Semiclassical model of electron dynamics

The Bloch theory extends the free electron theory of Sommerfeld in the equilibrium situation, by including periodic potentials to describe electrons.

To describe many properties due to electrons, one needs to go beyond equilibrium and describe dynamics of electrons.

The dynamical aspect of Sommerfeld model is essentially the Drude model except that now. $\langle v \rangle$ is replaced by v_F.

The approach behind the Drude model can be made more systematic and includes two important features: (i) semiclassical approximation and (ii) the relaxation-time approximation. Both of them are based on the Boltzman equation that is designed for describing non-equilibrium dynamics

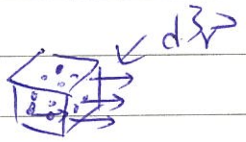
Boltzman equation

The classical theory of transport is based on the Boltzman equation and Hamilton equation of motion. In this approach, one defines the distribution function $f(\vec{r},\vec{p},t)$ as # of particles with position $\vec{r}$ & momentum $\vec{p}$ in the range $(\vec{r}, \vec{r}+d\vec{r})$ & $(\vec{p},\vec{p}+d\vec{p})$ at moment t.

In other words,

$$f(\vec{r},\vec{p},t)\,d^3\vec{r}\,d^3\vec{p} = \#\text{ of particles in } d^3\vec{r}\,d^3\vec{p}$$

centered at $(\vec{r},\vec{p})$ at moment t.



(For a single particle, f is then interpretated as probability density.)

Classically, $\vec{r}$ & $\vec{p}$ obey

$$\dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}}$$

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{r}} \qquad --- ①$$

In the absence of particle-particle collision, f obeys the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0$$

Here $\rho = f$, $\vec{v}$ is the velocity in the hyperspace formed by $\vec{r}, \vec{p}$, i.e., $\vec{v} = (\dot{\vec{r}}, \dot{\vec{p}})$, and $\vec{\nabla} = \left(\frac{\partial}{\partial \vec{r}}, \frac{\partial}{\partial \vec{p}}\right)$

$$\therefore \quad \frac{\partial f}{\partial t} + \nabla_r \cdot (\dot{\vec{r}} f) + \nabla_p \cdot (\dot{\vec{p}} f) = 0 \quad \cdots ②$$

Now $\nabla_r \cdot (\dot{\vec{r}} f) = \dot{\vec{r}} \cdot \nabla_r f(\vec{r}, \vec{p}) + (\nabla_r \cdot \dot{\vec{r}}) f$

$$\nabla_p \cdot (\dot{\vec{p}} f) = \dot{\vec{p}} \cdot \nabla_p f(\vec{r}, \vec{p}) + (\nabla_p \cdot \dot{\vec{p}}) f$$

$$\nabla_r \cdot \dot{\vec{r}} = \sum_k \frac{\partial}{\partial x_k} \dot{x}_k \underset{\substack{\uparrow \\ \text{eq.}①}}{=} \sum_k \frac{\partial^2 H}{\partial x_k \partial p_k}$$

$$\nabla_p \cdot \dot{\vec{p}} = \sum_k \frac{\partial}{\partial p_k} \dot{p}_k = -\sum_k \frac{\partial^2 H}{\partial p_k \partial x_k}$$

$$\therefore \quad (\nabla_r \cdot \dot{\vec{r}}) f + (\nabla_p \cdot \dot{\vec{p}}) f = 0$$

Eq. ② reduces to

$$\frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \vec{\nabla}_r f + \dot{\vec{p}} \cdot \vec{\nabla}_p f = 0$$

A reflection shows that the left part is $\frac{df}{dt}$. Therefore, in the absence of collision, if one follows the flow of particle in the hyperspace, f is invariant:

$$\frac{df(\vec{r}, \vec{p}, t)}{dt} = \frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial}{\partial \vec{r}} f + \dot{\vec{p}} \cdot \frac{\partial f}{\partial \vec{p}} = 0 \quad \cdots ③$$

This is so-called Liouville theorem.

In the presence of collisions, $\frac{df}{dt}$ no longer vanishes because particles originally have momentum $\vec{p}$ may be scattered into other $\vec{p}'$ and thus f is changed. Formally, we write

$$\frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \frac{\partial f}{\partial \vec{r}} + \dot{\vec{p}} \cdot \frac{\partial f}{\partial \vec{p}} = \left(\frac{\partial f}{\partial t}\right)_{coll} \quad \text{----} \quad ④$$

This is the Boltzman equation.

<u>Relaxation approximation</u> & <u>Drude model</u>

$\left(\frac{\partial f}{\partial t}\right)_{coll}$ is generally complicated and non-linear in f. We shall come back to its exact form later.

In the simplest approximation that is consistent with the Drude model, one approximates

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{f - f_0}{\tau} \quad \text{---} \quad ⑤$$

Here τ = relaxation time, f_0 = equilibrium distribution function. Classically, $f_0 = Ae^{-\beta E}$

With $\varepsilon = \frac{p^2}{2m} + U(r)$

Eq. ⑤ implies the distribution function will decay to equilibrium f_0 within a time scale τ:

$$\because \frac{\partial f_0}{\partial t}=0 \qquad \therefore \frac{\partial (f-f_0)}{\partial t} = -\frac{f-f_0}{\tau}$$

$$f = f_0 + (f(t=0)-f_0)\, e^{-t/\tau}$$

In the relaxation approximation, eq. ④ becomes

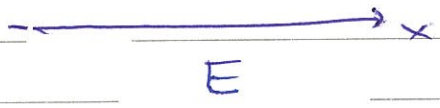
$$\frac{\partial f}{\partial t} + \vec{v}\cdot\frac{\partial f}{\partial \vec{r}} + \vec{F}\cdot\frac{\partial f}{\partial \vec{p}} = -\frac{f-f_0}{\tau} \quad \cdots ⑥$$

Classically, after the electric field $E\hat{x}$ is applied, locally, the energy reference point is μ, then $f_0 = e^{-\beta(\varepsilon-\mu)}$

In the steady state, $\frac{\partial f}{\partial t}=0$,

equilibrium f is established. $f=f_0$

∴ Eq. ⑥ becomes



$$v_x \frac{\partial f}{\partial x} + \frac{-eE}{m}\frac{\partial f}{\partial v_x} = -\frac{f-f_0}{\tau}$$

$$\therefore f = f_0 - v_x \tau \frac{\partial f_0}{\partial x} + \tau \frac{eE}{m}\frac{\partial f_0}{\partial v_x} + \cdots$$

--- ⑦

Here $\frac{\partial f_0}{\partial x} = \frac{d f_0}{d z}\frac{\partial z}{\partial x}$ $\quad z=\beta(\epsilon-\mu)$

$$= k_BT\frac{\partial f_0}{\partial \epsilon}\frac{\partial}{\partial x}\left[\frac{\epsilon-\mu}{k_BT}\right]$$

$$= -\frac{\partial f_0}{\partial \epsilon}\left[\frac{\epsilon}{T}\frac{\partial T}{\partial x} + T\frac{\partial}{\partial x}\left(\frac{\mu}{T}\right)\right]$$

$$= -\frac{\partial f_0}{\partial \epsilon}\left[\frac{\epsilon}{T}\frac{\partial T}{\partial x} - \frac{\mu}{T}\frac{\partial T}{\partial x}\right]$$

is linear in E & $\frac{\partial T}{\partial x}$.

∴ To linear order in E & $\frac{\partial T}{\partial x}$, lowest order terms in eq. ① are sufficient.

By writing $\frac{\partial f_0}{\partial v_x} = \frac{\partial f_0}{\partial \epsilon}\frac{\partial \epsilon}{\partial v_x} = m v_x\frac{\partial f_0}{\partial \epsilon}$,

we have

$$f = f_0 + \tau v_x\left(\frac{\partial f_0}{\partial \epsilon}\right)\left[\frac{\epsilon}{T}\frac{\partial T}{\partial x} + T\frac{\partial}{\partial x}\left(\frac{\mu}{T}\right) + eE\right] \quad \text{--- ②}$$

From eq. ②, one can calculate electric J^x & thermal current $\overset{\text{density}}{\wedge}$ J_u^x:

$$J^x = \int_0^\infty d\epsilon\, (-e v_x)\, \underbrace{g(\epsilon)}_{\text{density of states per volume}}\, f$$

$$J_u^x = \int_0^\infty d\epsilon\, (\epsilon v_x)\, g(\epsilon)\, f.$$

Here v_x has to be expressed in terms of ϵ.

It's clear that since f_0 is even in v_x, f_0 doesn't contribution J^x & J_u^x.

We find

$$J_x = \left[e^2 E + eT\frac{\partial}{\partial x}\left(\frac{\mu}{T}\right)\right]\int_0^\infty d\varepsilon\, v_x^2 \tau g(\varepsilon)\left(-\frac{\partial f_0}{\partial \varepsilon}\right)$$

$$+\frac{e}{T}\frac{\partial T}{\partial x}\int_0^\infty d\varepsilon\, v_x^2\, \varepsilon g(\varepsilon)\tau\left(-\frac{\partial f_0}{\partial \varepsilon}\right) \quad \cdots ⑨$$

Similarly,

$$J_u^x = -\left[eE + T\frac{\partial}{\partial x}\left(\frac{\mu}{T}\right)\right]\int_0^\infty d\epsilon\, \epsilon\, v_x^2 \tau g(\epsilon)\left(-\frac{\partial f_0}{\partial \epsilon}\right)$$

$$-\frac{1}{T}\frac{\partial T}{\partial x}\int_0^\infty d\epsilon\, \epsilon^2 v_x^2 \tau g(\epsilon)\left(-\frac{\partial f_0}{\partial \epsilon}\right) \quad \cdots ⑩$$

Classically, $-\frac{\partial f_0}{\partial \epsilon} = (-\beta f_0)$. $\quad (f_0 = A e^{-\beta(\epsilon-\mu)})$

Electric conductivity :-

set $\frac{\partial T}{\partial x} = 0$. $(\mu = \text{const.})$

$$\therefore J_x = e^2 E \tau \beta \underbrace{\int_0^\infty d\epsilon\, v_x^2 g(\epsilon) f_0}_{\substack{\| \\ n\langle v_x^2\rangle}}$$

$n = \#$ of electrons per volume

$$= e^2 E \tau \beta n \underbrace{\frac{1}{3}\langle v^2\rangle}_{\substack{\| \\ \frac{1}{3}\frac{2}{m}\langle\frac{1}{2}mv^2\rangle}}$$

$$\langle\tfrac{1}{2}mv^2\rangle = \tfrac{3}{2}k_B T$$

$$= \frac{ne^2E\tau}{m} \qquad \therefore \sigma = \frac{ne^2\tau}{m}, \text{ we recover}$$

the Drude formula with τ being the mean collision time.

Semiclassical approximation

The Boltzman equation is based on the probability of finding particles with $\vec{r}$ & $\vec{p}$ simultaneously. This is purely classical.

To extend it to include quantum nature of electrons, the partial success of Sommerfeld model seems to suggest that one can still use $\vec{r}$ & $\vec{p}$ to characterize electrons dynamically! Afterall, the Drude peak is observed experimentally.

The rationale for using ordinary classical mechanics to describe dynamical behavior is that if there is no need to localize the electron in the lengthscale comparable to interelectronic distance. This is justified if we describe the behavior of a wave packet of electron levels

$$\psi(\vec{r},t) = \sum_{k'} g(k') e^{i(\vec{k}'\cdot\vec{r} - \frac{\hbar k'^2}{2m}t)}$$

$$g(k') \simeq 0 \quad \text{for} \quad |k'-k| > \Delta k$$

where $\hbar\vec{k}$ and $\vec{r}$ are the mean momentum and position of the wave packet.

The accuracy of this description is limited by the uncertainty relation $\Delta x \Delta k \geq 1$.

∴ We must have $\Delta x \gg a$ (lattice spacing), $\Delta x \ll L$ (characteristic length of external perturbation E or $T(x)$)

For free electrons, in semi-classical approximation, one has

$$\dot{\vec{r}} = \frac{\hbar\vec{k}}{m} \qquad \text{--- ⑪}$$

$$\hbar\dot{\vec{k}} = (-e)\left[\vec{E} + \frac{1}{c}\vec{v}\times\vec{H}\right] \qquad \text{--- ⑫}$$

However, $f_0 = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$. This is exactly the Sommerfeld theory of metal.

In this case, both eqs. ⑨ & ⑩ are still valid except that one has to use the Fermi-Dirac distribution $f_0 = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$.

For 3D free electrons, $g(\epsilon) = \frac{3}{2}\frac{n}{\epsilon_F}\left(\frac{\epsilon}{\epsilon_F}\right)^{\frac{1}{2}} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{\frac{1}{2}}$

and we can replace v_x^2 by $\frac{1}{3}v^2 = \frac{2}{3}\frac{\epsilon}{m}$. $\epsilon = \frac{1}{2}mv^2$.

We can replace eqs. ⑨ ⑩ by

$$J_x = \left[e^2E + eT\frac{d}{dx}\left(\frac{\mu}{T}\right)\right]K_1 + \frac{e}{T}\frac{dT}{dx}K_2 \qquad \text{--- ⑬}$$

$$J_u^x = -\left[eE + T\frac{d}{dx}\left(\frac{\mu}{T}\right)\right]K_2 - \frac{1}{T}\frac{dT}{dx}K_3 \quad \cdots\cdots ⑭$$

Where

$$K_n = \frac{n}{m\epsilon_F^{3/2}}\int_0^\infty d\epsilon\left(-\frac{df_0}{d\epsilon}\right)\epsilon^{n+\frac{1}{2}}\tau$$

Electric conductivity:

The electric conductivity, as we have seen, is the same as the classical Drude model except that now we take τ to be ϵ-dependent! Therefore, $\tau = \tau(\epsilon)$ has to be inside the integral in K_n.

