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Solid state physics

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Contents

1 Semi-conductors **3**

1 Crystal and electronic structure . . . 3

1.1 Face-centered cubic lattice . . . 3

1.2 Diamond structure . . . 6

1.3 Bloch Theorem . . . 7

1.3.1 Band structure . . . 8

2 transport and charge carriers . . . 9

3 Thermal population of charge carriers . . . 11

4 Intrinsic semi-conductors . . . 13

5 Extrinsic semi-conductors . . . 14

6 Population of impurity levels in thermal equilibrium . . . 16

6.1 Thermal equilibrium carrier densities of impure semiconductors . . . 17

7 Non-homogeneous semi-conductors (n-p junction) . . . 20

8 Einstein relations . . . 26

9 Generation and recombination currents . . . 26

10 Rectification by an *np*-junction . . . 28

11 Some additional devices . . . 29

2 Magnetism **31**

1 Recall of basic concepts . . . 31

2 Diamagnetism . . . 33

2.1 Langevin approach . . . 34

2.2 Quantum treatment of diamagnetism . . . 35

3 Paramagnetism . . . 36

3.1 Classical treatment . . . 37

3.2 Quantum treatment . . . 38
3.3 Pauli's paramagnetism (metals) . . . 39
3.4 Diamagnetism of conduction electrons (Landau) . . . 41
4 Magnetic interactions . . . 41
4.1 Exchange interaction . . . 42
4.1.1 Effective Hamiltonians . . . 43
5 Molecular field (mean field), Pierre Weiss 1907 . . . 43
6 Stoner - Wohlfarth model for itinerant ferromagnetism . . . 45
7 Antiferromagnetism and ferrimagnetism . . . 47
8 Magnetic domains . . . 48

3 Superconductivity **50**
1 Phenomenology . . . 50
2 London equations (F. and H. London 1935) . . . 51
3 BCS Theory (Bardeen, Cooper, Schrieffer, 1957) . . . 54

Chapter 1

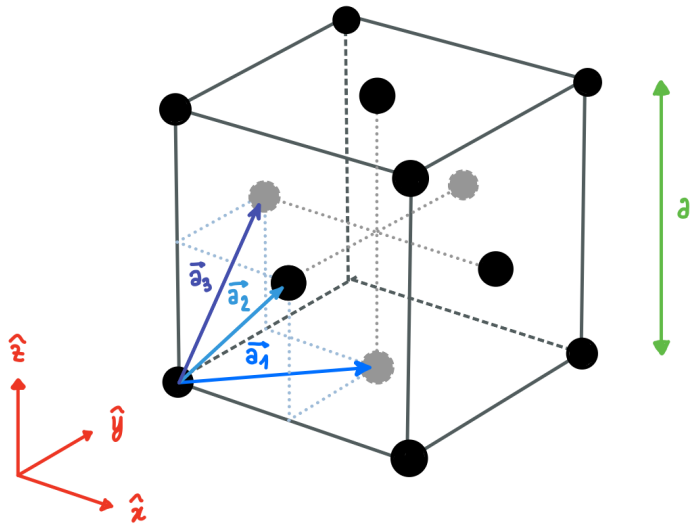
Semi-conductors

1 Crystal and electronic structure

1.1 Face-centered cubic lattice

A set of primitive vectors for the face-centered cubic lattice is

$$\vec{a}_1 = \frac{a}{2}(\hat{x} + \hat{y}), \qquad \vec{a}_2 = \frac{a}{2}(\hat{x} + \hat{z}), \qquad \vec{a}_3 = \frac{a}{2}(\hat{y} + \hat{z}).$$



A question can arise : what is the volume of the unit of the unit cell ?

$$v_c = |\vec{a}_1 \times \vec{a}_2 \cdot \vec{a}_3| = \frac{1}{4}a^3$$

Calculation :

$$\begin{aligned} v_c &= |\vec{a}_1 \times \vec{a}_2 \cdot \vec{a}_3| \\ &= \frac{a^3}{8} \left| \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \times \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right| \\ &= \frac{a^3}{8} \left| \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right| \\ &= \frac{a^3}{8} |-1-1| \\ &= \frac{a^3}{4} \end{aligned}$$

Remark : the smart way is to make the calculation of the number of atoms in the conventional cell :

$$\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$$

Where 1/8 and 1/2 is the sharing. One has to remember that the so-called *primitive cell* has one atom in it.

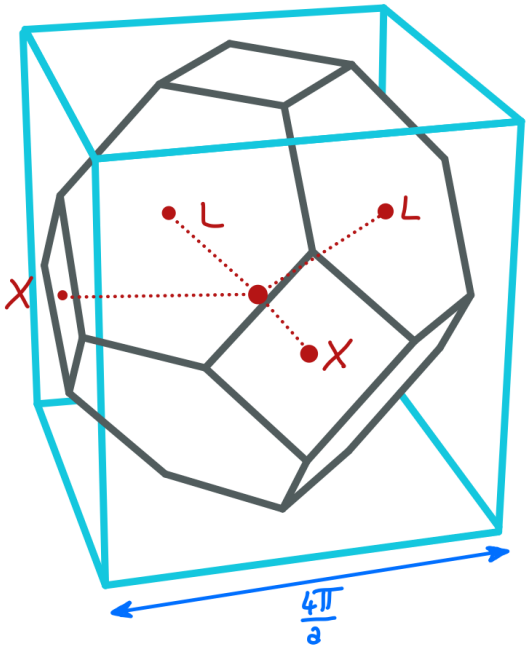
Reciprocal vector,

$$\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$$

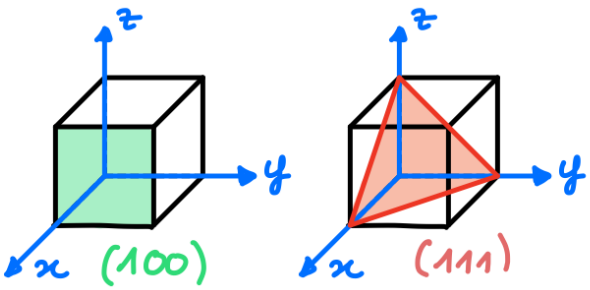
Thus,

$$\begin{cases} \vec{b}_1 = \dfrac{2\pi}{v_c}\vec{a}_2 \times \vec{a}_3 = \dfrac{2\pi}{a}(\hat{z} - \hat{y} - \hat{x}) \\ \vec{b}_2 = \dfrac{2\pi}{v_c}\vec{a}_3 \times \vec{a}_2 = \dfrac{2\pi}{a}(\hat{z} + \hat{y} - \hat{x}) \\ \vec{b}_3 = \dfrac{2\pi}{v_c}\vec{a}_1 \times \vec{a}_2 = \dfrac{2\pi}{a}(-\hat{y} - \hat{z} + \hat{x}) \end{cases}$$

The reciprocal vector are kind of the Fourier transform in space. The two spaces are dual of each others. The reciprocal space of the Face-Centered Cubic lattice is a Cubic Centered lattice.

