limits_{q \text{ in } 1^{st} BZ} d^3q \int_{-\infty}^{\infty} d\omega \, e^{i\vec{q}\cdot\vec{R}_i^0} e^{-i\omega t} (-\omega^2) M \vec{u}(\vec{q},\omega)$$

$$= -\int\limits_{q \in 1^{st} BZ} d^3q \int\limits_{q' \in 1^{st} BZ} d^3q' \int_{-\infty}^{\infty} d\omega \sum_j e^{i\vec{q}\cdot(\vec{R}_i^0 - \vec{R}_j^0)} e^{i\vec{q}'\cdot\vec{R}_j^0} e^{-i\omega t} \overleftrightarrow{D}(q) \cdot \vec{u}(\vec{q}',\omega)$$

↑ matrix product over coordinates

Do the ~~integral~~ summation

$$\sum_j e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0} = \delta(\vec{q}-\vec{q}')$$

Follows since $\{\vec{R}_j^0 + \vec{R}_0^0\} = \{\vec{R}_j^0\}$ since BL is closed under translation by any BL vector $\vec{R}_0^0$

$$\Rightarrow \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0} = \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot(\vec{R}_j^0 + \vec{R}_0^0)}$$

$$= e^{-i(\vec{q}'-\vec{q})\cdot\vec{R}_0^0} \sum_{R_j^0} e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_j^0}$$

$$\Rightarrow e^{i(\vec{q}'-\vec{q})\cdot\vec{R}_0^0} = 1 \text{ for any } \vec{R}_0^0 \text{ in BL}$$

$$\Rightarrow \vec{q}' - \vec{q} = \vec{K} \text{ in R.L.}$$

But since $\vec{q}, \vec{q}'$ both in 1^{st} BZ $\Rightarrow \vec{K} = 0$ and

$\vec{q} = \vec{q}'$ or the sum must vanish

$$\int_{1^{st} BZ} d^3q \int d\omega\, e^{i(\vec{q}\cdot\vec{R}_i^0 - \omega t)} (-\omega^2) M\, \vec{u}(\vec{q},\omega)$$

$$= -\int_{1^{st} BZ} d^3q\, d\omega\, e^{i(\vec{q}\cdot\vec{R}_i^0 - \omega t)} \overleftrightarrow{D}(\vec{q}) \cdot \vec{u}(\vec{q},\omega)$$

equate Fourier amplitudes to get

$$+\omega^2 M\, \vec{u}(\vec{q},\omega) = \overleftrightarrow{D}(\vec{q}) \cdot \vec{u}(\vec{q},\omega)$$

If the eigenvectors and eigenvalues of $\overleftrightarrow{D}(\vec{q})$ are $\vec{\epsilon}_1(\vec{q}), \vec{\epsilon}_2(\vec{q}), \vec{\epsilon}_3(\vec{q})$ and $\lambda_1(\vec{q}), \lambda_2(\vec{q}), \lambda_3(\vec{q})$

Then

$$+\omega_s^2 M = \lambda_s(\vec{q}) \qquad s = 1, 2, 3$$

$$\omega_s = \sqrt{\frac{\lambda_s(\vec{q})}{M}}$$

dispersion relation for elastic vibrations at wave vector $\vec{q}$, polarization $\vec{\epsilon}_s(\vec{q})$

We expect that in the <u>long wave length limit</u> we can expand

$$\overleftrightarrow{D}(\vec{q}) = \sum_i e^{-i\vec{q}\cdot\vec{R}_i} \overleftrightarrow{D}(\vec{R}_i)$$

$$\simeq \sum_i \left\{ 1 - i\vec{q}\cdot\vec{R}_i - \tfrac{1}{2}(\vec{q}\cdot\vec{R}_i)^2 \right\} \overleftrightarrow{D}(\vec{R})$$

$\sum_i \overleftrightarrow{D}(\vec{R}_i) = 0$ because if all $\vec{u}_i = \vec{u}_0$ a uniform displacement, then net force on ion i must vanish

$\sum_i \vec{R}_i \overleftrightarrow{D}(\vec{R}_i) = 0$ by inversion symmetry $\vec{R}_i \to -\vec{R}_i$
$\overleftrightarrow{D}(\vec{R}_i) = \overleftrightarrow{D}(-\vec{R}_i)$

so

$$\overleftrightarrow{D}(\vec{q}) \simeq -\frac{q^2}{2} \sum_{\vec{R}_i} (\hat{q}\cdot\vec{R}_i)^2 \overleftrightarrow{D}(\vec{R})$$

we assume this sum converges

$\Rightarrow \overleftrightarrow{D}(q) \propto q^2$

so $\lambda_s(\vec{q}) \propto q^2$ or $\lambda_s(\vec{q}) = A_s q^2$ for small $\vec{q}$

$\Rightarrow \quad \omega_s = \sqrt{\frac{A_s}{M}}\,|\vec{q}|$ with

$c_s = \sqrt{A_s/M}$ the speed of sound ~~for~~ for polarization s.

$\omega_s = c_s q$ for small $\vec{q}$

Also at small $\vec{q}$ we expect the spatial orientation of the B.L. to get "averaged over" and so the only directions of $\vec{q}$ and $\perp$ to $\vec{q}$. We thus expect the polarization vectors to become as $\vec{q} \to 0$

$\vec{\epsilon}_1(\vec{q}) = \hat{q}$ longitudinal sound mode, speed c_ℓ

$\left.\begin{array}{l}\vec{\epsilon}_2(\vec{q})\\ \vec{\epsilon}_3(\vec{q})\end{array}\right\} \perp \hat{q}$ transverse sound modes, speed c_{t1}, c_{t2}