By using the Sommerfeld expansion, one expands $F_n(\epsilon) \equiv \epsilon^{n+1/2}\tau(\epsilon)$

$$= F_n(\mu) + (\epsilon-\mu)F_n'(\mu) + \frac{1}{2!}(\epsilon-\mu)^2F_n''(\mu) + \cdots$$

and obtains

$$K_n = \left\{F_n(\mu)\int_0^\infty d\epsilon\left(-\frac{df_0}{d\epsilon}\right) + F_n'(\mu)\int_0^\infty d\epsilon\,(\epsilon-\mu)\left(-\frac{df_0}{d\epsilon}\right) + \frac{1}{2!}F_n''(\mu)\int_0^\infty d\epsilon\,(\epsilon-\mu)^2\left(-\frac{df_0}{d\epsilon}\right) + \cdots\right\}\frac{n}{m\epsilon_F^{3/2}}$$

$$= \frac{n}{m\epsilon_F^{3/2}}\left[\mu^{n+1/2}\tau(\mu) + \frac{\pi^2}{6}(k_BT)^2\frac{d^2}{d\epsilon^2}\left(\epsilon^{n+1/2}\tau(\epsilon)\right)\Big|_{\epsilon=\mu} + \cdots\right]$$

$\llcorner$ ⑮

Setting $\frac{dT}{dx}=0$, we get

$$J_x = e^2 E K_1$$

at $T=0$, $K_1 = \frac{n}{m\epsilon_F^{3/2}}\left[\epsilon_F^{\frac{3}{2}}\tau(\epsilon_F)\right]$

$$\therefore \quad J_x = \frac{ne^2\tau(\epsilon_F)}{m}E, \quad \sigma = \frac{n\,\tau(\epsilon_F)e^2}{m}$$

is determined by τ at $\epsilon=\epsilon_F$.

<u>Thermal conductivity :</u>

Setting $J_x=0$, eq. ⑬ implies

$$-\left(eE+T\frac{d}{dx}\left(\frac{\mu}{T}\right)\right]K_1 = \frac{1}{T}\frac{dT}{dx}K_2 .$$

Substituting the above into eq. ⑭, one gets

$$J_u^x = \frac{1}{T}\frac{dT}{dx}\frac{K_2}{K_1}K_2 - \frac{1}{T}\frac{dT}{dx}K_3$$

$$= -\frac{dT}{dx}\left(\frac{K_3K_1-K_2^2}{K_1T}\right)$$

$\therefore$ Thermal conductivity $\kappa = \frac{K_3K_1-K_2^2}{K_1T}$

Using eq. ⑮, $\left(\frac{\mu}{\epsilon_F}\right)^m = 1-\frac{\pi^2}{12}\left(\frac{k_BT}{\epsilon_F}\right)^2\cdot m+\cdots$,

and taking $\tau(\mu)\simeq\tau(\epsilon_F)$ (independant of ϵ),

One gets $K_1 \simeq \frac{n\tau(\epsilon_F)}{m}$

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$$K_2 = \frac{nZ\epsilon_F}{m}\left[1+\frac{5}{12}\pi^2\left(\frac{k_BT}{\epsilon_F}\right)^2\right]$$

$$K_3 = \frac{nZ\epsilon_F^2}{m}\left[1+\frac{7}{6}\pi^2\left(\frac{k_BT}{\epsilon_F}\right)^2\right]$$

then $k = k_B^2 \frac{\pi^2}{3}\frac{nZ}{m} T$ which recovers $\frac{k}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$ of the Sommerfeld model.

Semi-classical dynamics of Bloch electrons

To describe Bloch electrons, one uses $\vec{k}$ such that $\hbar\vec{k}$ = crystal momentum. The semiclassical dynamics describes wavepackets form by Bloch states:

$$\psi_n(\vec{r},t) = \sum_{k'} g_n(k-k')\psi_{nk'}(\vec{r})\, e^{-\frac{i}{\hbar}\varepsilon_n(k')t}$$

with $g_n(k-k') \simeq 0$ for $|k-k'| > \Delta k$

The wavepacket must be

(i) $\Delta x \gg a$ (lattice spacing)
(ii) $\Delta x \ll L$ L = characteristic length of $\phi(x) = -eEx$ or $T(x)$'s change.

Then the group velocity of the packet is

$$\vec{v}_n(k) = \frac{1}{\hbar} \nabla_k \varepsilon_n(k)$$

$$\therefore \dot{\vec{r}} = \frac{1}{\hbar} \nabla_k \varepsilon_n(k) \quad \text{for a fixed } n .$$

∴ The semiclassical description of Bloch electrons are

(i) The band index n is fixed, no interband transitions are allowed

(ii) $\dot{\vec{r}} = \vec{v}_n(\vec{k}) = \frac{1}{\hbar} \nabla_k \varepsilon_n(\vec{k})$

(iii) $\hbar \dot{\vec{k}} = -e\left(\vec{E} + \frac{1}{c} \vec{v}_n(\vec{k}) \times \vec{H}\right)$

(iv) $\vec{k}$ is restricted to 1st Brillouin zone.
$\vec{k}+\vec{G}$ & $\vec{k}$ describe the same electron.

with $f_0 = \dfrac{1}{e^{\beta(\varepsilon_n(k)-\mu)}+1}$

$\left(\times \dfrac{d^3\vec{k}}{(2\pi)^3} \times 2 = \# \text{of electron in } d^3\vec{k}\right)$

Validity: $e E a \ll \dfrac{[E_{gap}(k)]^2}{\varepsilon_F}$

$$\underset{\overset{\uparrow}{\frac{eH}{mc}}}{\hbar\omega_c} \ll \frac{(E_{gap}(k))^2}{\varepsilon_F}$$ (to prevent interband tunneling.)

(not easy to show, see Ashcroft & Mermin Appendix J.)

Physical origin of $\hbar\dot{\vec{k}} = \vec{F}$:

As we indicated, $\hbar\vec{k}$ is the crystal momentum, not the real momentum of the electron. Why is $\hbar\dot{\vec{k}} = \vec{F}$?

From the energy conservation, the change of electron's energy $\delta\epsilon = \vec{F}\delta t\cdot\vec{v}_n(k)$

$\because\ \delta\epsilon = \delta\vec{k}\cdot\nabla_k\epsilon_n(\vec{k})$ $\quad\therefore\ \delta\vec{k}\cdot\nabla_k\epsilon_n(\vec{k}) = \vec{F}\delta t\cdot\vec{v}_n(\vec{k})$

$$= \vec{F}\delta t\cdot\frac{1}{\hbar}\nabla_k\epsilon_n(\vec{k})$$

$$\therefore\ \hbar\frac{d\vec{k}}{dt} = \vec{F}$$

From the momentum conservation, $\vec{F}\Delta t = \Delta\vec{P}_e + \Delta\vec{P}_{lattice}$

$$\psi_k(\vec{r}) = \frac{1}{\sqrt{V}}\sum_G C_{k+G}\, e^{i(\vec{k}+\vec{G})\cdot\vec{r}}$$

$$\therefore\ \vec{P}_e = \frac{1}{V}\int d^3r\ \psi_k^*\frac{\hbar}{i}\nabla\psi_k = \frac{1}{V}\int d\vec{r}\sum_{GG'} C^*_{k+G}C_{k+G'} \times \hbar(\vec{k}+\vec{G}')e^{i(\vec{G}-\vec{G}')\cdot\vec{r}} = \sum_G \hbar(\vec{k}+\vec{G})\,|C_{k+G}|^2$$

$\therefore\ \Delta\vec{P}_e = \hbar\Delta\vec{k} + \sum_G \hbar\vec{G}\left(\nabla_k|C_{k+G}|^2\right)\cdot\Delta\vec{k}$ --- ⑯

On the other hand, an incident electron with momentum $\hbar\vec{k}$ will get reflected by the lattice to $\hbar(\vec{k}+\vec{G})$.

∴ The lattice acquires $-\hbar\vec{G}$ momentum!

∴ The momentum transferred to the lattice when $\vec{k}\to\vec{k}+\Delta\vec{k}$ is $\Delta\vec{P}_{lattice} = -\sum_G \hbar\vec{G}\underbrace{\left(\nabla_k|C_{k+G}|^2\right)}_{\text{Change of } \vec{k}+\vec{G} \text{ component}}\cdot\Delta\vec{k}$ -- ⑰

From eqs ⑯ & ⑰, $\therefore\ \Delta\vec{P}_e + \Delta\vec{P}_{lattice} = \hbar\Delta\vec{k}$

$\therefore\ \vec{F}\Delta t = \hbar\Delta\vec{k}$ even though $\hbar\vec{k}$ is crystal momentum!

Effective mass

The acceleration of a Bloch electron in band n is given by

$$\vec{a}_n = \frac{d\vec{v}_n}{dt} = \frac{1}{\hbar}\frac{d}{dt}\nabla_k E_n(k)$$

$$= \frac{1}{\hbar}\nabla_k\left[\nabla_k E_n(k)\right]\cdot\frac{d\vec{k}}{dt}$$

i.e. $a_n^i = \frac{1}{\hbar}\sum_j \frac{d}{dk_j}\frac{d}{dk_i}E_n(k)\,\frac{dk_j}{dt}$

$\because\ \hbar\frac{dk_j}{dt} = F_j$ (force)

$\therefore\ \frac{d\vec{v}_n}{dt} = (m_{eff})^{-1}\cdot\vec{F}$

with $(m_{eff})^{-1}_{ij} = \frac{1}{\hbar^2}\frac{d^2E_n(k)}{dk_i dk_j}$ being the effective mass tensor.

This is consistently with the perturbation theory (page 10-11, eq.㊳):

$$\varepsilon_k^{(n)} = \varepsilon_0^{(n)} + \frac{\hbar^2}{2}\vec{k}\cdot(m^*)^{-1}\cdot\vec{k}.$$

Filled bands & partial filled bands

For a crystal with inversion symmetry, $\varepsilon_n(-k)=\varepsilon_n(k)$.

$\therefore\ \vec{v}_n(k) = -\vec{v}_n(-\vec{k})$. In equilibrium, both $\vec{k}$ & $-\vec{k}$

are occupied, ∴ There is no current.

More rigorously,

electric current : $\vec{j} = (-e)\int \frac{d^3k}{(2\pi)^3} \times 2\, \vec{v}(k)$

$$= \frac{(-e)}{\hbar}\int \frac{d^3k}{4\pi^3}\frac{\partial \mathcal{E}(k)}{\partial \vec{k}}$$

heat current : $\vec{J}_u = \int \frac{d^3k}{4\pi^3}\mathcal{E}(k)\frac{1}{\hbar}\frac{\partial \mathcal{E}(\vec{k})}{\partial \vec{k}}$

$$= \frac{1}{2\hbar}\int \frac{d^3k}{4\pi^3}\frac{\partial \mathcal{E}^2(k)}{\partial \vec{k}}$$

Both currents are integrals over primitive cell of the gradient of some functions.

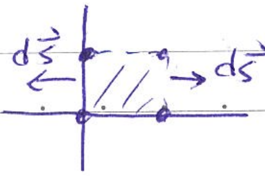
For any periodic function $f(\vec{r})$,

$$\int_{\substack{\text{primitive}\\ \text{cell}}} \vec{\nabla}\cdot(\vec{A}f)\, d\vec{r} = \int_{\text{Boundary}} d\vec{s}\cdot(\vec{A}f)$$

for any vector $\vec{A}$.

$\because \vec{\nabla}\cdot(\vec{A}f) = \vec{A}\cdot\vec{\nabla}f$ $\quad\therefore \int_{\substack{\text{Primitive}\\ \text{cell}}} \vec{\nabla}f\, d\vec{r} = \int_{\text{Boundary}} d\vec{s}\, f$

$\because$ f is periodic, f is the same on the boundary points with opposite $d\vec{s}$, e.g., square lattice



$\therefore \int d\vec{s}\, f = 0$, $\int \vec{\nabla} f\, d\vec{r} = 0$

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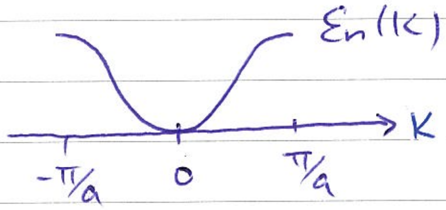
example: ·1D band



$$\int_{-\pi/a}^{\pi/a} dk \frac{\partial \varepsilon_n}{\partial k}$$

$$= \varepsilon_n(\tfrac{\pi}{a}) - \varepsilon_n(-\pi/a) = 0$$

Hence, for filled bands, both $\vec{J}$ & $\vec{J_u} = 0$

Only partial filled bands can carry electric & heat currents.

This is the situation of equilibrium.

In the presance of external fields, electrons become dynamical. In this case, the Liouville's theorem implies $\frac{df}{dt} = 0$. i.e., f is constant during the action of external fields between collisions. Hence $\underbrace{\text{the density}}_{\text{phase space}}$ $(\frac{1}{(2\pi)^3} \times 2)$ remains to be constant and is $\frac{1}{4\pi^3}$. Therefore, for semiclassical motion, external fields can't change the configration of a filled band. A filled band is still a filled band (i.e. all k's are occupied). ∴ $\vec{J}$ & $\vec{J_u}$ still vanish in the presance of external $\vec{E}$ & $\vec{B}$!

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Bloch oscillations

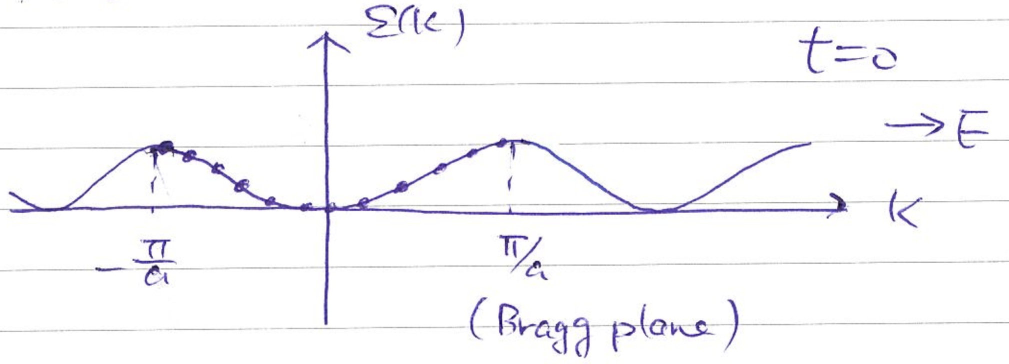
As we indicated in the above, the filled band is still filled under the action of electric field.

