

APPLIED SOLID STATE PHYSICS.

Prof. Siddhasatta Mahapatra.

Semiclassical Transport.

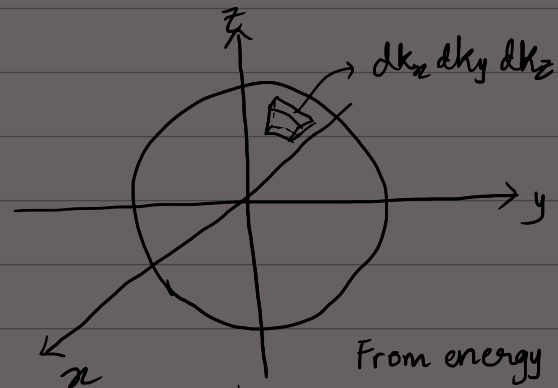
$$\vec{j} = nq\vec{v}$$

$$\vec{j}_q = \frac{q}{4\pi^3} \int_0^\infty d^3\vec{k} f(\vec{k}) \frac{1}{\hbar} \vec{\nabla}_k(\epsilon) \quad (1)$$

[Charge current]

from spin

$$n = \frac{2}{8\pi^3} \int_0^\infty f(\vec{k}) d^3\vec{k}$$



$$\vec{j}_E = nE\vec{v}$$

Energy associated with individual electron.

$$\vec{j}_E = \frac{1}{4\pi^3} \int_0^\infty f(\vec{k}) d^3\vec{k} \cdot \frac{1}{\hbar} \vec{\nabla}_k(\epsilon) \cdot \epsilon(\vec{k}) \quad (2)$$

[Energy current]

From energy band diagram, we know that -

$$v = \frac{1}{\hbar} \frac{\partial \epsilon}{\partial k}$$

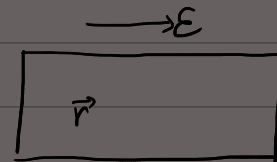
This can be generalised as shown in (1).

The standard expression for Note that $f(\vec{k})$, the distribution function, is valid iff the system is in equilibrium. So, now we'll try to derive this distribution f^n in the presence of an external field.

$$\frac{\partial f}{\partial t} + \frac{d\vec{k}}{dt} \cdot \vec{\nabla}_k f + \frac{d\vec{r}}{dt} \cdot \vec{\nabla}_r f = 0$$

$$\frac{1}{\hbar} \frac{\partial \vec{p}}{\partial t} = \frac{\vec{F}}{\hbar}$$

$$= \frac{\partial f}{\partial t} + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f + \vec{v}_k \cdot \vec{\nabla}_r f$$



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

There's something missing here... we've forgotten to take collisions into account, which are responsible for bringing the system into equilibrium.

$$\frac{\partial f}{\partial t} + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f + \vec{v}_k \cdot \vec{\nabla}_r f - \frac{\partial f}{\partial t} \Big|_{\text{collisions}} = 0$$

Said like a true physicist, and taken for granted, sire.

Operation	Notation	Description	Notational analogy	Domain/Range
Gradient	$\text{grad}(f) = \nabla f$	Measures the rate and direction of change in a scalar field.	Scalar multiplication	Maps scalar fields to vector fields.
Divergence	$\text{div}(\mathbf{F}) = \nabla \cdot \mathbf{F}$	Measures the scalar of a source or sink at a given point in a vector field.	Dot product	Maps vector fields to scalar fields.
Curl	$\text{curl}(\mathbf{F}) = \nabla \times \mathbf{F}$	Measures the tendency to rotate about a point in a vector field in \mathbb{R}^3 .	Cross product	Maps vector fields to (pseudo)vector fields.

$$\frac{\partial f}{\partial t} + \frac{\vec{F}}{h} \cdot \vec{\nabla}_k f + \vec{v}_k \cdot \vec{\nabla}_r f = \frac{\partial f}{\partial t} \Big|_{\text{coll.}}$$

→ Relaxation Time Approx. (the first & simplest approx)

$$\frac{\partial f}{\partial t} \Big|_{\text{collisions}} = -\frac{\delta f}{\tau} \quad \delta f = f - f^0 \quad \begin{matrix} \xrightarrow{\text{In equilibrium}} \\ (?) \end{matrix}$$

→ relaxation time

?? *

If there is a minute perturbation in the system, we can drop all the shitty terms & we'll be left with

$$\frac{df}{dt} = -\frac{f - f^0}{\tau} \quad (\text{In minute perturbation, the disturbance being momentary})$$

$$\frac{\partial f}{\partial t} + \frac{\vec{F}}{h} \cdot \vec{\nabla}_k f + \vec{v}_k \cdot \vec{\nabla}_r f = -\frac{\delta f}{\tau} = -\frac{(f - f^0)}{\tau} \quad [\text{Boltzmann transport eq.}]$$

$$f^0 = \frac{1}{1 + e^{(\epsilon - \mu)/k_B T}} \quad \beta = \frac{1}{k_B T}$$

$\mu = \text{chemical potential}$

Show that:

$$\frac{\partial f^0}{\partial \epsilon} = -\beta f^0 (1 - f^0)$$

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

$$\vec{\nabla}_k f^0 = -\beta f^0 (1 - f^0) h \vec{v}_k$$

We will now apply the simplest possible (practical) field: a const. electric field.

1

Const. electric field (external)

$$[\nabla_{\mathbf{k}} f = 0]$$

$$\cancel{\frac{\partial f}{\partial t}} + \frac{\vec{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f + \cancel{\vec{v} \cdot \nabla_{\mathbf{k}} f} = -\frac{\delta f}{\tau},$$

$$\vec{F} = q\vec{E}$$

$$\Rightarrow \frac{q\vec{E}}{\hbar} \cdot \nabla_{\mathbf{k}} f = -\frac{f - f_0}{\tau}$$

$$\Rightarrow -\frac{q\vec{E}\tau}{\hbar} \cdot \nabla_{\mathbf{k}} (f_0 + \delta f) = \delta f$$

** We will consider small perturbation, s.t. δf is independent of \mathbf{k} .

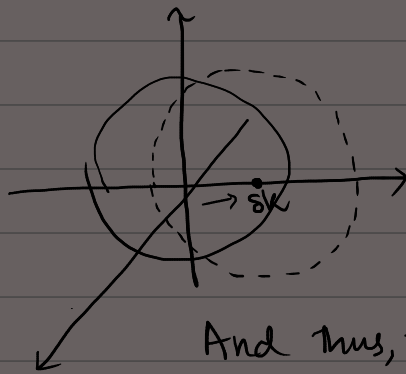
$$\Rightarrow -\frac{q\vec{E}\tau}{\hbar} \cdot \nabla_{\mathbf{k}} (f_0) = f - f_0$$

→ Is this a dot product?

$$\Rightarrow f = f_0 - \frac{q\vec{E}\tau}{\hbar} \cdot \nabla_{\mathbf{k}} (f_0) = f_0 + \delta\mathbf{k} \cdot \nabla_{\mathbf{k}} (f_0)$$

$$f(\mathbf{k}) = f_0(\mathbf{k} + \delta\mathbf{k}), \text{ where } \delta\mathbf{k} = -\frac{q\vec{E}\tau}{\hbar} = \frac{d\mathbf{k}}{dt} \delta t$$

→ Taylor's expansion.



The Fermi sphere effectively shifts to $\delta\mathbf{k}$. (Note that $\delta\mathbf{k}$ need not be along any single axes).

And thus, there was a current. Why so?

Earlier, we had a balanced Fermi sphere s.t. for every particle with a wavevector \vec{k} , we had a corresponding particle of wavevector $-\vec{k}$. Now, since the sphere has shifted, it is no longer balanced, and the corresponding net motion of the electrons constitutes a current in the material.

PROOFS.

Show that:

$$(i) \frac{\partial f^0}{\partial \epsilon} = -\beta f^0 (1-f^0) \quad \checkmark$$

$$f^0 = \frac{1}{1 + e^{(\epsilon - \mu)/k_B T}}$$

$$(ii) \vec{\nabla}_n f^0 = \left(\frac{\partial f}{\partial \epsilon} \right) \left[-\vec{\nabla} \mu - (\epsilon - \mu) \frac{\vec{\nabla} T}{T} \right] \quad \checkmark$$

$$(iii) \vec{\nabla}_k f^0 = -\beta f^0 (1-f^0) \hbar \vec{v}_k \quad \checkmark$$

$$\begin{aligned} (i) \quad \frac{\partial f^0}{\partial \epsilon} &= - \frac{1}{(1 + e^{(\epsilon - \mu)/k_B T})^2} \frac{1}{k_B T} e^{(\epsilon - \mu)/k_B T} \\ &= - \frac{1}{k_B T} \frac{1}{1 + e^{(\epsilon - \mu)/k_B T}} \frac{e^{(\epsilon - \mu)/k_B T}}{1 + e^{(\epsilon - \mu)/k_B T}} \\ &= -\beta f^0 (1-f^0) \end{aligned}$$

$$(ii) \quad \vec{\nabla}_n f^0 = - \frac{1}{(1 + e^{(\epsilon - \mu)\beta})^2} \vec{\nabla}_n \left(e^{(\epsilon - \mu)\beta} \right)$$

$$\vec{\nabla}_n \left(e^{(\epsilon - \mu)\beta} \right) = \vec{\nabla}_n \left(e^{(\epsilon - \mu)/k_B T} \right)$$

$$= e^{(\epsilon - \mu)\beta} \cdot \vec{\nabla}_n \left((\epsilon - \mu)/k_B T \right)$$

$$= e^{(\epsilon - \mu)\beta} \frac{\vec{\nabla}_n (\epsilon - \mu) \cdot k_B T - k_B \vec{\nabla}_n T \cdot (\epsilon - \mu)}{(k_B T)^2}$$

$$= e^{(\epsilon - \mu)\beta} \left(\frac{1}{k_B T} \left(\vec{\nabla}_n \epsilon - \vec{\nabla}_n \mu \right) - \frac{1}{k_B T^2} (\epsilon - \mu) \vec{\nabla}_n T \right)$$

$$= \frac{1}{k_B T} e^{(\epsilon - \mu)\beta} \left(-\vec{\nabla}_n \mu - (\epsilon - \mu) \frac{\vec{\nabla}_n T}{T} \right)$$

$$= \beta e^{(\epsilon - \mu)\beta} \left(-\vec{\nabla}_n \mu - (\epsilon - \mu) \frac{\vec{\nabla}_n T}{T} \right)$$

Substituting,

$$\vec{\nabla}_n f^0 = - \frac{1}{(1 + e^{(\varepsilon - \mu)\beta})^2} \beta e^{(\varepsilon - \mu)\beta} \left(-\vec{\nabla}_n \mu - (\varepsilon - \mu) \frac{\vec{\nabla}_n T}{T} \right)$$

$$= -\beta f_0 (1 - f_0) \left(-\vec{\nabla}_n \mu - (\varepsilon - \mu) \frac{\vec{\nabla}_n T}{T} \right)$$

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

Temp. gradient

mobility gradient

(iii) $\vec{\nabla}_k f^0 = - \frac{1}{(1 + e^{(\varepsilon - \mu)\beta})^2} \vec{\nabla}_k \left(e^{(\varepsilon - \mu)/k_B T} \right)$

$$\vec{v} = \frac{1}{\hbar} \vec{\nabla}_k \varepsilon$$

$$\vec{\nabla}_k \left(e^{(\varepsilon - \mu)/k_B T} \right) = e^{(\varepsilon - \mu)\beta} \vec{\nabla}_k \left(\frac{\varepsilon - \mu}{k_B T} \right)$$

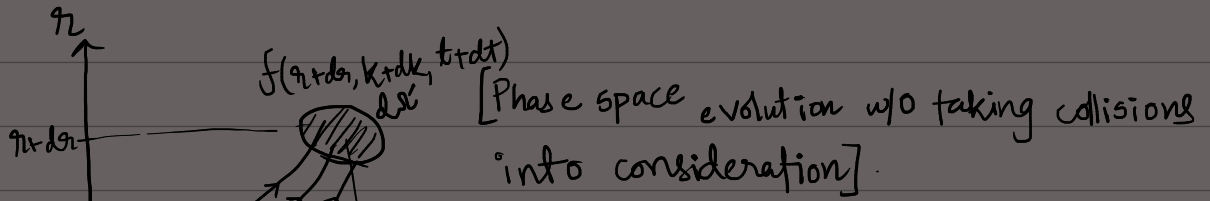
$$= e^{(\varepsilon - \mu)\beta} \frac{\vec{\nabla}_k (\varepsilon - \mu) \cdot k_B T - \vec{\nabla}_k (k_B T) \cdot (\varepsilon - \mu)}{(k_B T)^2}$$

$$= e^{(\varepsilon - \mu)\beta} \frac{1}{k_B T} \vec{\nabla}_k (\varepsilon)$$

$$= \beta e^{(\varepsilon - \mu)\beta} \hbar \vec{v}_k$$

$$\Rightarrow \vec{\nabla}_k f^0 = -\beta f_0 (1 - f_0) \hbar \vec{v}_k$$

Is μ necessarily independent of k ?



$$f(r+dr, k+dk, t+dt) dV' - f(r, k, t) dV = 0$$

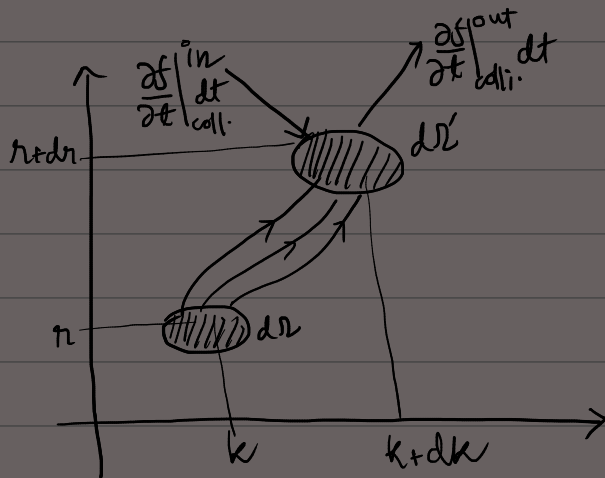
[in absence of collisions]

$$dr = v dt, \quad dk = \frac{F}{\hbar} dt$$

$$\Rightarrow f(r + \vec{v} dt, k + \frac{\vec{F}}{\hbar} dt, t + dt) dV' - f(r, k, t) dV = 0$$

Apply Taylor's expansion, and voila! You end up with the Boltzmann's eqn (w/o taking collisions into account.)

Apparently, dV' & dV are the same (during semiclassical transport), which is stated by some theorem.



$$f(\vec{r} + \vec{v} dt, \vec{k} + \frac{\vec{F}}{\hbar} dt, t + dt) = f(\vec{r}, \vec{k}, t)$$

[Non-collision BME]

$$f(\vec{r} + \vec{v} dt) = f(\vec{r}) + \vec{v} dt \cdot \vec{\nabla}_r f$$

$$f(\vec{k} + \frac{\vec{F}}{\hbar} dt) = f(\vec{k}) + \frac{\vec{F}}{\hbar} dt \cdot \vec{\nabla}_k f$$

$$f(t + dt) = f(t) + dt \cdot \frac{\partial f}{\partial t}$$

$$f(\vec{r} + \vec{v} dt, \vec{k} + \frac{\vec{F}}{\hbar} dt, t + dt) = f(\vec{r}, \vec{k}, t)$$

$$\Rightarrow \cancel{f(\vec{r}, \vec{k}, t)} + \vec{v} \cdot \vec{\nabla}_r f dt + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f dt + \frac{\partial f}{\partial t} dt = \cancel{f(\vec{r}, \vec{k}, t)}$$

$$\Rightarrow \vec{v} \cdot \vec{\nabla}_r f + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f + \frac{\partial f}{\partial t} = 0$$

Taking collisions into consideration, the final eqn is:

$$\vec{v} \cdot \vec{\nabla}_r f + \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f + \frac{\partial f}{\partial t} = \left. \frac{\partial f}{\partial t} \right|_{\text{colli.}}$$

Now, let's come back to our initial problem: finding currents.

$$\begin{aligned}
 \vec{j}_q &= \frac{q}{4\pi^3} \int d^3k \vec{v}_k f \\
 &= \frac{q}{4\pi^3} \int d^3k \left(\frac{q\vec{E}z}{\hbar} \cdot \vec{\nabla}_k f^0 \right) \vec{v}_k d^3k \\
 &= \frac{q^2}{4\pi^3} \int d^3k \left[(\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial k} \right) \right] \cdot \vec{E}
 \end{aligned}$$

$\rightarrow j_q = 0$ in eqn
 \rightarrow gives rise to the conductivity tensor.
 \rightarrow need not necessarily be const. As a zeroth-order approx., you can take it to be const.

Conductivity now looks something like this:

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}$$

In Drude model, the off-diagonal terms are all zero, and the diagonal terms are equal to $-\frac{ne^2\tau}{m}$. So, j_x depends on E_x only, and so on. We shall now show that our model indeed reduces to the Drude model under appropriate approx.

$$\frac{\vec{v}}{k} = \frac{\hbar \vec{k}}{m}$$

$$v_x = \frac{\hbar k_x}{m}, \quad v_y = \frac{\hbar k_y}{m}, \quad v_z = \frac{\hbar k_z}{m}$$

$$\frac{1}{4\pi^3} \int d^3k \rightarrow \int g(E) dE$$

$$\Rightarrow \vec{j} = \left(\frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial E} \right) \right) \cdot \vec{E}$$

$\rightarrow \sigma$ tensor

Show that if $k_i \neq k_j$, then

$\sigma_{i,j \neq i} = 0$. i.e. all the off-diagonal terms are null.

$$\Rightarrow \sigma_{ij} = q^2 \int \tau g(E) dE \left(\frac{\hbar^2}{m^*2} k_i k_j \right) \left(-\frac{\partial f^0}{\partial E} \right)$$

OR

$$\frac{q^2}{4\pi^3} \int \tau d^3k \left(\frac{\hbar^2}{m^*2} \right) k_i k_j \left(-\frac{\partial f^0}{\partial E} \right)$$

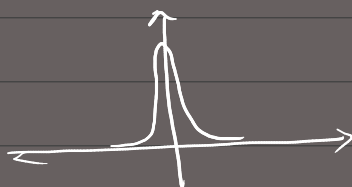
$$\text{So, } \sigma_{ii} = \frac{q^2}{4\pi^3} \int \tau d^3\vec{k} \left(\frac{\hbar}{m^*}\right)^2 k_i^2 \left(\frac{-\partial f_0}{\partial \epsilon}\right) \quad \langle k_i^2 \rangle = \frac{1}{3} k^2$$

$$= \frac{q^2}{4\pi^3 m} \int \tau d^3\vec{k} \left(\frac{\hbar^2 k^2}{2m}\right) \frac{2}{3} \left(\frac{-\partial f_0}{\partial \epsilon}\right)$$

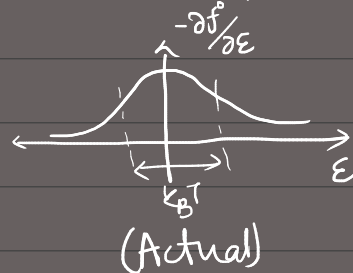
$$= \frac{q^2}{m} \int \tau g(\epsilon) \epsilon \frac{2}{3} \left(\frac{-\partial f_0}{\partial \epsilon}\right) d\epsilon$$

$$= \frac{2}{3} \frac{q^2}{m} \int \tau g(\epsilon) \epsilon \left(\frac{-\partial f_0}{\partial \epsilon}\right) d\epsilon \quad -\frac{\partial f_0}{\partial \epsilon} = \beta f_0(1-f_0)$$

ASSUMPTION: $-\frac{\partial f_0}{\partial \epsilon}$ can be written as a delta function.
(One hell of it, too)



$$-\frac{\partial f_0}{\partial \epsilon} = \delta(\epsilon - \mu)$$



We can neglect the broadening of $k_B T$ since at standard temp. values, $k_B T \ll E_F$ (or μ , for that matter). So, this approx is good enough to a respectable extent. At room temp., this gives us the electrical conductivity in the first order term (Drude conductivity).

$$\Rightarrow \sigma_{ii} = \frac{2q^2}{3m} \int \tau g(\epsilon) \epsilon \delta(\epsilon - \mu) d\epsilon \quad (m \text{ is } m^*, \text{ anyway})$$

Assume const. τ (as per Drude model)

$$\Rightarrow \sigma_{ii} = \frac{2q^2 \tau}{3m} \underbrace{g(\mu) \mu}_{\text{Now, calculate this!}}$$

$$\frac{4\pi k^2 dk}{4\pi^3} = g(\epsilon) d\epsilon, \quad \epsilon = \frac{\hbar^2 k^2}{2m}$$

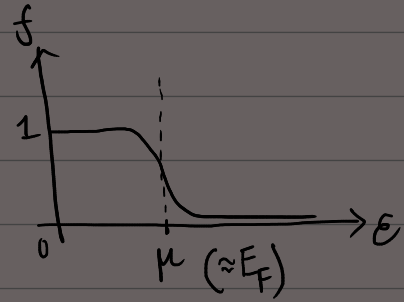
$$d\epsilon = \frac{\hbar^2}{m} k dk = \frac{\hbar^2}{m} \left(\frac{2m\epsilon}{\hbar^2}\right)^{1/2} dk$$

$$\Rightarrow dk = \frac{m}{\hbar^2} \left(\frac{\hbar^2}{2m\epsilon}\right)^{1/2} d\epsilon$$

Find $g(\epsilon)$ & plug it into the eqn, thereby showing that it does satisfy the Drude model.

$$\sigma_{ii} = \frac{2q^2}{3m} \int \tau g(\epsilon) \epsilon \delta(\epsilon - \mu) d\epsilon$$

$$= \frac{2q^2 \tau}{3m} \mu g(\mu)$$



We will assume that $f \approx 1$ for particles with energy $0 \leq \epsilon < \mu$ and $f \approx 0$ for the remaining particles.

$$n = \int_0^{\infty} g(\epsilon) f(\epsilon) d\epsilon$$

$$= \int_0^{\epsilon_F} g(\epsilon) d\epsilon + \int_{\epsilon_F}^{\infty} g(\epsilon) f(\epsilon) d\epsilon$$

$$= \int_0^{\epsilon_F} \frac{1}{\pi^2} \left(\frac{m}{\hbar^2} \right) \left(\frac{2m\epsilon}{\hbar^2} \right)^{1/2} d\epsilon = \frac{1}{\pi^2} \frac{m}{\hbar^2} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{\epsilon_F^{3/2}}{3/2} = \frac{1}{3\pi^2} \left(\frac{2m\epsilon_F}{\hbar^2} \right)^{3/2}$$

Now,

$$\sigma_{ii} = \frac{2q^2 \tau}{3m} \mu \cdot \frac{1}{\pi^2} \left(\frac{m}{\hbar^2} \right) \left(\frac{2m\mu}{\hbar^2} \right)^{1/2}$$

$$= \frac{q^2 \tau}{m} \left[\frac{1}{3\pi^2} \left(\frac{2m\mu^{3/2}}{\hbar^2} \right) \right] \rightarrow n$$

$$\Rightarrow \boxed{\sigma_{ii} = \frac{nq^2 \tau}{m}}$$

That's a helluva lot of assumptions we made back there, but boy, life's pretty fuckin' unfair.

$$\Rightarrow g(\epsilon) d\epsilon = \frac{4\pi k^2}{4\pi^3} \frac{m}{\hbar} \left(\frac{\hbar^2}{2m\epsilon}\right)^{1/2} d\epsilon \quad \text{[Continuation from } dk-d\epsilon \text{ relation]}$$

$$\Rightarrow g(\epsilon) = \frac{1}{2} \frac{2m\epsilon}{\hbar^2} \frac{m}{\hbar} \left(\frac{\hbar^2}{2m\epsilon}\right)^{1/2}$$

$$\Rightarrow g(\epsilon) = \frac{1}{2} \frac{m}{\hbar^2} \left(\frac{\hbar^2}{2m\epsilon}\right)^{1/2}$$

$$= \frac{1}{2} \frac{m}{\hbar} \left(\frac{2m\epsilon}{\hbar}\right)^{1/2}$$

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{bmatrix} \frac{ne^2\tau}{m^*} & 0 & 0 \\ 0 & \frac{ne^2\tau}{m^*} & 0 \\ 0 & 0 & \frac{ne^2\tau}{m^*} \end{bmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} \rightarrow \text{Drude model.}$$

② Const. \vec{E}, \vec{B} both are present (not necessarily \vec{E}^{\perp})

$$\vec{F} = q(\vec{E} + \vec{v}_k \times \vec{B})$$

$$\delta f = -\frac{q(\vec{E} + \vec{v}_k \times \vec{B})\tau}{\hbar} \cdot \vec{\nabla}_k f$$

$$\Rightarrow f = f_0 - \left(\frac{q\tau}{\hbar} (\vec{E} + \vec{v}_k \times \vec{B})\right) \cdot \vec{\nabla}_k f$$

Let's consider this part only: $(\vec{v}_k \times \vec{B}) \cdot \vec{\nabla}_k (f)$

$$= (\vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k (f_0 + \delta f)$$

$\vec{\nabla}_k f_0$ has a \vec{v}_k term. So, that particular term vanishes.

$$= (\vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k (\delta f) \quad \text{--- (1)}$$

In case of const. \vec{E} , we saw that δf can be written as: $\delta f = -\frac{q\tau}{\hbar} \vec{E} \cdot \vec{\nabla}_k f_0$