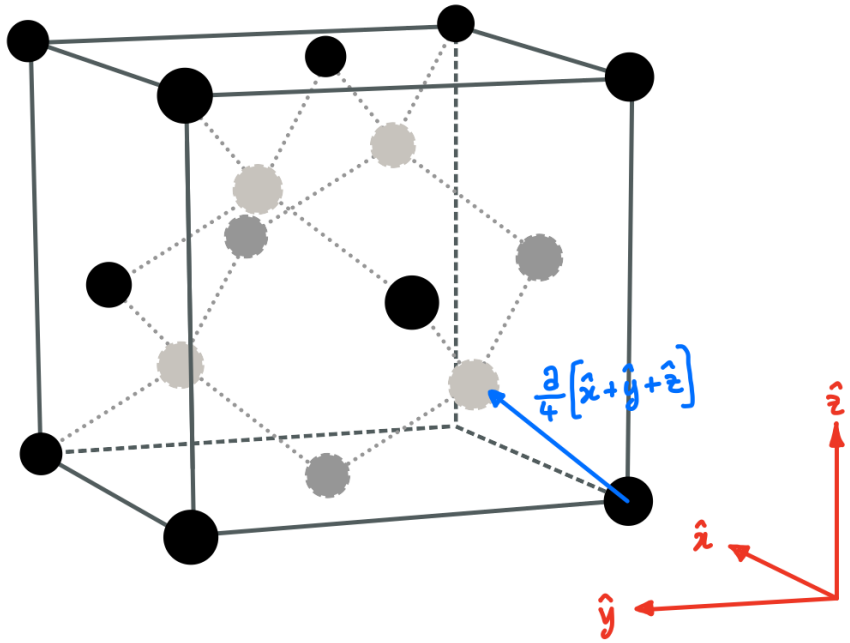


The size of the new cube has a length of $4\pi/a$. The Γ point is in the middle, X is from Γ to a face, L is from center to a vertex. X is in the plane (100) and L is in the plane (111)



1.2 Diamond structure

The diamond lattice (formed by the carbon atoms in a diamond crystal) consists of two interpenetrating face-centered cubic Bravais lattices, displaced along the body diagonal of the cubic cell by one quarter the length of the diagonal. It can be regarded as a face-centered cubic lattice with the two-point basis 0 and $(a/4)(\hat{x}+\hat{y}+\hat{z})$. The coordination number is 4. The diamond lattice is not a Bravais lattice,



Hence, the diamond is a face-centered cubic lattice with a basis $(0,0,0)$ and $(1/4,1/4,1/4)$. We have 8 atoms per conventional lattice.

> **Remark :** The *zinc-blende structure* is an example of two FCC lattices with two species.

1.3 Bloch Theorem

Now we put electrons in those cells.

Bloch Theorem :

Let ψ be the wavefunction. We are interested to know the wavefunction in an other cell as a function of the one in the first cell. If the lattice is periodic,

$$\begin{cases} \psi_{n,k}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n,k}(\vec{r}) \\ u_{n,k}(\vec{r}+\vec{R}) = u_{n,k}(\vec{r}) \end{cases}$$

$\vec{k}$ is the first Brillouin zone, $\vec{R}$ Bravais lattice vector, n the primitive cell and $u_{n,k}$ is a periodic function. We see indeed that the wavefunction is the same *up to a global phase*. Such a global phase keeps the physics the same indeed.

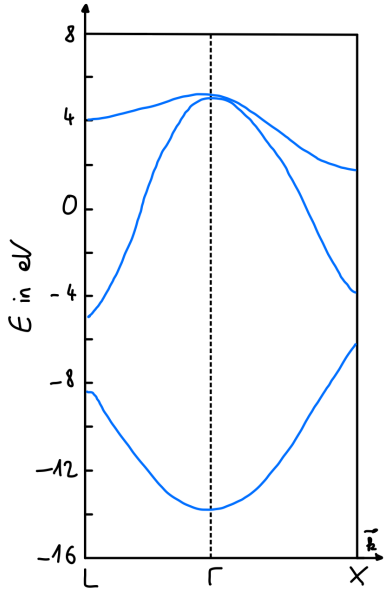
Remark : an equivalent formulation of Bloch Theorem is :

$$\psi_k(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_k(\vec{r})$$

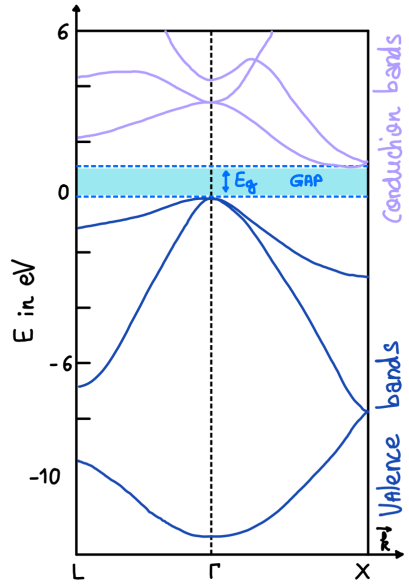
The two formulations are totally equivalent. The wavefunction is an eigenvector of the translation operator. Unitary operator has eigenvalues's modulus equal to 1, and hermitian opeartor has eigenvalues that are real.

1.3.1 Band structure

Carbon (C) has 8 electrons per unit cell. 4 occupied valence bands (2 spins per bond)

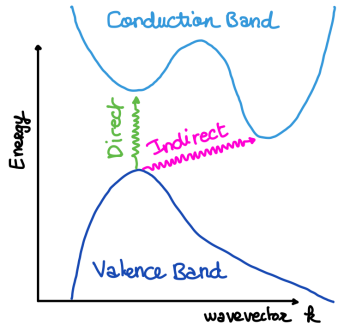


Silicon (Si) is also a diamond structure, with this time a gap between valence and conduction band,

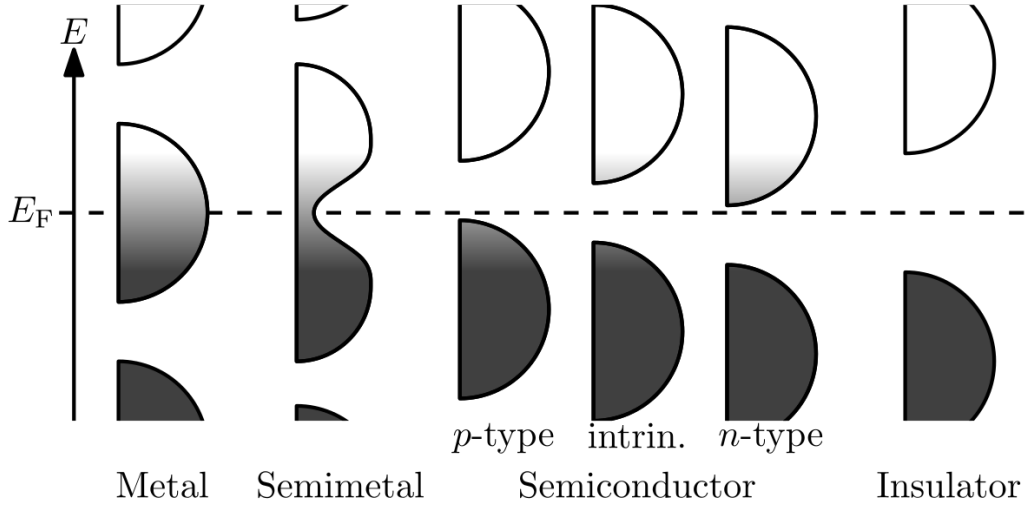


$$E_g = E_{\text{min}CB} - E_{\text{max}VV}$$

A *semi-conductor* is when with temperature, and electron can hop from the valence band to the conduction band.



If we have a so-called *direct gap*, $k_{\text{min}CB} = k_{\text{max}VV}$ otherwise it is called an *indrect gap* and thus $k_{\text{min}CB} \neq k_{\text{max}VV}$.



2 transport and charge carriers

When I say charge carriers, of course the one you are most used to is electrons. We are gonna explain the concept of holes.

At room temperature, the resistivity ρ, $\rho = \sigma^{-1}$ and σ is the conductivity. The resistance Ω is linked to the resistivity with $\Omega = \rho L/A$ where L is the length of the wire and A it's area. The resistivity is an intrinsic quantity and resistance an extrinsic quantity.

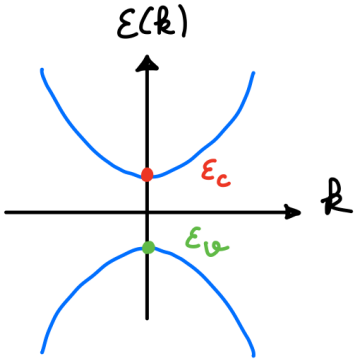
$$\begin{cases} \rho_{\text{semi-condcutor}} \sim 10^{9} \text{ Ohm.cm} \\ \rho_{\text{metal}} \sim 10^{-6} \text{ Ohm.cm} \\ \rho_{\text{insulator}} \sim 10^{22} \text{ Ohm.cm} \end{cases}$$

We recall Drude's conductivity,

$$\begin{cases} \sigma_{\text{metal}} = \dfrac{ne^2\tau}{m} \text{ decreases with } T \text{ because } \tau \text{ has a temperature dependency,} \\ \sigma_{\text{semi-conductor}} \text{ increases with temeperature,} \end{cases}$$

where n is the electron density, e is charge of electrons, m is the electron mass and proportional to the next time you have a collision τ. For semi-conductor, it increases because the electronic population depends on the temperature.