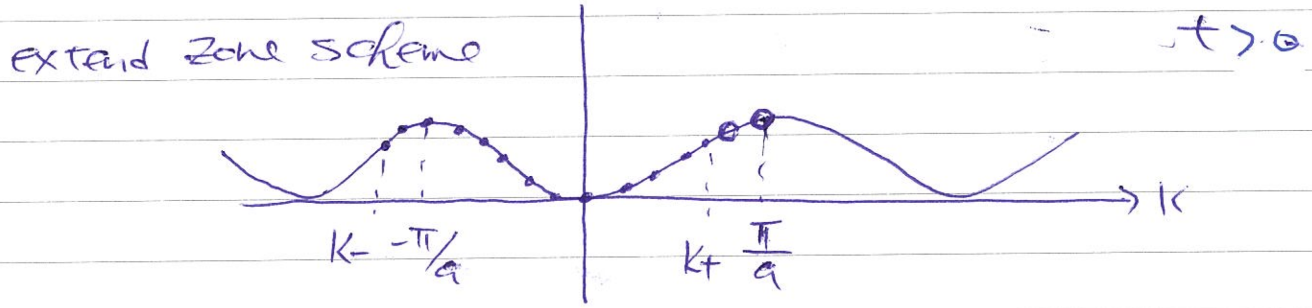
From the view of each state, one has

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E}$$

$$\therefore \vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}}{\hbar}t$$

$\therefore \vec{k}(t)$ is changing. In fact, all $\vec{k}$'s are shifting by the same amount. Therefore, the filled band is shifted as a whole, it is still filled:





One can shift two extra k near k_- back to k_+ so that it's still filled.

Since $v_n(\vec{k}) = \frac{1}{\hbar}\nabla_k \mathcal{E}(\vec{k})$, $\mathcal{E}(\vec{k})$ is periodic in $\vec{k}$. ∴ As t increases, $\vec{k}$ exceeds $-\pi/a$ $(-G/2)$, $v_n(\vec{k})$ simply goes to $v_n(+\pi/a)$. In other words, $\vec{k}$ should follow the reduced zone scheme and goes directly from $-\frac{\pi}{a}$ to $+\pi/a$, and then from π/a to $-\pi/a$ again and repeat to π/a,

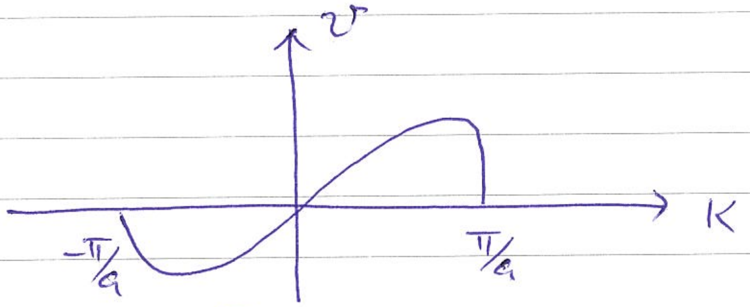
∴ Motion in $\vec{k}$ is periodic, & its velocity $\vec{v}_n(\vec{k})$ is also periodic.

This process is known as Bloch oscillation.

with $\frac{eET_B}{\hbar} = \frac{2\pi}{a}$ ∴ $T_B = \frac{2\pi\hbar}{eEa}$

$$\omega_B = \frac{eEa}{\hbar}$$

In the 1D excample as shown in the above, one has



Hence $\Delta x = \int_0^T v\,dt = 0$, electron has no net movement.

From the scattering point of view, as k increases and approaches $\frac{G}{2}$ (Bragg plane), the electron is likely to be Bragg-reflected back in the opposite direction. The extra momentum is provided by the lattice.

Therefore, a DC field can generate AC current.

Although the Bloch oscillation is reasonable for Bloch electrons, it is hard to observe it in real crystal. Typically, $T_B \sim 10^{-5}$ sec but collision time typically $\sim 10^{-14}$ sec at room temperature. Hence electrons experience enormous number of collisions & the oscillatory motion gets suppressed.

Therefore, to observe the Bloch oscillations, one often resorts to other lattices which are more perfect, such as optical (or superlattice by increasing a, i.e., reducing T_B) lattice formed by laser lights.

The observation of Bloch oscillations has been controversial. It's been much improved by the invention of superlattice of the semiconductor by Esaki & Tsu.

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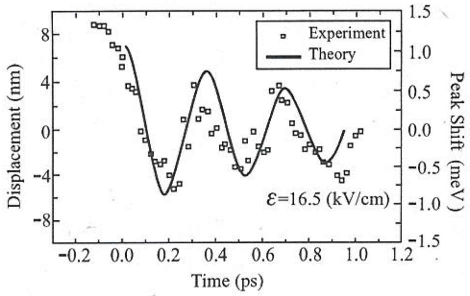
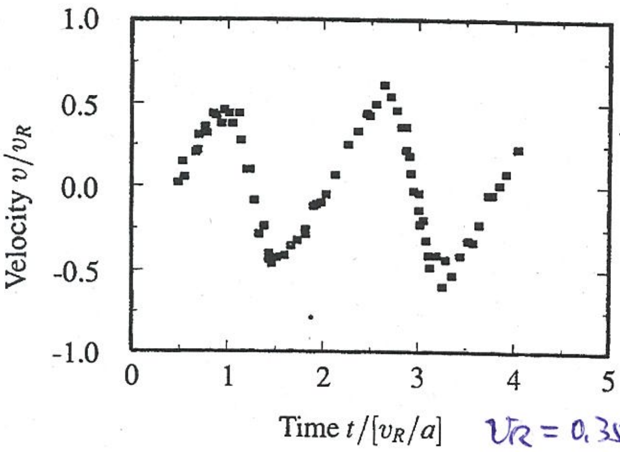
Experimental observation of Bloch oscillation



V.G. Lyssenko et. al.
Phys. Rev. Lett. 79, 301 (1997)

67Å/17Å superlattice.
GaAs $Al_{0.3}Ga_{0.7}As$



$v_R = 0.35 \text{ cm s}^{-1}$
$a = 0.85 \text{ m s}^{-2}$

Bloch oscillations of ultracold (cecium) atoms in an optical potential

M. Ben Dahan et. al. Phys. Rev. Lett. 76, 4508, 1996.

The potential is made to undergo uniform acceleration, but atoms oscillate rather than follow the potential.

Negative differential resistance

The Bloch oscillation is due to Bragg-reflection of electrons, which can also be exhibited as negative differential resistance in I-V curve. In the presence of collisions, one has $v_d = \int_0^\infty e^{-t/\tau} dv$, τ = mean-free time

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$\because \frac{d\vec{v}}{dt} = \vec{a} = \frac{1}{\hbar} \nabla_k \nabla_k \varepsilon_n(k) \cdot \frac{d\vec{k}}{dt}$

For isotropic crystals, one has $\hbar \frac{d\vec{k}}{dt} = -e\vec{E}$

$$dv = \frac{eE}{\hbar^2} \frac{\partial^2 \varepsilon(k)}{\partial k^2} dt$$

$$\therefore v_d = \frac{eE}{\hbar^2} \int_0^\infty \frac{\partial^2 \varepsilon(k)}{\partial k^2} e^{-t/\tau} dt$$

$\varepsilon(k)$ can be roughly approximated by sinusoidal functions : $\varepsilon(k) = \alpha - 2\beta \cos ka$

$\therefore \frac{\partial^2 \varepsilon(k)}{\partial k^2} = 2\beta a^2 \cos ka \qquad \frac{1}{m_{eff}} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2}\Big|_{k=0} = \frac{2\beta a^2}{\hbar^2}$

$$\therefore v_d = \frac{eE}{\hbar^2} 2\beta a^2 \, \mathrm{Re} \int_0^\infty e^{ika - t/\tau} dt$$

$k = k(0) - \frac{eE}{\hbar} t$, $\because$ the contribution of $k(0)$ to current $= 0$ (initially, there is no current),

$\therefore$ we may set $k(0)$ to zero.

$$\therefore v_d = \frac{eE}{m_{eff}} \mathrm{Re} \int_0^\infty e^{-t/\tau - i\frac{eEa}{\hbar}t} dt$$

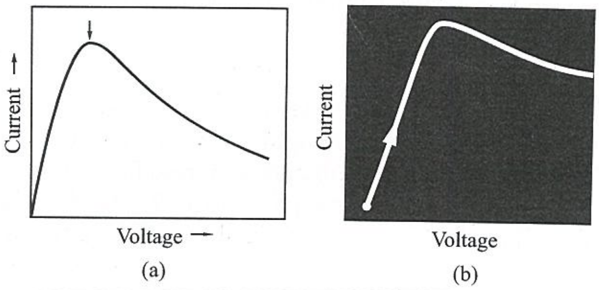
$$= \frac{eE}{m_{eff}} \mathrm{Re} \frac{1}{1/\tau + i\frac{eEa}{\hbar}} = \frac{eE}{m_{eff}} \frac{1/\tau}{(1/\tau)^2 + (\frac{eEa}{\hbar})^2}$$

$$= \frac{eE\tau}{m_{eff}} \left[1 + (\frac{eE\tau a}{\hbar})^2 \right]^{-1}, \quad \because T_B = \frac{2\pi\hbar}{eEa}$$

$$\therefore j = nev_d = \sigma_0 \left[1 + (\frac{2\pi\tau}{T_B})^2 \right]^{-1} E, \quad \sigma_0 = \frac{ne^2\tau}{m_{eff}}$$

∵ T_B depends on E, one sees that as $E\uparrow$, $T_B\downarrow$, eventually j reaches a maximum at $\frac{eE\tau a}{\hbar}=1$ and then j decreases. The reason why j decreases (this is negative differential resistance) is that when $T_B<\tau$, Bloch electrons can be Bragg-reflected so that current is reduced.

The experiment is difficult because usually $\tau \ll T_B$. However, in 1992, L. Esaki et.al. found that the superlattice can be used to exhibit a negative differential resistance:



(a)
(b)

Theoretical curve

experiment: (room temperature)
superlattice of 100 periods
GaAs well 60Å / $Ga_{0.5}Al_{0.5}As$
10Å

Ref. L. Esaki in Synthetic Modulated Structures edited by L.L. Chang & B.C. Giessen, Academic Press, Orlando (1985)

No.
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Concept of holes

One of the most important achievement of the semiclassical model is its explanation for the phenomena that carriers of crystals can have positive charges.

To understand how positive charges emerge, we start by noting that

$$(-e)\int_{\text{whole zone}} \frac{d^3k}{(2\pi)^3}\times 2\ v_n(k) = 0$$

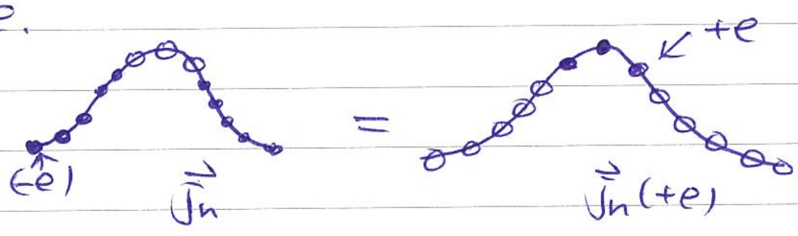
Since whole zone = occupied + unoccupied,

$$\therefore\ (-e)\left[\int_{\text{occupied}} \frac{d^3k}{4\pi^3}\ \vec{v}_n(k) + \int_{\text{unoccupied}} \frac{d^3k}{4\pi^3}\ \vec{v}_n(k)\right] = 0$$

$$\therefore\ \vec{j}_n = (-e)\int_{\text{occupied}} \frac{d^3k}{4\pi^3}\ \vec{v}_n(k)$$

$$= (+e)\int_{\text{unoccupied}} \frac{d^3k}{4\pi^3}\ \vec{v}_n(k)$$

i.e.



∴ Whenever it is convenient (especially when the band is nearly filled), one can think the current is carried by fictitious particles of (+e) filling the unoccupied k points!

These fictitious particles are called <u>holes</u>.

In this description, electrons are considered as <u>absence of holes</u>.

In addition to the calculation of current, the fictitious particles do behave as positive charges dynamically:

(i) $\vec{k}_h = -\vec{k}_e$, the crystal momentum of a hole is opposite to the crystal momentum of the unoccupied state.

The lattice is invariant under inversion $\vec{r} \to -\vec{r}$.

$\therefore$ if $\left(\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right)\psi_{\vec{k}}(\vec{r}) = \varepsilon_k \psi_{\vec{k}}(\vec{r})$

$$\left.\begin{array}{l} U(-\vec{r}) = U(\vec{r}) \\ \nabla_{-r}^2 = \nabla_r^2 \end{array}\right\} \quad \therefore \left[\frac{-\hbar^2}{2m}\nabla_{-r}^2 + U(-\vec{r})\right]\psi_k(-\vec{r}) = \varepsilon_k \psi_k(-\vec{r})$$

$$\Rightarrow \left(\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right)\psi_k(-\vec{r}) = \varepsilon_k \psi_k(-\vec{r})$$

Since $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r})$, $\therefore \psi_k(-\vec{r}) = e^{-i\vec{k}\cdot\vec{r}} u_k(-\vec{r})$

$\equiv e^{i(-\vec{k})\cdot\vec{r}}\, \hat{u}_{-k}(\vec{r})$ where $\hat{u}_{-k}(\vec{r}) \equiv u_k(-\vec{r})$ is periodic in $\vec{r}$.

$\therefore \psi_k(-\vec{r})$ can be labelled as $(-\vec{k})$ with the same energy ε_k!

$\therefore$ If $\vec{k}$ is present, so is $-\vec{k}$.

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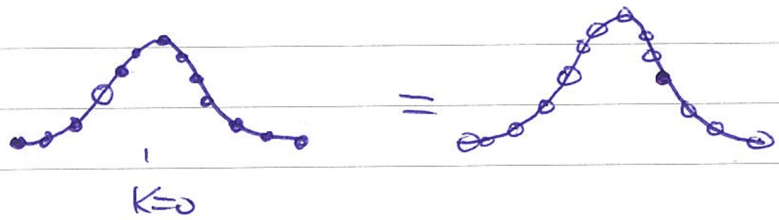
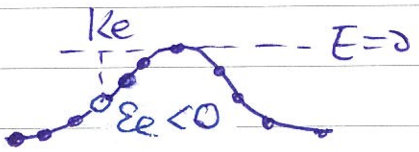
∴ $\sum_{\text{all zone}} \vec{k} = 0$. $\quad \sum_{\text{occupied}} \vec{k} = \sum_{\text{unoccupied}} (-\vec{k})$

∴ To calculate the total wave vector of the occupied states, we can equivalently calculate the unoccupied (holes) by assigning $(-\vec{k})$ to a hole.