In this case, we'll assume a priori that an equivalent ^{vector} field \vec{Z} exists s.t. $\delta f = -\frac{q\tau}{\hbar} \vec{Z} \cdot \vec{\nabla}_k f_0$. ($\Rightarrow -\frac{\delta f}{\tau} = \frac{q}{\hbar} \vec{Z} \cdot \vec{\nabla}_k f_0$, $(\vec{E} + \vec{v}_k \times \vec{B}) \cdot \vec{\nabla}_k f = \vec{Z} \cdot \vec{\nabla}_k f_0$)

Substituting in (1),

$$\vec{\nabla}_k (f_0(1-f_0))$$

$$= (1-f_0)\vec{\nabla}_k f_0 - f_0\vec{\nabla}_k f_0$$

Each of these yields a $\vec{\nabla}_k$ term whose dot product with $(\vec{\nabla}_k \times \vec{B})$ yields 0.

$$(\vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k \left(\frac{q\hbar}{\hbar} \vec{z} \cdot \vec{\nabla}_k f \right)$$

$$= (\vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k \left[\frac{\beta q \hbar}{\hbar} \vec{z} \cdot \vec{\nabla}_k f_0(1-f_0) \right]$$

$$= \beta q \hbar (\vec{\nabla}_k \times \vec{B}) \cdot \left[(\vec{z} \cdot \vec{\nabla}_k) (\vec{\nabla}_k f_0(1-f_0)) + f_0(1-f_0) (\vec{\nabla}_k (\vec{z} \cdot \vec{\nabla}_k)) \right]$$

dot product yields 0.

$$= \beta q \hbar (\vec{\nabla}_k \times \vec{B}) \cdot f_0(1-f_0) (\vec{\nabla}_k (\vec{z} \cdot \vec{\nabla}_k))$$

$$= \beta q \hbar f_0(1-f_0) (\vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k (\vec{z} \cdot \vec{\nabla}_k)$$

Due to presence of \vec{B} , we have an additional comp. in our velocity:

$$\vec{v}_k = \frac{\hbar \vec{k} - q\vec{A}}{m^*}$$

where \vec{A} is the vector potential generating the magnetic field.

$$\vec{\nabla}_k (\vec{z} \cdot \vec{v}_k) = \frac{\hbar \vec{z}}{m^*} \rightarrow \text{How?}$$

$$\text{Now, } (\vec{E} + \vec{\nabla}_k \times \vec{B}) \cdot \vec{\nabla}_k f = \vec{E} \cdot \vec{\nabla}_k f + \beta q \hbar f_0(1-f_0) (\vec{\nabla}_k \times \vec{B}) \cdot \frac{\hbar \vec{z}}{m^*}$$

$$\vec{z} \cdot \vec{\nabla}_k f_0 = \vec{E} \cdot \vec{\nabla}_k f_0 + \beta q \hbar f_0(1-f_0) (\vec{\nabla}_k \times \vec{B}) \cdot \frac{\hbar \vec{z}}{m^*}$$

Problematic point: δf neglected in case of \vec{E} , but in case of \vec{B} , it is responsible for the deviation.

$$\vec{z} \cdot \hbar \vec{\nabla}_k f_0(1-f_0) = \vec{E} \cdot \hbar \vec{\nabla}_k f_0(1-f_0) + (\vec{\nabla}_k \times \vec{B}) \cdot \beta q \hbar f_0(1-f_0) \frac{\hbar \vec{z}}{m^*}$$

$$\Rightarrow (\vec{E} - \vec{z}) \cdot \vec{\nabla}_k + \frac{q\hbar}{m^*} (\vec{\nabla}_k \times \vec{B}) \cdot \vec{z} = 0$$

$$\Rightarrow (\vec{E} - \vec{z}) \cdot \vec{\nabla}_k + \frac{q\hbar}{m^*} (\vec{B} \times \vec{z}) \cdot \vec{\nabla}_k = 0$$

I've forgotten the rules of vector algebra.

$$\Rightarrow \left((\vec{E} - \vec{z}) + \frac{q\hbar}{m^*} (\vec{B} \times \vec{z}) \right) \cdot \vec{\nabla}_k = 0$$

$$\Rightarrow \vec{E} = \vec{Z} - \left(\frac{q\tau}{m^*} \right) (\vec{B} \times \vec{Z})$$

$$\Rightarrow \vec{Z} = \frac{\vec{E} + \mu (\vec{B} \times \vec{E}) + \mu^2 (\vec{B} \cdot \vec{E}) \vec{E}}{1 + \mu^2 B^2}$$

$$\Rightarrow \vec{j} = \sigma \vec{Z} \rightarrow \text{Hall vector.}$$

Hall Effect: $\vec{B} = (0, 0, B_0)$, $\vec{E} = (E_x, E_y, 0)$

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{bmatrix} \sigma \\ \sigma \\ \sigma \end{bmatrix} \begin{pmatrix} Z_x \\ Z_y \\ Z_z \end{pmatrix}$$

Transform \vec{Z} to \vec{E}

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \begin{bmatrix} \sigma \\ \sigma \\ \sigma \end{bmatrix} \begin{pmatrix} E_x \\ E_y \\ 0 \end{pmatrix}$$

$$\vec{j} = \sigma \vec{E}$$

Magnetoconductance

Try to verify the Hall Effect using this relation.

$$\sigma = \frac{\sigma_0}{1 + (\mu B_0)^2} \begin{bmatrix} 1 & -\mu B_0 & 0 \\ \mu B_0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \text{ where } \sigma_0 = \frac{ne^2\tau}{m^*}$$

P.T.O.

$$\begin{aligned} \vec{j}_q &= \frac{q}{4\pi^3} \int d^3k \vec{v}_k f, \quad f = f_0 + \delta f = f_0 - \frac{q\tau}{\hbar} \vec{E} \cdot \vec{v}_k f_0 \\ &= \frac{q}{4\pi^3} \int d^3k \vec{v}_k \left(f_0 - \frac{q\tau}{\hbar} \vec{E} \cdot \vec{v}_k f_0 \right) \\ &= -\frac{q^2\tau}{4\pi^3\hbar} \int d^3k \vec{v}_k \left(\vec{E} \cdot \hbar \vec{v}_k \left(\frac{\partial f_0}{\partial \epsilon} \right) \right) \end{aligned}$$

$$\vec{j}_q = -\frac{q^2\tau}{4\pi^3\hbar} \left[\int d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f_0}{\partial \epsilon} \right) \right] \cdot \vec{E}$$

Gives us the same old σ_0 :
 $\sigma_0 = \frac{ne^2\tau}{m^*}$

$$\vec{E} \rightarrow \vec{E} \quad ??$$

$$\vec{E} = \frac{1}{1 + \mu^2 B_0^2} (\vec{E} + \mu(\vec{B} \times \vec{E}) + \mu^2(\vec{B} \cdot \vec{E})\vec{E})$$

$$\vec{B} \times \vec{E} = B_0 E_x \hat{y} - B_0 E_y \hat{x}$$

$$\vec{E} = \frac{1}{1 + \mu^2 B_0^2} (E_x \hat{x} + E_y \hat{y} + \mu B_0 E_x \hat{y} - \mu B_0 E_y \hat{x})$$

$$= \frac{1}{1 + \mu^2 B_0^2} ((E_x - \mu B_0 E_y) \hat{x} + (E_y + \mu B_0 E_x) \hat{y})$$

$$\vec{E} = \frac{1}{1 + \mu^2 B_0^2} (E_x (\hat{x} + \mu B_0 \hat{y}) + E_y (\hat{y} - \mu B_0 \hat{x}))$$

$\rightarrow z_x \hat{x} + z_y \hat{y} + z_z \hat{k}$

$$\vec{j} = \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & \sigma_0 & 0 \\ 0 & 0 & \sigma_0 \end{bmatrix} \begin{bmatrix} z_x \\ z_y \\ z_z \end{bmatrix}$$

$$\frac{1}{1 + \mu^2 B_0^2} \begin{bmatrix} z_x \\ z_y \\ z_z \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ 0 \end{bmatrix} = \begin{bmatrix} z_x \\ z_y \\ z_z \end{bmatrix}$$

$$\left(\frac{1}{1 + \mu^2 B_0^2} \begin{bmatrix} 1 & -\mu B_0 & 0 \\ \mu B_0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right) \begin{bmatrix} \sigma_0 & 0 & 0 \\ 0 & \sigma_0 & 0 \\ 0 & 0 & \sigma_0 \end{bmatrix}$$

TRANSFORMATION COMPLETE!

③ $\vec{E} = 0, \vec{B} = 0, \vec{\nabla}_r f \neq 0$

Examples: Semiconductor placed in a thermal gradient, or a semiconductor having a conc. gradient.

$$\frac{\partial f}{\partial t} + \underbrace{\vec{v}_k \cdot \nabla_n f}_{\text{drift}} + \frac{\vec{F}}{\hbar} \cdot \nabla_k f = -\frac{\delta f}{\tau}$$

$$\Rightarrow \vec{v}_k \cdot \nabla_n f = -\frac{\delta f}{\tau}$$

$$\Rightarrow \vec{v}_k \cdot \nabla_n f^0 = -\frac{\delta f}{\tau} \quad (\text{Assumption similar to const. } \vec{E} \text{ case})$$

$$\Rightarrow \left(\frac{\partial f^0}{\partial \epsilon_k} \right) \left[-\vec{\nabla}_r \mu(r) - (\epsilon_k - \mu) \frac{\vec{\nabla}_n T}{T} \right] \cdot \vec{v}_k = -\frac{\delta f}{\tau}$$

$$\Rightarrow \delta f = \tau \vec{v}_k \cdot \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) \left[-\vec{\nabla}_n \mu(r) - (\epsilon_k - \mu) \frac{\vec{\nabla}_n T}{T} \right]$$

$$\vec{j}_q = \frac{q}{4\pi^3} \int d^3k \vec{v}_k \delta f$$

$$\Rightarrow \vec{j}_q = \frac{q}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) \left[-\vec{\nabla}_n \mu - (\epsilon_k - \mu) \frac{\vec{\nabla}_n T}{T} \right]$$

$$= \frac{q^2}{4\pi^3} \left\{ \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) \cdot \left[\frac{-\vec{\nabla}_n \mu}{q} \right] \right. \quad \begin{array}{l} \text{current due to} \\ \text{gradient in chemical} \\ \text{pot. (which then is} \\ \text{equiv. to an } \vec{E}) \end{array} \\ \left. + \left\{ \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) (-\epsilon_k - \mu) \right\} \cdot \frac{\vec{\nabla}_n T}{T} \right]$$

current due to temp. gradient

Theoretically, we'll see that the effect of an electric field applied to the material can be taken into account by the gradient of electrochemical potential. In fact, doing a separate analysis for the \vec{E} is not necessary theoretically, but quite desirable practically.

$$\frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) \left[\frac{-\vec{\nabla}_n \mu}{q} + \frac{\vec{\nabla}_n \epsilon_k(r)}{q} + \vec{E} \right]$$

$$\vec{\nabla}_n (\epsilon_k(r)) = q \vec{\nabla}_k (\phi(r)) = -q \vec{E}$$

$$\begin{aligned} \therefore, \vec{j}_q &= \vec{\sigma} \left(-\frac{\vec{\nabla}_n \mu}{q} \right) + \left\{ \frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu) \right\} \cdot \left(-\frac{\vec{\nabla}_n T}{T} \right) \\ &= \vec{L}_{11} \left(-\frac{\vec{\nabla}_n \mu}{q} \right) + \vec{L}_{12} \left(-\frac{\vec{\nabla}_n T}{T} \right) \end{aligned}$$

$$\vec{L}_{11} = \vec{\sigma} = \vec{L}^{(0)}$$

$$\vec{L}_{12} = \frac{\vec{L}^{(1)}}{qT}, \text{ where } \vec{L}^{(\alpha)} = \frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)^\alpha$$

$$\begin{array}{l} \text{charge current} \leftarrow \\ \text{heat current} \leftarrow \end{array} \begin{array}{l} \vec{j}_q \\ \vec{j}_Q \end{array} = \begin{bmatrix} \vec{L}_{11} & \vec{L}_{12} \\ \vec{L}_{21} & \vec{L}_{22} \end{bmatrix} \begin{array}{l} -\frac{\vec{\nabla}_n \mu}{q} \\ -\vec{\nabla}_n T \end{array}$$

→ I believe this is now the most generalised form possible. (with the possible exception of \vec{B} , which was left out in this case).

$$\vec{L}^{(\alpha)} = \frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)^\alpha$$

$$\Rightarrow L_{xx}^{(\alpha)} = \frac{q^2}{4\pi^3} \int \tau d^3k \left(\frac{\hbar}{m^*} \right)^2 \frac{k^2}{3} \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)^\alpha \quad [L_{ij} = 0, \text{ for } i \neq j]$$

$$= \frac{2q^2}{3m^{*2}} \int \tau g(\epsilon) \epsilon \left(\frac{-\partial f^0}{\partial \epsilon} \right) (\epsilon - \mu)^\alpha d\epsilon$$

Take $\alpha=0 \Rightarrow$

$$\sigma = L^{(0)} = \frac{2q^2 \tau}{3m^{*2}} \int \underbrace{g(\epsilon_k) \epsilon_k}_{\Theta(\epsilon)} \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) d\epsilon_k$$

$$\begin{aligned} \int_0^\infty \Theta(\epsilon) \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon &= -\cancel{\Theta(\epsilon) f^0} \Big|_0^\infty + \int_0^\infty \Theta'(\epsilon) f^0 d\epsilon \\ &= \int_0^\infty \Theta'(\epsilon) f^0 d\epsilon \end{aligned}$$

Imp. expansion
in condensed
matter physics.

Behold the Sommerfeld expansion:

$$\int_{-\infty}^{\mu} H(\epsilon) f^0(\epsilon) d\epsilon = \int_{-\infty}^{\mu} H(\epsilon) d\epsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\epsilon) \Big|_{\epsilon=\mu}$$

In our case, $H(\epsilon) = \Theta'(\epsilon) = g(\epsilon) + \epsilon g'(\epsilon)$; $g(\epsilon) = \alpha \sqrt{\epsilon}$

$$\begin{aligned} H'(\epsilon) &= g'(\epsilon) + \epsilon g''(\epsilon) + g'(\epsilon) \\ &= 2g'(\epsilon) + \epsilon g''(\epsilon) \end{aligned}$$

$$\begin{aligned} \Rightarrow \sigma &= \frac{2q^2 \tau}{3m^*} \left[\int_0^{\mu} (\alpha \sqrt{\epsilon} + \epsilon \cdot \frac{1}{2} \alpha \epsilon^{-1/2}) d\epsilon + \frac{\pi^2}{6} (k_B T)^2 \frac{3\alpha}{4} \epsilon^{-1/2} \Big|_{\epsilon=\mu} \right] \\ &= \frac{2q^2 \tau}{3m^*} \left[\frac{3}{2} \frac{\alpha \mu^{3/2}}{3/2} + \frac{\pi^2}{6} (k_B T)^2 \frac{3\alpha}{4} \mu^{-1/2} \right] \\ &= \frac{2q^2 \tau}{3m^*} \left[\frac{3n}{2\mu^{3/2}} \mu^{3/2} + \frac{\pi^2}{6} (k_B T)^2 \frac{3}{4} \frac{3n}{2\mu^{3/2}} \mu^{1/2} \right] \\ &= \left(\frac{nq^2 \tau}{m^*} \right) \left[1 + \frac{\pi^2 (k_B T)^2}{8 \mu^2} \right] \\ \sigma_0 &\leftarrow \left(\frac{nq^2 \tau}{m^*} \right) \end{aligned}$$

$$\Rightarrow \sigma = \sigma_0 \left(1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 \right) \Rightarrow \overleftrightarrow{\sigma} = \overleftrightarrow{\sigma}_{11}$$

We know that conductivity in metals has a strong dependence on temp, which does not appear to be so from this expression. So where is that dependence coming from? That particularly strong dependence is due to ' τ '. τ depends on T much more strongly, and its effect is more than sufficient to drown out the ^{weaker} effect of this term.

$$\overleftrightarrow{L}_{12} = \frac{q^2}{4\pi^3} \int \tau d^3k (\vec{v}_k \otimes \vec{v}_k) \left(-\frac{\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)$$

$$\Rightarrow L_{12}^{(1)} = \frac{2q^2 \tau}{3m^*} \int g(\epsilon) \epsilon \left(-\frac{\partial f^0}{\partial \epsilon} \right) (\epsilon - \mu) d\epsilon$$

$$= \frac{2q^2 \tau}{3m^*} \left[\int_0^\infty \underbrace{g(\epsilon) \epsilon^2}_{\Theta(\epsilon)} \left(-\frac{\partial f^0}{\partial \epsilon} \right) d\epsilon - \mu \int_0^\infty g(\epsilon) \epsilon \left(-\frac{\partial f^0}{\partial \epsilon} \right) d\epsilon \right]$$

$\underbrace{\hspace{10em}}_{L_{12}^{(0)}}$

$$\int_0^\infty H(\epsilon) f^0(\epsilon) d\epsilon = \int_0^\mu H(\epsilon) d\epsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\epsilon) \Big|_{\epsilon=\mu}$$

$$= \frac{5}{2} \alpha \frac{\mu^{5/2}}{5/2} + \frac{\pi^2}{6} (k_B T)^2 \frac{15}{4} \alpha \mu^{1/2}$$

$$= \alpha \mu^{5/2} + \frac{5}{8} \pi^2 (k_B T)^2 \alpha \mu^{1/2}$$

$$\Rightarrow L_{12}^{(1)} = \frac{2q^2 \tau}{3m^*} \left(\alpha \mu^{5/2} + \frac{5}{8} \pi^2 (k_B T)^2 \alpha \mu^{1/2} - \alpha \mu^{5/2} - \frac{\pi^2}{8} \frac{(k_B T)^2}{\alpha \mu^{1/2}} \right)$$

$$= \frac{2q^2 \tau}{3m^*} \left(\frac{1}{2} \pi^2 (k_B T)^2 \mu^{1/2} \alpha \right)$$

$$= \frac{2}{5} \frac{q^2 \tau}{m^*} \frac{1}{2} \pi^2 (k_B T)^2 \mu^{1/2} \frac{3n}{2\mu^{3/2}}$$

$$= \frac{n q^2 \tau}{m^*} \frac{\pi^2 (k_B T)^2}{2\mu}$$

$$\Rightarrow L_{12}^{(1)} = \sigma_0 \frac{\pi^2 (k_B T)^2}{2\mu}$$

Set $\vec{v}_0 = 0$, and '5' relates the gradient in temp to the gradient in chemical pot.

$$\Rightarrow S \text{ (Seebeck coefficient)} = \frac{\overleftrightarrow{L}_{12}}{\overleftrightarrow{L}_{11}} = \frac{4\mu}{qT} \left(\frac{1}{1 + \frac{8}{\pi^2} \left(\frac{\mu}{k_B T} \right)^2} \right)$$

$$L^{11} = \mathcal{L}^{(0)}$$

$$L^{21} = T L^{12} = -\frac{1}{e} \mathcal{L}^{(1)}$$

$$L^{22} = \frac{1}{e^2 T} \mathcal{L}^{(2)}$$

→ Aiyyo, this made my day!

→ Heat current, \vec{j}_Q

$$dQ = T ds$$

$$\text{But } Tds = dU - \mu dN$$

$$\Rightarrow dQ = dU - \mu dN$$

$$\Rightarrow \vec{j}_Q = \vec{j}_E - \mu \vec{j}_N \quad \text{Number current, or simply the flux of particles.}$$

$$\Rightarrow \vec{j}_Q = \frac{1}{4\pi^3} \int d^3k \vec{v}_k \epsilon_k \delta f - \frac{\mu}{4\pi^3} \int d^3k \vec{v}_k \delta f,$$

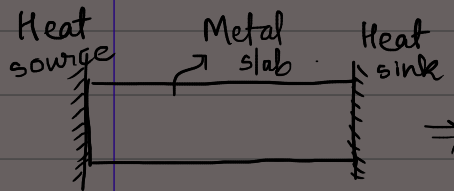
$$\delta f = \tau \vec{v}_k \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) \left[-\vec{\nabla}_n \mu - (\epsilon_k - \mu) \frac{\vec{\nabla}_n T}{T} \right]$$

$$\frac{1}{q} \left\{ \frac{q^2}{4\pi^3} \int \tau d^3k \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\vec{v}_k \otimes \vec{v}_k) (\epsilon_k - \mu) \right\} \left(-\frac{\vec{\nabla}_n \mu}{q} \right)$$

$$+ \frac{1}{q^2 T} \left\{ \frac{q^2}{4\pi^3} \int \tau d^3k \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\vec{v}_k \otimes \vec{v}_k) (\epsilon_k - \mu)^2 \right\} (-\vec{\nabla}_n T) = \vec{j}_Q$$

$$\Rightarrow \vec{j}_Q = \overleftrightarrow{L}_{21} \left(\frac{-\vec{\nabla}_n \mu}{q} \right) + \overleftrightarrow{L}_{22} (-\vec{\nabla}_n T)$$

$$= \overleftrightarrow{L}_{21} \vec{E} + \overleftrightarrow{L}_{22} (-\vec{\nabla} T)$$



⇒ Insulated electrically, so $\vec{j}_Q = 0$. However, the presence of a heat source & sink enables flow of heat current.

Show that the thermal coeff., $\vec{K} = (\overleftrightarrow{L}_{22} - \overleftrightarrow{L}_{21} \vec{E})$.

$\vec{j}_Q = \vec{K} (-\vec{\nabla} T)$ [by definition] ⇒ Use the above result, and it's pretty much a no-brainer.

→ Seebeck coefficient for the free electron gas :-

$$S = \frac{\vec{L}_{12}}{\vec{L}_{11}}, \quad \vec{L}_{11} = \vec{L}^{(0)}, \quad \vec{L}_{12} = \frac{\vec{L}^{(1)}}{qT}$$

$$\vec{L}^{(\alpha)} = \frac{q^2}{4\pi^3} \int \tau d^3\vec{k} (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)^\alpha$$

$$\vec{L}_{ij}^{(\alpha)} = 0 \text{ for } i \neq j \text{ (No proof available :))}$$

Calculated beforehand $\vec{L}_{ii}^{(0)} = \frac{q^2}{4\pi^3} \int \tau d^3\vec{k} (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right)$

$$g(\epsilon) = \lambda \sqrt{\epsilon}$$

$$= \frac{2q^2}{3m} \int \tau g(\epsilon) \epsilon \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon$$

$$= \frac{2q^2 \tau \lambda}{3m} \int \epsilon^{3/2} \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon$$

$$= \frac{2q^2 \tau \lambda}{3m} \left[-\epsilon^{3/2} f^0 \Big|_0^\infty + \frac{3}{2} \int \epsilon^{1/2} f^0 d\epsilon \right]$$

$$= \frac{q^2 \tau \lambda}{m} \int \epsilon^{1/2} f^0 d\epsilon$$

$$\vec{L}_{ii}^{(1)} = \frac{q^2}{4\pi^3} \int \tau d^3\vec{k} (\vec{v}_k \otimes \vec{v}_k) \left(\frac{-\partial f^0}{\partial \epsilon_k} \right) (\epsilon_k - \mu)$$

$$= \frac{2q^2}{3m} \int \tau (\epsilon - \mu) g(\epsilon) \epsilon \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon$$

$$= \frac{2q^2 \tau \lambda}{3m} \left[\int \epsilon^{5/2} \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon - \mu \int \epsilon^{3/2} \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon \right]$$

$$\int \epsilon^{5/2} \left(\frac{-\partial f^0}{\partial \epsilon} \right) d\epsilon = -\epsilon^{5/2} f^0 \Big|_0^\infty + \int \frac{5}{2} \epsilon^{3/2} f^0 d\epsilon \quad \vec{L}_{ii}^{(0)}$$

$$\Rightarrow \vec{L}_{ii}^{(1)} = \frac{2qz\lambda}{3m} \left[\frac{5}{2} \int \epsilon^{3/2} f^0 d\epsilon - \mu \frac{3}{2} \int \epsilon^{1/2} f^0 d\epsilon \right]$$

$$\Rightarrow \vec{L}_{12} = \frac{2qz\lambda}{3mT} \left[\frac{5}{2} \int \epsilon^{3/2} f^0 d\epsilon - \mu \frac{3}{2} \int \epsilon^{1/2} f^0 d\epsilon \right]$$

$$\Rightarrow S = \frac{\vec{L}_{12}}{\vec{L}_{11}} = \frac{\frac{2qz\lambda}{3mT} \left[\frac{5}{2} \int \epsilon^{3/2} f^0 d\epsilon - \mu \frac{3}{2} \int \epsilon^{1/2} f^0 d\epsilon \right]}{\frac{qz\lambda}{m} \int \epsilon^{1/2} f^0 d\epsilon}$$

$$= \frac{2}{3qT} \left[\frac{5}{2} \frac{\int \epsilon^{3/2} f^0 d\epsilon}{\int \epsilon^{1/2} f^0 d\epsilon} - \frac{3}{2} \mu \right]$$

$$\Rightarrow S = \frac{1}{qT} \left[\frac{5}{3} \frac{\int \epsilon^{3/2} f^0 d\epsilon}{\int \epsilon^{1/2} f^0 d\epsilon} - \mu \right]$$

→ Transforming this into Fermi integral form brings about the extra $k_B T$ term:

Is Sommerfeld expansion valid only under this condition?