The electrons close to the bottom of the conduction band,



$$\epsilon(k) = \epsilon_c + \hbar^2 \left(\frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3} \right)$$

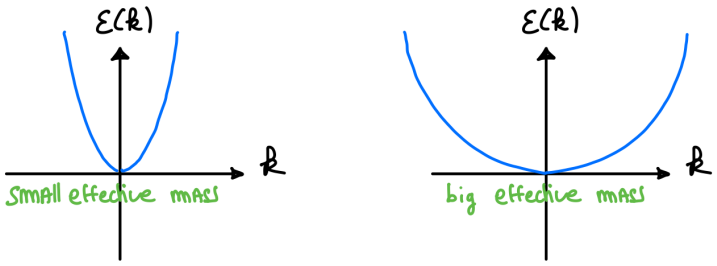
for a direct gap.

> **Remark :** In the case of an indirect gap, you have to make an expansion near a k-point that is not the Γ point.

We can define the *effective mass*,

$$m_i = \hbar^2 \left(\frac{\partial^2 \epsilon}{\partial k_i^2} \right)^{-1}$$

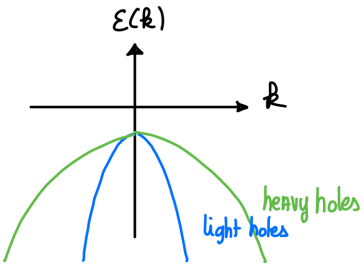
If we apply a magnetic or electric field, the electron's acceleration will be given by its effective mass.



If we have holes close to the maximum of the valence band, a *hole* is a missing electron in the valence band,

$$\epsilon(k) = \epsilon_v - \hbar^2 \left(\frac{k_1^2}{2m_1} + \frac{k_2^2}{2m_2} + \frac{k_3^2}{2m_3} \right)$$

If we have multiple valence band,



$$k_h = k_e, \qquad \epsilon_h = -\epsilon_k$$

hence, we can assign the charge $+e$ to the hole.

For GaAs,

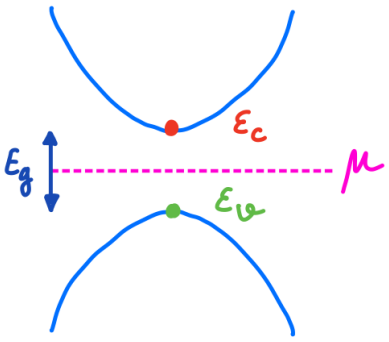
$$\begin{cases} m_e = 0.06 m_0 \\ m_{eh} = 0.08 m_0 \\ m_{hh} = 0.5 m_0 \end{cases}$$

For Si,

$$\begin{cases} m_{eh} = 0.16 m_0 \\ m_{hh} = 0.49 m_0 \end{cases}$$

where m_0 is the free electron mass.

3 Thermal population of charge carriers



The Fermi energy divides the state between an occupied and unoccupied zone. At $T = 0$, it is equal to the chemical potential. We impose that $\epsilon_v < \mu < \epsilon_c$ and $E_g = \epsilon_c - \epsilon_v$. We will assume that $\epsilon_c - \mu \gg k_B T$ and $\mu - \epsilon_v \gg k_B T$. Thus, $E_g \gg k_B T$.

Electronic density in the conduction band,

$$n_c(T) = \int_{\epsilon_c}^{+\infty} \mathrm{d}\epsilon g_c(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

where $g_c(\epsilon)$ is the electron density in the conduction band and μ the chemical potential.

Hole density in the valence band,

$$p_v(T) = \int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon) \left(1 - \frac{1}{e^{\beta(\epsilon-\mu)} + 1}\right) = \int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon) \frac{1}{e^{\beta(\mu-\epsilon)} + 1}$$

We remind ourselves the Taylor expansion,

$$\begin{cases} \dfrac{1}{e^{\beta(\epsilon-\mu)} + 1} \approx e^{-\beta(\epsilon-\mu)} & \text{for } \epsilon > \epsilon_c \\ \dfrac{1}{e^{\beta(\mu-\epsilon)} + 1} \approx e^{-\beta(\mu-\epsilon)} & \text{for } \epsilon < \epsilon_v \end{cases}$$

Thus,

$$\begin{cases} n_c(T) = \displaystyle\int_{\epsilon_c}^{+\infty} g_c(\epsilon) e^{-(\epsilon-\mu)/k_B T} = e^{-(\epsilon_c-\mu)/k_B T} N_c(T) \\ p_v(T) = \displaystyle\int_{-\infty}^{\epsilon_v} g_v(\epsilon) e^{-(\mu-\epsilon)/k_B T} = e^{-(\mu-\epsilon_v)/k_B T} P_v(T) \end{cases}$$

With,

$$\begin{cases} N_c(T) = \displaystyle\int_{\epsilon_c}^{+\infty} \mathrm{d}\epsilon g_c(\epsilon) e^{-(\epsilon-\epsilon_c)/k_B T} \\ P_v(T) = \displaystyle\int_{-\infty}^{\epsilon_v} \mathrm{d}\epsilon g_v(\epsilon) e^{-(\epsilon_v-\epsilon)/k_B T} \end{cases}$$

$$g_{c,v}(\epsilon) = \sqrt{2|\epsilon - \epsilon_{c,v}|} \frac{m_{c,v}^{3/2}}{\hbar^3 \pi^2}$$

Where $m_c^3 = m - 1 m_2 m_3$ and $m_v^3 = m_1' m_2' m_3'$. We are using the free gas density of states because we are only in the vicinity of the bottom/top of the bands, and so, with the exponential factor that is going to go to 0 quick, we are not making a big mistake in that approximation. And so we get the integrals,

$$\begin{aligned} N_c(T) &= \frac{m_c^{3/2}}{\hbar^3 \pi^2} \int_{\epsilon_c}^{+\infty} \mathrm{d}\epsilon \sqrt{2(\epsilon - \epsilon_c)} e^{-(\epsilon-\epsilon_c)/k_B T} \qquad x = \sqrt{\frac{\epsilon - \epsilon_c}{k_B T}} \\ &= \frac{m_c^{3/2}}{\hbar^3 \pi^2} (2k_B)^{3/2} \int_0^{+\infty} \mathrm{d}x x e^{-x^2} \\ &= \frac{1}{4} \left(\frac{2 m_c k_B T}{\pi \hbar^2}\right)^{3/2} \end{aligned}$$

And with the same method,

$$P_v(T) = \frac{1}{4}\left(\frac{2m_v k_B T}{\pi\hbar^2}\right)^{3/2}$$

And with numbers,

$$\begin{cases} N_c(T) = 2.5\left(\dfrac{m_c}{m_0}\right)^{3/2}\left(\dfrac{T}{300\text{ K}}\right)^{3/2} \times 10^{19}\text{ cm}^{-3} \\ P_v(T) = 2.5\left(\dfrac{m_v}{m_0}\right)^{3/2}\left(\dfrac{T}{300\text{ K}}\right)^{3/2} \times 10^{19}\text{ cm}^{-3} \end{cases}$$

And finally,

$$\begin{cases} n_c(T) = e^{-(\epsilon_c-\mu)/k_B T} N_c(T) \\ p_v(T) = e^{-(\mu-\epsilon_v)/k_B T} P_v(T) \end{cases}$$

We remark that N_c and P_v do not depend on the chemical potential, hence if we calculate $n_c \times p_v$, this quantity is independent of the chemical potential.

Action-mass law,

$$\begin{aligned} n_c(T) \times p_v(T) &= N_c(T)P_v(T)e^{-(\epsilon_c-\epsilon_v)/k_B T} \\ &= N_c(T)P_v(T)e^{-E_g/k_B T} \\ &= \frac{1}{2}\left(\frac{k_B T}{\pi\hbar^2}\right)^3 (m_c m_n)^{3/2} e^{-E_g/k_B T} \end{aligned}$$

4 Intrinsic semi-conductors

Intrinsic semi-conductors is when there is a negligible quantity of impurities. Meaning that the only carriers are coming from the semi-conductor.