(ii) $\mathcal{E}_h(k_h) = -\mathcal{E}_e(k_e)$

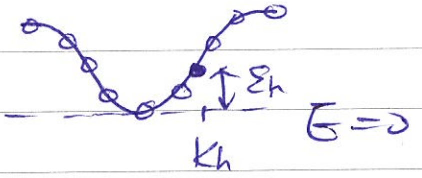
If we take the energy zero point at the max energy,



the energy of a hole ($\mathcal{E}_h$)

= the work one needs to remove the electron that occupies the position of the hole

∴ $\mathcal{E}_h = 0 - (\mathcal{E}_e) > 0$
$\quad = -\mathcal{E}_e$



(iii) $\vec{v}_h = \vec{v}_e$

$$\vec{v} = \frac{1}{\hbar}\nabla_k \mathcal{E}(k) \quad \therefore \vec{v}_h = \frac{1}{\hbar}\frac{d}{d\vec{k}}\mathcal{E}_h(\vec{k})\Big|_{\vec{k}=\vec{k}_h}$$

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$$= \frac{1}{\hbar}\frac{d}{d(-\vec{k}_e)}\mathcal{E}_n(\vec{k}_h) = -\frac{1}{\hbar}\frac{d}{d\vec{k}_e}[\mathcal{E}_n(\vec{k}_e)]$$

$k_h = -k_e$

$$= \frac{1}{\hbar}\frac{d}{d\vec{k}_e}\mathcal{E}_n(\vec{k}_e) = \vec{v}_e$$

∴ e & hole have the same velocity so that they carry opposite current because of their opposite charges.

(iv) eq. of motion

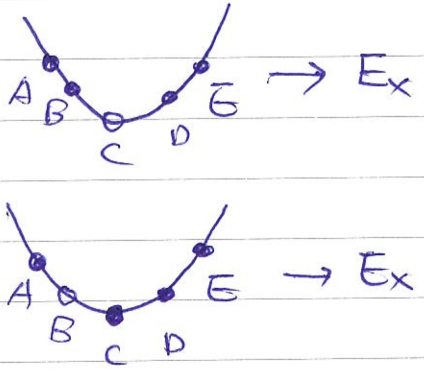
$$\because \ \hbar\frac{d\vec{k}_e}{dt} = (-e)\left(\vec{E} + \frac{1}{c}\vec{v}_e \times \vec{H}\right), \quad \vec{k}_h = -\vec{k}_e,\ \vec{v}_h = \vec{v}_e$$

$$\therefore \ \hbar\frac{d(-\vec{k}_h)}{dt} = (-e)\left(\vec{E} + \frac{1}{c}\vec{v}_h \times \vec{H}\right)$$

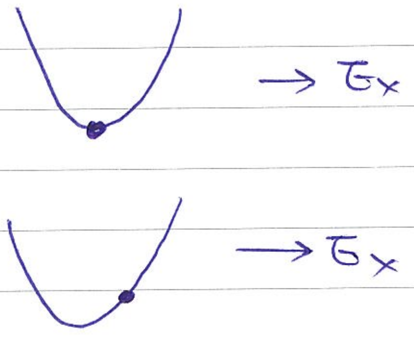
$$\therefore \ \hbar\frac{d\vec{k}_h}{dt} = (+e)\left(\vec{E} + \frac{1}{c}\vec{v}_h \times \vec{H}\right)$$

Dynamically, a hole behaves exactly as a particle carrying a positive charge.

e.g.



picture of electrons



picture of a hole

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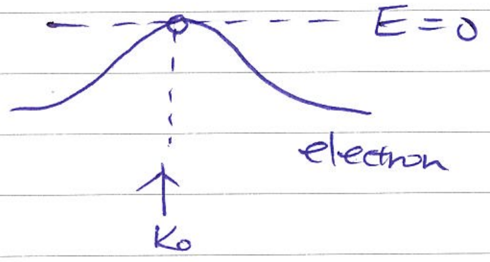
(V) effective mass of a hole

Near filled band

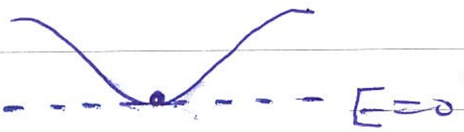


$$\varepsilon(k) \simeq \varepsilon(k_0) - A(k-k_0)^2$$

$$A \equiv \frac{\hbar^2}{2m^*}, \qquad \left(\frac{1}{m^*}\right)_{ij} = \frac{-1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_i \partial k_j}\bigg|_{k=k_0}$$

Hole :

$\Rightarrow$



$$\therefore \left(\frac{1}{m_{hole}}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_i \partial k_j}\bigg|_{k=k_0}$$

The above hole picture is particularly useful when one deals with nearly filled band! In this description, # of degrees is largely reduced! For a half-filled band, such as a metal, it is a half mixture of holes & electrons, it is not very useful to use the hole picture.

In full quantum treatment, one can also extend the hole description by particle-hole transformation : $c^{\dagger}_{i\sigma} \rightarrow d_{i\sigma}$, $c_{j\sigma} \rightarrow d^{\dagger}_{j\sigma}$

$d^{\dagger}$ = creation a hole and obeys the same Fermi-Dirac statistics.

Semiclassical motion in uniform magnetic/electric fields

In the presence of $\vec{E}$ & $\vec{H}$ fields, $\left\{\begin{matrix}\vec{K}\\ \vec{r}\end{matrix}\right.$ changes and obeys

$$\hbar\dot{\vec{K}} = -e\left(\vec{E} + \frac{1}{c}\vec{v}_n \times \vec{H}\right)$$

$$\vec{v}_n = \dot{\vec{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(K)}{\partial \vec{K}}$$

Since $\vec{v}_n$ is expressible in $\vec{K}$, the semi-classical motion can be described in the K space.

For instance, in a uniform $\vec{H}$ field,

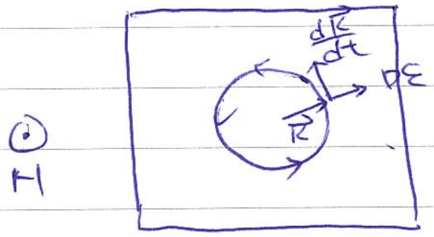
$$h\dot{\vec{K}} = -\frac{e}{c}\vec{v}_n \times \vec{H} = \frac{-e}{\hbar c}\vec{\nabla}_K \varepsilon(K) \times \vec{H}$$

$$\Delta\vec{K} \propto \vec{\nabla}\varepsilon \times \vec{H} \qquad \therefore \Delta\vec{K} \perp \vec{\nabla}\varepsilon,\ \Delta\vec{K} \perp \vec{H}$$

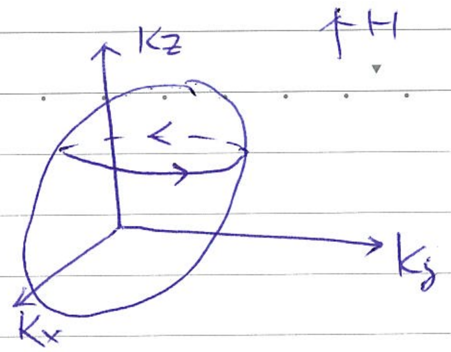
$\because$ $\vec{\nabla}\varepsilon \perp$ surface of constant energy

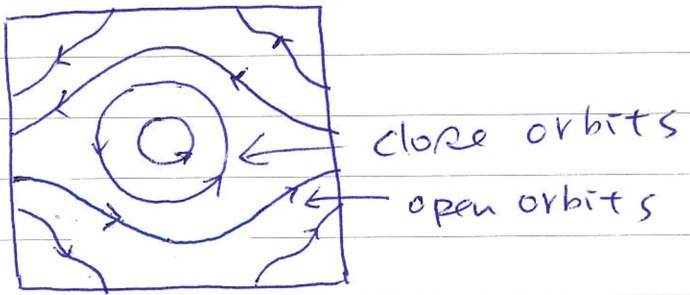
$\therefore$ $\vec{K}$ moves in the surface of constant energy. $\left(\frac{d\varepsilon}{dt} = \nabla_K\varepsilon \cdot \frac{d\vec{K}}{dt} = 0\right)$

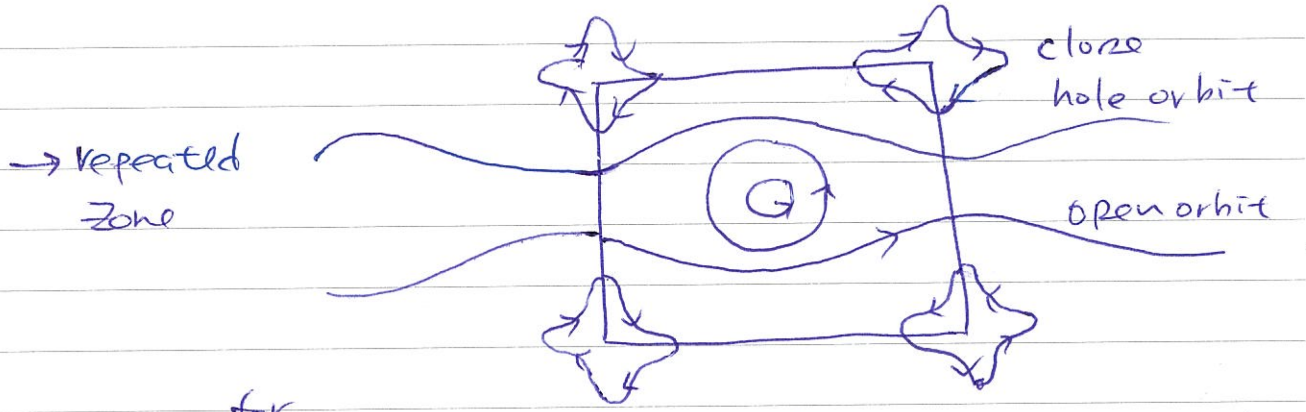
examples:



11-30







Note that for open orbits, the motion is still periodic!

∴ We can have closed electric orbits
closed hole orbits
open orbits } in kspace.

Quantized semiclassical dynamics

For closed orbits, by applying the Bohr-Sommerfeld quantization condition, the energy is quantized.

Through the semi-classical quantization, quantum effects can be also included.

$$\oint \vec{P_\perp}\cdot d\vec{r_\perp} = 2\pi\hbar\,(n+\gamma) \quad , \quad n=0,1,2,3\ldots$$

$P_\perp, r_\perp$ are momentum & position along the orbit that are perpendicular to $\vec{H}$.
$0\le\gamma\le 1$ is the Maslove index (for extra phase) often being ½. In the current problem, one can set $\gamma=0$.

In the presence of magnetic field

$$\vec{H}=\nabla\times\vec{A}\ , \quad \therefore \quad \vec{P_\perp} = \hbar\vec{K_\perp} - \frac{e}{c}\vec{A_\perp}$$

$$\because \quad \hbar\dot{\vec{K}} = \frac{e}{c}\vec{v}\times\vec{H}$$

$$\dot{\vec{K_\perp}} = \frac{-e}{\hbar c}|v_\perp| B$$

$$\vec{K_\perp} = \frac{e\vec{H}}{\hbar c}\times\vec{r_\perp} + \text{constant}.$$

Choose origin of $\vec{r_\perp}$ so that constant $=0$

$$\therefore \quad \vec{K_\perp} = \frac{e}{\hbar c}\vec{H}\times\vec{r_\perp}$$

$$\oint \vec{P_\perp}\cdot d\vec{r_\perp} = \frac{e}{c}\vec{H}\cdot\underbrace{\oint \vec{r_\perp}\times d\vec{r_\perp}}_{\substack{2\times\text{area of}\\ \text{orbit in real space}\\ A(\varepsilon,K_z)}} - \frac{e}{c}\underbrace{\oint \vec{A}\cdot d\vec{r_\perp}}_{\substack{\int \nabla\times\vec{A}\cdot d\vec{S}\\ = H\cdot\text{area of orbit}}}$$

$$= \frac{e}{c}H\cdot A(\varepsilon,k_z) = 2\pi\hbar(n+\gamma) \quad (\text{set } \vec{H}=H\hat{z})$$

$\because \vec{K_\perp} = \frac{e\vec{H}}{\hbar c}\times\vec{r_\perp}$. $\therefore$ the area of orbit in K space

$$= S(\varepsilon,k_z) = \left(\frac{eH}{\hbar c}\right)^2 A(\varepsilon,k_z)$$

$\therefore S(\epsilon, k_z) \cdot \frac{eH}{c} \left(\frac{\hbar c}{eH}\right)^2 = (n+\gamma)(2\pi\hbar)$

$$S(\epsilon, k_z) = \frac{2\pi eH}{\hbar c}(n+\gamma) \quad \text{--} \quad (18)$$

i.e. area of orbit in k space is quantized!

example

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \quad \text{(free electron)}$$

$S(\varepsilon, k_z) = \pi k_\perp^2$, $\quad k_\perp^2 = k^2 - k_z^2 = \frac{2m\varepsilon}{\hbar^2} - k_z^2$

$$\therefore \pi\left(\frac{2m\varepsilon}{\hbar^2} - k_z^2\right) = \frac{2\pi eH}{\hbar c}(n+\gamma)$$

$$\varepsilon = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c (n+\gamma) \qquad \omega_c = \frac{eH}{mc}$$

$\llcorner$ - (19) $\quad$ = cyclotron frequency

if $\gamma = \frac{1}{2}$ $\Rightarrow$ ε is exactly the same as results of full quantum treatment.

Known as Landau levels

Wannier - Stark Ladder

The Bloch oscillation due to the electric field also implies that new quantization of energy can be formed in large E field.

In the presence of $\vec{E}$ field,

$$\vec{k}(t) = \vec{k}(0) - \frac{e\vec{E}t}{\hbar} \qquad \because \dot{\vec{r}} = \frac{\partial \varepsilon(k)}{\hbar \partial \vec{k}} = \vec{v}$$

$\therefore$ when $\vec{k}(t) = -\vec{k}(0)$, $\dot{\vec{r}}(t)$ also flips sign because $\mathcal{E}(-K) = \mathcal{E}(K)$.