For $\beta\mu \gg 1$ ($\mu \gg k_B T$),

$$\int_0^{\mu} \epsilon^{3/2} f^0 d\epsilon = \int_0^{\mu} \epsilon^{3/2} d\epsilon + \frac{\pi^2}{6} (k_B T)^2 \frac{3}{2} \mu^{1/2}$$

$$= \frac{2}{5} \mu^{5/2} + \frac{\pi^2}{4} (k_B T)^2 \mu^{1/2}$$

$$\int_0^{\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_0^{\mu} H(\epsilon) d\epsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\mu)$$

$$\int \epsilon^{1/2} f^0 d\epsilon = \frac{2}{3} \mu^{3/2} + \frac{\pi^2}{6} (k_B T)^2 \frac{1}{2} \mu^{1/2} = \frac{2}{3} \mu^{3/2} + \frac{\pi^2}{12} (k_B T)^2 \mu^{1/2}$$

$$\Rightarrow S = \frac{1}{qT} \frac{5}{3} \left[\frac{\frac{2}{5} \mu^{5/2} + \frac{\pi^2}{4} (k_B T)^2 \mu^{1/2} - \frac{2}{5} \mu^{5/2} - \frac{\pi^2}{20} (k_B T)^2 \mu^{1/2}}{\frac{2}{3} \mu^{3/2} + \frac{\pi^2}{12} (k_B T)^2 \mu^{1/2}} \right]$$

$$= \frac{1}{qT} \frac{5}{3} \frac{\frac{1}{5} \pi^2 (k_B T)^2 \mu^{1/2}}{\frac{2}{3} \mu^{3/2}}$$

$$\Rightarrow 5 = \frac{\pi^2}{2} \frac{k_B T}{\mu} \left(\frac{k_B T}{\mu} \right)$$

(I don't remember fundamental thermo, so yeah, this is more like rote learning for me)

$$\rightarrow \text{Energy per unit volume} = \int_0^{\infty} \epsilon g(\epsilon) f^0(\epsilon) d\epsilon$$

$$C_v^{el} = \frac{\partial U(T)}{\partial T} = \frac{\partial}{\partial T} \int_0^{\infty} \epsilon g(\epsilon) f^0(\epsilon) d\epsilon$$

$$= \int_0^{\infty} \epsilon g(\epsilon) \frac{\partial f^0}{\partial T} d\epsilon$$

$$\text{Now, } n = \int_0^{\infty} g(\epsilon) f^0(\epsilon) d\epsilon \quad [\text{Independent of } T]$$

$$\frac{\partial n}{\partial T} = 0 = \int_0^{\infty} g(\epsilon) \frac{\partial f^0}{\partial T} d\epsilon$$

Man, you gotta be kidding me, did we just add a 0 term to the ϵ^n !?

$$\Rightarrow C_v^{el} = \frac{\partial U}{\partial T} - \mu \frac{\partial n}{\partial T}$$

$$\Rightarrow C_v^{el} = \int_0^{\infty} (\epsilon - \mu) g(\epsilon) \frac{\partial f^0}{\partial T} d\epsilon$$

Specific heat capacity of e^- gas, can be evaluated numerically ...

→ Phonon scattering:
(Most significant source of scattering.) $\frac{1}{\tau} \propto T^5$ for $T \ll T_D$ (Debye temp.)
 $\frac{1}{\tau} \propto T$ for $T \gg T_D$

Electron-electron scattering: Pretty weak mode of scattering, evident only at very low temps. when phonon scattering is very low.

$$\frac{1}{\tau_{e-e}} \propto T^2$$

Impurity scattering: Independent of temperature, and is responsible for the "intrinsic" resistance of the material, which does not vanish even at $T=0K$.

Semiconductors.

→ $\hbar\vec{k}$ is not the real momentum of the electron in a periodic potential (it is not the eigenvalue of Bloch's equation).

$$\psi_{n,\vec{k}}(\vec{r}) = u_n(\vec{r}) e^{i\vec{k}\cdot\vec{r}}$$

$$-i\hbar\vec{\nabla}_n \psi_{n,\vec{k}}(\vec{r}) = \hbar\vec{k} \psi_{n,\vec{k}}(\vec{r}) - \vec{\nabla}_n u_n(\vec{r}) \cdot e^{i\vec{k}\cdot\vec{r}}$$

⇒ Not an eigenvector of momentum operator

This is the so-called "crystal momentum", which provides us a direct framework to help account for the effects of external forces on an e^- in the crystal, w/o having to worry about the internal forces acting on it.

→ The Hamiltonian in presence of an external electric field, \vec{E} :

↳ Intrinsic periodic potential.

$$H = \frac{p^2}{2m} + V(x) + eEx$$

$$\psi(x, k, t=0) = \psi_0$$

Time evolution of the wavefunction:

$$\psi(x, k, t) = e^{-i\hat{H}t/\hbar} \psi_0$$

$$= e^{-i\left[\frac{p^2}{2m} + V(x) + eEx\right]t/\hbar} \psi_0$$

Since the particle experiences a periodic potential in the lattice, we can safely assume that it obeys Bloch's wavefunction.

$$\psi(x+na, k, t) = e^{-it/\hbar \left\{ \frac{\hat{p}^2}{2m} + V(x+na) + eE(x+na) \right\}} e^{ik_0 a} \psi_0$$

$$= e^{-it/\hbar \left\{ \frac{\hat{p}^2}{2m} + V(x) + eEx \right\}} e^{-ieaEt/\hbar} e^{ik_0 a} \psi_0$$

$$= e^{ia\left(k_0 - \frac{eEt}{\hbar}\right)} \psi(x, k, t)$$

Bloch's wavefunction:

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u(\vec{r}),$$

where $u(\vec{r} + n\vec{a}) = u(\vec{r})$
for $n \in \mathbb{Z}$.

$$\Rightarrow k(t) = k_0 - \frac{eEt}{\hbar}$$

$$\Rightarrow \frac{d}{dt}(\hbar k) = -eE \quad !!!$$

But what if \vec{E} is position dependent? That situation can't be resolved as such...

$$m^* = \hbar^2 / \partial^2 E / \partial k^2$$

$$\rightarrow \vec{a} = \frac{d}{dt} \vec{v}$$

$$= \frac{d}{dt} \left[\frac{1}{\hbar} \vec{\nabla}_k \epsilon_k \right]$$

Effective mass is a tensor because it can exhibit directional dependence.

$$a_i = \frac{d}{dt} (v_i(k_j)) \quad (??)$$

$$= \frac{\partial v}{\partial k_j} \frac{dk_j}{dt}$$

$$\rightarrow M_{ij}^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

$$= \frac{1}{\hbar} \frac{\partial^2 E}{\partial k_i \partial k_j} \cdot \frac{\vec{F}_j}{\hbar}$$

$$\rightarrow \psi = u_{\vec{k}(x)} e^{i\vec{k}x}$$

$$\Rightarrow p|\psi\rangle = -i\hbar \frac{\partial \psi}{\partial x} = \hbar k |\psi\rangle + (-i\hbar) \frac{\partial u_{\vec{k}}}{\partial x} e^{i\vec{k}x}$$

$$\Rightarrow p|\psi\rangle = \hbar k |\psi\rangle + e^{i\vec{k}x} p|u_{\vec{k}}\rangle$$

$$\Rightarrow p|\psi\rangle = e^{i\vec{k}x} (p + \hbar k) |u_{\vec{k}}\rangle \quad [\because \psi = e^{i\vec{k}x} u_{\vec{k}}]$$

$$\left(\frac{p^2}{2m} + V(x) \right) |\psi\rangle = E |\psi\rangle \quad [\text{Hamiltonian}]$$

$$\text{Now, } p|\psi\rangle = e^{i\vec{k}x} (p + \hbar k) |u_{\vec{k}}\rangle$$

$$\Rightarrow p(p|\psi\rangle) = p \left(e^{i\vec{k}x} (p + \hbar k) |u_{\vec{k}}\rangle \right) = -i\hbar \frac{\partial}{\partial x} \left(e^{i\vec{k}x} (p + \hbar k) |u_{\vec{k}}\rangle \right)$$

$$\Rightarrow p^2 |\psi\rangle = e^{i\vec{k}x} \hbar k (p + \hbar k) |u_{\vec{k}}\rangle + e^{i\vec{k}x} p (p + \hbar k) |u_{\vec{k}}\rangle$$

$$\Rightarrow p^2 |\psi\rangle = e^{i\vec{k}x} \left[(p + \hbar k)^2 |u_{\vec{k}}\rangle \right]$$

Substituting in the Hamiltonian,

$$e^{i\vec{k}x} \left(\frac{(p + \hbar k)^2}{2m} |u_{\vec{k}}\rangle + V \right) |u_{\vec{k}}\rangle = e^{i\vec{k}x} E |u_{\vec{k}}\rangle$$

$$\Rightarrow H|u_k\rangle = E|u_k\rangle$$

Differentiating on both sides,

$$\Rightarrow H \frac{\partial}{\partial k}|u_k\rangle + \frac{\hbar}{m}(p + \hbar k)|u_k\rangle = \frac{\partial E}{\partial k}|u_k\rangle + E \frac{\partial}{\partial k}|u_k\rangle$$

This step is suspicious, but hey, if only I had another option!

Taking expectation values,

$$\langle u_k | H \frac{\partial}{\partial k} | u_k \rangle + \frac{\hbar}{m} \langle u_k | p + \hbar k | u_k \rangle = \frac{\partial E}{\partial k} \langle u_k | u_k \rangle + E \langle u_k | \frac{\partial}{\partial k} | u_k \rangle$$

\downarrow operator \downarrow some factor

$$\Rightarrow \frac{\hbar}{m} \langle \psi | p | \psi \rangle = \frac{\partial E}{\partial k} \quad [\because p | \psi \rangle = e^{i k a} (p + \hbar k) | u_k \rangle]$$

$$\Rightarrow \langle \psi | \frac{p}{m} | \psi \rangle = \frac{1}{\hbar} \frac{\partial E}{\partial k}$$

The so-called 'group velocity' of the electronic wavefunction.

Expectation value of velocity associated with 'crystal momentum'.

→ Effective mass & the E-k diagram:

$$m^* a = \hbar k$$

Now, $a = \frac{dv}{dt} = \frac{dv}{dk} \frac{dk}{dt} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \cdot \hbar k$ (Much better, convincing method mathematically than simply assuming free particle & writing shit).

$$\Rightarrow a = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \cdot \frac{m^*}{\hbar} a$$

$$\Rightarrow m^* = \frac{\hbar^2}{\partial^2 E / \partial k^2}$$

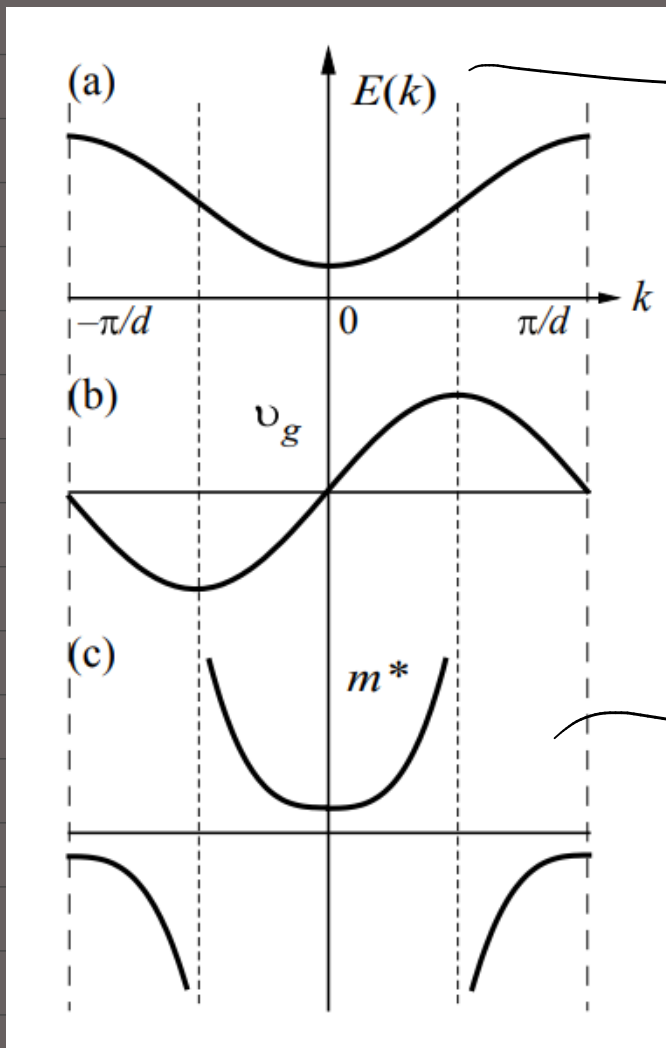
[I believe we're using the actual mass in TISE/Hamiltonian, but here it's a transition to m^* in order to apply plain old Newtonian mech.]



Near the 1st Brillouin zone, we can approximate the graph to be a parabola.

$$E(k) = E_0 - A(k - k_0)^2$$

sign (& magnitude) of A depends on sign (& magnitude) of m^* .



→ a cosine function

→ $m^* \propto \sec(kd)$, so there's a discontinuity at $k = \frac{\pi}{2d}$.
Theoretically, it means e^- can have -ve effective mass!

As shown in Fig. 3.21b, the resultant group velocity is not a constant within the first Brillouin zone. Rather, it oscillates from zero to a maximum, then going through a minimum and back up to maximum again. Since the zone boundaries $\pm\pi/d$ are equivalent using the periodicity of k -space, the zero velocity at the zone boundaries corresponds to the standing wave nature of the electron waves due to Bragg reflections. Furthermore,

This velocity oscillation is equivalent to a mass change at critical points in k -space shown in Fig. 3.21c. The electron mass has a constant positive value near the zone center but becomes negative on the zone boundary. One unusual property of the effective mass is that at wave vectors corresponding to the maximum and minimum velocities, the effective mass goes to infinite. This marks the point where a deceleration must begin to slow down the electron. The other peculiar property is that the effective mass has regions in which it is negative. A negative m^* means that the acceleration resulting from the externally applied electric field is in a direction opposite to that of the applied field; this is the effect of electron reflection due to the periodic crystal lattice.

→ Trajectory of e^- in presence of \vec{B} in real space & k -space.

Show that:

① $\frac{d\epsilon_k}{dt} = 0,$

② $\frac{dk_{||}}{dt} = 0$

$\parallel \rightarrow$ parallel to \vec{B} .

$$\hbar \dot{\vec{k}} = (-e) \vec{v}_k \times \vec{B}$$

$$\vec{v}_k = \dot{\vec{r}} = \frac{1}{\hbar} \nabla_k \epsilon_k$$

$$\vec{v}_k = \dot{\vec{r}} = \dot{\vec{r}}_{||} + \dot{\vec{r}}_{\perp}$$

$$\Rightarrow \hat{B} \times \hbar \dot{\vec{k}} = (-e) \hat{B} \times (\vec{v}_k \times \vec{B})$$

$$= (-e) [(\hat{B} \cdot \vec{B}) \vec{v}_k - (\hat{B} \cdot \vec{v}_k) \vec{B}]$$

$$= (-e) [B \vec{v}_k - \dot{r}_{||} \vec{B}]$$

$$= (-e) B [\dot{\vec{r}}_{\perp} - \dot{r}_{||}]$$

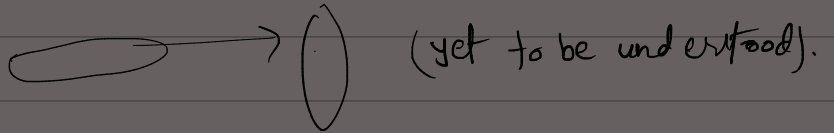
$$= (-e) B \dot{\vec{r}}_{\perp}$$

Component of vel. \parallel to \vec{B} is constant

$$\hat{B} \cdot (\dot{\vec{r}}_{||} + \dot{\vec{r}}_{\perp}) = \hat{B} \cdot \dot{\vec{r}}_{||} = \dot{r}_{||}$$

$$\Rightarrow \dot{\vec{r}}_{\perp} = -\frac{\hbar}{eB} \hat{B} \times \dot{\vec{k}}$$

$$\Rightarrow \vec{r}_{\perp}(t) - \vec{r}_{\perp}(0) = -\frac{\hbar}{eB} \hat{B} \times (\vec{k}(t) - \vec{k}(0))$$



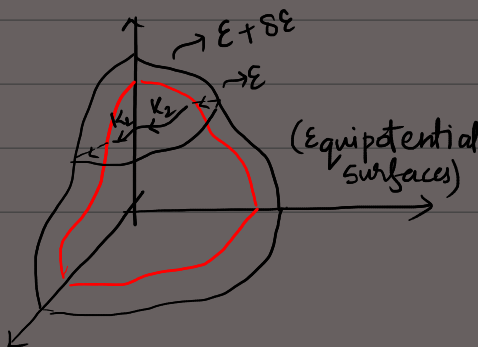
Time taken to travel from one pt. to another in the k -space trajectory.

$$t_2 - t_1 = \int_{t_1}^{t_2} dt = \int_{k_1}^{k_2} \frac{dk}{|\dot{\vec{k}}|}$$

$$\frac{eB}{\hbar^2} |\nabla_k \epsilon_k| \Delta(\vec{k})$$

(Derive this)

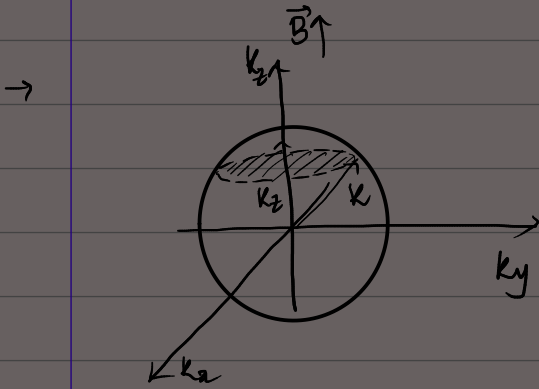
$$= \frac{\hbar^2}{eB} \int \frac{dk}{|\nabla_k \epsilon_k|}$$



$$\delta E = \nabla_k \epsilon_k \cdot \Delta(\vec{k}) = |\nabla_k \epsilon_k|_{\perp} \cdot \Delta(\vec{k})$$

$$\Rightarrow t_2 - t_1 = -\frac{\hbar^2}{eB} \frac{1}{\delta E} \int_{k_1}^{k_2} \Delta(\vec{k}) dk$$

$$\Rightarrow \Delta t = -\frac{\hbar^2}{eB} \frac{\partial(A, k_u)}{\partial \mathcal{E}} (\delta \mathcal{E} \rightarrow 0).$$



$$T = -\frac{\hbar^2}{eB} \frac{\partial}{\partial \mathcal{E}} \left[\pi(k_x^2 - k_z^2) \right]$$

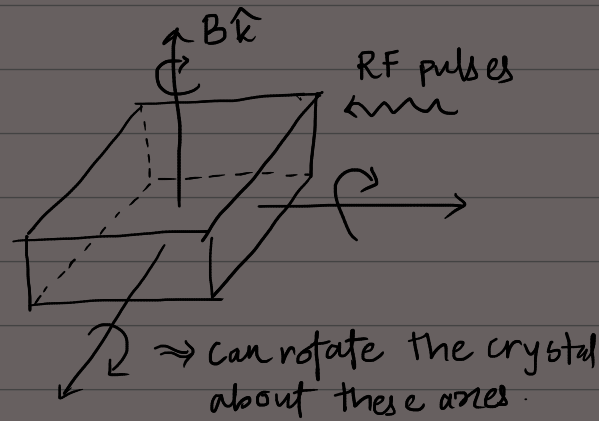
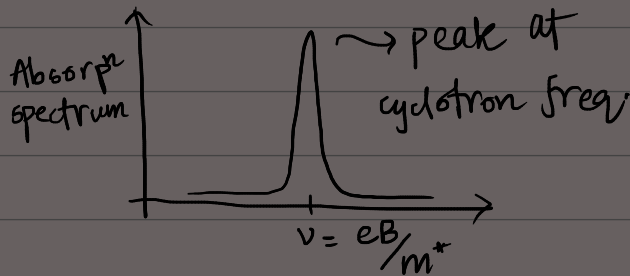
$$= -\frac{\hbar^2}{eB} \frac{\partial}{\partial \mathcal{E}} \left[\pi \left(\frac{2m\mathcal{E}}{\hbar^2} - k_z^2 \right) \right]$$

$$= -\frac{\hbar^2}{eB} \pi \cdot \frac{2m}{\hbar^2} \quad (\text{What about the -ve sign, bruv?})$$

$$\boxed{T = \frac{2\pi m}{eB}}, \quad \boxed{\omega_c = eB/m} \quad (\text{cyclotron freq.})$$

→ How to determine effective mass in a semiconductor?

Cyclotron Resonance Technique:



Just a side note.

Consider a free e^- undergoing cyclotron motion in presence of \vec{B} . Quantum mechanically, we'll see that e^- will occupy quantized energy states known as 'Landau levels'. So, shining an RF pulse of a particular freq; will excite the e^- from a lower energy level to a higher one.

$$\vec{E} = E_0 e^{i\omega t} \hat{x}$$

$$\vec{B} = B_0 \hat{z}$$

$$F_x = qE_0 e^{i\omega t} + qB_0 v_y, \quad F_y = -qB_0 v_x, \quad F_z = 0.$$

$$\Rightarrow m^* \ddot{x} = qE_0 e^{i\omega t} + qB_0 v_y, \quad m^* \ddot{y} = -qB_0 v_x$$

$$\Rightarrow \ddot{x} = \frac{qE_0}{m^*} e^{i\omega t} + \underbrace{\left(\frac{qB_0}{m^*}\right)}_{\omega_c} v_y, \quad \ddot{y} = -\underbrace{\left(\frac{qB_0}{m^*}\right)}_{\omega_c} v_x$$

$$\ddot{x} = \frac{qE_0}{m^*} e^{i\omega t} + \omega_c \dot{y}, \quad \ddot{y} = -\omega_c \dot{x}$$

Trial solⁿ: $x = x_0 e^{i\omega t}, \quad y = y_0 e^{i\omega t}$

$$y_0 = \left(\frac{i\omega}{\omega_c}\right) x_0, \quad x_0 = \frac{qE_0/m^*}{\omega^2 - \omega_c^2}$$

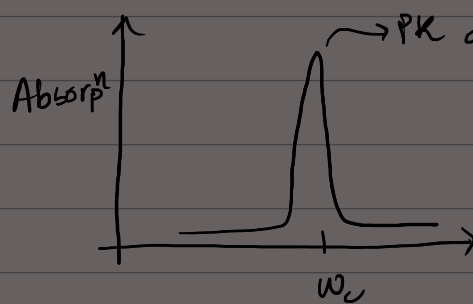
$$\Rightarrow y_0 = \left(\frac{i\omega}{\omega_c}\right) \left(\frac{qE_0/m^*}{\omega^2 - \omega_c^2}\right)$$

The Fermi surface is spherical in direct band-gap materials, so it doesn't matter which direction \vec{E} & \vec{B} are being applied, as long as they're orthogonal to each other.

For resonance,

$$\omega = \omega_c$$

At resonance, e^- absorbs max. energy from the RF field.



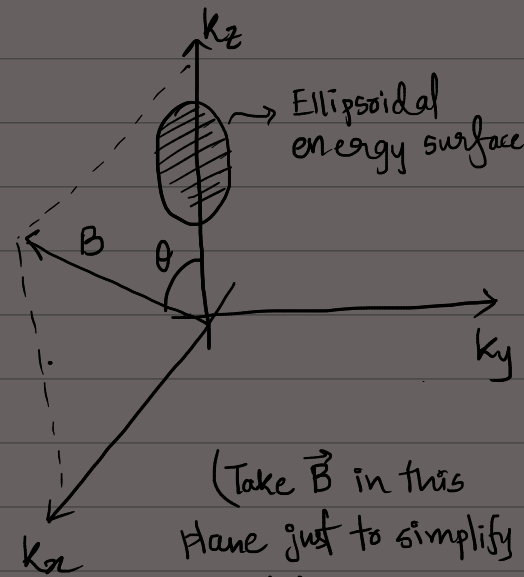
$$x(t) = x_0 e^{i\omega t}$$

$$y(t) = i x_0 e^{i\omega t}$$

For direct band-gap semiconductors, we'll get 2 peaks (e^- & h) or at most 3 peaks (e^- + light h + heavy h). What happens in an indirect band-gap semiconductor like Si?

$$\vec{B} = B_0 \sin\theta \hat{i} + B_0 \cos\theta \hat{k}$$

$$\vec{E} = E_0 e^{i\omega t} \hat{j}$$



(Take \vec{B} in this plane just to simplify stuff)

$$m_{\perp} \ddot{x} = q(\dot{y} B_z - \dot{z} B_y) + qE_x$$

$$m_{\perp} \ddot{y} = q(\dot{z} B_x - \dot{x} B_z) + qE_y$$

$$m_{\parallel} \ddot{z} = q(\dot{x} B_y - \dot{y} B_x) + qE_z$$

$$\ddot{x} = \omega_{\perp} \dot{y} \cos\theta, \quad \omega_{\perp} = eB_0/m_{\perp}$$

$$\ddot{y} = \omega_{\perp} \dot{z} \sin\theta - \omega_{\perp} \dot{x} \cos\theta + \frac{qE_0}{m_{\perp}^*} e^{i\omega t}$$

$$\ddot{z} = -\omega_{\parallel} \dot{y} \sin\theta, \quad \omega_{\parallel} = eB_0/m_{\parallel}$$

$$x_0 = \frac{qE_0}{m_{\perp}^*} \frac{i \omega_{\perp} \cos\theta}{(\omega^2 - \omega_{\perp}^2 \cos^2\theta - \omega_{\perp} \omega_{\parallel} \sin^2\theta)}, \quad [\text{Correspond to trial solns.}]$$

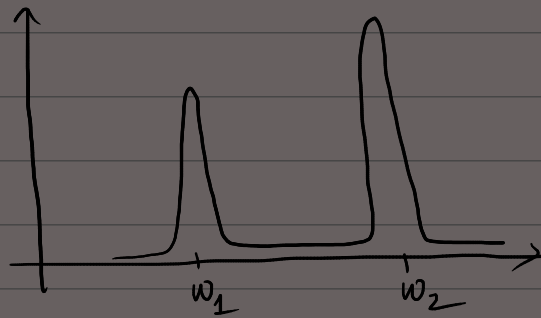
$$y_0 = \frac{qE_0}{m_{\perp}^*} \frac{1}{(\omega^2 - \omega_{\perp}^2 \cos^2\theta - \omega_{\perp} \omega_{\parallel} \sin^2\theta)}$$

$$z_0 = -\frac{qE_0}{m_{\parallel}^*} \frac{i \omega_{\parallel} \sin\theta}{\omega(\quad)}$$

→ Just a foolish thought: Since ω_{\perp} & ω_{\parallel} are constants, we can have resonance at any θ ... and that sounds extremely foolish. How do we argue that prominent resonance peaks are only observed at $\theta=0, \pi/2$ only?