And so, in this situation, $n_c(T) = p_v(T) = n_i(T)$.

$$\begin{aligned} n_i(T) &= (N_c(T)P_v(T))^{1/2} e^{-E_g/2k_B T} \\ &= \frac{1}{4}\left(\frac{2k_B T}{\pi\hbar^2}\right)^{3/2} (m_c m_v)^{3/4} e^{-E_g/2k_B T} \end{aligned}$$

$$n_c(T) = N_c(T)e^{-\beta(\epsilon_c-\mu_i)} = p_v(T) = P_v(T)e^{-\beta(\mu_i-\epsilon_v)}$$

And so we can make the calculation of μ_i,

$$e^{-\beta(\epsilon_c-\epsilon_v+2\mu_i)} = \frac{P_v(T)}{N_c(T)}$$

And so,

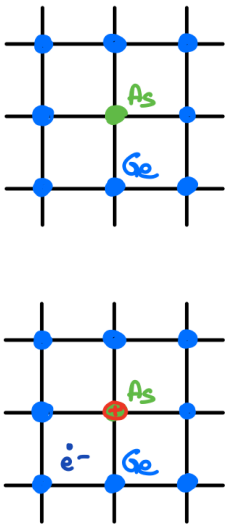
$$\begin{aligned}\mu_i &= \frac{1}{2}\left(\epsilon_c + \epsilon_v + k_B T \ln\left(\frac{P_v(T)}{N_c(T)}\right)\right) \\ &= \epsilon_v + \frac{1}{2}E_g + \frac{3}{4}k_B T \ln\left(\frac{m_v}{m_c}\right)\end{aligned}$$

at $T = 0$, the chemical potential μ_i is the middle of the gap. At room temperature, the chemical potential stays close to $\mu_i(T = 0) = (\epsilon_c + \epsilon_v)/2$ because $m_v/m_c \simeq 1$ and $E_g \gg k_B T$. So our hypothesis are consistent with what we get here.

5 Extrinsic semi-conductors

If impurities contribute a significant fraction of the conduction band electrons and/or valence band holes, one speaks of an extrinsic semiconductor.

Impurities that contribute to the carrier density of a semiconductor are called donors if they supply additional electrons to the conduction band, and acceptors if they supply additional holes to (*i.e.*, capture electrons from) the valence band. Consider, for example, the case of substitutional impurities in a group IV semi- conductor. Suppose that we take a crystal of pure germanium, and replace an occasional germanium atom by its neighbor to the right in the periodic table, arsenic. The germanium ion has charge $4e$ and contributes four valence electrons, while the arsenic ion has charge $5e$ and contributes five valence electrons. If, to a first approximation, we ignore the difference in structure between the arsenic and germanium ion cores, we can represent the substitution of an arsenic atom for a germanium atom by a slightly less drastic modification, in which the germanium atom is not removed, but an additional fixed positive charge of e is placed at its site, along with an additional electron.



The electron will be bound to the positive ion, with a binding energy much smaller than in the Hydrogen atom.

i) The electric field is reduced by the effect of the dieletric constant ($\kappa \sim 16$).

ii) The effective mass of the electron in the semi-conductor is of the order of ~ 0.1 of the free electron mass.

For the Hydrogen atom, the binding energy is

$$\epsilon_{\text{Binding}} = 1 \text{ Ry} = 15.6 \text{ eV} = \frac{m_0 e^4}{2\hbar^2}$$

For the donor level, the binding energy is

$$\epsilon_{\text{Binding}} = \frac{m^\star}{m_0}\frac{1}{\kappa^2}\frac{m_0 e^4}{2\hbar^2} = \frac{m^\star}{m_0}\frac{1}{\kappa^2} \times 13.6 \text{ eV} \ll 13.6 \text{ eV}$$

where $m^\star$ is the effective mass of the electron in the semi-conductor. Using $m^\star/m_0 \sim 0.1$ and $\kappa \sim 16$, we get $\epsilon_{\text{Binding}} \sim 5.3$ meV. The level of the impurity (donor ϵ_d) is very close to the minimum of the conduction band, $\epsilon_c - \epsilon_d \ll E_g$.

Bohr radius,

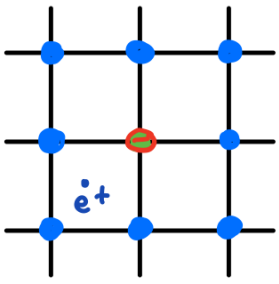
$$a_0 = \frac{\hbar^2}{me^2} = 0.52 \text{ Å}$$

Radius for the donor,

$$r_0 = \frac{m}{m^\star}\kappa\frac{\hbar^2}{me^2} \sim 100 \text{ Å} \gg a_0$$

At $T = 300$ K, $k_B T = 26$ meV.

For acceptor levels it is the same idea as with the donors one, but instead of a positive site, it is a negative site, and with a hole in the lattice and not an electron,



If impurities contribute a significant fraction of the conduction band electrons and/or valence band holes, one speaks of an extrinsic semiconductor. Because of these added sources of carriers in the density of conduction band electrons need no longer be equal to the density of valence band holes, thus,

$$n_c - p_v = \Delta n \neq 0$$

Since the law of mass action,

$$n_c p_v = n_i^2$$

holds regardless of the importance of impurities. Thus we can express the carrier density in the extrinsic case in terms of their intrinsic values n_i and the deviation Δn from intrinsic behavior,

$$\begin{cases} n_c = +\frac{1}{2}\Delta n + \frac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2} \\ p_v = -\frac{1}{2}\Delta n + \frac{1}{2}\sqrt{(\Delta n)^2 + 4n_i^2} \end{cases}$$

The quantity $\Delta n/n_i$, which measure the importance of the impurities as a source of carriers, can be given a particularly simple expression as a function of chemical potential μ,

$$n_c = e^{\beta(\mu-\mu_i)} n_i, \qquad p_v = e^{-\beta(\mu-\mu_i)} n_i$$

Therefore,

$$\Delta n = n_c - p_v = n_i \left(e^{\beta(\mu-\mu_i)} - e^{-\beta(\mu-\mu_i)} \right) = 2n_i \sinh(\beta(\mu - \mu_i))$$

So,

$$\frac{\Delta n}{n_i} = 2\sinh(\beta(\mu - \mu_i))$$

If Δn is not much larger than n_i, then μ is close to μ_i. If $|\Delta n| \gg n_i$, if $\Delta n > 0$, then $n_c \simeq \Delta n$ and it is called a n-type, and if $\Delta n < 0$ then $p_v \simeq -\Delta n$ and it is called a p-type.

6 Population of impurity levels in thermal equilibrium

We assume that the density of impurities is low enough that the interaction of electrons (or holes) bound at different impurity sites is negligible. The mean number of electrons (or holes) there would be if there were only a single (at most) impurity. For simplicity we assume that the impurity introduces only a single one-electron orbital level.

Donor Level : If we ignored electron-electron interactions the level could either be empty, could contain one electron of either spin, or two electrons of opposite spins. However, the Coulomb repulsion of two localized electrons raises the energy of the doubly occupied level so high that double occupation is essentially prohibited. Quite generally, the mean number of electrons in a system in thermal equilibrium is given by:

$$\langle n \rangle = \frac{\sum_j N_j e^{-\beta(E_j - \mu N_j)}}{\sum_j e^{-\beta(E_j - \mu N_j)}}$$

where the sum is over all states of the system, E_j and N_j, are the energy and number of electrons in state j, and μ is the chemical potential. In the present case the system is a single impurity

with just three states: one with no electrons present which makes no contribution to the energy, and two with a single electron present of energy ϵ_d. Therefore,

$$\langle n \rangle = \frac{2e^{-\beta(\epsilon_d-\mu)}}{1+2e^{-\beta(\epsilon_d-\mu)}} = \frac{1}{\frac{1}{2}e^{\beta(\epsilon_d-\mu)}+1}$$

If there are N_d impurities per unit volume,

$$n_d = \frac{N_d}{\frac{1}{2}e^{\beta(\epsilon_d-\mu)}+1}$$

where n_d is the number of electrons coming from the impurities.