Evidently, v is also periodic.

$\therefore$ $\vec{r}$ is also periodic!

Starting from $K=0$ to $K=G$ (1D, $\frac{2\pi}{a}$), then K flips to 0, forming a periodic orbit.

Semiclassical quantization:

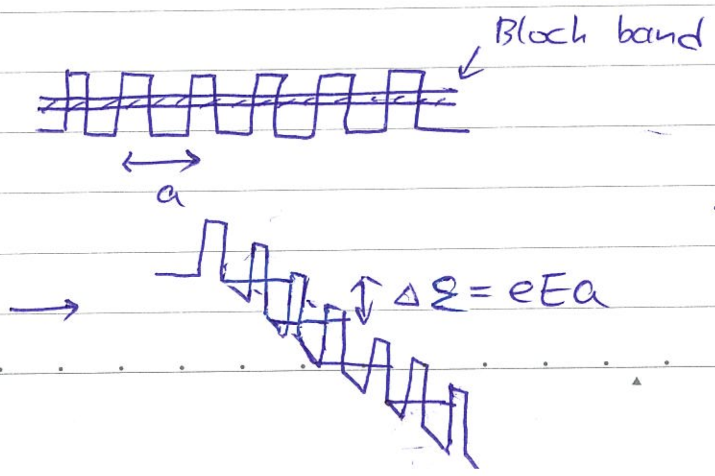
$$\int_0^{G} \hbar\vec{K}\cdot d\vec{r} = 2\pi n\hbar \quad n=1,2,\ldots$$

$$|||$$

$$\hbar G\langle\vec{r}\rangle$$

$$\therefore \langle\vec{r}\rangle_n = \frac{2\pi}{G}\times n$$

In other words, in the presence of strong $\vec{E}$ field, electrons get localized in space with spacing $\frac{2\pi}{G}\sim a$. Since $U=-eEx$, $\therefore$ different n corresponding to different $\langle x\rangle_n$ and different energy as indicated below:



$$\mathcal{E}_n = eEa\cdot n$$

These equally spaced energy levels are called Wannier-Stark ladders

In reality, this effect is almost impossible to be observed in real crystals as

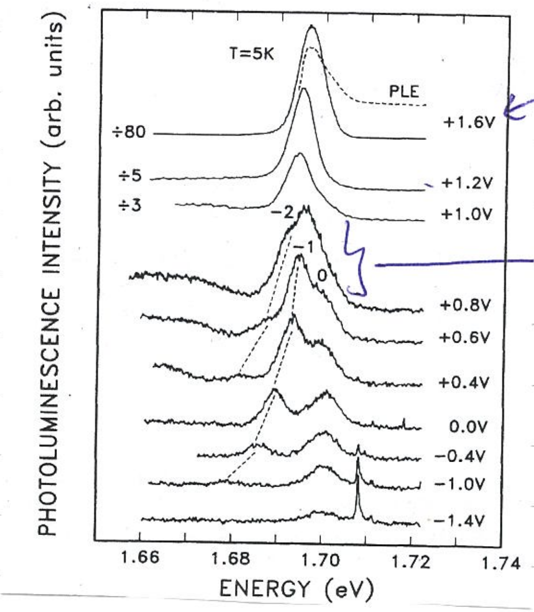
$a \sim 2Å$ for semiconductors, with $\mathcal{E} \sim 10^4 V/cm$

$e\mathcal{E}a \sim 0.2 meV$ is very small.

However, for superlattice, $a \sim 100 Å$,

$e\mathcal{E}a \sim 10 meV$ can be observed.

In this case, one can see extra optical transitions.



no bias

extra peaks

E.E. Mendez et al.
Phys. Rev. Lett. 60
2426, 1988

GaAs/GaAlAs multilayers.

Cyclotron resonance & cyclotron effective mass

In the presence of E.M. field, transitions can occur among different quantized semiclassical orbits.

If we can make a transition from

$n \to n+1$ (Cyclotron resonance), we have (using ⑱)

$$S(\varepsilon_n, k_z) = \frac{2\pi eH}{\hbar c}(n+\gamma)$$

$$-)\ S(\varepsilon_{n+1}, k_z) = \frac{2\pi eH}{\hbar c}(n+1+\gamma)$$

$$\therefore (\varepsilon_{n+1} - \varepsilon_n)\frac{dS}{d\varepsilon} = \frac{2\pi eH}{\hbar c}$$

For free electrons, $\varepsilon_{n+1} - \varepsilon_n = \hbar\omega_c$ with $\omega_c = \frac{eH}{mc}$. However, for Bloch electrons, we define $\varepsilon_{n+1} - \varepsilon_n = \hbar\omega_c(\varepsilon, k_z)$, with $\omega_c(\varepsilon, k_z)$ being now dependent on orbit (ε, k_z).

$\omega_c = \frac{eH}{m^* c}$, m^* is cyclotron effective mass.

We get

$$\omega_c(\varepsilon, k_z) = \frac{2\pi eH}{\hbar^2 c}\left[\frac{dS(\varepsilon, k_z)}{d\varepsilon}\right]^{-1} = \frac{eH}{m^* c}$$

$$m^*(\varepsilon, k_z) = \frac{\hbar^2}{2\pi}\frac{dS(\varepsilon, k_z)}{d\varepsilon}.$$

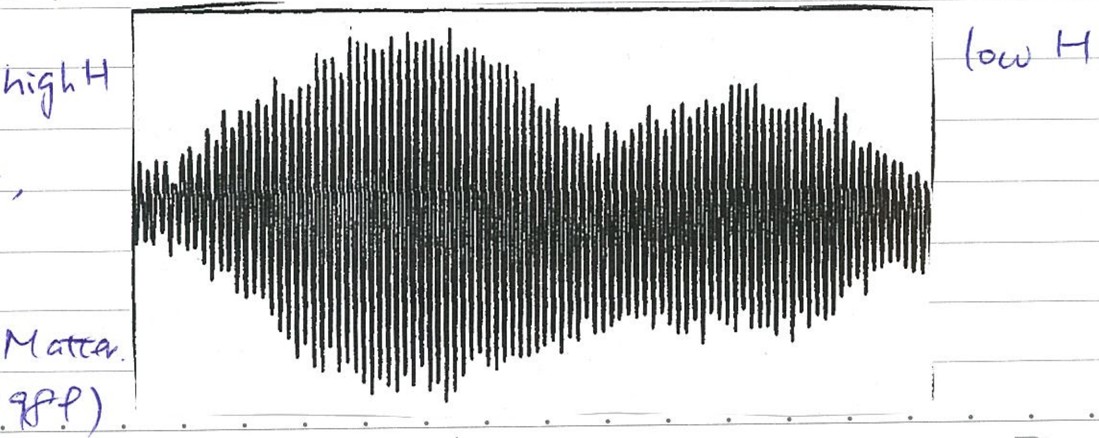
Therefore, by measuring the transition frequency (frequency of absorbed light), one can determine $m^*(\varepsilon, k_z)$, i.e., $\frac{dS(\varepsilon, k_z)}{d\varepsilon}$.

The de Haas-van Alphen effect

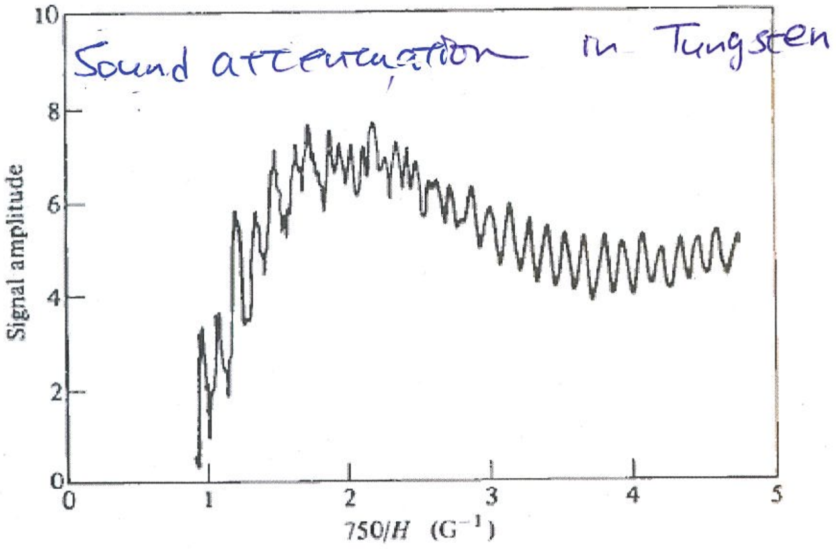
de Haas and van Alphen found that the M/H of metals (bismuth) oscillates as
↑
Magnetization

a function of H in 1930. Since then, careful experiments around 1960 show that $\chi = \frac{dM}{dH}$ (magnetic susceptibility) of many metals show oscillatory behavior and display regularity in period of $1/H$. These are now called de Haas-van Alphen oscillations.

Similar oscillatory behavior has been also observed in conductivity (Shubnikov-de Hass effect), sound attenuation, magnetoresistance, etc. See figures in below.

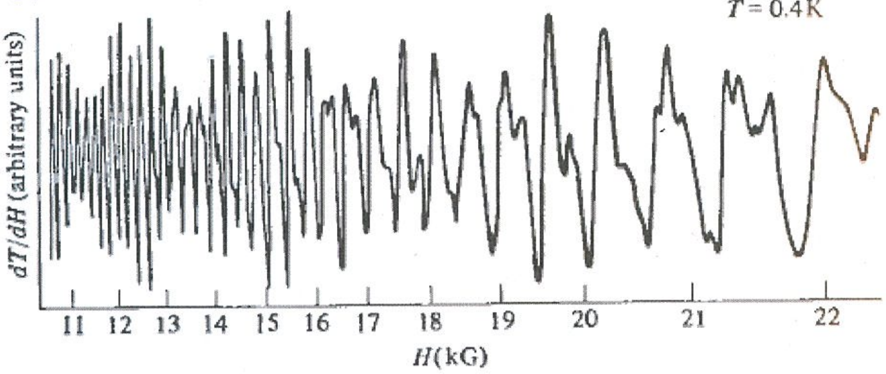


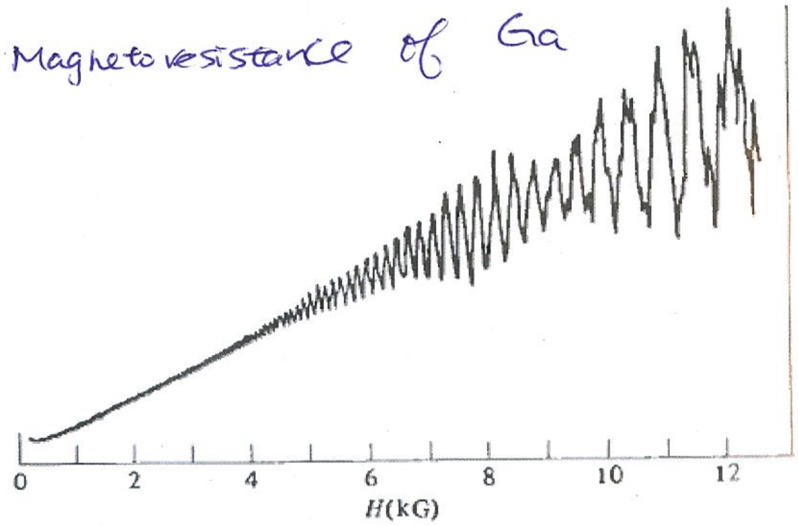
M.B. Hunt, et. al. J. Phys. Condense. Matter. 1, 6588(1989)



Sound attenuation in Tungsten

of Sb





Magnetoresistance of Ga

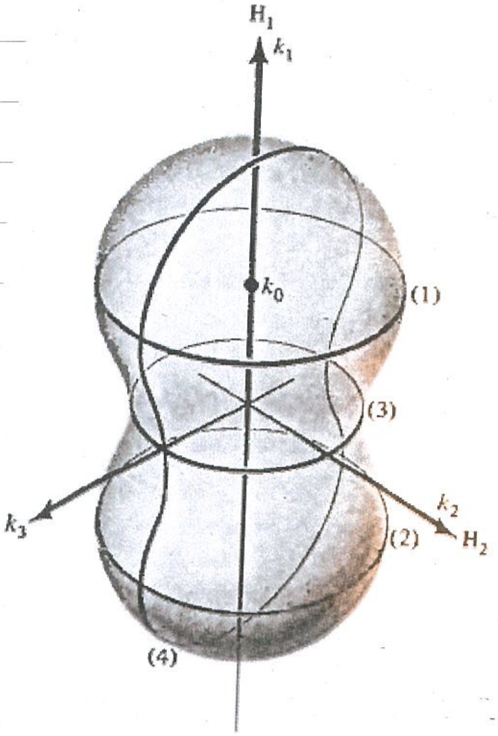
Origin of oscillatory phenomena & Fermi surface measurement

Onsager (1952) pointed out the key to understand the oscillatory behavior by stating

$$\Delta \frac{1}{H} = \frac{2\pi e}{\hbar c} \frac{1}{S_e} \quad \cdots\cdots \text{⑳}$$

S_e = any extremal cross-sectional area of Fermi surface in a plane normal to H.

example:



1, 2, 3 are the extreme cross sections when $\vec{H} \parallel k_1$

4 is the extreme cross section when $\vec{H} \parallel k_2$.

Using this relation, D. Shoenberg turned the oscillatory behavior into a powerful probe for measuring the Fermi surface.