At resonance, $\omega^2 = \omega_{\perp}^2 \cos^2 \theta + \omega_{\perp} \omega_{\parallel} \sin^2 \theta$

Now, m_{\perp} & m_{\parallel} can't be found from this case, given an arbitrary θ . However, since we can rotate the crystal, we can align the \vec{B} along energy surface along z-axis (technically, along a crystal plane) such that $\theta=0$. If $\theta=0$ for z-axis, this will mean $\theta=\pi/2$ for the energy surfaces along x- & y-axes → this will mean that we'll get two peaks.



$$\omega_1 = \omega_{\perp} = \frac{eB_0}{m_{\perp}}$$

$$\omega_2 = \omega_{\parallel} = \frac{eB_0}{\sqrt{m_{\perp} m_{\parallel}}}$$

Higher peak at ω_2 since \vec{B} is \perp^n to 4 cigars, while it is \parallel^k to only 2 cigars.

The same experiment will give us an absorption spectrum for holes too. However, hole masses can't be distinguished directionally (m_{\perp} & m_{\parallel}), so their absorption peak won't change as θ changes. We'll have two peaks, one each for the light & heavy holes.

→ We have defined two masses (m_{\perp} & m_{\parallel}) for e's as well as for holes (m_{\perp} & m_{\parallel}). So how do we reconcile these two masses to obtain a single effective mass for the analytic purposes?

① Density of states (DOS) effective mass:
let's start with holes!

$$\begin{aligned}
 P_0 &= P_e + P_h \\
 &= \mu_v^e e^{-(E_F - E_v)\beta} + \mu_v^h e^{-(E_F - E_v)\beta} \\
 &= 2 \left[(2\pi m_e^* k_B T)^{3/2} + (2\pi m_h^* k_B T)^{3/2} \right] e^{-(E_F - E_v)\beta} \\
 \Rightarrow & \boxed{m^{(DOS)}^{3/2} = m_L^{*3/2} + m_h^{*3/2}}
 \end{aligned}$$

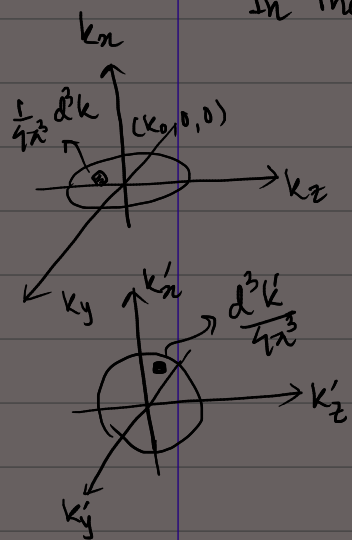
Now, let's consider electrons.

$$E = \frac{\hbar^2}{2m_{||}} (k_x - k_{x0})^2 + \frac{\hbar^2}{2m_{\perp}} (k_y^2 + k_z^2) \quad \rightarrow \text{Life isn't as easy here because of the ellipsoidal surface.}$$

Do a co-ordinate transformation -

$$\begin{aligned}
 k'_x &= \sqrt{\frac{m_0}{m_{||}}} (k_x - k_{x0}), \quad k'_y = \sqrt{\frac{m_0}{m_{\perp}}} k_y, \quad k'_z = \sqrt{\frac{m_0}{m_{\perp}}} k_z \\
 E - E_c &= \frac{\hbar^2}{2m_0} [k_x'^2 + k_y'^2 + k_z'^2] \quad [m_0 = m_e^{(DOS)}]
 \end{aligned}$$

In the k -space, transformation wouldn't change the DOS.



$$\Rightarrow \frac{1}{4\pi^3} d^3k' = \frac{1}{4\pi^3} d^3k = g(E) dE$$

$$\Rightarrow d^3k' = d^3k$$

$$\Rightarrow \boxed{m_0^3 = m_{\perp}^2 m_{||}} \Rightarrow \boxed{m_e^{(DOS)} = (m_{\perp}^2 m_{||})^{1/3}}$$

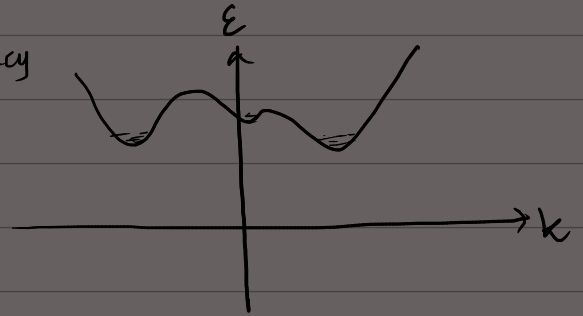
Our e DOS now reads as:

$$g(E) = \frac{4\sqrt{2} m_0^{3/2}}{\hbar^3} (E - E_c)$$

② Conductivity effective mass:

For electrons,

$$\sigma = \sum_{i=1}^6 \sigma_i \quad \text{Valley degeneracy}$$



$n_i = \frac{n_0}{6}$
 [Each valley contributes equally to e⁻ conc.]

$$= \sum \frac{n_i e^2 \tau}{m_i^*}$$

$$= \frac{n_0}{6} \sum \frac{e^2 \tau}{m_i^*}$$

$$= \frac{n_0 e^2 \tau}{6 m^*} \times 2 \left\{ \begin{bmatrix} m_n^{-1} & 0 & 0 \\ 0 & m_{\perp}^{-1} & 0 \\ 0 & 0 & m_{\perp}^{-1} \end{bmatrix} + \begin{bmatrix} m_{\perp}^{-1} & 0 & 0 \\ 0 & m_n^{-1} & 0 \\ 0 & 0 & m_{\perp}^{-1} \end{bmatrix} + \begin{bmatrix} m_{\perp}^{-1} & 0 & 0 \\ 0 & m_{\perp}^{-1} & 0 \\ 0 & 0 & m_n^{-1} \end{bmatrix} \right\}$$

We would want to reduce this into -

$$\sigma = n_0 e^2 \tau \begin{bmatrix} m_c^{-1} & 0 & 0 \\ 0 & m_c^{-1} & 0 \\ 0 & 0 & m_c^{-1} \end{bmatrix}$$

$$\Rightarrow \frac{1}{m_c^*} = \frac{1}{3} \left(\frac{2}{m_{\perp}} + \frac{1}{m_n} \right)$$

→



Direct bandgap semiconductors
 eg. GaAs, InAs
 → useful for optoelectronics



Indirect bandgap semiconductors
 eg. Si, Ge
 → useful in logic devices

→ $E(k) = E_c + \frac{\hbar^2 k^2}{2m_c^*}$ → effec. mass in CB.

$E(k) = E_v - \frac{\hbar^2 k^2}{2m_v^*}$ → effec. mass in VB.

→ Density of states (DOS) in C.B. & V.B.:

$g_c(E) = \frac{\sqrt{2}(m_c^*)^{3/2}}{\hbar^3 \pi^2} \sqrt{E - E_c} = \zeta_c \sqrt{E - E_c}$ → DOS effec. mass

$g_v(E) = \frac{\sqrt{2}(m_v^*)^{3/2}}{\hbar^3 \pi^2} \sqrt{E_v - E} = \zeta_v \sqrt{E_v - E}$

Now, $f(E) = \frac{1}{1 + e^{(E - E_F)\beta}} \approx e^{-(E - E_F)\beta}$ [Boltzmann's approx.]

Intrinsic hole conc., $n_o = \int_{E_c}^{\infty} g_c(E) f(E) dE$

$= \zeta_c \int_{E_c}^{\infty} e^{-(E - E_c)\beta} \sqrt{E - E_c} dE$

$= \zeta_c \frac{e^{-(E_c - E_F)\beta}}{\beta^{3/2}} \int_0^{\infty} \sqrt{x} e^{-x} dx \rightarrow \Gamma(3/2)$

$= 2 \left(\frac{2\pi m_c^* k_B T}{\hbar^2} \right)^{3/2} e^{-(E_c - E_F)\beta}$

is it h or only h?

$n_o = U_c e^{-(E_c - E_F)\beta}$

Similarly, $p_o = \int_{-\infty}^{E_v} g_v(E) \sqrt{E_v - E} dE \Rightarrow p_o = U_v e^{-(E_F - E_v)\beta}$

→ For an intrinsic semiconductor, $n_0 = p_0 = n_i(T)$

$$\Rightarrow n_0 p_0 = n_i^2 = n_c n_v \exp\left(\frac{E_c - E_v}{k_B T}\right)$$

$$\Rightarrow n_i^2 = n_c n_v \exp\left(\frac{E_g}{k_B T}\right)$$

$$\Rightarrow n_i = \sqrt{n_c n_v} \exp\left(\frac{E_g}{2k_B T}\right)$$

The product of $n \cdot p$ stays the same even for a doped semiconductor (under eq. of) since doping will merely change the E_F , but the end expression will anyways still be the same.

→ For an intrinsic semiconductor,

$$n_0 = p_0$$

$$\Rightarrow n_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = n_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

$$\Rightarrow E_F = \frac{1}{2}(E_c + E_v) + \frac{1}{2} k_B T \ln\left(\frac{n_c}{n_v}\right) \text{ [Rearrange]}$$

Note that the same expression doesn't apply to a doped material since $n \neq p$ then

$$\Rightarrow E_F = \frac{1}{2}(E_c + E_v) + \frac{3}{4} k_B T \ln\left(\frac{m_c^*}{m_v^*}\right)$$

→ Excitons: It is a quasiparticle which represents the bound state of an electron & its corresponding hole. Excitons are formed when the material absorbs a photon with energy lower than the bandgap energy. This $e-h$ pair now form a Coulomb-interacting pair, with properties analogous to a hydrogenic atom.

The recombination time for such a pair is much higher as compared to other time scales, so it qualifies as a quasi-particle.

Some interesting threads on excitons:

<https://physics.stackexchange.com/questions/588395/energy-of-exciton-formation-in-semiconductors?rq=1>

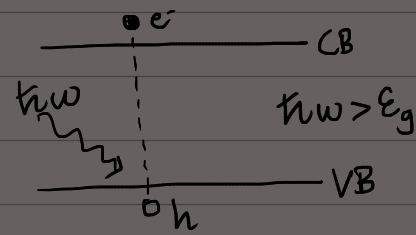
<https://physics.stackexchange.com/questions/586890/excitons-increase-in-absorption/586972#586972>

→ Total energy of an electrostatically bound e⁻-h pair:

$$E_{\text{tot}} = E_c + \frac{\hbar^2 k_e^2}{2m_e^*} + E_v + \frac{\hbar^2 k_h^2}{2m_h^*}$$

consider $E_v = 0$, $\Rightarrow E_c = E_g$

$$\Rightarrow E_{\text{tot}} = E_g + \frac{\hbar^2 k_e^2}{2m_e^*} + \frac{\hbar^2 k_h^2}{2m_h^*}$$



Hamiltonian of the e⁻-h pair, $H = H_e + H_h$

$$= \left\{ \frac{p_e^2}{2m_e^*} + \frac{p_h^2}{2m_h^*} - \frac{e^2}{4\pi\epsilon_0 k |\mathbf{r}_e - \mathbf{r}_h|} \right\} \psi(\vec{r}_e, \vec{r}_h)$$

$$\vec{\pi} = \vec{\pi}_e - \vec{\pi}_h, \quad \mu = \frac{m_e^* m_h^*}{m_e^* + m_h^*}, \quad M = m_e^* + m_h^*$$

$$\vec{p} = -i\hbar \vec{\nabla}_h, \quad \vec{P} = -i\hbar \vec{\nabla}_R$$

Transforming the Hamiltonian, we obtain:

$$\Rightarrow (E - E_g) \psi(\vec{R}, \vec{\pi}) = \left(\frac{p^2}{2M} + \frac{p^2}{2M} - \frac{e^2}{4\pi\epsilon_0 k r} \right) \psi(\vec{R}, \vec{\pi})$$

Solⁿ to $\psi(\vec{R}, \vec{\pi})$ is of the form $\chi(\vec{R}) \cdot \phi(\vec{\pi})$, where

$$\chi(\vec{R}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{R}}, \quad \left(\frac{p^2}{2M} - \frac{e^2}{4\pi\epsilon_0 k r} \right) \phi(\vec{\pi}) = E_e \phi(\vec{\pi})$$

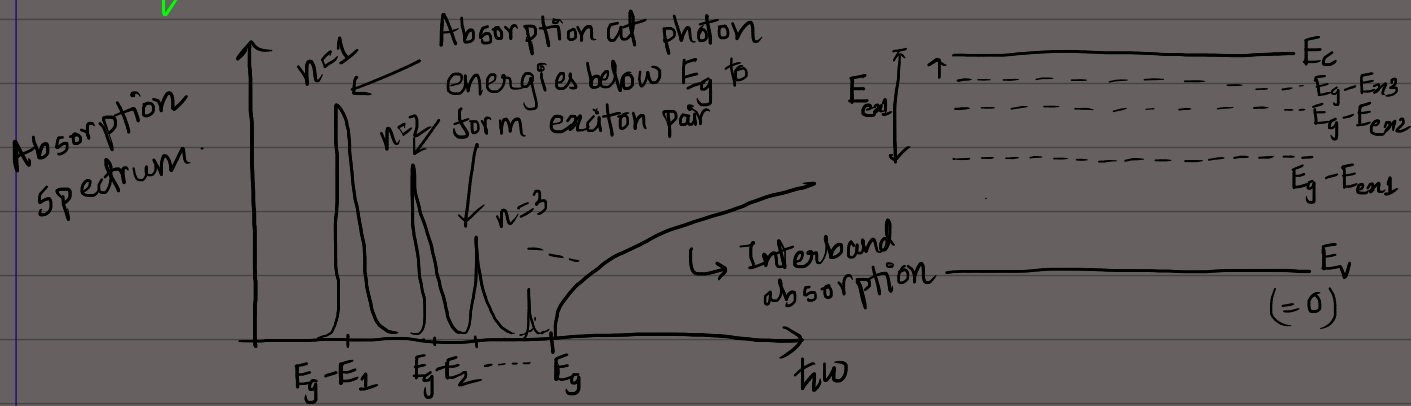
Solⁿ to H-atom problem.

$$\Rightarrow \phi_0(r) = \frac{1}{\sqrt{\pi(a_0^{\text{ex}})^3}} e^{-r/a_0^{\text{ex}}}$$

$$a_0^{\text{ex}} = \frac{4\pi\epsilon_0 k \hbar^2}{\mu e^2} \rightarrow \text{Exciton Bohr radius}$$

$$E_{\text{ex}} = \frac{-\mu e^4}{2(4\pi\epsilon_0 k)^2 \hbar^2} = \left[-\frac{\mu R_H}{m_0 k^2} \right] \rightarrow \text{Analogous to ground state energy of Bohr system?}$$

A slight digression, but a necessary one, considering that excitons are not quite well-understood.



- The absorption that occurs in the material when the material is supplied with photonic energy less than the bandgap energy may go into creating excitons.
- These excitons can have various binding energies which depend on n .
- In reference to Image 1, I take the $n = 1$ absorption line. Such an exciton will have binding energy equal to $E_{ex 1}$. When I supply the material with a photon of energy equal to $\hbar\omega = E_g - E_{ex 1}$, the material will absorb this photon and this energy will go into creating an exciton that has a quantum number $n = 1$.
- As we increase the energy that we supply to the material in the form of photonic energy we can force the material to form excitons with $n = 2$ (using photon energy of $\hbar\omega = E_g - E_{ex 2}$), $n = 3$ (using photon energy of $\hbar\omega = E_g - E_{ex 3}$) and so on (Image 2).
- Overall, when you supply specific photonic energies less than the bandgap, you get characteristic absorption in the material at specific energies corresponding to exciton formation. When you supply energy equal to or greater than the bandgap energy you get interband absorption, with electron transfer occurring directly from the valence band to the conduction band, no excitons form at these energies.

I have consulted a book by Mark Fox on Optical Properties of Solids, and it states:

"The absorption of a photon by an inter-band transition in a semiconductor or insulator creates an electron in the conduction band and hole in the valence band. The oppositely charged particles are created at the same point in space and can attract each other through their mutual Coulomb interaction... Moreover, if the conditions are satisfied, a bound electron-hole pair can be formed. This neutral bound pair is called an exciton."

My understanding is - We first need to supply $E > E_g$ for excitons to form. Once excitons exist in a material, they facilitate the absorption of photons with $E < E_g$, specifically at energies corresponding to $n=2, n=3$ etc. If the material has not been initially supplied with photons of $E > E_g$, with the material containing no excitons then why do we see an additional absorption response (red lines in figure below) apart from the $\alpha \sim \sqrt{E - E_g}$ response we normally observe? I'm confused because I saw spectra such as one below, I don't expect to see absorption below the band gap - we aren't supplying E_g for excitons to form.

I thought that the idea of a spectra is that you provide photons energy from 0 eV to final energy value greater than E_g , starting from low energy and sweep into higher energies.

- ▲ The e-h pair that is created can be either free, or bound. If the bound state is formed, you don't need to create a free pair and have it become bound, it just directly forms the bound state. - Jon Custer Oct 13, 2020 at 20:27
- ▲ Once a bound state e-h pair is formed (I understand that group velocity of electron and hole needs to be the same) then if you again supply energy to this exciton then it would break apart? I read that the position E_g corresponds to where the bound exciton has been ionized to a free e-h pair, and from the graph ^ it would seem that this is correct - the excitons are gone after you supply E_g to them. To me this seems strange that supplying a bound exciton with what seems like an arbitrary energy (E_g) to form the free e-h. Would the exciton not dissociate when binding energy is provided? - Aleksejus Pacalovas Oct 13, 2020 at 21:43
- ▲ Does an absorption spectra at energies of peaks ($n = 2, n = 3$, ie lower than bandgap energy) simply indicate the formation of bound states (and hence absorption of photons) or do you need to supply $E = E_g$ for bound states to form? - Aleksejus Pacalovas Oct 13, 2020 at 21:43
- ▲ You can directly form the bound state supplying the appropriate energy that is less than the band gap. - Jon Custer Oct 13, 2020 at 21:57
- ▲ Ok, would I be correct in saying that a bound exciton therefore would exist under the conduction band edge (since we provide the appropriate energy less than the band gap), while on the other hand a free exciton pair would have a hole in the valence band and an electron in the conduction band? - Aleksejus Pacalovas Oct 13, 2020 at 22:18
- ▲ The pair of electron in the CB and a hole in the VB is not bound - there is no binding energy tying them together. By definition, a bound exciton has an energy below the band gap. - Jon Custer Oct 13, 2020 at 22:20

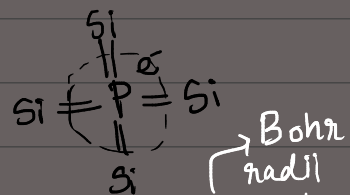
Anyways, total energy of the exciton = $E_g + \frac{\hbar^2 k^2}{2M} - \frac{\mu R_H}{m_0 k^2}$ → what is this now?

→ Intrinsic semiconductors: (in eqb.)

Doping a semiconductor doesn't necessarily mean that the dopants will contribute to the carrier conc., irrespectively of the environment. The dopants' ionization is purely a thermal phenomenon, and it will donate (or accept) e⁻s at a respectable scale only if the thermal energy is above a certain threshold.

Let us consider P, a n-type dopant in Si lattice. The extra e⁻ donated by P is said to be bound to the P as if it is a hydrogenic system (don't ask for justification, it's just a model to get a qualitative feel). If that is true, then-

$$\left\{ \frac{-\hbar^2}{2m_e^*} \nabla^2 - \frac{e^2}{4\pi\epsilon_0 \kappa r} \right\} \psi = E \psi$$



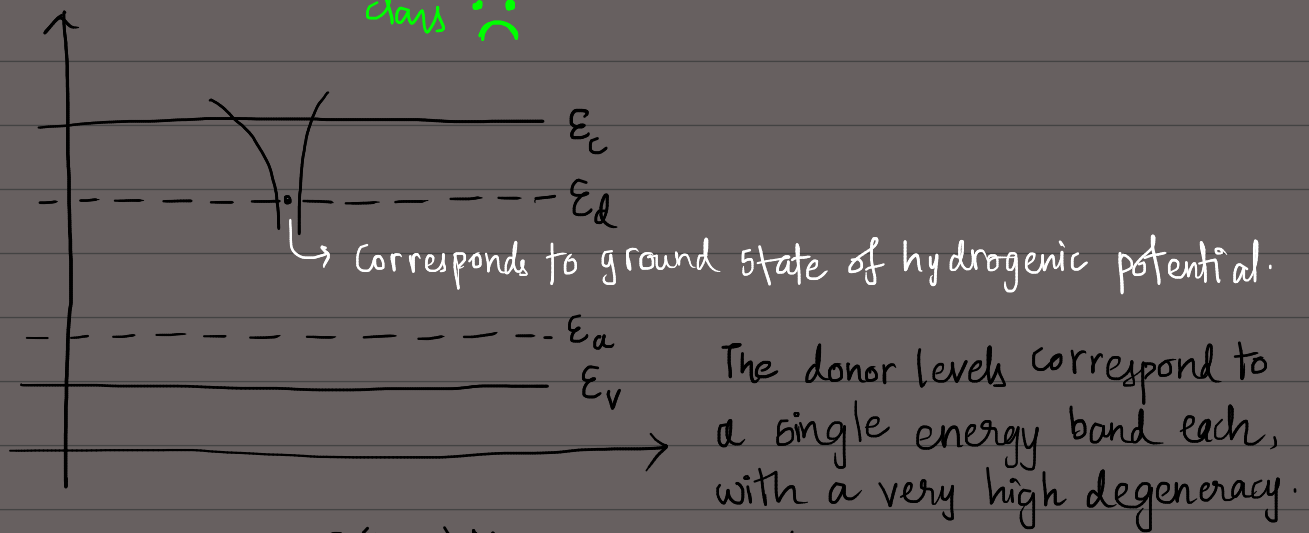
Ground state: $\psi_0(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$, $a_0^* = \frac{4\pi\epsilon_0 \kappa \hbar^2}{m_e^* e^2}$ when bound to donor

$$E = \frac{-m_e^* e^4}{2(4\pi\epsilon_0 \kappa)^2 \hbar^2} = \frac{-m_e^* R_H}{m_0 \kappa^2}$$

→ Ground state energy (donor level)

∵ $m_e^* < m_0$ & $\kappa > 1$ for semiconductors, a_0^* is usually in the range of nm, which means that it is much larger than inter-atomic distance. Thus, the dopant electronic orbit covers multiple unit cells at the same time.

How? WHY!? Man, I shouldn't have f*ckin' slept in that class :-)



$$g(E_d) = 8(E - E_d) N_D, \quad g(E_a) = 8(E - E_a) N_A$$

To be filled up only after understanding the theory

For donor energy level,

$$n_d / N_D = \frac{1}{1 + \frac{1}{2} e^{(E_d - E_f)\beta}}$$

For acceptor energy level,

$$n_a / N_A = \frac{1}{1 + \frac{1}{4} e^{(E_f - E_a)\beta}}$$

→ Due to additional degeneracy

Boltzmann approx.
 $(E_f - E_d)$ large $\Rightarrow p_a = 4 N_A e^{-(E_f - E_d)\beta}$
 $(E_d - E_f)$ large $\Rightarrow n_d = 2 N_D e^{-(E_d - E_f)\beta}$

(Just so as to avoid confusion)

→ N_D : doping density, n_d : e's bound to donors,
 n : e's in conduction band, N_D^+ : ionized donor density

→ Shallow donors: Donors that are nearly 100% ionized at room temp.

Fraction of un-ionized donors ←

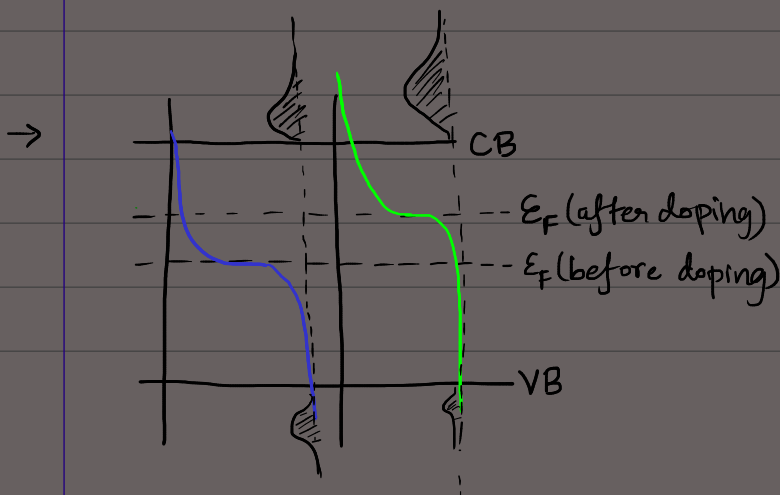
$$\frac{n_d}{n_d + n} = \frac{1}{1 + \frac{n}{n_d}} = \frac{1}{1 + \frac{N_C e^{-(E_C - E_F)\beta}}{2N_D e^{-(E_D - E_F)\beta}}}$$

$$= \frac{1}{1 + \frac{N_C}{2N_D} e^{-(E_C - E_D)\beta}}$$

From our simple hydrogenic dopant model, it would appear that the gap b/w E_C & E_D does not vary with dopant material (E_D is the ground state, & its energy is merely a scaled version of Rydberg energy - which is dependent on effec. mass, & which ideally, should not depend on the dopant material).