> **Remark :** What happen at $T = 0$? At $T = 0$, the chemical potential is in-between ϵ_d and ϵ_c, thus, $\epsilon_d - \mu < 0$ and so, $n_d\big|_{T=0} = N_d$. But, if $\epsilon_d - \mu \gg k_B T$ then $n_d/N_d \ll 1$, $n_d \simeq 2N_d e^{-\beta(\epsilon_d-\mu)}$.

Recall,

$$\begin{aligned} n_c &= \int_{\epsilon_c}^{\infty} \mathrm{d}\epsilon \frac{g(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} \\ &\simeq e^{-\beta(\epsilon_c-\mu)} N_c(T) \end{aligned}$$

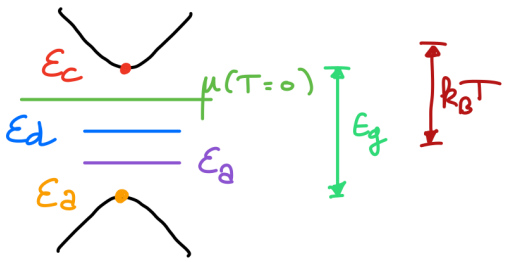
And so,

$$\frac{n_d}{n_c} = \frac{2N_d}{N_c} \underbrace{e^{\beta(\epsilon_c-\epsilon_d)}}_{\lesssim 1} \ll 1$$

the $\lesssim$ is if $\epsilon_c - \epsilon_d \ll k_B T$. Thus we get, $N_d \sim 10^{16}$ cm^{-3} and $N_c \sim 10^{19}$ cm^{-3}.

6.1 Thermal equilibrium carrier densities of impure semiconductors

Consider a semiconductor doped with N_d donor impurities and N_a acceptor impurities per unit volume. Suppose $N_d \geq N_a$.



In thermal equilibrium at temperature T the electrons will be redistributed among these levels, but since their total number remains the same, the number of electrons in conduction band or donor levels, $n_c + n_d$, must exceed its value at $T = 0$, $N_d - N_a$ by precisely the number of empty levels (*i.e.*, holes), $p_v + p_a$, in the valence band and acceptor levels:

$$n_c + n_d = N_d - N_a + p_v + p_a$$

Suppose that

$$\begin{cases} \epsilon_d - \mu \gg k_B T \\ \mu - \epsilon_a \gg k_B T \end{cases}$$

$$\frac{n_d}{N_d} \simeq 2e^{-\beta(\epsilon_d - \mu)} \ll 1$$

Also $p_a \ll N_d$

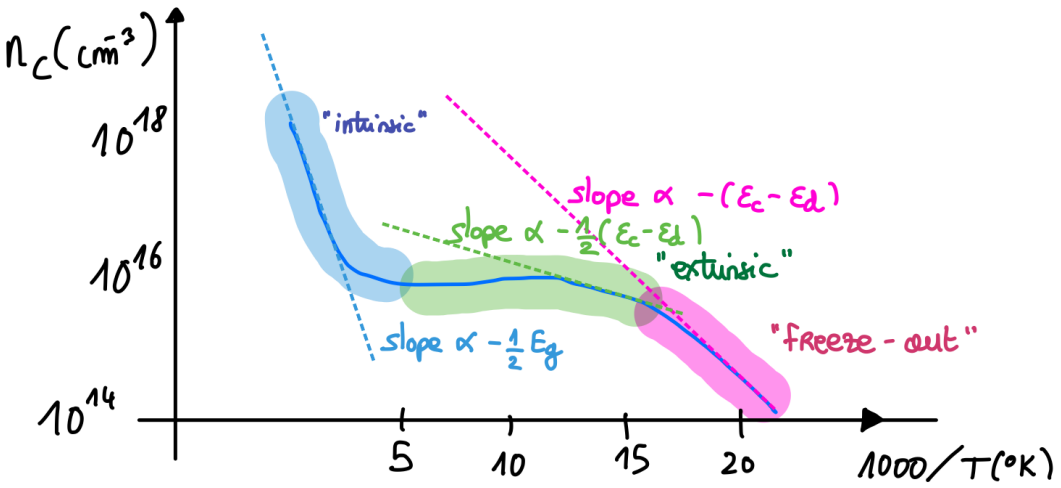
$$\Delta n = n_c - p_v = N_d - N_a + p_a - n_d \simeq N_d - N_a$$

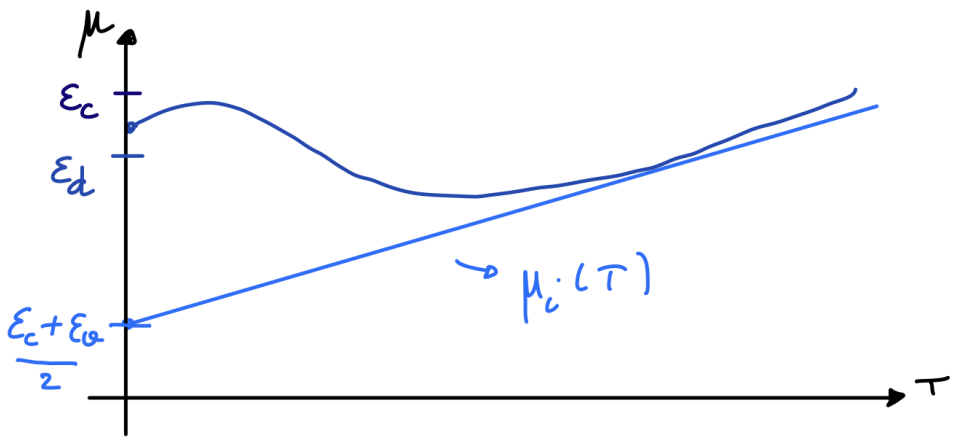
$$\begin{cases} n_c = +\frac{1}{2}(N_d - N_a) + \frac{1}{2}\sqrt{(N_d - N_a)^2 + 4n_i^2} \\ p_v = -\frac{1}{2}(N_d - N_a) + \frac{1}{2}\sqrt{(N_d - N_a)^2 + 4n_i^2} \end{cases}$$

For a considerable range of carrier concentrations in the extrinsic regime,

$$\begin{cases} n_c \simeq N_d - N_a \\ p_v \simeq \dfrac{n_i^2}{N_d - N_a} \ll 1 \end{cases}$$

Most of electrons are in the conduction band and participate to transport.





$$\frac{\Delta n}{n_i} = 2\sin(\beta(\mu - \mu_i))$$

n-doping $N_a = 0$, if we can neglect p_v,

$$\begin{aligned} n_c &= N_d - n_d \\ &= N_d\left(1 - \frac{1}{\frac{1}{2}e^{\beta(\epsilon_d-\mu)}+1}\right) \\ &= \frac{N_d}{1+2e^{\beta(\mu-\epsilon_d)}} \\ &= N_c e^{-\beta(\epsilon_c-\mu)} \end{aligned}$$

Thus,

$$N_d = \left(1+2e^{\beta(\mu-\epsilon_d)}\right) N_c e^{-\beta(\epsilon_c-\mu)}$$

$$N_c e^{-\beta(\epsilon_c-\mu)} + 2N_c e^{-\beta(\epsilon_c-\mu)} e^{\beta(\mu-\epsilon_d)} - N_d = 0$$

$$N_c e^{\beta(\mu-\epsilon_d)} e^{\beta(\epsilon_d-E_c)} + 2N_c e^{2\beta(\mu-\epsilon_d)} e^{\beta(\epsilon_d-\epsilon_c)} - N_d = 0$$

We can multiply by $e^{\beta(\epsilon_c-\epsilon_d)}/2N_c$,

$$\left(e^{\beta(\mu-\epsilon_d)}\right)^2 + \frac{1}{2}\left(e^{\beta(\mu-\epsilon_d)}\right) - \frac{1}{2}\frac{N_d}{N_c}e^{\beta(\epsilon_c-\epsilon_d)} = 0$$

$$\mu(T) = \epsilon_d + k_B T \ln\left(\frac{1}{4}\left(-1+\left(1+\frac{8N_d}{N_c}e^{\beta(\epsilon_c-\epsilon_d)}\right)^{1/2}\right)\right)$$

$$e^{\beta(\mu-\epsilon_d)} = \frac{1}{4}\left(-1+\left(1+\frac{8N_d}{N_c}e^{\beta(\epsilon_c-\epsilon_d)}\right)^{1/2}\right)$$