To understand the de Haas-van Alphen effect, one first realizes that it can not be classical: since classically, the effect of H is to change $\vec{p}$ into $\vec{p}-\frac{e}{c}\vec{A}$, in classical statistical mechanics, one has

$$Z = \int \Pi d\vec{r_i}\, \Pi d\vec{p_i}\ e^{-\sum \frac{1}{2m_i}(\vec{p_i}-\frac{e}{c}\vec{A_i})^2 + U(r_1, r_2, \ldots r_N))}.$$

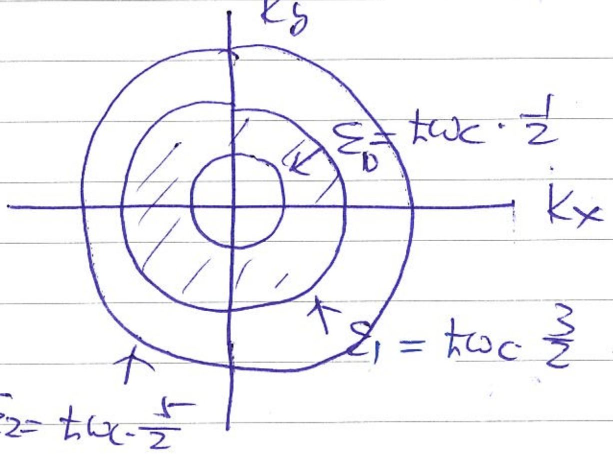
By changing the integration $\int d\vec{p_i} \rightarrow \int d(\vec{p_i}-\frac{e}{c}\vec{A_i})$, one sees that the effect of $\vec{H}$ is completely gone. Hence classically, there is no effect of H. (theorem by Bohr and van Leeuwen)

Therefore, the origin of de Haas-van Alphen effect is quantum. However, to solve the full quantum problem with a uniform magnetic field is really a formidable task. Nonetheless, semiclassical quantization provides a simple way to under the effect. To understand it, one needs to understand that there are degeneracy associated with each Landau level :

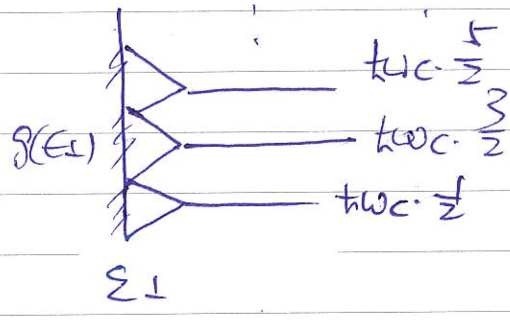
$$\varepsilon = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c\left(n+\frac{1}{2}\right)$$

Before H is turned on, $\varepsilon = \frac{\hbar^2 k_z^2}{2m} + \underbrace{\frac{\hbar^2(k_x^2+k_y^2)}{2m}}_{\varepsilon_\perp}$

There are many (k_x, k_y) points between $\hbar\omega_c(n+\frac{1}{2})$:



These states are collapsed into $\hbar\omega_c(n+\frac{1}{2})$:

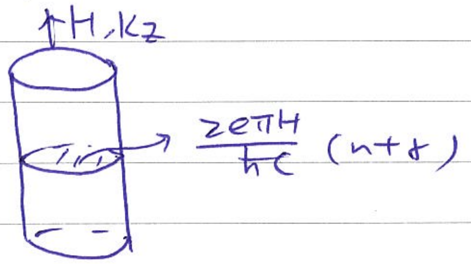


∴ Each Landau level's degeneracy = $\hbar\omega_c$

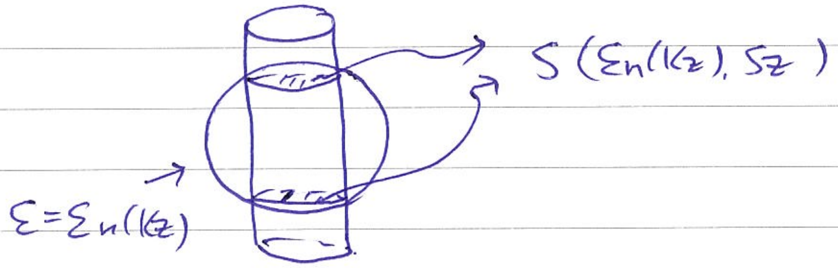
In addition, for a fixed n^{th}, k_z can be changed.

One has : area of orbit $= S(\epsilon_n^{(k_z)}, k_z) = \frac{2\pi e H}{\hbar c}(n+\gamma)$
$= \text{fixed}.$

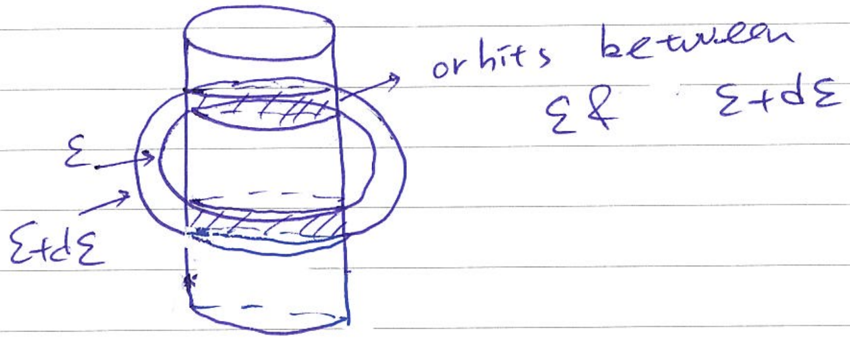
Which can be represented as a cylinder



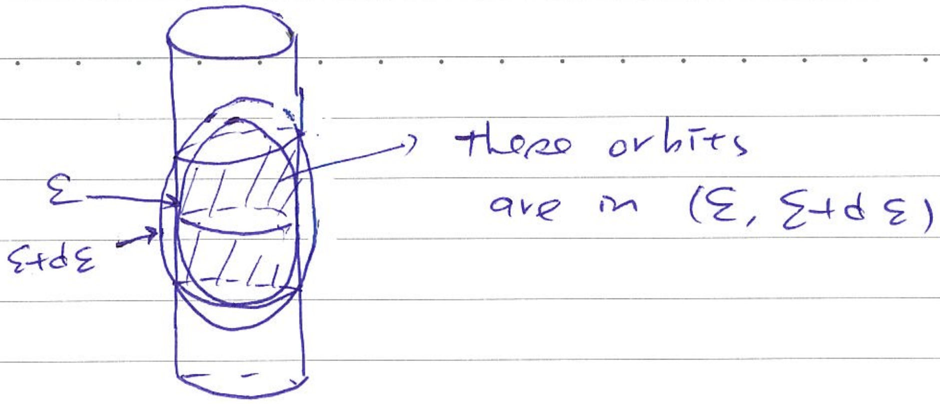
The nth level is the intersection of the above cylinder with ε surface



As kz changes, $\varepsilon_n(k_z)$ also changes. The density of intersecting orbits also changes. To see it, consider two energy surfaces ε, ε+dε. The available orbits (with different kz) are shown in below.



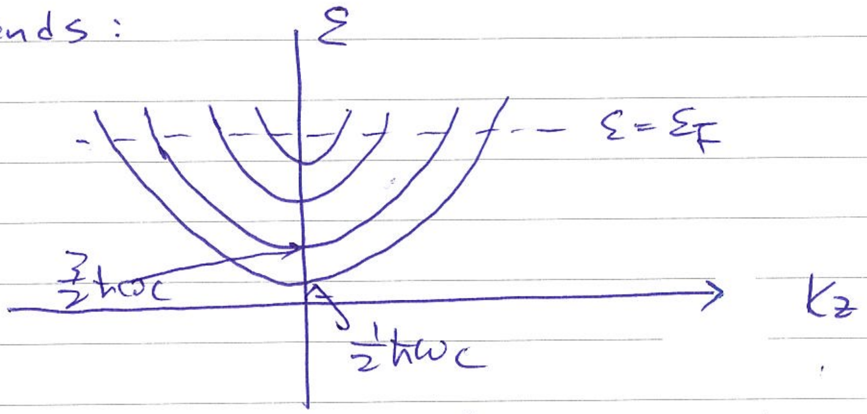
It is clear that if the orbit that intersects with ε is extremal, $g(\varepsilon)\,d\varepsilon$ is much enhanced (is actually singular, see below)



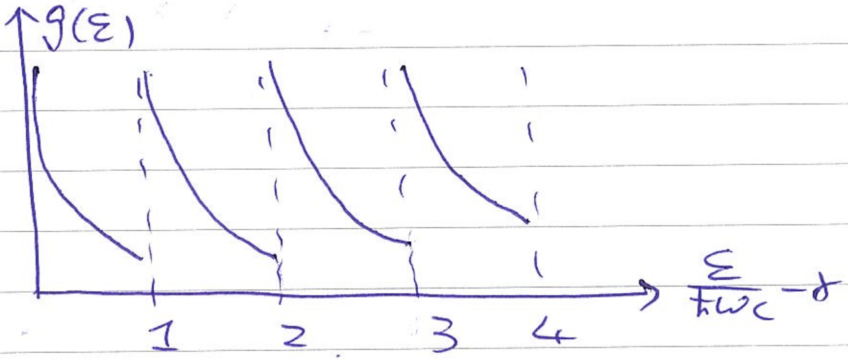
Take free electrons as an example.

$$\varepsilon = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c(n+\gamma) \qquad \gamma = 1/2$$

For fixed n & H, one has 1D parabolic bands:



The density of states $g(\varepsilon)$ due to availble k_z ~~is~~ diverges at $\frac{1}{2}\hbar\omega_c$, $\frac{3}{2}\hbar\omega_c$, . . .



It's clear that for extrem orbits, $g(\varepsilon)$ is divergent. As H increases, $\hbar\omega_c$ ↑ distance between Landau levels increases.

Some levels float up and cross $\varepsilon = \varepsilon_F$. Right before & after crossing ε_F, "total energy" E of the electrons goes down, and then E increases again until the next level floats across ε_F.

Hence E is a periodic function of H.

Obviously, since the density of states determines the response of the system, the largest response can be represented by extremal orbits when $g(\varepsilon_F) = \infty$.

$$\therefore \frac{2\pi e H}{\hbar c}(n+\gamma) = \underset{\uparrow}{S_e}$$

area of Fermi surface extremo orbits.

& $\Delta \frac{1}{H} = \frac{2\pi e}{\hbar c}\frac{1}{S_e}$.

This is the key result by Onsager (eq.⑳)

Therefore, any quantity that depends on the density of states at $\varepsilon = \varepsilon_F$ would show oscillatory behavior characterized by eq.⑳ at $T=0$

For finite T, it is clear that the spreading due to temperature, K_BT, has to be small in comparison to $\hbar\omega_c$.

For free electrons, $\omega_c = \frac{eH}{mc}$, it requires $H \sim 10^4\,G$, $T \sim$ a few K to see the oscillatory behavior.

Semiclassical theory of conduction for Bloch electrons.

The Boltzman equation can be generalized to describe the Bloch electrons.

In this case, one uses $\vec{r}$ & $\vec{k}$ (crystal momentum) as the variables. so that eq. ④ becomes

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{1}{\hbar} \frac{\partial}{\partial \vec{k}} f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

$\llcorner$ - - ㉑

$f = f(\vec{r}, \vec{k}, t)$

In general, $\left(\frac{\partial f}{\partial t}\right)_{coll.}$ needs not to take the relaxation-time approximation.

From the view of quantum mechanics, collision rate is described by the scattering probability which is defined to be

$$\frac{W_{\vec{k},\vec{k}'}\,dt\,d\vec{k}'}{(2\pi)^3}$$

as the probability in dt (between t & t+dt) that an electron with wavenumber $\vec{k}$ is scattered into $d^3\vec{k}'$ around $\vec{k}'$.

In other words, $W_{\vec{k},\vec{k}'}$ is the transition rate from $\vec{k}$ to $\vec{k}'$.

By taking Pauli exclusion principle & occupation f into consideration, one has

$$\left(\frac{df(\vec{k})}{dt}\right)^{out}_{coll} = -\int \frac{d^3\vec{k}'}{(2\pi)^3}\, W_{\vec{k},\vec{k}'}[1-f(\vec{k}')]\,f(k) \quad \text{--- ㉒}$$

Similarly, there are also electrons scattered into $\vec{k}$ from other $\vec{k}'$. Hence

$$\left(\frac{df(\vec{k})}{dt}\right)^{in}_{coll} = \int \frac{d^3\vec{k}'}{(2\pi)^3}\, W_{\vec{k}',\vec{k}}\, f(\vec{k}')(1-f(\vec{k})) \quad \text{--- ㉓}$$

Therefore, generally, $\left(\frac{df}{dt}\right)_{coll}$ can be expressed in terms of $W_{\vec{k},\vec{k}'}$

$$\left(\frac{df(\vec{k})}{dt}\right)_{coll} = -\int \frac{d^3\vec{k}'}{(2\pi)^3} \left\{ W_{k,k'}f(k)(1-f(k')) - W_{k',k}f(\vec{k}')(1-f(\vec{k})) \right\} \quad \text{--- ㉔}$$

Equations ㉑ & ㉔ are the general Boltzman equations.

If the scattering can be described by a potential $V(\vec{r})$ (for instance, dilute impurities), the transition rate is

$$W_{\vec{k},\vec{k}'} = \frac{2\pi}{\hbar} \delta(\varepsilon_k - \varepsilon_{k'}) \, |\langle k | V | k' \rangle|^2$$

(Fermi's Golden rule in Q.M.)

It's clear from this particular example that we have (i) $W_{kk'} = W_{k'k}$ (detailed balancing) (ii) $\varepsilon_k = \varepsilon_{k'}$ (this is only the case for elastic scattering).

The detailed balance is a general property as long as $\langle k | V | k' \rangle = \langle k' | V | k \rangle^*$, V is real. In this case, one gets

$$\left(\frac{d f(\vec{k})}{dt} \right)_{coll} = - \int \frac{d^3 k'}{(2\pi)^3} W_{k,k'} \left(f(\vec{k}) - f(\vec{k}') \right)$$

in which the quadratic term gets cancelled and the Boltzman equation is linear in f.

In general, if there are electron-electron interactions, $W_{k,k'}$ also depends on f, then the Boltzman is no longer linear in f.

In the relaxation time approximation, one approximates eq. ㉒ by $-\frac{f(k)}{\tau(k)}$; i.e.

$$\left(\frac{df(k)}{dt}\right)^{out}_{coll} = -\frac{f(k)}{\tau(k)};$$

while one approximates eq. ㉓ by $\frac{f^0(k)}{\tau(k)}$; i.e.,

$$\left(\frac{df(k)}{dt}\right)^{in}_{coll} = \frac{f^0(k)}{\tau(k)}$$

so that $\left(\frac{df}{dt}\right)_{coll} = -\frac{1}{\tau(k)}\left(f(k)-f^0(k)\right)$.

where $f^0(k) = \frac{1}{e^{\beta(\mathcal{E}(k)-\mu)}+1}$ with local temperature T & μ.