At room temp., order of $(E_C - E_D)\beta \approx 1$.

$$\therefore, \frac{n_d}{n + n_d} \approx \frac{1}{1 + \frac{N_C}{2N_D}} \quad N_C \sim 10^{19} \text{ cm}^{-3} \text{ @ } 300\text{K}.$$



So how exactly does E_F vary with doping?

charge-neutrality condⁿ.

(complete ionization)

$$p - n + N_D^+ - N_A^- + p_a - n_d = 0$$

$p_a = n_d = 0$ (assuming complete ionization at near-room temp.)

$$\Rightarrow p - n + N_D - N_A = 0$$

$$\Rightarrow u_v e^{-(E_f - E_v)\beta} - u_c e^{-(E_c - E_f)\beta} + N_D - N_A = 0$$

$$e^{E_f\beta} = \alpha e^{-E_c\beta} = \beta_c e^{+E_v\beta} = \beta_v$$

$$\Rightarrow \frac{u_v \beta_v}{\alpha} - u_c \beta_c \alpha + N_D - N_A = 0$$

$$\Rightarrow \alpha^2 - \frac{\alpha(N_D - N_A)}{u_c \beta_c} - \frac{u_v \beta_v}{u_c \beta_c} = 0$$

$$\Rightarrow \alpha = \left[\frac{N_D - N_A}{2u_c \beta_c} + \sqrt{\left(\frac{N_D - N_A}{2u_c \beta_c}\right)^2 + \frac{u_v \beta_v}{u_c \beta_c}} \right]$$

$$\Rightarrow \frac{E_f}{k_B T} = \ln(\quad)$$

Now, $\ln(a + \sqrt{a^2 + x^2}) = \ln a + \sinh^{-1}\left(\frac{x}{a}\right)$

$$\Rightarrow E_f = \frac{E_c + E_v}{2} + k_B T \ln\left(\frac{m_n^*}{m_p^*}\right)^{\frac{3}{4}} + k_B T \sinh^{-1}\left[\frac{(N_D - N_A)}{2\sqrt{u_c u_v} e^{-E_f\beta/2}}\right]$$

$$\Rightarrow E_f = E_{F_i} + k_B T \sinh^{-1}\left[\frac{N_D - N_A}{2n_i}\right]$$

$\sinh^{-1}(x) = \pm \ln|x|$ if x large.

$$\Rightarrow E_f = E_{F_i} \pm k_B T \ln\left|\frac{N_D - N_A}{2n_i}\right|$$

(Incomplete ionization)

Just so as to simplify stuff, we assume it is a n-type semiconductor at a low temp.

$$\cancel{p} - n + N_D^+ - \cancel{N_A} + \cancel{p} - n_d = 0$$

$$\Rightarrow n - N_D + n_d = 0$$

$$\Rightarrow n_c e^{-(E_c - E_f)\beta} - N_D + \frac{N_D}{1 + \frac{1}{2} e^{(E_d - E_f)\beta}} = 0$$

we're considering low temp, so Boltzmann approx. is not valid.

$$\Rightarrow n_c e^{-(E_c - E_f)\beta} - N_D \frac{1}{1 + 2e^{-(E_d - E_f)\beta}} = 0$$

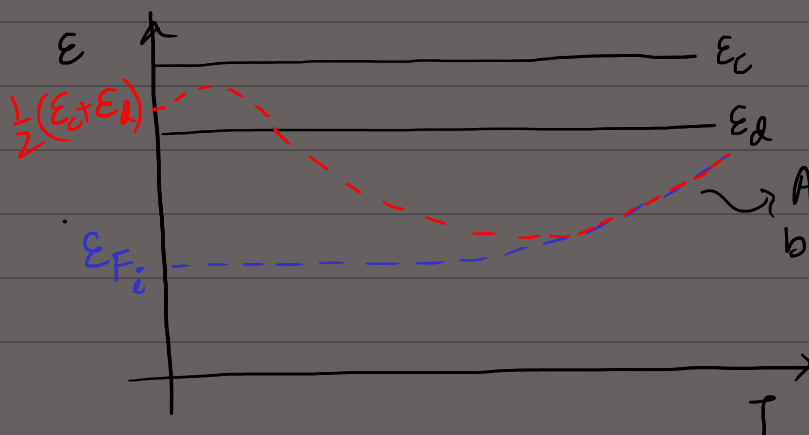
$$\Rightarrow n_c e^{-(E_f - E_c)\beta} + 2n_c e^{-(E_c + E_d - 2E_f)\beta} - N_D = 0.$$

$$\beta_c = e^{-E_c\beta}, \quad \beta_d = e^{-E_d\beta}, \quad \alpha = e^{+E_f\beta}$$

$$\Rightarrow \alpha^2 + \frac{\alpha}{2\beta_d} - \frac{N_D}{2n_c\beta_c\beta_d} = 0$$

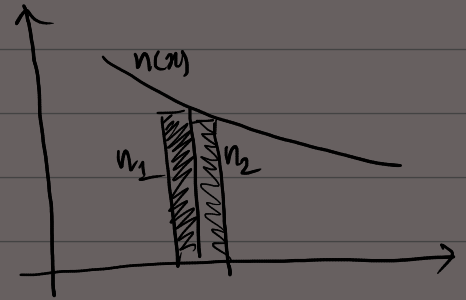
$$\Rightarrow E_f = \frac{E_c + E_d}{2} + \frac{1}{2} k_B T \ln\left(\frac{N_D}{2n_c}\right) - k_B T \sinh^{-1}\left(\sqrt{\frac{n_c}{8N_D}} e^{-E_g\beta/2}\right)$$

At $T=0K$, E_f is midway b/w E_c & E_d



→ Derivation of drift-diffusion current in a semiconductor.

(For a more detailed discussion, refer to Streetman & Banerjee or my 505 report).



$$\phi_n(x) = \frac{\bar{L}}{\tau} \frac{n_1 - n_2}{2}$$

$$n_1 - n_2 = \frac{n(x) - n(x + \Delta x)}{\Delta x} \bar{L}$$

$$\Rightarrow \phi_n(x) = \frac{-\bar{L}}{2\tau} \frac{dn(x)}{dx} \rightarrow D_n \text{ (diff. coefficient)}$$

$$\Rightarrow J_n(x) = (-q) \left(-D_n \frac{dn}{dx} \right), \quad \phi_p = q \left(-D_p \frac{dp}{dx} \right)$$

$$\Rightarrow J_{\text{diff}} = q \left(D_n \frac{dn}{dx} - D_p \frac{dp}{dx} \right) \quad [\text{diffusion component of current}]$$

$$J_{\text{drift}} = (nq\mu_n + pq\mu_p) E \quad [\text{drift component of current}]$$

$$\Rightarrow J_{\text{tot}} = q \left(D_n \frac{dn}{dx} - D_p \frac{dp}{dx} \right) + (nq\mu_n + pq\mu_p) E$$

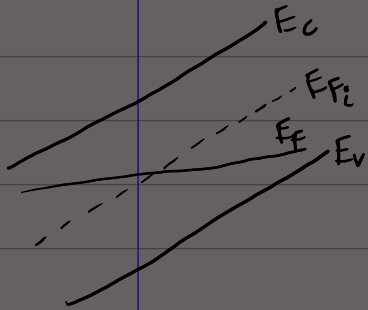
$$J_n = q \left(D_n \frac{dn}{dx} + n\mu_n E \right),$$

$$J_p = q \left(-D_p \frac{dp}{dx} + p\mu_p E \right)$$



Einstein Relation

Consider the sample to be in equilibrium, so that $J_n = J_p = 0$.



∵ the sample is in eqb., E_F is constant throughout

$$\Rightarrow p(x) \mu_p e E(x) = e D_p \frac{dp(x)}{dx}$$

$$\Rightarrow E(x) = \frac{D_p}{\mu_p} \frac{1}{p(x)} \frac{dp(x)}{dx} = \frac{D_p}{\mu_p} \frac{d \ln(p(x))}{dx}$$

$$\begin{aligned} p(x) &= u_v e^{-(E_F - E_v)\beta} \\ &= \underbrace{u_v e^{-(E_{F_i} - E_v)\beta}}_{n_i} e^{-(E_F - E_{F_i})\beta} \\ &= n_i e^{-(E_F - E_{F_i})\beta} \rightarrow \text{dependent on } x. \end{aligned}$$

$$\Rightarrow E(x) = \frac{1}{k_B T} \frac{D_p}{\mu_p} \left\{ \frac{d}{dx} (E_F - E_{F_i}(x)) \right\}$$

$$\Rightarrow E(x) = \frac{1}{k_B T} \frac{D_p}{\mu_p} \frac{d}{dx} (-E_{F_i}(x)) \quad \left[E(x) = \frac{d}{dx} \left(\frac{E(x)}{e} \right) \right]$$

$$\Rightarrow \frac{D_p}{\mu_p} \frac{e}{k_B T} = 1 \Rightarrow \boxed{\frac{D_p}{\mu_p} = \frac{k_B T}{q}}, \quad \boxed{\frac{D_n}{\mu_n} = \frac{k_B T}{q}}$$

necessarily an internal field arising from inhomogeneity of the sample, since no ext. \vec{E} is being applied in eqb.

This idea relates to the derivation we did in BTE, wherein the electric field can be ^{equivalently} represented by a gradient of the chemical potential.

[For homogenous semiconductors, s.t. there is no gradient in carrier conc. at eqp.]

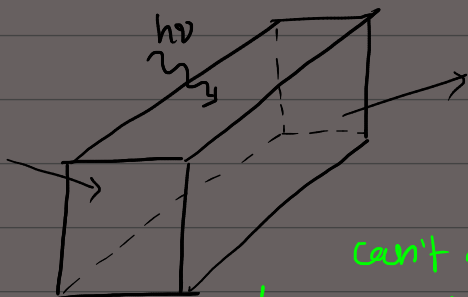


→ Continuity Equation :

Generalised continuity equation: $\frac{dp}{dt} + \vec{\nabla} \cdot \vec{j}_p = 0$

Sources or sinks inside the volume

charge flowing into & out of the volume



For semiconductors, we have some additional terms:

can't g_p & r_p terms be absorbed into $\frac{dp}{dt}$ itself?

$$\frac{dp}{dt} = -\vec{\nabla} \cdot \vec{j}_p + g_p - r_p$$

↓
↓
 generation rate of holes recomb. rate of holes

For a sample in both eq^m & steady state: $g_{n_0} = g_{p_0} = r_{n_0} = r_{p_0}$

For a sample not in eq^m, but in steady state: $g_n = g_p = r_n = r_p$

τ_{n_0}, τ_{p_0} : carrier lifetimes.

Rate of recombination in a ^{unit} volume containing only 1 electron = $\frac{1}{\tau_{n_0}}$

$$\Rightarrow r_{n_0} = \frac{n_0}{\tau_{n_0}}, \quad r_n = \frac{n}{\tau_n}$$

$$r_{p_0} = \frac{p_0}{\tau_{p_0}}, \quad r_p = \frac{p}{\tau_p}$$

Since charge accumulation is to be avoided in steady state, when current is constant.

Substituting all this stuff,

No. density, so drop the charge term.

$$\frac{dp}{dt} = -\vec{\nabla} \cdot \vec{j}_p + g_p - r_p$$

$$\begin{aligned} \vec{\nabla}(n) &= \vec{\nabla}(n_0 + \delta n) = \vec{\nabla}(\delta n) \\ g_n &= g_{n_0} + g'_n \\ g_p &= g_{p_0} + g'_p \end{aligned}$$

$$= -\vec{\nabla} \cdot (p \mu_p \vec{E} - D_p \vec{\nabla} p) + g_p - r_p$$

$$= D_p \nabla^2 p - \mu_p \vec{\nabla} \cdot (p \vec{E}) + g_p - \frac{p}{\tau_p}$$

||| 1/4

$$\frac{dn}{dt} = D_n \nabla^2 n + \mu_n \vec{\nabla} \cdot (n \vec{E}) + g_n - \frac{n}{\tau_n}$$

we haven't equated g'_n & g'_p yet.

→

$$\textcircled{I} \Rightarrow \partial_p \nabla^2(\delta p) - \mu_p [\vec{E} \cdot \vec{\nabla}(\delta p) + p \vec{\nabla} \cdot \vec{E}] + g'_p - \left(\frac{p}{\tau_p} - \frac{p_0}{\tau_{p0}} \right) = \frac{d(\delta p)}{dt}$$

$$\textcircled{II} \partial_n \nabla^2(\delta n) + \mu_n [\vec{E} \cdot \vec{\nabla}(\delta n) + n \vec{\nabla} \cdot \vec{E}] + g'_n - \left(\frac{n}{\tau_n} - \frac{n_0}{\tau_{n0}} \right) = \frac{d(\delta n)}{dt}$$

$$\vec{\nabla} \cdot \vec{E} = \frac{e}{\epsilon} [p - n + N_D - N_A + p_a - n_d]$$

Assumptions:

(i) $\delta p = \delta n$

(ii) $g'_n = g'_p$

(iii) $n = \frac{n_0 + \delta n}{\tau_n}, p = \frac{p_0 + \delta p}{\tau_p}$

$$\textcircled{I} \times n \mu_n + \textcircled{II} \times p \mu_p = \frac{n \mu_n \partial_p + p \mu_p \partial_n}{n \mu_n + p \mu_p} \nabla^2(\delta p) - \left(\frac{\mu_n \mu_p (n_0 - p_0)}{n \mu_n + p \mu_p} \right) (\vec{E} \cdot \vec{\nabla}(\delta p)) + g' - \left(\frac{p_0 + \delta p}{\tau_p} - \frac{p_0}{\tau_{p0}} \right) = \frac{\partial(\delta p)}{\partial t}$$

→ μ^* (Ambipolar mobility)

Using Einstein's relation,

$$\delta n - \delta p \ll n_0, p_0$$

$$\frac{n \mu_n \partial_p + p \mu_p \partial_n}{n \mu_n + p \mu_p} = \frac{(n+p) \partial_n \partial_p}{n \partial_n + p \partial_p} = \mathcal{D}^* \text{ (Ambipolar diff. coeff.)}$$

$$\Rightarrow \mathcal{D}^* \nabla^2(\delta p) - \mu^* \vec{E} \cdot \vec{\nabla}(\delta p) + g' - \frac{\delta p}{\tau} = \frac{\partial}{\partial t} (\delta p),$$

$$\mathcal{D}^* \nabla^2(\delta n) + \mu^* \vec{E} \cdot \vec{\nabla}(\delta n) + g' - \frac{\delta n}{\tau} = \frac{\partial}{\partial t} (\delta n)$$

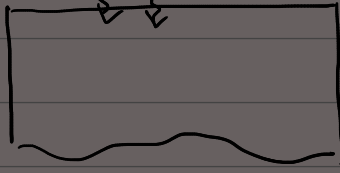
→ Low Injection Regime: Consider an n-type SC wherein $n_0 = 10^{15} \text{ cc}$, and $p_0 = n_i^2 / n_0 \approx 10^5 \text{ cc}$. $\delta n = \delta p = 10^{11} \text{ cc}$.

$$n = n_0 + \delta n \approx n_0, \quad p = p_0 + \delta p \approx \delta p$$

$$\tau_n \neq \tau_{n0}, \quad \tau_p \approx \tau_{p0}$$

For excess carriers, $\tau = \begin{cases} \tau_{p0} & \text{in n-type SC} \\ \tau_{n0} & \text{in p-type SC} \end{cases}$

(Uniform along the entire length of SC sample).



$t=0$, Δp holes & Δn e⁻s.

Case-I

Light pulse at $t=0$ (along entire length)

$$-\frac{\delta p}{\tau} = \frac{\partial (\delta p)}{\partial t} \Rightarrow \delta p = \Delta p e^{-t/\tau}$$

$$\Rightarrow p = p_0 + \Delta p e^{-t/\tau}$$

Case-II

Continuous illumination along entire length of SC.

$$g' - \frac{\delta p}{\tau} = 0 \Rightarrow \delta p = g'\tau \quad \left[\frac{\partial (\delta p)}{\partial t} = 0 \right]$$

$$n = n_0 + \delta n = n_0 + \delta p = n_0 + g'\tau$$

$$g' = 10^{13} \text{ EHP}/\mu\text{s}/\text{cm}^3, \quad \tau_{n0} = \tau_{p0} = 2 \mu\text{s}$$

$$n_0 = 10^{15} \text{ cm}^{-3}, \quad p_0 = 2.25 \times 10^5 \text{ cm}^{-3}$$

$$np = (n_0 + \delta n)(p_0 + \delta p)$$

$$= (10^{15} + 2 \times 10^3) (2.25 \times 10^5 + 2 \times 10^3)$$

$$\approx 2 \times 10^{23} \text{ cm}^{-6} \neq n_i^2 = n_0 p_0$$

This implies that we can no longer express n' as per it's old formula: $n \neq n_i e^{(E_F - E_{Fi})/\beta}$. We would still like to express n' in a format similar to this, so we introduce a 'quasi-Fermi level'.

$$n = n_i e^{(F_n - E_{Fi})/\beta}, \quad p = n_i e^{(E_{Fi} - F_p)/\beta}$$

$$J_n(x) = q \mu_n n(x) E(x) + q D_n \frac{dn(x)}{dx}$$

$$\frac{dn(x)}{dx} = \frac{d}{dx} \left[n_i e^{(F_n(x) - E_{F_2}(x)) / k_B T} \right]$$

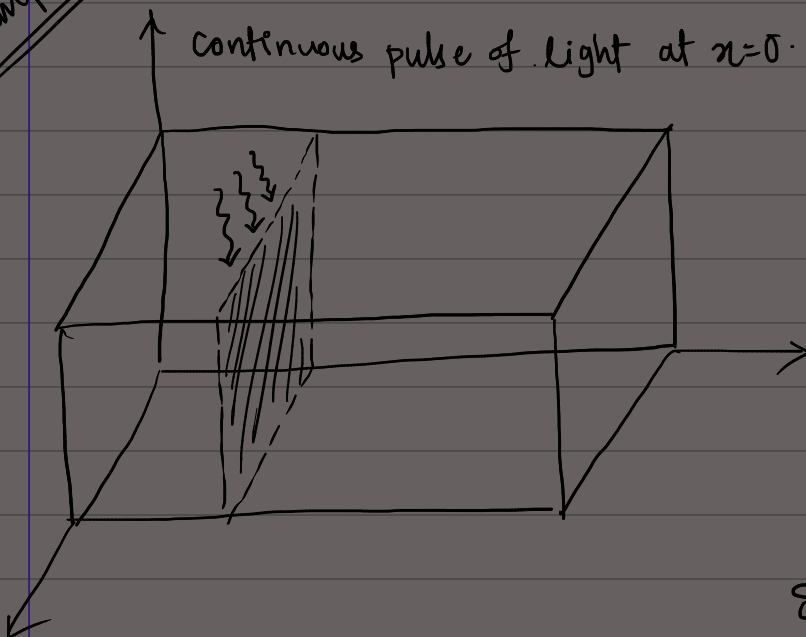
$$= \frac{n(x)}{k_B T} \left[\frac{dF_n(x)}{dx} - \frac{dE_{F_2}(x)}{dx} \right]$$

$$= \frac{n(x)}{k_B T} \left[\frac{dF_n(x)}{dx} - eE \right]$$

$$\Rightarrow J_n(x) = \mu_n n(x) \frac{dF_n(x)}{dx}$$

\Rightarrow At eqb, since we do not have a current in the bulk, there is no gradient in the Fermi level.

Example:



$$D_p \frac{\partial^2 (\delta p)}{\partial x^2} - \frac{\delta p}{\tau_p} + g' = 0$$

$$\delta p_+(x) = p_+(x) - p_0 = A_+ e^{x/L_p} + B_+ e^{-x/L_p}$$

$$\delta p_-(x) = p_-(x) - p_0 = A_- e^{-x/L_p} + B_- e^{x/L_p}$$

$$\delta p_{\pm} \rightarrow 0 \text{ as } x \rightarrow \pm\infty$$

$$A_+ = B_- = 0.$$

$$J_{p+}(x) = -D_p \frac{\partial}{\partial x} (\delta p_+) = \frac{A_0 D_p}{L_p} e^{-x/L_p}$$

$$\delta p_+(x=0) = \delta p_-(x=0) = A_- = B_+ = A_0$$

$$J_{p-}(x) = -A_0 \frac{D_p}{L_p} e^{x/L_p}$$

$$\delta p(x) = \begin{cases} A_0 e^{-x/L_p}, & x > 0 \\ A_0 e^{x/L_p}, & x < 0. \end{cases}$$

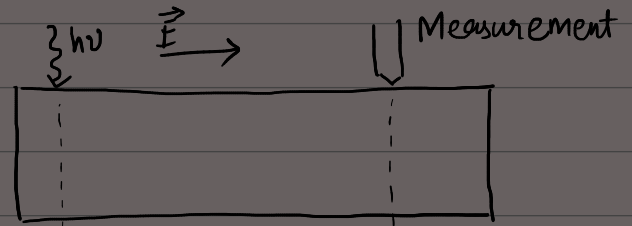
$$J_{p+}(0) - J_{p-}(0) = \frac{2A_0 D_p}{L_p} \rightarrow \text{Carrier generated/time/area.}$$

→ Haynes-Shockley Experiment :

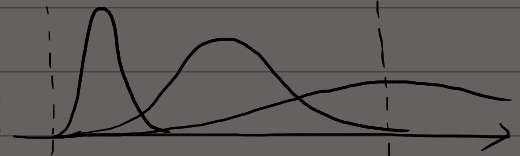
Is the 'input' to the sample a light pulse? Otherwise the results won't make any sense.

In Hall Effect measurements, we obtain the conc. and mobility of majority carriers only. So, how can we determine the corresponding parameters for the minority carriers?

(Unlike the prev. example, we're applying an external \vec{E} here, so the solution is diff.)



μ can be determined using the time taken by the packet to travel across the given length.