$k_BT \ll \epsilon_c - \epsilon_d$ imply that

$$\mu(T) \simeq \frac{\epsilon_c+\epsilon_d}{2} + \frac{k_BT}{2}\ln\left(\frac{N_d}{2N_c}\right)$$

$$\mu(T=0) = \frac{\epsilon_c+\epsilon_d}{2}$$

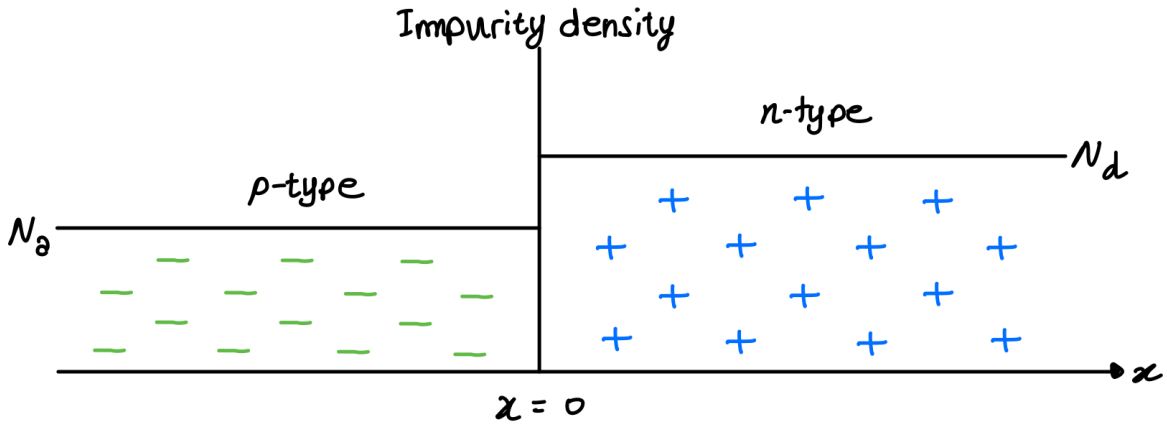
μ increase with the temperature, since $N_c(T) \sim T^{3/2}$ as long as N_c remains smaller than N_d. When $N_c \geq N_d$ we have μ that decrease.

$\epsilon_c - \epsilon_d < k_BT \ll E_g$, thus,

$$\mu(T) = \epsilon_c - k_BT\ln\left(\frac{N_c}{N_d}\right)$$

if $k_BT \simeq E_g$, then we are in the intrinsic regime.

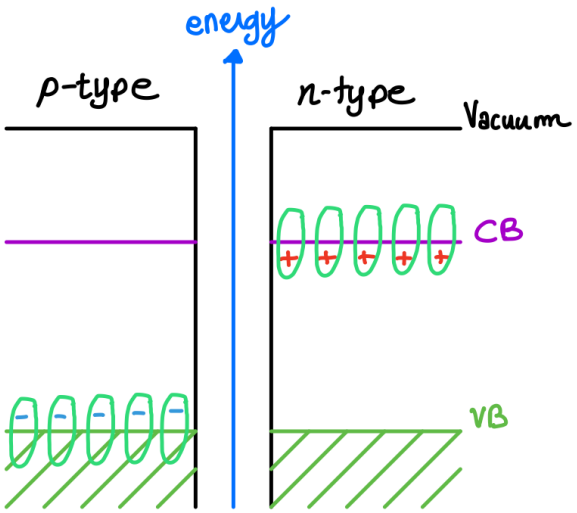
7 Non-homogeneous semi-conductors (n-p junction)



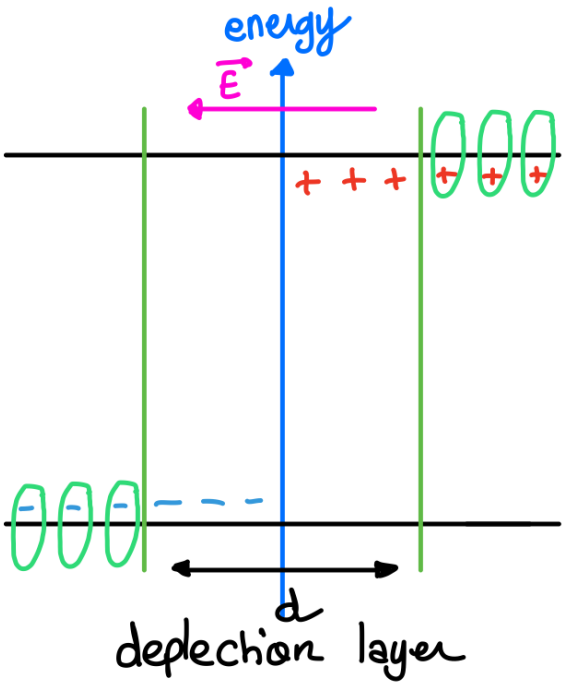
$$N_d(x) = \begin{cases} N_d & x>0 \\ 0 & x<0 \end{cases} \qquad N_a(x) = \begin{cases} 0 & x>0 \\ N_a & x<0 \end{cases}$$

We assume we are in the extrinsic regime carriers in the conduction band for $x > 0$ and in the valence band ($x < 0$). We assume an abrupt junction

The electric field stops the charge transfer



When we make contact,



The electric field stops the charge transfer.

$\phi(x)$ the electrostatic potential. We will mix quantum mechanics (band structure) with classical mechanics. If $\phi(x)$ varies slowly with x, we can take it (for each x) as a constraint that we add

to the electron's energy with the hypothesis of a Maxwell's distribution,

$$\begin{cases} n_c(x) = N_c(T) \exp\left\{ -\dfrac{[\epsilon_c - e\phi(x) - \mu]}{k_B T} \right\} \\ p_v(x) = P_v(T) \exp\left\{ -\dfrac{[\mu - \epsilon_v + e\phi(x)]}{k_B T} \right\} \end{cases}$$

The potential $\phi(x)$ must be determined self-consistently. Far away on the n-side the density of conduction band electrons is very nearly equal to the density N_d of donors, while far away on the p-side the density of valence band holes is very nearly equal to the density N_a of acceptors:

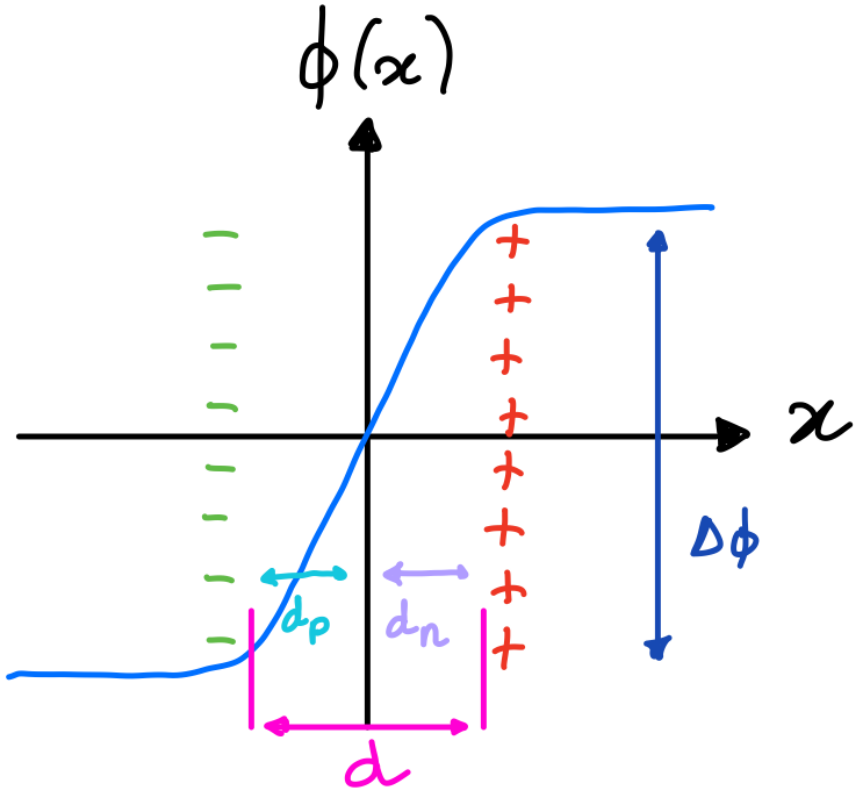
$$\begin{cases} N_d = n_c(+\infty) = N_c(T) \exp\left\{ -\dfrac{[\epsilon_c - e\phi(+\infty) - \mu]}{k_B T} \right\} \\ N_a = p_v(-\infty) = P_v(T) \exp\left\{ -\dfrac{[\mu - \epsilon_v + e\phi(-\infty)]}{k_B T} \right\} \end{cases}$$