Eq. ㉑ becomes

$$\frac{\partial f}{\partial t} + \dot{\vec r}\cdot\frac{\partial f}{\partial \vec r} + \dot{\vec k}\cdot\frac{\partial f}{\partial \vec k} = -\frac{1}{\tau(k)}\left(f-f^0\right)\cdots\ \text{㉕}$$

With

$$\left.\begin{aligned}\dot{\vec r} &= \frac{\partial \mathcal{E}}{\hbar\,\partial \vec k} = \vec v\\ \hbar\dot{\vec k} &= -e\vec E - \frac{e\vec v}{c}\times\vec H.\end{aligned}\right\}\ \text{㉕}-1$$

To solve eq. ㉕, we first realize that

$$\frac{df}{dt} = -\frac{1}{\tau(k)}(f - f^0) \quad \text{in the relaxation}$$

← .. ㉖

approximation.

In other words, if we follow particles, we will find that the total # of particles in $d^3\vec{r}\, d^3\vec{k}$ decays.

Eq. ㉖ can be solved, we find

$$f(\vec{r},\vec{k},t) = \int_{-\infty}^{t} dt'\, f^0(\vec{r},\vec{k},t)\, e^{-\frac{t-t'}{\tau(k)}} \quad .. ㉗$$

$\because\ dt'\, e^{-\frac{t-t'}{\tau(k)}} = d\, e^{-\frac{t-t'}{\tau(k)}}$, by integrating by part, we can rewrite eq. ㉗ as

$$f(\vec{r},\vec{k},t) = f^0(\vec{r},k,t) - \int_{-\infty}^{t} dt'\, e^{-\frac{t-t'}{\tau(k)}} \frac{df^0}{dt'} \quad -- ㉘$$

Here we write $\frac{df^0}{dt'}$ as $\frac{df^0}{dt'}$ to remind us that the derivative on t' only acts on t' of $f^0(r,k,t')$

Now, in the absence of collisions, one has ← -- ㉙

$$\frac{df^0}{dt'} + \dot{\vec{r}}(t') \cdot \frac{\partial f^0(\vec{r}(t'),\vec{k}(t'),t')}{\partial \vec{r}} + \dot{\vec{k}}(t') \cdot \frac{\partial f^0(\vec{r}(t'),\vec{k}(t'),t')}{\partial \vec{k}'} = 0$$

where $\vec{r}(t)$ & $\vec{k}(t)$ are solutions to eqs ㉕-1.

There fore, we find

$$f(\vec r,\vec k,t) = f^0(\vec r,\vec k,t) - \int_{-\infty}^{t} dt'\, e^{-\frac{t-t'}{\tau(k)}} \left[\dot{\vec r}(t')\cdot\frac{\partial}{\partial \vec r} + \dot{\vec k}(t')\cdot\frac{\partial}{\partial \vec k}\right] f^0$$

with $\vec r(t')$ & $\vec k(t')$ being solutions to eqs. (25)-1

with b.c. $\vec r(t)=\vec r$, $\vec k(t)=\vec k$.

Now, $f^0(\vec r,\vec k,t) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$ with $\varepsilon=\varepsilon(k)$,

$T=T(\vec r)$, & $\mu=\mu(\vec r)$, one has

$$\frac{\partial f^0}{\partial \vec r} = \frac{\partial f^0}{\partial \varepsilon}\left[-\vec\nabla\mu - (\varepsilon-\mu)\frac{\vec\nabla T}{T}\right]$$

$$\frac{\partial f^0}{\partial k} = \frac{\partial f^0}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial k} = \frac{\partial f^0}{\partial \varepsilon}(\hbar\vec v)$$

Hence

$$f(\vec r,\vec k,t) = f^0(\vec r,\vec k,t) + \int_{-\infty}^{t} e^{-\frac{t-t'}{\tau(k)}}\, dt'$$

$$\times\left[\left(\frac{\partial f^0}{\partial\varepsilon}\right)\vec v\cdot\left(-e\vec E-\vec\nabla\mu - \frac{\varepsilon-\mu}{T}\vec\nabla T\right)\right] \quad \text{L}\cdots(30)$$

$(\vec v\cdot \frac{e}{c}\vec v\times\vec H = 0)$

Eq. (30) generalizes eqs. (7), (8), (9), (10).

In the case when the semiclassical dynamics is slow in comparison to $\tau(k)$, one takes $\left(\frac{\partial f^0}{\partial\varepsilon}\right)\vec v\cdot(-e\vec E-\vec\nabla\mu$

$- \frac{\varepsilon-\mu}{T}\vec{\nabla} T)$ out of the integral in eq. ㉚.

$$\because \int_{-\infty}^{t} e^{-\frac{t-t'}{\tau(k)}}\, dt' = \tau(k)$$

Eq. ㉚ $\Rightarrow$ $f(\vec{r},\vec{k},t) = f^0(\vec{r},\vec{k},t) + \tau_k \vec{v}\cdot$

$$\left\{ e\vec{E} + \vec{\nabla}\mu + \frac{\varepsilon-\mu}{T}\vec{\nabla} T \right\} \frac{\partial f^0}{\partial \varepsilon}$$

— ㉚-1

which recovers eq. ⑧.

In general, one has to use eq. ㉚ to keep effects due to the lattice.

DC electrical conductivity

If T & μ are uniform (weak $\vec{E}$), we get: f is independent of t & $\vec{r}$

$$f(k) = f^0(k) + \int_{-\infty}^{t} e^{-\frac{t-t'}{\tau(k)}}\, dt' \left(\frac{+\partial f^0}{\partial \varepsilon}\right) \vec{v}\cdot e\vec{E}$$

$$= f^0(k) - e\vec{E}\cdot\vec{v}(\vec{k})\,\tau_k \left(-\frac{\partial f^0}{\partial \varepsilon}\right)$$

$$\vec{j} = \int (-e) \frac{d^3k}{(2\pi)^3} \vec{v}(k) f$$

$$= \sum_n e^2 \int \frac{d^3k}{4\pi^3} \tau_n(k) \vec{v}_n(k) (\vec{E}\cdot\vec{v}_n(k)) \left(\frac{\partial f^0}{-\partial \varepsilon}\right)_{\varepsilon=\varepsilon_n(k)}$$

$$\equiv \sum_n \overleftrightarrow{\sigma}^n \cdot \vec{E} \equiv \overleftrightarrow{\sigma}\cdot\vec{E}$$

$\because \left(-\frac{\partial f^0}{\partial \varepsilon}\right)_{\varepsilon=\varepsilon_n(k)} = 0$ except that $\varepsilon \hat{=} \mu + O(k_B T)$.

$\therefore$ Filled bands don't contribute! Only the partial filled band contributes!

In a metal, $\underset{(\sim 1eV)}{\mu} \gg k_B T$, to $\left(\frac{k_B T}{\varepsilon_F}\right)^2$,

$$\left(-\frac{\partial f^0}{\partial \varepsilon}\right) = \delta(\varepsilon - \varepsilon_F) \quad (\text{i.e. } T \simeq 0)$$

$\therefore$ $\tau(k)$ can be replaced by $\tau(\varepsilon_F)$.

$$\therefore \sigma = e^2 \tau(\varepsilon_F) \int \frac{d^3\vec{k}}{4\pi^3} \vec{v}(k) \underbrace{\vec{v}(k) \left(-\frac{\partial f^0}{\partial \varepsilon}\right)}_{\substack{\| \\ -\frac{1}{\hbar}\frac{\partial f}{\partial \vec{k}}}}$$

$$= e^2 \tau(\varepsilon_F) \int \frac{d^3\vec{k}}{4\pi^3 \hbar} \frac{\partial}{\partial \vec{k}}[\vec{v}(\vec{k})] f^0$$

$$\therefore \sigma_{\alpha\beta} = \frac{e^2 \tau(\varepsilon_F)}{\hbar^2} \int_{\text{occupied}} \frac{d^3\vec{k}}{4\pi^3} \frac{\partial^2 \varepsilon}{\partial k_\alpha \partial k_\beta}.$$

$$\because \varepsilon(k) = \varepsilon^0 + \frac{\hbar^2}{2} \vec{k} \cdot (m^*)^{-1} \cdot \vec{k}$$

$$\therefore \sigma_{\alpha\beta} = e^2 \tau(\varepsilon_F) \int_{\text{occupied}} \frac{d^3\vec{k}}{4\pi^3} (m^*)^{-1}_{\alpha\beta} \quad \text{: (electron picture)}$$

$$= e^2 \tau(\varepsilon_F) \int_{\text{unoccupied}} \frac{d^3\vec{k}}{4\pi^3} -(m^*)^{-1}_{\alpha\beta} \quad \text{(hole picture)}$$

(hole : $m^* \to -m^*$)

Clearly, in the isotropic case & m^* being independent of $\vec{k}$, $(m^*)^{-1}_{\alpha\beta} = \frac{1}{m^*}\delta_{\alpha\beta}$ for occupied k, one has

$$\sigma_{\alpha\beta} = \frac{e^2\tau(\varepsilon_F)}{m^*} \underbrace{\int \frac{d^3k}{4\pi^3}}_{n} \delta_{\alpha\beta}$$

$$= \frac{ne^2\tau(\varepsilon_F)}{m^*}\delta_{\alpha\beta}$$

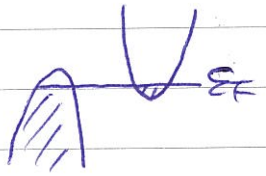
∴ This is the same as the Drude formula except that m is replaced by an effective mass m^*

However, if $(m^*)^{-1}_{\alpha\beta} = -\frac{1}{m_h^*}\delta_{\alpha\beta}$ and is independent of k for unoccupied levels, one gets

$$\sigma_{\alpha\beta} = \frac{n_h e^2 \tau}{m_h^*}$$

In this case, the charge carrier is positive and σ is determined by density of holes.

In the case of semi-metals, we have both electrons & holes. This is the two-band model that was discussed in HW. 4 but it is a natural outcome of semiclassical theory of Bloch electrons.



Hall effects (in high field)

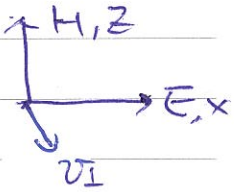
(H~10^4 G.)

In the high fields, $\omega_c \tau \gg 1$ i.e. $T_c \ll \tau$,

One can neglect impurities.

From $\hbar \dot{\vec{k}} = -e\vec{E} - \frac{e}{c}\vec{v}\times\vec{H}$, one has

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



$$= -\frac{e}{c}\vec{v}_\perp H^2$$

with $\vec{v}_\perp \perp \vec{H}$.

$$\therefore \vec{v}_\perp = -\frac{\hbar c}{e}\frac{\vec{H}\times\dot{\vec{k}}}{H^2} - c\frac{\vec{H}\times\vec{E}}{H^2} \quad \cdots (31)$$

Eq. (30) becomes $(\vec{v}_\perp \perp \vec{E})$

$$f - f^0 = \int_{-\infty}^{t} e^{-\frac{t-t'}{\tau}} \underbrace{\frac{c\hbar}{e}\frac{\vec{H}\times\dot{\vec{k}}}{H^2}\cdot e\vec{E}}_{\frac{c\hbar\dot{\vec{k}}}{H^2}\cdot(\vec{E}\times\vec{H})} \left(-\frac{\partial f^0}{\partial \varepsilon}\right) dt'$$

$$= \frac{c\hbar}{H^2}(\vec{E}\times\vec{H})\left(-\frac{\partial f^0}{\partial \varepsilon}\right)\cdot(\vec{k} - \langle\vec{k}\rangle) \quad \cdots (32)$$

where we have performed integration by parts:

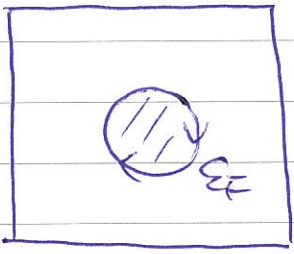
$$\int_{-\infty}^{t} e^{-\frac{t-t'}{\tau}}\dot{\vec{k}}\,dt' = \vec{k}\,e^{-t-t'/\tau}\Big|_{-\infty}^{t}$$

$$-\int_{-\infty}^{t}\frac{1}{\tau}e^{-\frac{t-t'}{\tau}}\vec{k}(t')\,dt'$$

$$= \vec{k} - \langle\vec{k}\rangle$$

For closed orbits & $T_c << \tau$
(see below)

$\because \vec{k}(T_c) \simeq \vec{k}(0)$



The integral $\int_{-\infty}^{t} e^{-\frac{t-t'}{\tau}} \vec{k}(t')\, dt'$ also has value for orbits with $t' \sim t$ & not a complete a cycle.

For other t', $\int dt' = 0$ due to $\vec{k}(T_c) \simeq \vec{k}(0)$

For the last incomplete cycle, $\int dt'\, k(t')$
$\sim T_c \vec{k}$

$\therefore \langle \vec{k} \rangle \sim \frac{T_c}{\tau} \vec{k} << \vec{k}$ can be neglected! --- ㉝

$\therefore f - f^0 = \frac{\hbar c}{H^2} (\vec{E} \times \vec{H}) \cdot \vec{k} \left(-\frac{\partial f^0}{\partial \varepsilon} \right)$ --- ㉞

$\therefore$ If All obits on Fermi surface are closed,

$$\vec{J} = (-e) \int \frac{d^3k}{4\pi^3} \underbrace{\underset{\underset{\frac{\partial \varepsilon_k}{\partial \hbar \vec{k}}}{\uparrow}}{\vec{v}_k} \left(-\frac{\partial f^0}{\partial \varepsilon_k} \right)}_{-\frac{\partial f^0}{\partial \hbar \vec{k}}} \frac{\hbar c}{H^2} (\vec{E} \times \vec{H}) \cdot \vec{k}$$

$$= \frac{+ec}{H^2} \int \frac{d^3k}{4\pi^3} \frac{\partial}{\partial \vec{k}} \left[f^0 \vec{k} \cdot (\vec{E} \times \vec{H}) \right]$$

$$- \frac{ec}{H^2} \vec{E} \times \vec{H} \int \frac{d^3k}{4\pi^3} f^0 \quad \text{---} \ ㉟$$

∵ all orbits on the Fermi surfaces are closed. If one can choose the B.Z. boundary to be unoccupied. where $f^0 = 0$

, the 1st term in eq. ㉟ $= 0$

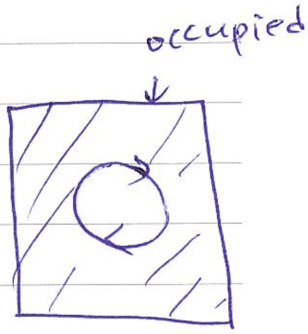
$$\int \frac{d^3k}{4\pi^3} f^0 = n$$

$$\vec{J} = -\frac{nec}{H^2} \vec{E} \times \vec{H}$$

On the other hand, if the B.Z. boundaries. are occupied, replace f^0 in $\frac{df^0}{d\varepsilon_k}$ by $\frac{df^0 - 1}{d\varepsilon_k}$, one gets

$$\vec{J} = \frac{ec}{H^2} \vec{E} \times \vec{H} \int \frac{d^3k}{4\pi^3}(1 - f^0)$$

$$= \frac{n_h ec}{H^2} \vec{E} \times \vec{H}$$



∴ The Hall coefficient

$$R \equiv \frac{E_y}{H J_x} = -\frac{1}{nec} \quad \text{or} \quad \frac{1}{n_h ec}$$

electron-like hole-like

The explanation of hole-like behavior for the Hall coefficient is one of the successes for the semi-classical approach.