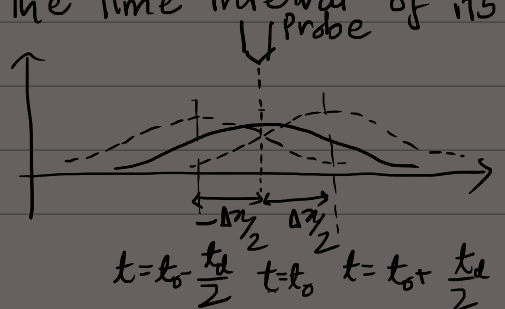
The dispersion of the Gaussian packet is related to the diffusion coefficient in the material.

$$\frac{\partial \langle \delta p \rangle}{\partial t} = D_p \frac{\partial^2 \langle \delta p \rangle}{\partial x^2} \rightarrow \text{We are assuming negligible recombination } (\tau_p \gg \tau)$$

$$\delta p(x,t) = \left[\frac{AP}{2\sqrt{\pi D_p t}} \right] e^{-x^2/4D_p t} \quad \begin{matrix} \downarrow \\ v_d \end{matrix}$$

The measurement device cannot measure δp 'spatially', but rather 'temporally'. So basically what happens is that when the wave packet passes the probe, we would measure its amplitude [btw when the wave packet's peak passes the probe, it will be the maximum reading for experiment, so we won't have any problem in identifying that]. The FWHM of the wave packet and the time interval of its passage can be documented by our probe reading.

$$(\Delta x)^2 = 16 D_p t_d$$

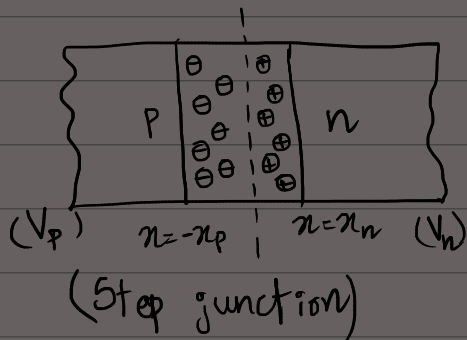


$$\Delta x = \Delta t \cdot v_d = \Delta t \cdot \frac{L}{t_d}$$

It is true that there will be some distortion in the wave packet as it passes the probe, however, we can ignore such a minor distortion.

$$\left(\Delta t \cdot \frac{L}{t_d} \right)^2 = 16 \Delta_p t_d$$

→ p-n junctions: [Man, I'm done with p-n junction derivations]



$$\frac{dE(x)}{dx} = \frac{q}{\epsilon} [p - n + N_D - N_A]$$

For $0 < x \leq x_n$,

$$\frac{dE(x)}{dx} = \frac{qN_D}{\epsilon}$$

$$E(x) = \frac{qN_D}{\epsilon} x + C,$$

$$E(x_n) = 0.$$

$$\Rightarrow E(x) = \frac{qN_D}{\epsilon} (x - x_n)$$

For $-x_p \leq x < 0$,

$$\frac{dE(x)}{dx} = -\frac{qN_A}{\epsilon}$$

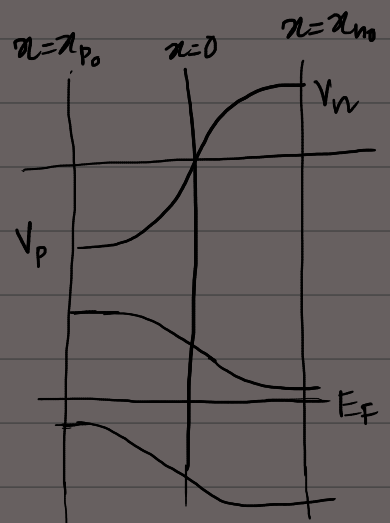
$$\Rightarrow E(x) = -\frac{qN_A}{\epsilon} (x + x_p)$$

$$V(x_n) = \int \frac{qN_D}{\epsilon} (x_{n0} - x_n) dx = -\frac{qN_D}{2\epsilon} (x_{n0} - x_n)^2 + C$$

$$V(x_{n0}) = V_n$$

$$\Rightarrow V(x_n) = V_n - \frac{qN_D}{2\epsilon} (x_{n0} - x_n)^2$$

$$V(x_p) = \int \frac{qN_A}{\epsilon} (x_p + x_p) dx = V_p + \frac{qN_A}{2\epsilon} (x_p + x_p)^2$$



Built-in potential, $\phi_b = V_n - V_p$

$$= \frac{1}{2} |E_m| (x_{n0} + |x_{p0}|) = \frac{1}{2} \frac{qN_D x_{n0}}{\epsilon} (W)$$

$$= \frac{1}{2} \frac{q N_D}{\epsilon} \frac{N_A}{N_A + N_D} W^2$$

$$\Rightarrow \phi_b = \frac{q}{2\epsilon} \frac{N_A N_D}{N_A + N_D} W^2$$

$$\Rightarrow W = \left[\frac{2\epsilon}{q} \left(\frac{1}{N_A} + \frac{1}{N_D} \right) \phi_b \right]^{\frac{1}{2}}$$

Now, $J_n(x) = J_p(x) = 0$ [in equilibrium]

$$q \mu_p p(x) E(x) - q D_p \frac{dp(x)}{dx} = 0$$

$$\Rightarrow -\frac{dV(x)}{dx} = \frac{D_p}{\mu_p} \frac{d \ln(p(x))}{dx}$$

$$\Rightarrow \int_{V_p}^{V_n} dV(x) = -\frac{D_p}{\mu_p} \int_{x_p}^{x_n} d \ln(p(x))$$

$$\Rightarrow V_n - V_p = -\frac{k_B T}{q} \ln \left[\frac{p_n(x_n)}{p_p(x_p)} \right]$$

$$\Rightarrow \phi_b = \frac{k_B T}{q} \ln \left(\frac{N_A N_D}{n_i^2} \right)$$

$\rightarrow n_i^2 / N_D$

$$p_{n0} = p_{p0} e^{-q\phi_b / k_B T}$$

$$n_{p0} = n_{n0} e^{-q\phi_b / k_B T}$$

→ Apply a potential V_a across the diode.

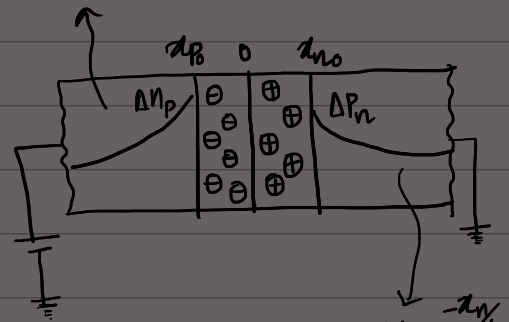
$$P_{n0} = P_{p0} e^{-q\phi_b/k_B T}$$

$$P_n = P_p e^{-q(\phi_b - V_a)/k_B T} \rightarrow \approx P_{p0}, \text{ since } \Delta P_p/P_{p0} \text{ is negligible (majority carrier)}$$

$$\Rightarrow P_n \approx P_{p0} e^{-q(\phi_b - V_a)/k_B T}$$

$$\Rightarrow P_n = P_{n0} e^{qV_a/k_B T}$$

$$\delta P(x_p) = \Delta P(x_{p0}) e^{-x_p/L_p}$$



$$\delta P(x_n) = \Delta P(x_{n0}) e^{-x_n/L_n}$$

This is also a kind of injection of carriers, much similar to the optical method.

$$\Delta P_n = P_{n0} (e^{qV_a/k_B T} - 1)$$

$$\Delta n_p = n_{p0} (e^{qV_a/k_B T} - 1)$$

$$I_p(x_n) = -qA D_p \frac{d}{dx_n} \delta P(x_n) = \frac{qA D_p}{L_p} \Delta P_n e^{-x_n/L_n} = \frac{qA D_p}{L_p} \delta P(x_n)$$

$$\text{Similarly, } I_n(x_p) = -qA D_n \frac{d}{dx_p} \delta n(x_p)$$

$$\Rightarrow I_p(x_n=0^+) - I_n(x_p=0^-) = I(0) = qA \left[\frac{D_p}{L_p} P_{n0} + \frac{D_n}{L_n} n_{p0} \right] (e^{qV_a/k_B T} - 1)$$

$$\Rightarrow I = I_0 (e^{qV_a/k_B T} - 1)$$

Junction capacitance, $C_j = \left| \frac{dQ}{dV_a} \right|$

(it's kinda AC capacitance)

$$Q = qAN_D x_{n0} = qAN_A |x_{p0}|$$

$$= qA \frac{N_A N_D}{N_A + N_D} (W) \rightarrow \text{dependent on } V_a$$

On solving,

$$\frac{1}{C_j^2} = \frac{4}{A^2} \frac{(\phi_b - V_a)}{2qE} \left[\frac{1}{N_D} + \frac{1}{N_A} \right]$$

MAGNETISM IN MATTER.

→ $\vec{B} = \mu_0 \vec{H}$ in A/m. [In free space, $\vec{M} = 0$]

\downarrow
in T

If $\vec{M} \neq 0$, $\vec{B} = \mu_0 (\vec{M} + \vec{H})$

If $\vec{M} = \chi \vec{H}$ (Linear medium)
↳ susceptibility

⇒ $\vec{B} = \mu_0 (1 + \chi) \vec{H} = \mu_0 \mu_r \vec{H}$
↳ rel. permeability.

χ → dimensionless

$\chi_g = \chi / \rho$ → density of material [m³/kg]

$\chi_m = \chi V_m$ [m³/mol]
↳ molar volume

→ $|\vec{L}| = \sqrt{l(l+1)} \hbar$

$|\vec{\mu}_L| = \hbar \gamma \sqrt{l(l+1)} = \mu_B \sqrt{l(l+1)}$

$\mu_L^z = -m_l \mu_B$, $\mu_s^z = -g m_s \mu_B$ → e- g-factor [2.0023]

$E_s = -\vec{\mu} \cdot \vec{B} = -\mu_z B = g \mu_B m_s B$

$E_L = \mu_B m_l B$

$\mu_B = \frac{e \hbar}{2m}$ [Bohr magneton]

→ Hamiltonian of an e- in presence of a magnetic field.

[B=0] $H_i = \frac{p_i^2}{2m} + V_i$

[B ≠ 0] $H_i = \frac{(p_i + |e| \hbar \vec{A})^2}{2m} + V_i + g \mu_B \vec{B} \cdot \vec{S}_i$
→ This is a stand-alone term, and is not a part of any other term in the Hamiltonian.

$H = \sum_{i=1}^Z H_i = \sum_i \left\{ \frac{(p_i + |e| \hbar \vec{A}(\vec{r}_i))^2}{2m} + V_i \right\} + \sum_i g \mu_B \vec{B} \cdot \vec{S}_i$

$S = \sum S_i$, $\hbar \vec{L} = \sum_{i=1}^Z (\vec{r}_i \times \vec{p}_i)$

Show that:

$H = \sum_{i=1}^Z \left(\frac{p_i^2}{2m} + V_i \right) + \mu_B (\vec{L} + g \vec{S}) \cdot \hat{B} + \frac{e^2}{8m} \sum_{i=1}^Z (\vec{B} \times \vec{r}_i)^2$

Paramagnetic term Diamagnetic term.

Given $\vec{B} = (0, 0, B)$ ⇒ $\hat{B} \times \vec{r}_i = (-y_i, x_i, 0)$
⇒ $(\hat{B} \times \vec{r}_i)^2 = (x_i^2 + y_i^2) B^2$

$$\begin{aligned} \Rightarrow H &= \sum_i H_i = \sum_i \left\{ \frac{(\vec{p}_i + e\vec{A}(\vec{r}_i))^2}{2m} + V_i \right\} + \sum_i g \mu_B \vec{B} \cdot \vec{S}_i \\ &= \sum_i \left(\frac{p_i^2}{2m} + V_i \right) + \sum_i \frac{e^2}{2m} A^2(\vec{r}_i) + \sum_i \frac{e}{m} \vec{p}_i \cdot \vec{A}(\vec{r}_i) \end{aligned}$$

$\vec{A} = -\frac{1}{2}(\vec{r} \times \vec{B})$ for a uniform magnetic field.

$$\Rightarrow H = \sum_i \left(\frac{p_i^2}{2m} + V_i \right) + \sum_i \frac{e^2}{2m} \frac{1}{4} (\vec{r} \times \vec{B})^2 + \sum_i g \mu_B \vec{B} \cdot \vec{S}_i + \sum_i \frac{2e}{m} \vec{p}_i \cdot \vec{A}(\vec{r}_i)$$

$$\vec{p} \cdot \vec{A}(\vec{r}) = \vec{p} \cdot \left(-\frac{1}{2}(\vec{r} \times \vec{B}) \right) = \frac{1}{2} \vec{B} \cdot (\vec{r} \times \vec{p})$$

$$\Rightarrow H = \sum_i \left(\frac{p_i^2}{2m} + V_i \right) + \frac{e^2}{8m} \sum_i (\vec{B} \times \vec{r}_i)^2 + \mu_B (\vec{L} + g\vec{S}) \cdot \vec{B}$$

$$\Rightarrow H = \sum_i \left(\frac{p_i^2}{2m} + V_i \right) + \frac{e^2}{8m} \sum_i B^2 (x_i^2 + y_i^2) + \mu_B (\vec{L} + g\vec{S}) \cdot \vec{B}$$

My quantum formalism is shit, so you're gonna have to manage with this.

Can we follow a perturbative approach for this problem?

For $B = 1\text{T}$, terms in $B \approx 10^{-4}\text{eV}$
 terms in $B^2 \approx 10^{-8}\text{eV}$. } These orders of magnitude justify considering energy perturbations.

$$\Delta E = \underbrace{\mu_B \langle n | \vec{B} \cdot (\vec{L} + g\vec{S}) | n \rangle}_{\text{Paramagnetic}} + \underbrace{\mu_B^2 \sum_i \frac{|\langle n | \vec{B} \cdot (\vec{L} + g\vec{S}) | n' \rangle|^2}{E_n - E_{n'}}}_{\text{Van-Vleck Paramagnetism}} + \underbrace{\frac{e^2 B^2}{8m} \langle n | \sum_i (x_i^2 + y_i^2) | n \rangle}_{\text{Diamagnetic}}$$

$\rightarrow \Delta E_D = \frac{e^2 B^2}{8m} \frac{2}{3} \langle n | \sum_i r_i^2 | n \rangle$ [Assuming a spherical system?]

$M = -n \frac{\partial F}{\partial B} \xrightarrow{\text{Helmholtz free energy}} \approx -n \frac{\partial U}{\partial B} = -n \frac{e^2 B}{6m} \sum_i \langle n | r_i^2 | n \rangle$

no. of atoms per unit volume, $(N/V \text{ ofc, as per book})$, $F = U - TS \xrightarrow{\text{can we neglect the entropy of the system while using } M = -n \frac{\partial F}{\partial B}}$

$\chi = \frac{\partial M}{\partial H} = \mu_0 \frac{\partial M}{\partial B} = -\frac{n e^2 \mu_0}{6m} \sum_i \langle r_i^2 \rangle$ susceptibility is -ve, which agrees with diamagnetic behavior.

Typical χ 's : Water, $\chi = -9.0 \times 10^{-6}$
 NaCl, $\chi = -7.2 \times 10^{-6}$
 Cu, $\chi = -1.1 \times 10^{-6}$

$\rightarrow \vec{L}, \vec{S} \Rightarrow$ We'd like to use $\vec{J} = \vec{L} + \vec{S}$ for the paramagnetic term instead.

$\left. \begin{matrix} \mu_B m_L B \\ g \mu_B m_S B \end{matrix} \right\} g_J \mu_B m_J B$ (where g_J has been chosen appropriately).
 \rightarrow total magnetic quantum number

Partition function, $Z = \sum_{m_J=-J}^{+J} e^{(m_J g_J \mu_B B / k_B T)}$

$$\alpha = \frac{g_J \mu_B B}{k_B T} \Rightarrow Z = \sum_{-J}^{+J} e^{m_J \alpha}$$

$$\Rightarrow \langle m_J \rangle = \frac{\sum_{m_J} m_J e^{m_J \alpha}}{Z}$$

$$= \frac{1}{Z} \frac{\partial Z}{\partial \alpha}$$

$$\Rightarrow M = n g_J \mu_B \langle m_J \rangle$$

$$= \frac{n g_J \mu_B}{Z} \frac{\partial Z}{\partial \alpha}$$

$$= \frac{n g_J \mu_B}{Z} \frac{\partial Z}{\partial B} \frac{\partial B}{\partial \alpha}$$

$$= n k_B T \frac{\partial (\ln Z)}{\partial B}$$

$$Z = a + ar + ar^2 + \dots + ar^{M-1}, \text{ where } a = e^{-J\alpha}, r = e^{\alpha}, M = 2J+1$$

$$\Rightarrow Z = \frac{a(1-r^M)}{1-r} = \frac{\sinh[(2J+1)\alpha/2]}{\sinh[\alpha/2]} \rightarrow \text{Verify!}$$

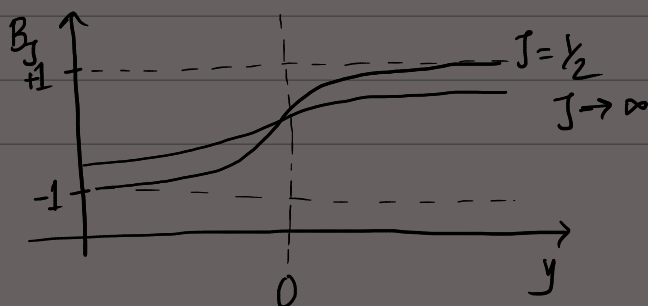
Substituting,

$$M = n g_J \mu_B J [B_J(y)], \quad [y = \alpha J]$$

$$\text{where } B_J(y) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J} y\right) - \frac{1}{2J} \coth\left(\frac{y}{2J}\right)$$



Brillouin function



Ex: $J = \frac{1}{2}$, $g_J = 2$, $B = 1T \rightarrow y \approx 2 \times 10^{-3}$ @ RT

Don't forget that this is quite a large number.

So, $B_J(y)$ for small y : $B_J(y) \approx \frac{(J+1)y}{3J} + O(y^3)$ -ve sign

Now, $M = n g_J \mu_B J [B_J(y)]$

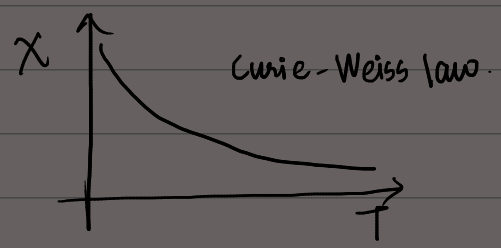
Don't forget all this analysis is for the case of paramagnets. Note that there is nothing here in these equations that suggest the strong interaction forces operating within a ferromagnet.

$$= n g_J \mu_B J \frac{(J+1)y}{3J}$$

$$= \frac{n g_J \mu_B J}{3k_B T} (J+1) g_J \mu_B B$$

$$= \frac{n \mu_{eff}^2 B}{3k_B T}, \text{ where } \mu_{eff} = g_J \mu_B \sqrt{J(J+1)}$$

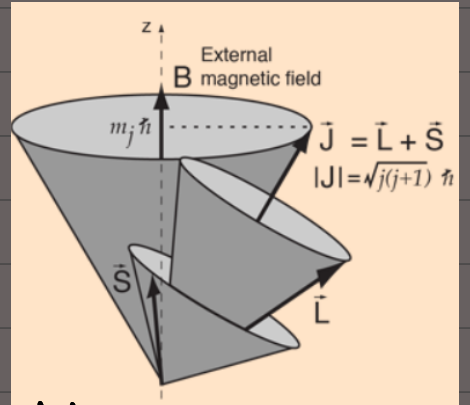
$\Rightarrow \chi = \frac{n \mu_{eff}^2 \mu_0}{3k_B T}$



→ How to determine g_J ?

$$\left. \begin{aligned} \Delta E_{spin} &= -g \mu_B m_s B \\ \Delta E_{orbital} &= -\mu_B m_L B \end{aligned} \right\} \Delta E = -g_J \mu_B m_J B$$

Now, $\Delta E = -\mu_B (\vec{L} + g\vec{S}) \cdot \vec{B}$ & $\vec{J} = \vec{L} + \vec{S}$



↳ by definition.

Well, the issue with this model is that \vec{L} & \vec{S} are indeterminate as far as their directions are concerned (since their z-components are known exactly). We can deal with this problem by considering the projections of vectors along \vec{J} (i.e. by considering \vec{J} as our reference axis).

$$\begin{aligned} \Rightarrow \Delta E &= \frac{e}{2m} (\vec{L} + g\vec{S}) \cdot \vec{J} \quad \left(\frac{\vec{B} \cdot \vec{J}}{J} \right) \\ &= \frac{e}{2m} \frac{(\vec{L} + g\vec{S}) \cdot (\vec{L} + \vec{S})}{J^2} J_z B \\ &= \frac{e}{2m} \frac{(L^2 + gS^2 + (g+1)\vec{L} \cdot \vec{S})}{J^2} m_J \hbar B \end{aligned}$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$\Rightarrow J^2 = L^2 + S^2 + 2\vec{L} \cdot \vec{S}$$

$$\Rightarrow \vec{L} \cdot \vec{S} = \frac{1}{2} (J^2 - L^2 - S^2)$$

Substituting in the previous result,

$$\Rightarrow \Delta E = \mu_B \frac{(L^2 + gS^2 + (g+1) \frac{1}{2} (J^2 - L^2 - S^2))}{J^2} m_J B$$

$$= \left(\frac{g+1}{2} + \frac{g-1}{2} \frac{S^2 - L^2}{J^2} \right) m_J \mu_B B$$

$$\Rightarrow \Delta E = \left(\frac{g+1}{2} + \frac{g-1}{2} \frac{S(S+1) - L(L+1)}{J(J+1)} \right) m_J \mu_B B$$

For $g \approx 2$,

$$\Rightarrow \Delta E = \left(\frac{3}{2} + \frac{1}{2} \frac{S(S+1) - L(L+1)}{J(J+1)} \right) m_J \mu_B B$$

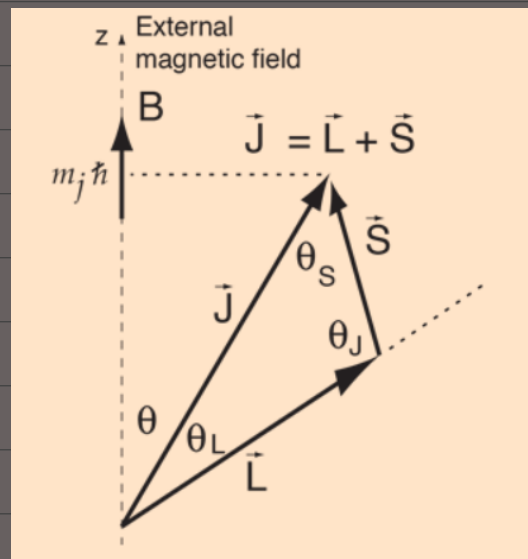
$\hookrightarrow g_J$ (Landé g-factor)

Term symbol: $^{2S+1}L_J \rightarrow$ for S, L, J

$$n \leq 2L+1, \quad n > 2L+1,$$

$$J = |L-S|, \quad J = |L+S|$$

\hookrightarrow is denoted by alphabets, check out with the reference.



→ Consider the interaction energy b/w two dipoles -

$$E = \frac{\mu_0}{4\pi} \left[\vec{\mu}_1 \cdot \vec{\mu}_2 - \frac{3}{r^3} (\vec{\mu}_1 \cdot \vec{r})(\vec{\mu}_2 \cdot \vec{r}) \right]$$

A back of the envelope estimation with $\mu_1 = \mu_2 = \mu_B$ & $r \approx 1 \text{ \AA}$ reveals that interaction energy is of the order 10^{-23} J , equivalent to 1 K in the Boltzmann scale. However, the ferromagnetic ordering of solids is broken only at high temperatures, upto $700\text{--}800 \text{ K}$. So, something much more stronger than mere electrostatic interaction is at play here. Turns out that this force is not of magnetic origin at all, but is rather a quantum mechanical phenomena.

Owing to time constraints, I shall omit the calculations leading to the derivation of the exchange energy term in a hydrogen molecule (this has been amply covered in the notes uploaded in the course drive & in Blundell too). Anyways, the final Hamiltonian for the hydrogen molecule is given by -

$$\hat{H} = \frac{(E_S + 3E_T)}{4} - \frac{(E_S - E_T)}{2} (2\vec{S}_1 \cdot \vec{S}_2) \quad \left[\vec{S}_1 \cdot \vec{S}_2 = S(S+1) - \frac{3}{2} \right]$$

↗ exchange constant.

or

$$\hat{H} = K - J \left(\frac{1}{2} + 2\vec{S}_1 \cdot \vec{S}_2 \right), \quad \text{s.t. } E_S = K + J, \quad E_T = K - J$$

Ultimately, the perturbation in the Hamiltonian of the system due to exchange interaction is given by -

$$\hat{H}_{\text{spin}} = -2J(\vec{S}_1 \cdot \vec{S}_2)$$

If $J > 0$, the triplet state is favoured and if $J < 0$, the singlet state is preferred.

Now, we shall generalize the result to a many-body system, which forms the foundation for the Heisenberg model.

$$\hat{H} = -\sum_{i,j} J_{ij} (\vec{S}_i \cdot \vec{S}_j) + g\mu_B \sum_i \vec{S}_i \cdot \vec{B}$$

↳ 2 has been omitted since we're double-counting

→ The Heisenberg Ferromagnet.

Consider a set of magnetic ions located at Bravais lattice sites, \vec{R} , and described by the Heisenberg Hamiltonian -

Considering this factor is pretty much dependent on the author. For our analyses, we have dropped the $\frac{1}{2}$ factor henceforth.

$$\hat{H} = -\frac{1}{2} \sum_{\vec{R}, \vec{R}'} S(\vec{R}) \cdot S(\vec{R}') J(\vec{R}-\vec{R}') - g\mu_B \sum_{\vec{R}} S_z(\vec{R})$$

$$J(\vec{R}-\vec{R}') = J(\vec{R}'-\vec{R}) \geq 0.$$

The ground state for this system is when all the spins S_n are parallel to the magnetic field and to each other. We shall show that such a state is indeed an eigenvector of the given Hamiltonian. (namely, their z-components)

$$|0\rangle = \prod_{\vec{R}} |S\rangle_{\vec{R}}, \text{ where } S_z(\vec{R}) |S\rangle_{\vec{R}} = S |S\rangle_{\vec{R}}$$

Now consider the ladder operator corresponding to the spin of the particle -

$$S_{\pm}(\vec{R}) = S_x(\vec{R}) \pm i S_y(\vec{R})$$

which have the property -

$$S_{\pm}(\vec{R}) |S_z\rangle_{\vec{R}} = \sqrt{(S \mp S_z)(S \pm S_z + 1)} |S_z \pm 1\rangle_{\vec{R}}$$

$$\text{Now, } S_x = \frac{1}{2}(S_+ + S_-), \quad S_y = \frac{1}{2i}(S_+ - S_-)$$

$$\Rightarrow S(\vec{R}) \cdot S(\vec{R}') = S_x(\vec{R}) S_x(\vec{R}') + S_y(\vec{R}) S_y(\vec{R}') + S_z(\vec{R}) S_z(\vec{R}')$$

$$= \frac{1}{4} (S_+(\vec{R}) + S_-(\vec{R})) (S_+(\vec{R}') + S_-(\vec{R}')) - \frac{1}{4} (S_+(\vec{R}) - S_-(\vec{R})) (S_+(\vec{R}') - S_-(\vec{R}')) + S_z(\vec{R}) S_z(\vec{R}')$$

$$= \frac{1}{2} (S_+(\vec{R}) S_-(\vec{R}') + S_-(\vec{R}) S_+(\vec{R}')) + S_z(\vec{R}) S_z(\vec{R}')$$

Substituting in the Hamiltonian, we get -

$$H = - \sum_{R, R'} \left[\frac{1}{2} \{ S_+(\vec{R}') S_-(\vec{R}) + S_-(\vec{R}') S_+(\vec{R}) \} + S_z(\vec{R}') S_z(\vec{R}) \right] J(\vec{R} - \vec{R}') - g \mu_B B \sum_R S_z(\vec{R})$$

→ Apply this, and observe that the product of the eigenvalues turns out to be zero. In general, this term can be dropped.

$$\Rightarrow H = - \sum_{R, R'} \left[\frac{1}{2} S_-(\vec{R}') S_+(\vec{R}) + S_z(\vec{R}') S_z(\vec{R}) \right] J(\vec{R} - \vec{R}') - g \mu_B B \sum_R S_z(\vec{R})$$

→ observe that $S_+(\vec{R}') |S_z\rangle_{R'} = 0$.

$$\Rightarrow H |0\rangle = \left[- \sum_{R, R'} S_z(\vec{R}') S_z(\vec{R}) J(\vec{R} - \vec{R}') - g \mu_B B \sum_R S_z(\vec{R}) \right] |0\rangle$$

$$= \left[-S^2 \sum_{R, R'} J(\vec{R} - \vec{R}') - N g \mu_B B S \right] |0\rangle$$

→ The corresponding eigenvalue.