Since the entire crystal is in thermal equilibrium, the chemical potential does not vary with position. In particular, the same value of μ appears in either of those equations, this immediately requires that the total potential drop across the junction be given by

$$e\phi(+\infty) - e\phi(-\infty) = \epsilon_c - \epsilon_v + k_B T \ln\left[\frac{N_d N_a}{N_c(T) P_v(T)} \right]$$

That can we written,

$$e\Delta\phi = E_g + k_B T \ln\left[\frac{N_d N_a}{N_c(T) P_v(T)} \right]$$



d is of the order of $10^2 \sim 10^4$ Åand si much larger than the region of dopant's variation.

$$\left.\begin{aligned} \nabla \cdot \vec{E} &= \frac{4\pi\rho}{\epsilon} \\ \vec{E} &= -\nabla\phi \end{aligned}\right\} \nabla^2\phi = -\frac{4\pi\rho}{\epsilon}$$

Poisson's equation (in CGS)

$$\begin{cases} n_c(x) = N_d \exp\left\{-\dfrac{e(\phi(+\infty) - \phi(x))}{k_B T}\right\} \\ p_v(x) = N_a \exp\left\{-\dfrac{e(\phi(x) - \phi(-\infty))}{k_B T}\right\} \end{cases}$$

But, what is $\rho(x)$?

$$\rho(x) = e(N_d(x) - n_c(x)) - e(N_a(x) - p_v(x))$$

where $e(N_d(x) - n_c(x))$ is the non compensated charge for $x > 0$.

$$\begin{cases} x > d_n \longrightarrow \phi(x) \approx \phi(+\infty), & n_c \approx N_d, & \rho(x) \approx 0 \\ x < d_p \longrightarrow \phi(x) \approx \phi(-\infty), & p_v \approx N_a, & \rho(x) \approx 0 \end{cases}$$

$$\begin{cases} 0 < x < d_n \longrightarrow n_c(x) & \approx 0, \\ -d_p < x < 0 \longrightarrow p_v(x) & \approx 0, \end{cases} \qquad e\Delta\phi \approx E_g \gg k_B T, \qquad \begin{matrix} \rho(x) \approx eN_d \\ \rho(x) \approx -eN_a \end{matrix}$$

$$\nabla^2\phi = \frac{4\pi\rho}{\epsilon} = \begin{cases} 0, & x > d_n, \\ -\dfrac{4\pi e N_d}{\epsilon}, & d_n > x > 0, \\ \dfrac{4\pi e N_a}{\epsilon}, & 0 > x > -d_p, \\ 0, & -d_p > x. \end{cases}$$

This immediately integrates to give

$$\phi(x) = \begin{cases} \phi(+\infty), & x > d_n, \\ \phi(+\infty) - \left(\dfrac{2\pi e N_d}{\epsilon}\right)(x - d_n)^2, & d_n > x > 0, \\ \phi(-\infty) + \left(\dfrac{2\pi e N_a}{\epsilon}\right)(x + d_p)^2, & 0 > x > -d_p, \\ \phi(-\infty), & -d_p > x. \end{cases}$$

Continuity of ϕ' at $x = 0$ implies that

$$N_d d_n = N_a d_p$$

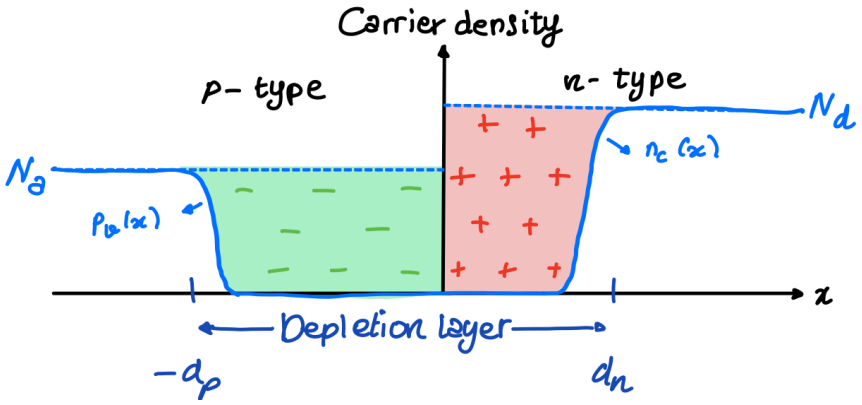
which is just the condition that the excess of positive charge on the n-side of the junction be equal to the excess of negative charge on the p-side. Continuity of ϕ at $x = 0$ requires that

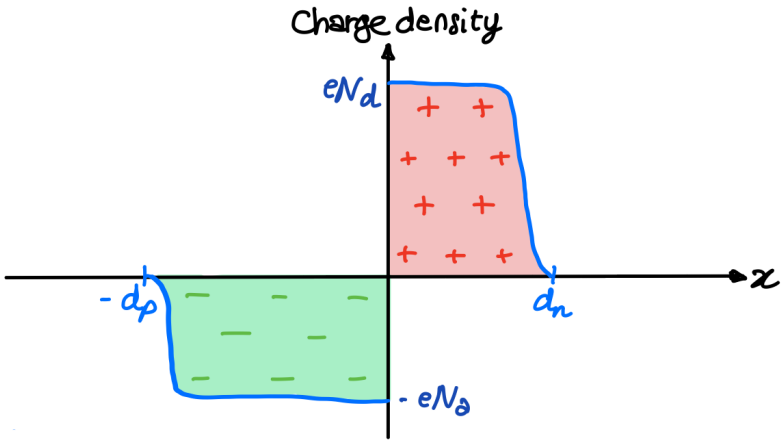
$$\left(\frac{2\pi e}{\epsilon}\right)(N_d d_n^2 + N_a d_p^2) = \phi(+\infty) - \phi(-\infty) = \Delta\phi.$$