Magnetoresistance

The Hall effect implies

$$\sigma \propto \begin{pmatrix} \tilde{\sigma}_0 & R/H \\ -R/H & \tilde{\sigma}_0 \end{pmatrix}.$$

As indicated, $\langle \vec{k} \rangle \sim \frac{T_c}{\tau} \vec{k}$. Here due to the acceleration of E, $\vec{k} \parallel \hat{E}$

$$\therefore \langle \vec{k} \rangle \sim \frac{T_c}{\tau} \vec{E}$$

$\tilde{\sigma}_0 \sim c \frac{T_c}{\tau} \frac{R}{H}$ $\quad c =$ some constant

$$\therefore \sigma \propto \begin{pmatrix} c \frac{T_c}{\tau} \frac{R}{H} & R/H \\ -R/H & c \frac{T_c}{\tau} \frac{R}{H} \end{pmatrix}$$

$\because T_c \sim \frac{1}{H}$, this is consistent with the Drude model $\quad \sigma = \frac{\sigma_0}{1+(\omega_c \tau)^2} \begin{pmatrix} 1 & -\omega_c \tau \\ \omega_c & 1 \end{pmatrix}$

In the strong field limit $\omega_c \tau >> 1$.

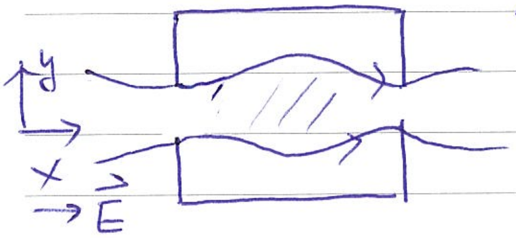
Because $\sigma_{xx} \sim \frac{1}{H^2} \sim \sigma_{yy}$, $\sigma_{xy} \sim \frac{1}{H}$

$$\Rightarrow \rho = \sigma^{-1} = \frac{1}{\underbrace{\sigma_{xx}\sigma_{yy} - \sigma_{xy}^2}_{\sim H^2}} \begin{pmatrix} \sigma_{xx} & +\sigma_{xy} \\ -\sigma_{xy} & \sigma_{yy} \end{pmatrix}$$

$\therefore \rho_{xx}$ (magnetoresistance) is H independent!

Magnetoresistance due to open orbits

In the presence of open orbits (i.e. $a \neq b$), the above analysis doesn't work.



$\vec{k}$ changes abruptly when it hits the zone boundary.

Hence $\vec{k}$ is not continuous and the above analysis fails.

The difference between open & closed orbits is that $\because \dot{\vec{r}} = \frac{1}{\hbar}\nabla_k \varepsilon_k$, $\vec{j} \perp$ energy countor,

For open orbits, ε_k countor $\sim$ flat, $\therefore \vec{j}$ (real space) $\sim$ fixed direction (+ some minor wiggling due to $\vec{H}$).
This is completely different from close orbits in which the Lorentz force deflects the electron effectively to prevent electrons in gaining energy from $\vec{E}$!

For the above figure, $\vec{j} \parallel \hat{y}$. $\therefore$ one expects that in high field, $\sigma_{yy} = s\sigma_0$. $s = $ const,

while for other directions, σ_{xx} behaves the same

$$\therefore \sigma \sim \begin{pmatrix} \frac{1}{H^2} & -\frac{R}{H} \\ +\frac{R}{H} & s \end{pmatrix} \qquad \vec{j} = \sigma \cdot \vec{E}, \quad j_y = \frac{R}{H}E_x + sE_y = 0$$

$$\therefore j_x = \frac{1}{H^2}E_x - \frac{R}{H}E_y = \left(\frac{1}{H^2} + s\frac{R^2}{H^2}\right)E_x, \quad \rho_x \sim H^2!$$

In other words, along the direction of open orbit,

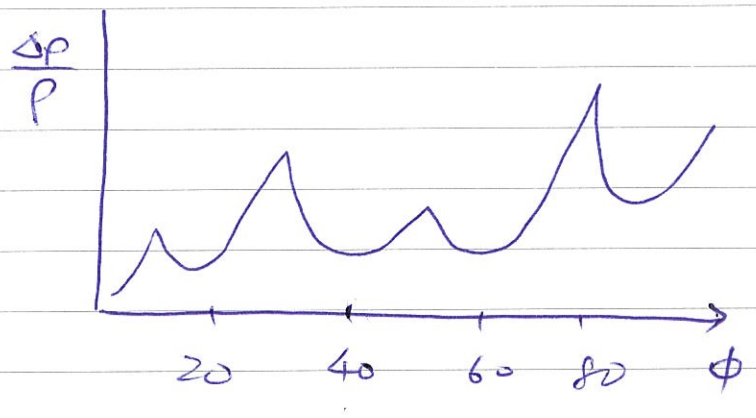
ρ can grow as H^2 !

On the other hand, if $j_x = 0$. $\frac{1}{H^2}E_x = \frac{R}{H}E_y$

$j_y = \frac{R}{H}E_x + SE_y = (R^2+S)E_y$. $\rho_y \to$ const

Hence magnetoresistance (transverse $H \perp j$) can serve as a probe for open orbits on Fermi surface.

The noble metals have open orbits and their magnetoresistance shows peaks for H along particular directions where currents of open orbits ⊥ H can occur.



H = 2.35T along [0,01] of Silver

Mixed electric & thermal transports

As in the Sommerfeld model, one can apply the relaxation approximation to find the thermal transport.

Eq. ㉚-1 is essentially the same as eq ⑧ for Sommerfeld model.

$$f = f^{\circ} + \tau_k \vec{v} \cdot \left\{ e\vec{E} + \vec{\nabla}\mu + \frac{\varepsilon - \mu}{T} \vec{\nabla} T \right\} \frac{\partial f^{\circ}}{\partial \varepsilon}.$$

Therefore, eqs. ⓔ & ⑩ can be generalized to

$$\vec{J} = L^{11} \vec{G} + L^{12} \left(-\frac{\nabla T}{T} \right) \qquad --- ㊱$$

$$\vec{J_u} = L^{21} \vec{G} + L^{22} \left(-\frac{\nabla T}{T} \right) \qquad --- ㊲$$

$$\vec{G} \equiv \vec{E} + \vec{\nabla}\mu / e$$

$$L^{11}_{\alpha\beta} = e^2 \tau_F \int \frac{d^3k}{4\pi^3} v_\alpha v_\beta \, \delta(\varepsilon_F - \varepsilon_k) \equiv \sigma_{\alpha\beta}(\varepsilon_F)$$

$$L^{12} = L^{21}, \quad L^{12}_{\alpha\beta} = -e \int \frac{d^3k}{4\pi^3} \tau_k \frac{\partial f^{\circ}}{\partial \varepsilon} v_\alpha v_\beta (\varepsilon_k - \mu)$$

$$L^{22}_{\alpha\beta} = \int \frac{d^3k}{4\pi^3} \tau_k \left(-\frac{\partial f^{\circ}}{\partial \varepsilon} \right) v_\alpha v_\beta (\varepsilon_k - \mu)^2$$

Using the fact that $-\frac{\partial f^{\circ}}{\partial \varepsilon} \simeq \delta(\varepsilon_k - \varepsilon_F)$ for $T \ll T_F$ and Sommerfeld expansion, One finds

$$L^{12}_{\alpha\beta} = -\frac{1}{e}\int d\varepsilon \left(-\frac{\partial f^0}{\partial \varepsilon}\right)(\varepsilon-\mu)\,\sigma_{\alpha\beta}(\varepsilon) = \frac{-\pi^2}{e3}(k_B T)^2\,\sigma'_{\alpha\beta}(\varepsilon_F)$$

$$\left.\begin{aligned} L^{22}_{\alpha\beta} &= \frac{1}{e^2}\int d\varepsilon \left(-\frac{\partial f^0}{\partial \varepsilon}\right)(\varepsilon-\mu)^2\,\sigma_{\alpha\beta}(\varepsilon) \\ &= \frac{1}{e^2}\frac{\pi^2}{3}(k_B T)^2\,\sigma_{\alpha\beta}(\varepsilon_F) \end{aligned}\right\} \quad ⑶⑻$$

Wiedemann-Franz Law

As in the model of Sommerfeld, setting $\vec{J}=0$ in ㊱, we get

$$\vec{G} = L^{11^{-1}} L^{12}\frac{\nabla T}{T}$$

$$\therefore \vec{J}_u = \left(L^{21}L^{11^{-1}}L^{12} - L^{22}\right)\frac{\nabla T}{T} \equiv -K\,\nabla T$$

Using eqs. ㊳, L^{21} & $L^{21} \sim O(k_B^2 T^2)$ $\therefore$ the 1st term can be neglected.

$$K = \frac{L^{22}}{T} + O(T^2)$$

$$\therefore K_{\alpha\beta} = \frac{\pi^2}{3}\frac{k_B^2 T}{e^2}\sigma_{\alpha\beta}$$, this recovers The Wiedemann-Franz Law

Thermopower - Seebeck effect

(Seebeck coefficient: Θ, α or S)

$$\vec{J}=0, \quad \vec{G} = \underbrace{L^{11^{-1}}L^{12}\frac{1}{T}}_{\Theta}\,\vec{\nabla} T, \quad \therefore \Theta = L^{11^{-1}}L^{12}/T \quad ㊴$$

$$= -\frac{\pi^2}{3e}k_B^2 T\,\sigma^{-1}\sigma'$$

Which now depends on σ' & σ^{-1}!

$$\because\ \sigma(\varepsilon) = e^2\tau(\varepsilon)\int\frac{d^3k}{4\pi^3}\,\vec{v}\,\vec{v}\cdot\delta(\varepsilon-\varepsilon_k)$$

$$\frac{d\sigma}{d\varepsilon} = \frac{\tau'(\varepsilon)}{\tau(\varepsilon)}\sigma(\varepsilon) + e^2\tau(\varepsilon)\int\frac{d^3\vec{k}}{4\pi^3}\,\vec{v}\,\underbrace{\underset{\substack{\uparrow\\ \frac{1}{\hbar}\frac{d\varepsilon_k}{d\vec{k}}}}{\vec{v}}\;\underbrace{\delta'(\varepsilon-\varepsilon_k)}_{\left(-\frac{\partial}{\partial\varepsilon_k}\delta\right)}}_{-\frac{1}{\hbar}\frac{\partial}{\partial\vec{k}}\delta(\varepsilon-\varepsilon_k)}$$

Integration by parts, we get

$$\sigma' = \frac{\tau'}{\tau}\sigma + \frac{e^2\tau}{4\pi^3}\int d^3\vec{k}\,\delta(\varepsilon_F-\varepsilon_k)\,(m^*)^{-1}(k)$$

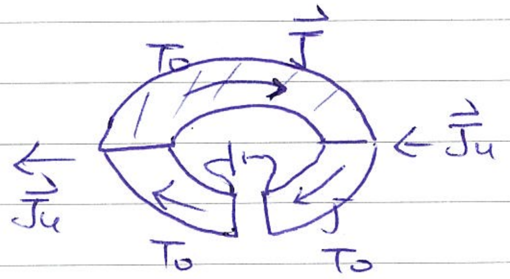
$\therefore$ If τ's ε dependence is not important, sign of Q is determined by that of effective mass averaged over the Fermi surface.

hole-like $\Rightarrow$ $Q>0$. electron-like, $Q<0$

In real expts, Q is not a valuable probe of electronic properties due to it is difficult to an accurate measurement of the electronic part. (phonons can also affect the transport of thermal energy.)

Peltier effect

In a bimetallic circuit as shown in below,



if an electric current $\vec{J}$ is set up & circuit is kept at a constant T_0, than heat will be created & absorbed at junctions.

This is becauso an isothermal electric current in a metal is accompanied by a thermal current.

$$\vec{J_u} = \Pi \vec{J} \quad \cdots \text{(40)}, \quad \Pi = \text{Peltier Coefficients}$$

From eqs. (36) & (37),

$$\vec{J_u} = L^{21} L^{11^{-1}} \vec{J}, \quad \therefore \Pi = L^{21} L^{11^{-1}}$$

From eq. (39), it's clear that

$$\Pi = T\theta \quad \text{if } [L^{12}, L^{11}] = 0$$

Eq. (40) is for one metal. For different metals, Π is different. Hence if $\vec{J}$ is the same, $\vec{J_u}$ is different and it thus results in releaso & absorb of heat in junctions.

Figure of merit Z

To characterize the potential efficiency of a material in the performance of thermoelectric device, one uses Z to indicate its potential. Here

$$Z = \frac{\sigma \alpha^2}{K}$$

σ = conductivity
K = thermal conductivity
α = thermal power.

$\because [Z] = \frac{1}{T}$

$\therefore$ It's often to use ZT as dimensionless figure of merit.

$ZT = 1$ is considered to be good.

Best ZT reported $= 2 \sim 3$

$ZT = 3\text{-}4 \Rightarrow$ compete with mechanic generation and refrigeration in efficiency.