Note that the Hamiltonian we were dealing with is the result of a "perturbation", so this eigenvalue now represents the decrease in ground state energy of the system due to exchange interaction (i.e. assuming $J(\vec{R} - \vec{R}') \geq 0$ of $<$).

$$E_0 = -S^2 \sum_{R, R'} J(\vec{R} - \vec{R}') - N g \mu_B B S$$

At zero temperature, the ferromagnet is in its ground state, and the magnetization density is given by $M = g \mu_B \frac{N}{V} S$. At low temperatures, we can expect contribution from some low-lying excited states too, the

simplest of these being the case when only one of the e 's in the lattice has spin down, while all others are spin up.

$$|R\rangle = \frac{1}{\sqrt{25}} S_-(\vec{R}) |0\rangle$$

spin down at \vec{R}
↑ position.

Something interesting happens when $S_-(\vec{R}) S_+(\vec{R}')$ operates on $|R\rangle$.

$$\begin{aligned} S_-(\vec{R}') S_+(\vec{R}) |R\rangle &= S_-(\vec{R}') \sqrt{25} |s\rangle_R (\dots) \\ &= 25 |s-1\rangle_{R'} (\dots) \\ &= 25 |R'\rangle \end{aligned}$$

The operator simply swaps the spin down location from \vec{R} to \vec{R}' !

Does this have any physical significance, or is it just a mere mathematical construct? Because, energetically, the system is identical after all...

$$S_z(\vec{R}') |R\rangle \begin{cases} S |R\rangle, & \vec{R}' \neq \vec{R} \\ (S-1) |R\rangle, & \vec{R}' = \vec{R} \end{cases}$$

$$H = -\sum_{R,R'} \left[\frac{1}{2} S_-(\vec{R}') S_+(\vec{R}) + S_z(\vec{R}') S_z(\vec{R}) \right] J(\vec{R}-\vec{R}') - g\mu_B B \sum_R S_z(\vec{R})$$

$$\Rightarrow H |R\rangle = E_0 |R\rangle + g\mu_B B |R\rangle + 5 \sum_{R'} J(\vec{R}-\vec{R}') (|R\rangle - |R'\rangle)$$

↳ ground state energy

As can be seen, $|R\rangle$ is not an eigenstate for the Hamiltonian. One can instead create appropriate L-C's of $|R\rangle$ to form eigenstates for H .

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_R e^{i\vec{k}\cdot\vec{R}} |R\rangle$$

Using result of previous analysis,

$$E_k = E_0 + g\mu_B B + 5 \sum_R J(\vec{R}) (1 - e^{i\vec{k}\cdot\vec{R}})$$

Use $J(-\vec{R}) = J(\vec{R})$
to obtain -

$$E_k - E_0 = 25 \sum_R J(\vec{R}) \sin^2\left(\frac{1}{2}\vec{k}\cdot\vec{R}\right) + g\mu_B B$$

Just a flesh wound!

$$H = - \sum_{R,R'} \left[\frac{1}{2} S_-(\vec{R}') S_+(\vec{R}) + S_z(\vec{R}') S_z(\vec{R}) \right] J(\vec{R}-\vec{R}') - g \mu_B B \sum_R S_z(\vec{R})$$

$$H|R\rangle = ?$$

$$-g \mu_B B \sum_R S_z(\vec{R}) \Rightarrow -g \mu_B B (NS - 1) |R\rangle$$

$$- \sum_{R,R'} \frac{1}{2} S_-(\vec{R}') S_+(\vec{R}) J(\vec{R}-\vec{R}') \Rightarrow -S \sum_{R'} J(\vec{R}-\vec{R}') |R\rangle$$

$$- \sum_{R,R'} S_z(\vec{R}') S_z(\vec{R}) J(\vec{R}-\vec{R}') \Rightarrow -S^2 \sum_{R,R'} J(\vec{R}-\vec{R}') |R\rangle + S \sum_{R'} J(\vec{R}-\vec{R}') |R\rangle$$

$$\Rightarrow H|R\rangle = E_0 |R\rangle + g \mu_B B |R\rangle + S \sum_{R'} J(\vec{R}-\vec{R}') (|R\rangle - |R'\rangle)$$

To give a physical interpretation of the state $|k\rangle$ we note the following:

1. Since $|k\rangle$ is a superposition of states in each of which the total spin is diminished from its saturation value NS by one unit, the total spin in the state $|k\rangle$ itself has the value $NS - 1$.
2. The probability of the lowered spin being found at a particular site R in the state $|k\rangle$ is $|\langle k|R\rangle|^2 = 1/N$; i.e., the lowered spin is distributed with equal probability among all the magnetic ions.
3. We define the transverse spin correlation function in the state $|k\rangle$ to be the expectation value of

$$\mathbf{S}_1(\mathbf{R}) \cdot \mathbf{S}_1(\mathbf{R}') = S_x(\mathbf{R})S_x(\mathbf{R}') + S_y(\mathbf{R})S_y(\mathbf{R}'). \quad (33.26)$$

A straightforward evaluation (Problem 4) gives

$$\langle k | \mathbf{S}_1(\mathbf{R}) \cdot \mathbf{S}_1(\mathbf{R}') | k \rangle = \frac{2S}{N} \cos [\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')], \quad \mathbf{R} \neq \mathbf{R}'. \quad (33.27)$$

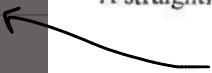
$$S_x = \frac{1}{2}(S_+ + S_-), \quad S_y = \frac{1}{2i}(S_+ - S_-)$$

$$S_x(\vec{R}) S_x(\vec{R}') + S_y(\vec{R}) S_y(\vec{R}') = \frac{1}{4} (S_+(\vec{R}) + S_-(\vec{R})) (S_+(\vec{R}') + S_-(\vec{R}')) - \frac{1}{4} (S_+(\vec{R}) - S_-(\vec{R})) (S_+(\vec{R}') - S_-(\vec{R}'))$$

$$= \frac{1}{2} S_+(\vec{R}) S_-(\vec{R}') + \frac{1}{2} S_-(\vec{R}) S_+(\vec{R}')$$

$$= \left(\frac{1}{2} S_+(\vec{R}') S_-(\vec{R}) \right) + \frac{1}{2} S_-(\vec{R}') S_+(\vec{R})$$

Next, we shall try to prove this result:



$$\langle k | S_{\perp}(\vec{R}) S_{\perp}(\vec{R}') | k \rangle = \langle k | \frac{1}{2} S_{-}(\vec{R}') S_{+}(\vec{R}) | k \rangle$$

$$S_{-}(\vec{R}) S_{+}(\vec{R}') \left(\frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} |R\rangle \right) =$$

$$\langle k | = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{k} \cdot \vec{R}} \langle R | \quad | k \rangle = \frac{1}{\sqrt{N}} \left(\dots + e^{i\vec{k} \cdot \vec{R}} |R'\rangle + e^{i\vec{k} \cdot \vec{R}'} |R\rangle \right)$$

$$e^{i\vec{k} \cdot (\vec{R} - \vec{R}')}$$

Thus on the average each spin has a small transverse component, perpendicular to the direction of magnetization, of size $(2S/N)^{1/2}$; the orientations of the transverse components of two spins separated by $\vec{R} - \vec{R}'$ differ by an angle $\vec{k} \cdot (\vec{R} - \vec{R}')$.

The microscopic magnetization in the state $|k\rangle$ suggested by these facts is pictured in Figure 33.7. One describes the state $|k\rangle$ as a state containing a spin wave (or "magnon") of wave vector \vec{k} and energy $\mathcal{E}(\vec{k})$ (Eq. (33.25)).

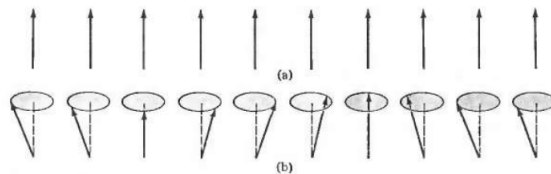


Figure 33.7
Schematic representations of the orientations in a row of spins in (a) the ferromagnetic ground state and (b) a spin wave state.

5.1 Ferromagnetism

A ferromagnet has a spontaneous magnetization even in the absence of an applied field. All the magnetic moments lie along a single unique direction.¹ This effect is generally due to exchange interactions which were described in the previous chapter. For a ferromagnet in an applied magnetic field \mathbf{B} , the appropriate Hamiltonian to solve is

$$\hat{\mathcal{H}} = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + g\mu_B \sum_j \mathbf{S}_j \cdot \mathbf{B}, \quad (5.1)$$

and the exchange constants for nearest neighbours will be positive in this case, to ensure ferromagnetic alignment. The first term on the right is the Heisenberg exchange energy (see eqn 4.7). The second term on the right is the Zeeman energy (see eqn 1.35). To keep things simple to begin with, let us assume² that we are dealing with a system in which there is no orbital angular momentum, so that $L = 0$ and $J = S$.

5.1.1 The Weiss model of a ferromagnet

To make progress with solving eqn 5.1 it is necessary to make an approximation. We define an effective molecular field at the i^{th} site by

$$\mathbf{B}_{\text{mf}} = - \frac{2}{g\mu_B} \sum_j J_{ij} \mathbf{S}_j. \quad (5.2)$$

being present. Notice that the alignment of these magnetic moments gives rise to the internal molecular field that causes the alignment in the first place, so that this is something of a 'chicken-and-egg' scenario. At low temperature the magnetic order is self-sustaining. As the temperature is raised, thermal fluctuations begin to progressively destroy the magnetization and at a critical temperature the order will be destroyed. This model is known as the Weiss model of ferromagnetism.

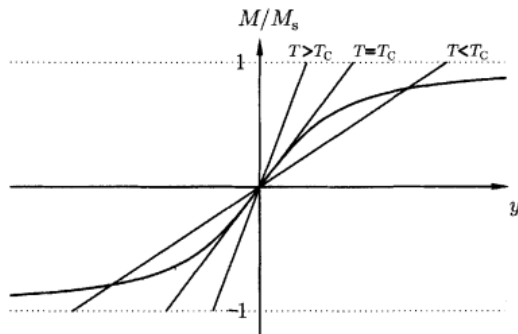
To find solutions to this model, it is necessary to solve simultaneously the equations

$$\frac{M}{M_s} = B_J(y) \quad (5.6)$$

(see eqn 2.38) and

$$y = \frac{gJ\mu_B J(B + \lambda M)}{k_B T} \quad (5.7)$$

(see eqn 2.37). Without the λM term due to the molecular field, this would be identical to our treatment of a paramagnet in Section 2.4.3.



These equations can be solved graphically. First, we restrict our attention to the case of $B = 0$, so that $M = k_B T y / gJ\mu_B J\lambda$. Hence the straight line produced by plotting M against y has a gradient which is proportional to temperature T as illustrated in Fig. 5.2. For high temperature, there is no simultaneous solution of eqns 5.6 and 5.7 except at the origin where $y = 0$ and $M_s = 0$. This situation changes when the gradient of the line is less than that of the Brillouin function at the origin. At low temperatures there are then three solutions, one at $M_s = 0$ and another two for M_s at \pm some non-zero value. It turns out that when the curve is less steep than the Brillouin function at the origin, the non-zero solutions are stable and the zero-solution is unstable. (If the system has $M_s = 0$ for $T < T_C$, any fluctuation, no matter how small, will cause the system to turn into either one of the two stable states.) Thus below a certain temperature, non-zero magnetization occurs and this grows as the material is cooled. The substance thus becomes magnetized, even in the absence of an external field. This spontaneous magnetization is the characteristic of ferromagnetism.

The temperature at which the transition occurs can be obtained by finding when the gradients of the line $M = k_B T y / gJ\mu_B J\lambda M_s$ and the curve $M = M_s B_J(y)$ are equal at the origin. For small y , $B_J(y) = (J + 1)y / 3J + O(y^3)$.

Now focus on the i^{th} spin. Its energy is due to a Zeeman part $g\mu_B \mathbf{S}_i \cdot \mathbf{B}$ and an exchange part. The total exchange interaction between the i^{th} spin and its neighbours is $-2 \sum_j J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, where the factor of 2 is because of the double counting.³ This term can be written as

$$-2S_i \cdot \sum_j J_{ij} \mathbf{S}_j = -g\mu_B \mathbf{S}_i \cdot \mathbf{B}_{\text{mf}}. \quad (5.3)$$

Hence the exchange interaction is replaced by an effective molecular field \mathbf{B}_{mf} produced by the neighbouring spins. The effective Hamiltonian can now be written as

$$\hat{\mathcal{H}} = g\mu_B \sum_i \mathbf{S}_i \cdot (\mathbf{B} + \mathbf{B}_{\text{mf}}) \quad (5.4)$$

which now looks like the Hamiltonian for a paramagnet in a magnetic field $\mathbf{B} + \mathbf{B}_{\text{mf}}$. The assumption underpinning this approach is that all magnetic ions experience the same molecular field. This may be rather questionable, particularly at temperatures close to a magnetic phase transition, as will be discussed in the following chapter. For a ferromagnet the molecular field will act so as to align neighbouring magnetic moments. This is because the dominant exchange interactions are positive. (For an antiferromagnet, they will be negative.)

Since the molecular field measures the effect of the ordering of the system, one can assume that

$$\mathbf{B}_{\text{mf}} = \lambda \mathbf{M} \quad (5.5)$$

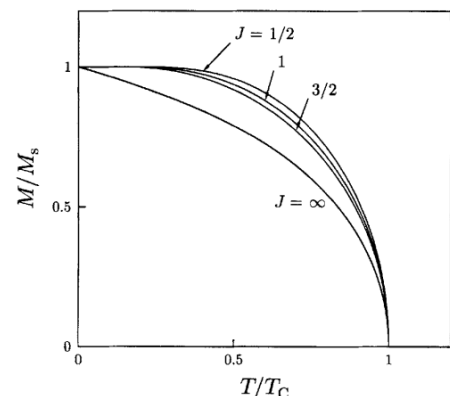
where λ is a constant which parametrizes the strength of the molecular field as a function of the magnetization. For a ferromagnet, $\lambda > 0$. Because of the large Coulomb energy involved in the exchange interaction, the molecular field is often found to be extremely large in ferromagnets.

We are now able to treat this problem as if the system were a simple paramagnet placed in a magnetic field $\mathbf{B} + \mathbf{B}_{\text{mf}}$. At low temperature, the moments can be aligned by the internal molecular field, even without any applied field

The transition temperature, known as the Curie temperature T_C , is then defined by

$$T_C = \frac{gJ\mu_B(J+1)\lambda M_s}{3k_B} = \frac{n\lambda\mu_{\text{eff}}^2}{3k_B}. \quad (5.8)$$

The molecular field $B_{\text{mf}} = \lambda M_s$ is thus $3k_B T_C / gJ\mu_B(J+1)$ and so for a ferromagnet with $J = \frac{1}{2}$ and $T_C \sim 10^3$ K, $B_{\text{mf}} = k_B T_C / \mu_B \sim 1500$ T. This is an enormous effective magnetic field and reflects the strength of the exchange interaction.



5.1.2 Magnetic susceptibility

Applying a small B field at $T \geq T_C$ will lead to a small magnetization, so that the $y \ll 1$ approximation for the Brillouin function can be used. Thus

$$\frac{M}{M_s} \approx \frac{gJ\mu_B(J+1)}{3k_B} \left(\frac{B + \lambda M}{T} \right) \quad (5.9)$$

so that

$$\frac{M}{M_s} \approx \frac{T_C}{\lambda M_s} \left(\frac{B + \lambda M}{T} \right). \quad (5.10)$$

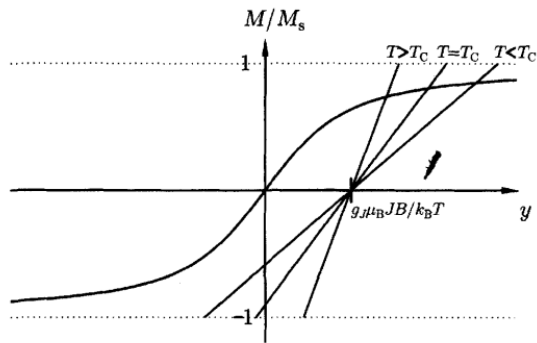
This can be rearranged to give

$$\frac{M}{M_s} \left(1 - \frac{T_C}{T} \right) \approx \frac{T_C B}{\lambda M_s} \quad (5.11)$$

so that

$$\chi = \lim_{B \rightarrow 0} \frac{\mu_0 M}{B} \propto \frac{1}{T - T_C} \quad (5.12)$$

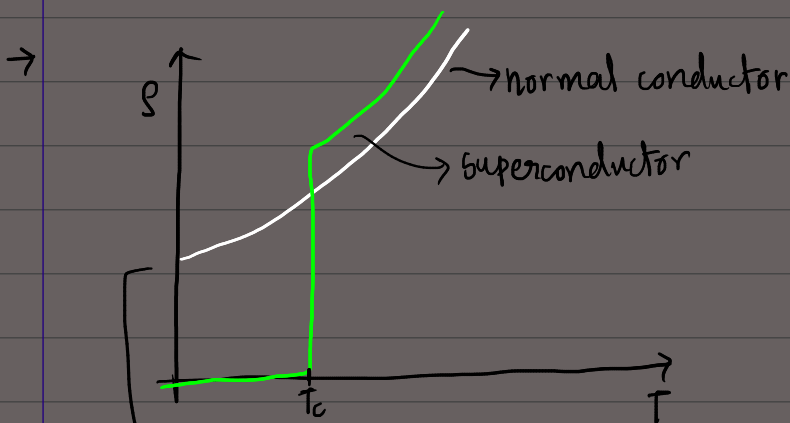
which is known as the Curie Weiss law.



SUPERCONDUCTIVITY

→ Resistance goes to zero as temp. decreases, and magnetic field is expelled from the material. This is what distinguishes a superconductor from say, a theoretically ultra-pure conductor at $T=0K$.

→ When a material goes from being a normal insulator/conductor to being a superconductor, it essentially undergoes a phase transition. Consequently there is an 'order parameter' associated with the superconductive state.



→ This finite resistivity is due to impurities in the lattice, and will go to zero as the material approaches a perfect conductor-kind state. There, however is a diff. b/w a perfect conductor & a superconductor.

Setup for measurement:

$$\vec{B} < \vec{B}_c$$

$$T < T_c \downarrow$$



$$\vec{B} = \mu_0 \vec{H}$$

$$V = -\frac{d\phi}{dt} = L \frac{dI}{dt} + IR = 0$$

$$\Rightarrow I = I_0 e^{-\frac{t}{RL}}$$

$R \rightarrow 0, I \rightarrow$ flattens out.

Decrease the temp. & magnetic field to a point s.t. $\vec{B} < \vec{B}_c$ & $T < T_c$, and switch off the magnetic field. A current is induced in the coil, which would persist for a supposedly 'infinite' period of time if the material is superconductive now.

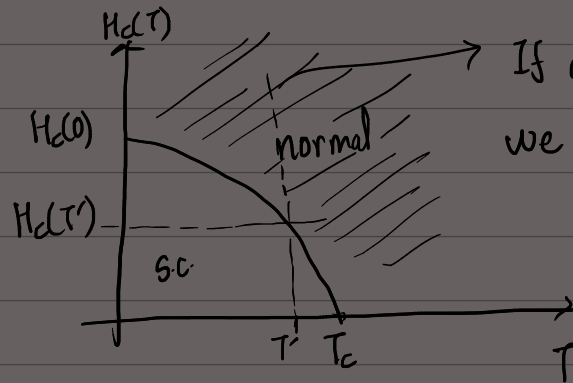
(SQUID magnetometer)

Hg $T_c = 4.2\text{K}$

Pb $T_c = 7\text{K}$

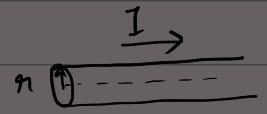
NbN $T_c \leq 16\text{K}$

$$H_c(T) = H_c(0) \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$



If at $T=T'$, applied field $> H_c(T')$, we won't observe superconductivity.

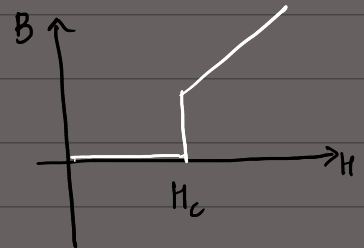
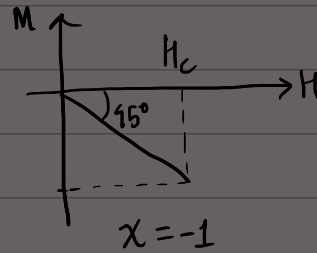
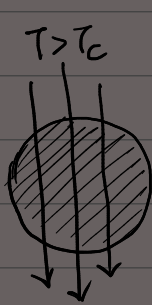
$$I_c = I_0 \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$



$$B = \frac{\mu_0 I}{2\pi r}$$

$$B \leq B_c \Rightarrow I_c \leq 2\pi r H_c$$

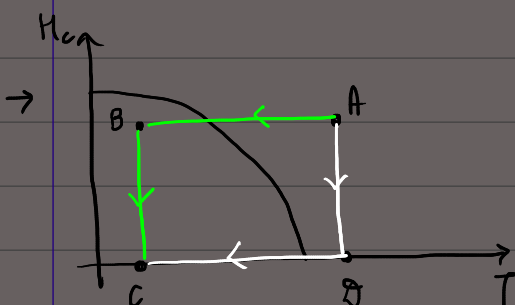
→



The superconductor does not completely expel the magnetic field from its bulk, rather the magnetic field penetrates to a very small, yet finite depth inside the material (known as London penetration depth).



Meissner-Ochsenfeld effect.



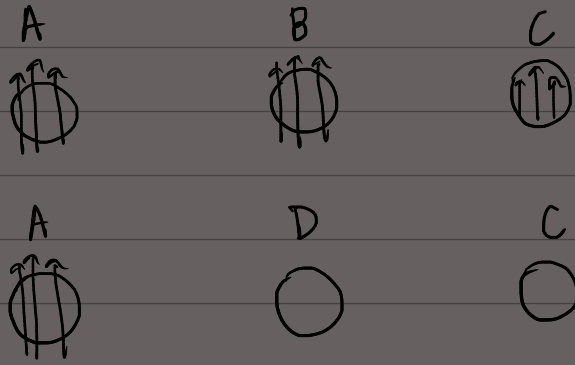
$$\vec{J} = \sigma \vec{E}$$

For a perfect conductor, $\sigma \rightarrow \infty$ & for finite \vec{J} ,

$$\vec{E} = 0.$$

$$\text{Now, } \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \Rightarrow \frac{\partial \vec{B}}{\partial t} = 0$$

$\Rightarrow \vec{B}$ is constant, but not necessarily zero.

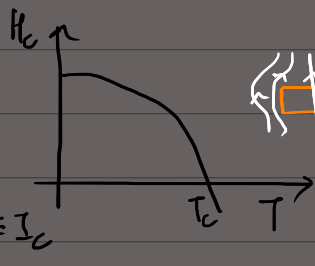


(A contradiction for a perfect conductor (C state not the same). In a superconductor, $\vec{B} = 0$ at B point.)

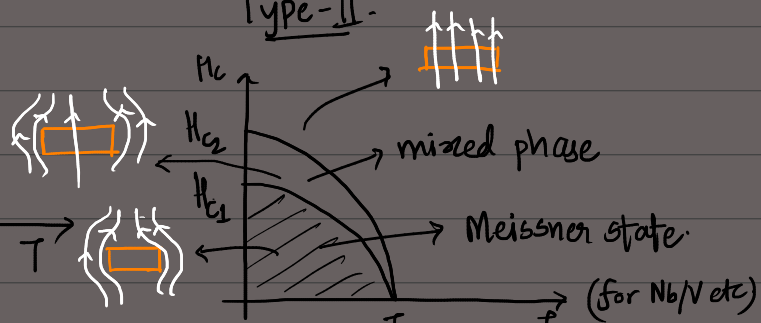
→

Type-I

$\rho = 0$
 $\vec{B} = 0$
 $\forall T \leq T_c, H \leq H_c, I \leq I_c$
 (except Nb/V)

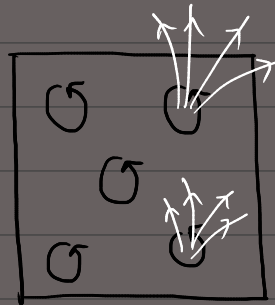


Type-II



(In the Meissner state, it's a regular s.c. with the properties same as type-I).

In the mixed phase, magnetic flux starts penetrating the material due to formation of 'vortices'.



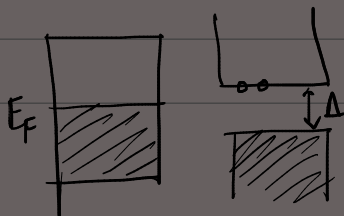
So, the vortices are points where essentially the material starts to revert back to its normal state.

Each vortex encloses a flux quantum,

$$\phi_0 = \frac{h}{2e} = 2.07 \times 10^{-15} \text{ T}\cdot\text{m}^2$$

	B_{c2}	T_c
Nb ₃ Ge	38 T	23 K
Nb ₃ Sn	21.3 T	18 K
V ₃ Si	23.5 T	16.9 K

The vortices can form a lattice (if they are not pinned down by impurities) & have also been imaged as such!



$$2\Delta(T=0) = 3.52 k_B T_c$$

- Isotope effect. (First indication that phonons are involved in superconductive phenomena).
 $T_c \propto M^{-\beta}$
 $\beta = 0.5$ usually.



→ LONDON THEORY (Two-fluid model).

$$n = n_s + n_n \rightarrow \text{normal } e\text{'s}$$

↳ superconductive $e\text{'s}$

$$\vec{j}_n = \frac{n_n e^2 \tau}{m} \vec{E} = \sigma_n \vec{E}$$

$$\vec{j}_s = -n_s e v_s \Rightarrow \frac{d\vec{j}_s}{dt} = -n_s e \frac{dv_s}{dt} = -n_s e \left(\frac{-e\vec{E}}{m} \right) = \frac{n_s e^2}{m} \vec{E}$$

(No scattering during superconductivity, i.e. $\tau \rightarrow \infty$)

$$\text{let } \frac{1}{\lambda_L} = \frac{n_s e^2}{m}$$

$$\frac{d}{dt} (\vec{\nabla} \times \vec{j}_s) = \lambda_L^{-1} (\vec{\nabla} \times \vec{E}) = -\lambda_L^{-1} \left(\frac{\partial \vec{B}}{\partial t} \right)$$

$$\Rightarrow \frac{d}{dt} (\lambda_L \vec{\nabla} \times \vec{j}_s + \vec{B}) = 0$$

$$\Rightarrow \lambda_L (\vec{\nabla} \times \vec{j}_s) = -\vec{B} + C(\vec{\pi})$$

Now, $C(\vec{r})$ need not necessarily be zero, and there is no physical argument which can justify otherwise. However, London theory "forced" $C(\vec{r})$ to be zero (the justification for this will be provided later).

WTF? $\vec{J}_s = 0$, $C(\vec{r}) = 0$.

$$\Rightarrow \vec{E} = \lambda_L \frac{d\vec{J}_s}{dt} \quad (\text{1st London eqn}),$$

$$\vec{\nabla} \times \vec{J}_s = -\frac{\vec{B}}{\lambda_L} \quad (\text{2nd London eqn})$$

Now, $\vec{\nabla} \times \vec{B} = \mu_0 \vec{J}_s$

(Why not consider $\vec{J}_{\text{tot}} = \vec{J}_s + \vec{J}_n$ here?)

$$\Rightarrow \vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = \mu_0 (\vec{\nabla} \times \vec{J}_s)$$

$$\Rightarrow \vec{\nabla} (\vec{\nabla} \cdot \vec{B}) - \nabla^2 \vec{B} = -\frac{\mu_0}{\lambda_L} \vec{B}$$

$$\Rightarrow \boxed{\nabla^2 \vec{B} - \frac{\mu_0}{\lambda_L} \vec{B} = 0}$$

|||, it can be shown that -

$$\boxed{\nabla^2 \vec{J}_s - \frac{\mu_0}{\lambda_L} \vec{J}_s = 0}$$

$$-\nabla^2 \vec{B} = \mu_0 (\underbrace{\vec{\nabla} \times \vec{J}_s}_{-\vec{B}/\lambda_L} + \underbrace{\vec{\nabla} \times \vec{J}_n}_{\vec{\nabla} \times (\epsilon_0 \vec{E})})$$

$$\vec{\nabla} \times \vec{E} = -\partial \vec{B} / \partial t$$

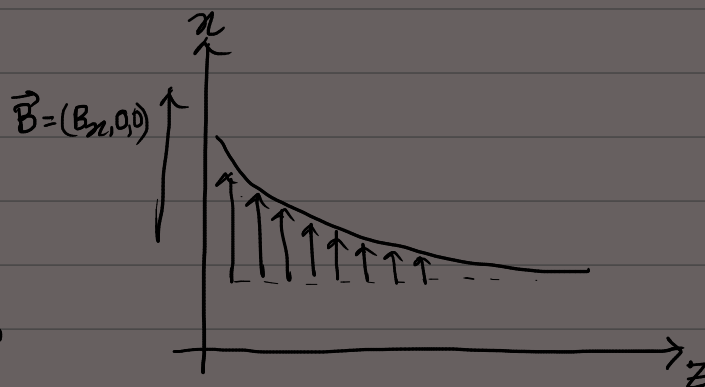
$$\nabla^2 \vec{B} - \frac{\mu_0}{\lambda_L} \vec{B} - \frac{\partial \vec{B}}{\partial t} = 0$$

can this be set to 0?

$$\vec{B} = (B_x, 0, 0)$$

$$\frac{\partial^2 B_x}{\partial x^2} - \frac{\mu_0}{\lambda_L} B_x = 0$$

$$\Rightarrow B_x = B_{x0} e^{-z/\lambda_L}$$



$$\lambda_L = \sqrt{\frac{m}{\mu_0 n_s e^2}}$$

London penetration depth.

Reason for dropping $c(\vec{\pi})$: "Rigidity of the superconducting state"

$$\vec{\nabla} \times \vec{j}_s = -\frac{\vec{B}}{\lambda_L} = -\frac{\nabla \times \vec{A}}{\lambda_L} \Rightarrow \vec{j}_s = -\frac{\vec{A}}{\lambda_L}$$

$$\vec{\nabla} \cdot \vec{A} = 0 \quad [\text{London gauge}]$$

$$\Rightarrow \vec{\nabla} \cdot \vec{j}_s = 0.$$

The question, basically, is that can I still claim that in the presence of a magnetic field, expectation value of the perturbed momentum is still zero?

$$\langle \psi | \hat{P} | \psi \rangle = 0 \quad (\text{for a system at ground state})$$

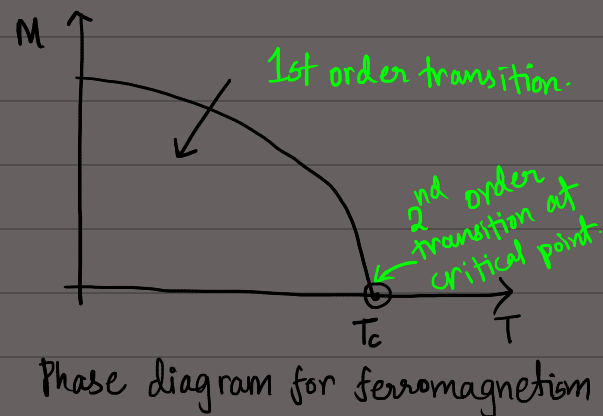
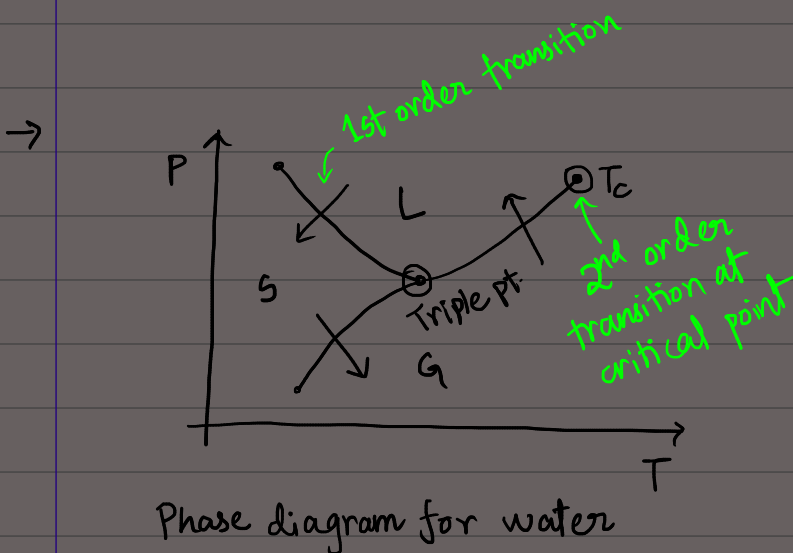
$$\langle \psi | \hat{P} - e\vec{A} | \psi \rangle = 0$$

$$\langle \psi | \vec{v} - \frac{e\vec{A}}{m} | \psi \rangle = 0$$

$$\Rightarrow \langle \vec{v} \rangle = \frac{e\langle \vec{A} \rangle}{m}$$

$$\vec{j}_s = -ne\langle \vec{v} \rangle = -\frac{ne^2\langle \vec{A} \rangle}{m} \frac{1}{\lambda_L}$$

$$\langle \vec{A} \rangle = \int \psi^* \vec{A} \psi d^3\vec{r}$$



$$dG = -S dT + V dP + \mu dN$$

$$G = U - TS + PV$$

$$\begin{aligned}
 dG &= dU - T dS - S dT + P dV + V dP \\
 &= \{T dS - P dV + \mu dN\} - T dS - S dT + P dV + V dP \\
 &= -S dT + V dP + \mu dN
 \end{aligned}$$

Assuming no change in number of particles, ($dN=0$)

$$dG = -S dT + V dP$$

$$S = -\left(\frac{\partial G}{\partial T}\right)_{P,N}, \quad V = \left(\frac{\partial G}{\partial P}\right)_{T,N}$$

1st order transition: G is continuous, 1st deriv. of G is disconti.

2nd order transition: G is continuous, 1st derivative of G is also continuous, but the 2nd derivative is discontinuous.

$$C_P = -T \frac{\partial^2 G}{\partial T^2}$$

For magnetic materials,

$$U = (S, \vec{M})$$

$$T = \frac{\partial U}{\partial S}, \quad \vec{H} = \frac{1}{\mu_0 V} \frac{\partial U}{\partial \vec{M}}$$

$$G(T, \vec{H}) = U - TS - \mu_0 V \vec{H} \cdot \vec{M}$$

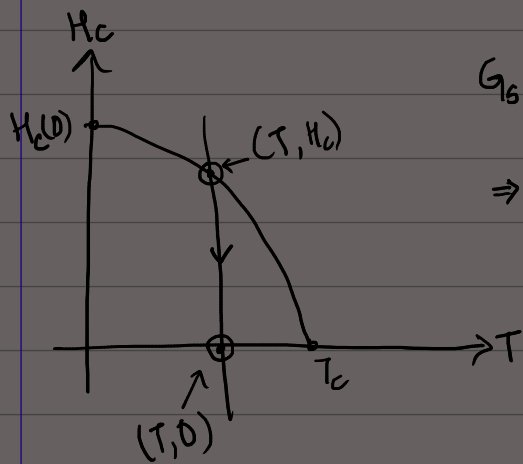
$$\Rightarrow dG = -S dT - \mu_0 V \vec{M} \cdot d\vec{H}$$

$$S = -\frac{\partial G}{\partial T}, \quad \vec{M} = -\frac{1}{\mu_0 V} \frac{\partial G}{\partial \vec{H}}, \quad \chi = -\frac{1}{\mu_0 V} \left(\frac{\partial^2 G}{\partial H^2}\right)$$

→ Condensation energy:

There must be a free energy advantage for the system to "condense" into the superconducting state.

So, second order transition occurs only when we cross the $(T_c, 0)$ point?



$$\begin{aligned}
 G_S(T, H_c) - G_S(T, 0) & \\
 \Rightarrow \int dG &= - \int_0^{H_c} \mu_0 V \vec{M} \cdot d\vec{H}_c \\
 &= - \int_0^{H_c} \mu_0 V (-\vec{H}_c) \cdot d\vec{H}_c \\
 &= \frac{\mu_0 H_c^2 V}{2}
 \end{aligned}$$

For a normal material, $G_N(T, H_c) - G_N(T, 0) \approx 0$.
 H_c is in the range of mT , so assuming material to be paramagnetic (ferromagnetic materials do not go superconductive), $M \approx 0$.

$$\Rightarrow G_S(T, 0) - G_N(T, 0) = -\frac{\mu_0 H_c^2 V}{2} \quad \left[\text{Note that it's a 1st order transition, so } G_N(T, H_c) = G_S(T, H_c) \right]$$

ex: Consider Nb, with $T_c = 9\text{K}$, $H_c = 160\text{kA m}^{-1}$, $B_c = 0.2\text{T}$
 $\Rightarrow CE = 16.5\text{ kJ/m}^3 \Rightarrow CE = 2\text{ eV/atom}$.

→ GINZBERG-LANDAU (GL) THEORY.

The GL theory is built upon a more general theory of second-order phase transitions developed by Landau. In his theory, Landau introduced the concept of order parameter to describe the change in symmetry of the system. For example, consider a ferromagnet - above the Curie temp., it has no magnetic moment. But below the Curie temp., it develops a spontaneous magnetic moment. In this case, the magnetization \vec{M} behaves as an order parameter for the system.

Similarly, for superconductors, GL proposed an order parameter ψ , characterizing the superconducting state in the same manner as \vec{M} does for the ferromagnetic state.

The main features of GL theory are-

$$\textcircled{1} \quad \Psi = \begin{cases} 0 & , T > T_c \\ \Psi(T) \neq 0 & , T < T_c \end{cases}$$

$\textcircled{2}$ Ψ should be a complex quantity, $\Psi = |\Psi| e^{i\theta}$ [idea borrowed from superfluidity]
 The results of GL theory can be derived from BCS theory, and in such a case, it turns out that $|\Psi|^2$ is the density of Cooper pairs (from BCS theory).

$\textcircled{3}$ Free energy of the superconductor depends smoothly on Ψ and $|\Psi|$.

$\textcircled{5}$ F_s can be expanded on powers of $|\Psi|$ since $\Psi \rightarrow 0$ at T_c .

\leftarrow superconducting state free energy $\quad \rightarrow$ normal state free energy

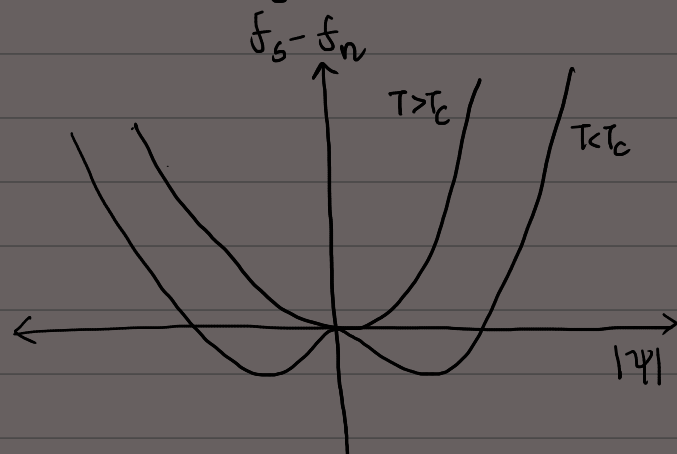
$$f_s(T) = f_n(T) + a(T) |\Psi|^2 + \frac{1}{2} b(T) |\Psi|^4$$

$a(T)$ & $b(T)$ are temp. dependent phenomenological constants.

$b(T) > 0$ otherwise $f_s(T)$ will not have any minimum;
 If $a(T) > 0 \quad |\Psi|_{\min} = |\Psi(0)|$
 $a(T) < 0 \quad |\Psi|_{\min}^2 = -\frac{a(T)}{b(T)}$

Phenomenologically, we define-

$a(T) < 0, T > T_c$
 $a(T) > 0, T < T_c$



If $a(T) > 0$, $\Psi(T) = 0$ is the minimum free energy solution, which is the normal state, after all. As $a(T) \downarrow$, we get a min. free energy solution with $\Psi \neq 0$ at $a(T) < 0$. $\Rightarrow a(T) = 0$ represents a transition point, and the temp. at which $a(T) = 0$ gives us the critical temperature, T_c .

Expanding $a(T)$ & $b(T)$ near T_c using Taylor's expansion-

$$a(T) = a(T_c) + \dot{a}(T-T_c) + \dots = \dot{a}(T-T_c)$$

$$b(T) = b(T_c) + \dots = b$$

$$|Y| = \begin{cases} (\dot{a}/b)^{1/2} (T_c - T)^{1/2}, & T < T_c \\ 0, & T > T_c \end{cases} \quad (\text{in the vicinity of } T=T_c, \text{ right?})$$

Substitute the value of $|Y|$ into the expression of free energy-

$$f_s(T) - f_n(T) = -\frac{\dot{a}^2 (T-T_c)^2}{b} + \frac{b}{2} \frac{\dot{a}^2 (T-T_c)^2}{b^2}$$

$$= -\frac{\dot{a}^2 (T_c - T)^2}{2b}$$

$$= -M_0 H_c^2 / 2 \quad (\text{condensation energy}).$$

$$\Rightarrow H_c = \frac{\dot{a}}{(M_0 b)^{1/2}} (T_c - T) \quad [\text{near } T_c]$$

The entropy per unit volume, $S_s(T) - S_n(T) = \frac{\partial}{\partial T} (f_s(T) - f_n(T)) = -\frac{\dot{a}^2}{b} (T_c - T)$

At T_c , there is no discontinuity in the entropy or latent heat, which corresponds to a second-order thermodynamic phase transition.

$$\text{Now, } C_v = T \frac{dS}{dT} \Rightarrow C_{v_s} - C_{v_n} = \begin{cases} T \dot{a}^2 / b, & T < T_c \\ 0, & T > T_c \end{cases}$$

So, the heat capacity has a discontinuity of $\Delta C_v = T_c \dot{a}^2 / b$ at T_c . Note that while this does not agree with the difference b/w exponential & linear portions of C_v observed experimentally, still the existence of the discontinuity validates the existence of phase transition.

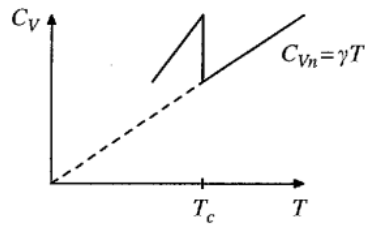


Fig. 4.4 Specific heat of a superconductor near T_c in the GL model. Above T_c the specific heat is given by the Sommerfeld theory of metals, $C_{Vn} = \gamma T$. At T_c there is a discontinuity and a change of slope.

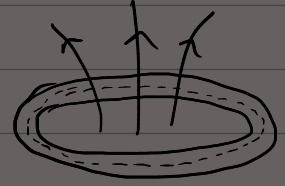
Note that GL theory can be used reliably only in the neighborhood of T_c .

→ To get the \vec{r} dependence of the order parameter (inhomogeneous systems), we need to include another term in $f_s(T)$:

$$f_s(T, \vec{r}) = f_n(T) + a(T) |\psi(\vec{r})|^2 + \frac{b(T)}{2} |\psi(\vec{r})|^4 + \frac{\hbar^2}{2m^*} |\nabla \psi(\vec{r})|^2$$

$$\vec{j}_s = -\frac{\vec{A}}{\lambda_L} + \frac{\hbar}{2m} \nabla \theta$$

$$\Rightarrow \nabla \theta = \frac{2m\vec{A}}{\hbar} + \frac{2m\lambda_L}{\hbar} \vec{j}_s$$



Consider a contour as shown inside the superconducting ring.

$$\oint_C \nabla \theta = \frac{2m}{\hbar} \oint_C \vec{A} \cdot d\vec{l} + \frac{2m\lambda_L}{\hbar} \oint_C \vec{j}_s \cdot d\vec{l}$$

\vec{j}_s lies at the surface of the ring, so the contour integral goes to zero.

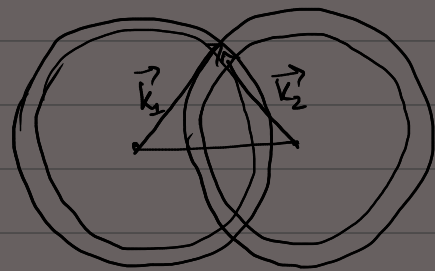
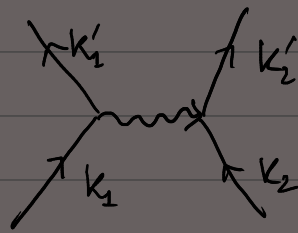
$$\Rightarrow \theta_1 - \theta_2 = \frac{2m\lambda_L}{\hbar} \oint_C \vec{j}_s \cdot d\vec{l} + \frac{2m}{\hbar} \oint_S (\nabla \times \vec{A}) \cdot d\vec{S}$$

$$\Rightarrow \theta_1 - \theta_2 = \frac{2m}{\hbar} \oint_S \vec{B} \cdot d\vec{S}$$

$$[\Phi = n\Phi_0] = \frac{2m}{\hbar} \Phi = \pm 2n\pi \quad (\text{flux through the superconducting ring is quantized})$$

Bardeen-Shockley-Cooper (BCS) theory:

→ Formation of Cooper pairs



(\vec{q} : momentum of phonon)

$$\vec{k}_1 - \vec{q} = \vec{k}_1'$$

$$\vec{k}_2 + \vec{q} = \vec{k}_2'$$

$$\Rightarrow \vec{k}_1 + \vec{k}_2 = \vec{k}_1' + \vec{k}_2' = \vec{k}$$

For max. prob. of collision,
 $k_1 = -k_2$

$$k_F < k < \sqrt{\frac{(E_F + \hbar\omega_p) 2m}{\hbar^2}}$$

Attractive potential b/w the two e's.

$$-\frac{\hbar^2}{2m} [\nabla_1^2 + \nabla_2^2] \Psi(\vec{r}_1, \vec{r}_2) + V(\vec{r}_1, \vec{r}_2) \Psi(\vec{r}_1, \vec{r}_2) = E \Psi(\vec{r}_1, \vec{r}_2)$$

$\hookrightarrow (E + 2\varepsilon_F^0)$

$$\phi_{\vec{k}} = \frac{1}{\sqrt{L^3}} e^{i\vec{k} \cdot \vec{r}} \quad (\text{Free-electron state})$$

Consider a toy wavefunction for the two-particle state:

$$\frac{1}{L^3} e^{i\vec{k}_1 \cdot \vec{r}_1} \cdot e^{i\vec{k}_2 \cdot \vec{r}_2} = \frac{1}{L^3} e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)}$$

But this ain't symmetric. So, the two-particle wavefunction finally looks like-

$$\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{L^3} \left(\frac{e^{i\vec{k} \cdot \vec{r}_1} + e^{-i\vec{k} \cdot \vec{r}_1}}{\sqrt{2}} \right) |S\rangle \quad (\vec{r} = \vec{r}_1 - \vec{r}_2)$$

\hookrightarrow singlet spin

$$\Psi(\vec{r}) = \frac{1}{L^3} \sum_{\vec{k}} g(\vec{k}) e^{i\vec{k} \cdot \vec{r}}$$

$$g(\vec{k}) = 0 \text{ for } k < k_F \text{ \& } k > \sqrt{\frac{2m(E_F + \hbar\omega_D)}{\hbar^2}}$$

Multiply by $e^{-i\vec{k} \cdot \vec{r}}$ & integrate over space

$$\frac{\hbar^2 k^2}{m} g(\vec{k}) + \frac{1}{L^3} \sum_{\vec{k}'} g(\vec{k}') V_{\vec{k}\vec{k}'} = (E + 2\varepsilon_F^0) g(\vec{k})$$

$$\text{where } V_{\vec{k}\vec{k}'} = \int V(\vec{r}) e^{-i(\vec{k} - \vec{k}') \cdot \vec{r}} d^3\vec{r}$$

$$\Rightarrow \left\{ -\frac{\hbar^2 k^2}{m} + E + 2\varepsilon_F^0 \right\} g(\vec{k}) = -A \quad \text{where } A = \frac{V_0}{L^3} \sum_{\vec{k}'} g(\vec{k}')$$

$$V_{\vec{k}\vec{k}'} = -V_0 \quad (V_0 > 0)$$

$$\varepsilon_F^0 < \frac{\hbar^2 k^2}{2m} < \varepsilon_F^0 + \hbar\omega_D$$

$$= 0, \text{ otherwise.}$$

$$\sum_{\mathbf{k}} g(\mathbf{k}) = \frac{V_0}{L^3} \sum_{\mathbf{k}} \frac{-A}{\left(\frac{\hbar^2 \mathbf{k}^2}{2m} + \varepsilon + 2\varepsilon_F^0 \right)}$$

$$\frac{V_0}{L^3} \sum_{\mathbf{k}} \frac{1}{\left(\frac{\hbar^2 \mathbf{k}^2}{2m} - \varepsilon - 2\varepsilon_F^0 \right)} = 1.$$

$$\sum_{\mathbf{k}} \rightarrow \frac{L^3}{8\pi^3} \int d^3\mathbf{k} \quad (\text{No spin multiplicity})$$

$$\begin{aligned} \sum_{\mathbf{k}} g(\mathbf{k}) &= V_0 \int_{\varepsilon_F^0}^{\varepsilon_F^0 + \hbar\omega_D} g(E) dE \frac{1}{2E - \varepsilon - 2\varepsilon_F^0} (= 1) \\ &= V_0 g(\varepsilon_F^0) \int_{\varepsilon_F^0}^{\varepsilon_F^0 + \hbar\omega_D} \frac{dE}{2E - \varepsilon - 2\varepsilon_F^0} (= 1) \\ &= \frac{1}{2} V_0 g(\varepsilon_F^0) \ln\left(\frac{\varepsilon - 2\hbar\omega_D}{\varepsilon} \right) (= 1) \end{aligned}$$

$$\Rightarrow \varepsilon = \frac{2\hbar\omega_D}{1 - e^{2/V_0 g(\varepsilon_F^0)}}$$

In the limit of $V_0 g(\varepsilon_F^0) \ll 1$ (weak interaction)

$$\varepsilon \simeq -2\hbar\omega_D e^{-2/V_0 g(\varepsilon_F^0)}$$