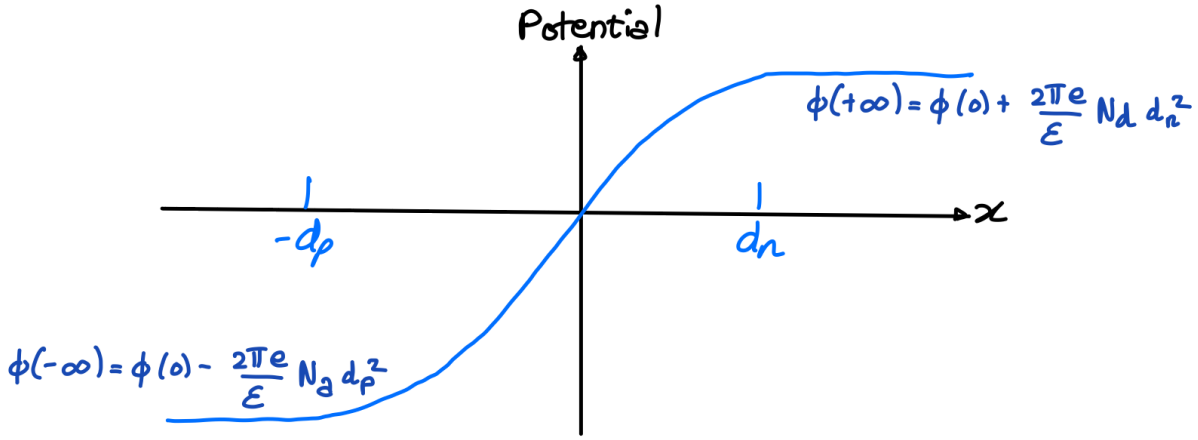
And so,

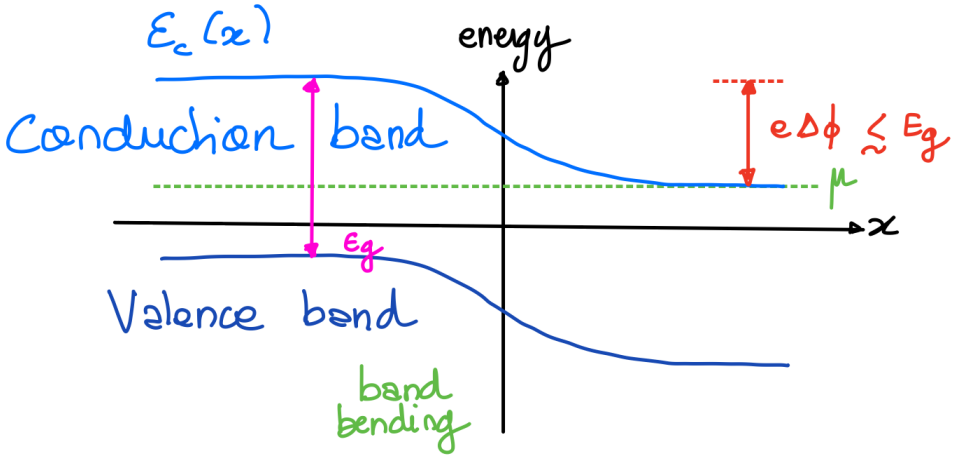
$$d_{n,p}\left(\frac{(N_a/N_d)^{\pm 1}}{(N_a + N_d)}\frac{\epsilon\Delta\phi}{2\pi e}\right)^{1/2}$$

$N_a, N_d \sim 10^{14} \sim 10^{18}$ cm^{-3} imply that $d_n \sim d_p \sim 10^2 \sim 10^4$ Å.




Charge density
eNd
- dp
dn
x
- eNa


Potential
φ(+∞) = φ(0) + 2πe/ε Nd dn²
-dp
dn
x
φ(-∞) = φ(0) - 2πe/ε Na dp²


Ec(x)
energy
Conduction band
eΔφ ≲ Eg
μ
x
Eg
Valence band
band bending

8 Einstein relations

$$\vec{j_e} = -e\vec{J_e}$$

where $\vec{j_e}$ is the current density and $\vec{J_e}$ is the electrical current.

$$\vec{J_e} = -\mu_n n_c \vec{E} - D_n \nabla n_c$$

the first term is the conduction current 'driven by the electric field $\vec{E}$ and the second one is the diffusion current (Fick's law) driven by a gradient of the concentration. This D_n is a diffusion coefficient. Uniform density,

$$\vec{j_e} = -e\vec{J_e} = \sigma\vec{E} = e\mu_n n_c \vec{E}$$

So the mobility μ,

$$\mu_n = \frac{\sigma}{en_c} = \frac{e\tau}{m_e} \qquad\qquad \sigma = \frac{e^2 n_c \tau}{m_e}$$

where σ is the conductivity.

For holes we have,

$$\vec{J_h} = \mu_p p_v \vec{E} - D_p \nabla p_v$$

At equilibrium $\vec{J_e} = 0$,

$$\mu_n n_c \vec{E} \cdot \hat{x} = -\mu_n \frac{\partial \phi}{\partial x} N_c(T) \exp\left(-\frac{\epsilon_c - e\phi(x) - \mu}{k_B T}\right) = -D_n \frac{\partial n_c}{\partial x} = -D_n \frac{e}{k_B T} \frac{\partial \phi}{\partial x} N_c(T) \exp\left(-\frac{\epsilon_c - e\phi(x) - \mu}{k_B T}\right)$$

and so we get,

$$\mu_n = \frac{eD_n}{k_B T}$$

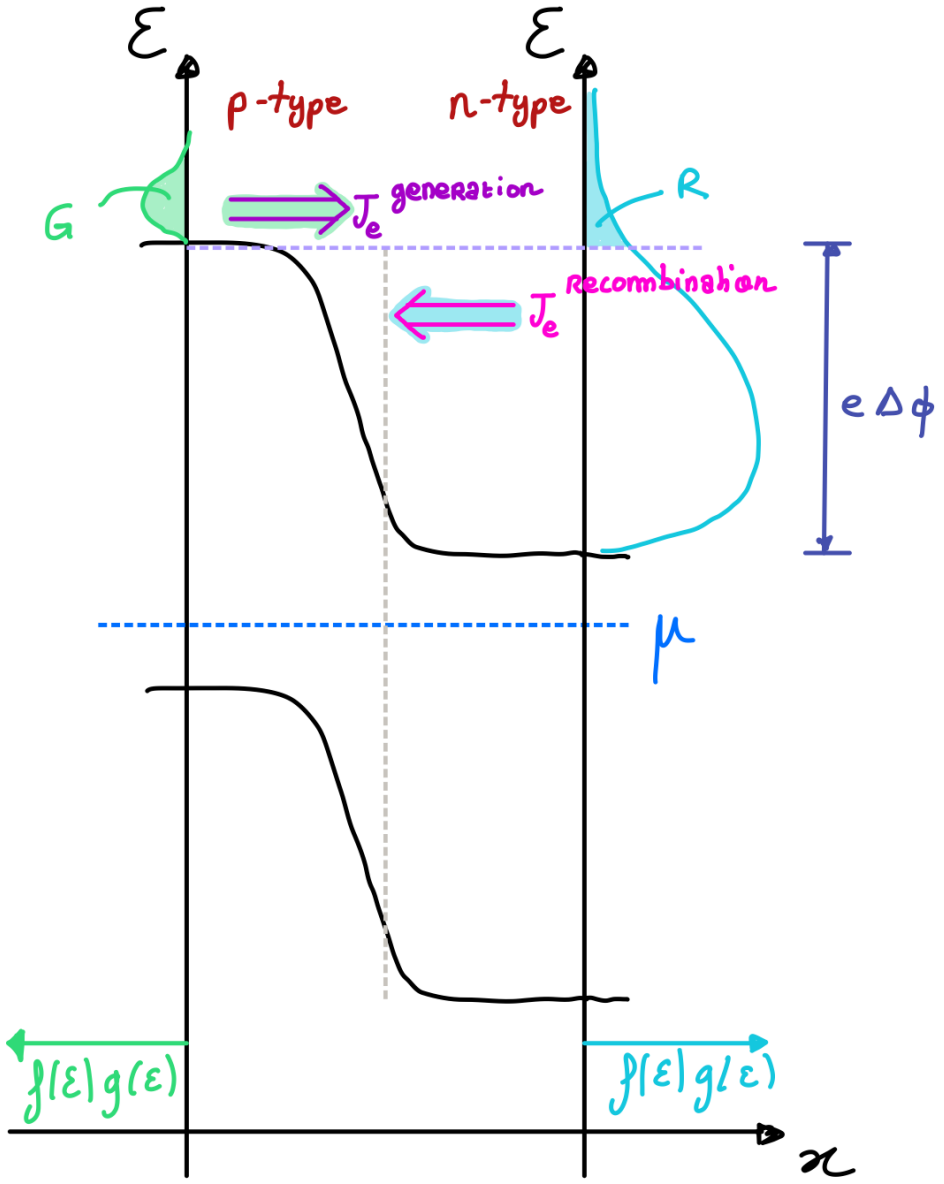
And if we do the same for holes we get,

$$\mu_p = \frac{eD_p}{k_B T}$$

those two are the well known *Einstein's relations*.

9 Generation and recombination currents

At equilibrium, generation of electron-hole pairs through thermal excitation balanced by the recombination (under a time τ_r).



G : minority electrons generated in the p-part, they are taken to the n-part by the field : $J_e^{\text{generation}}$. R : only electrons with energy $> e\phi$ may go to the p part : $J_e^{\text{recombination}}$.

The recombination current,

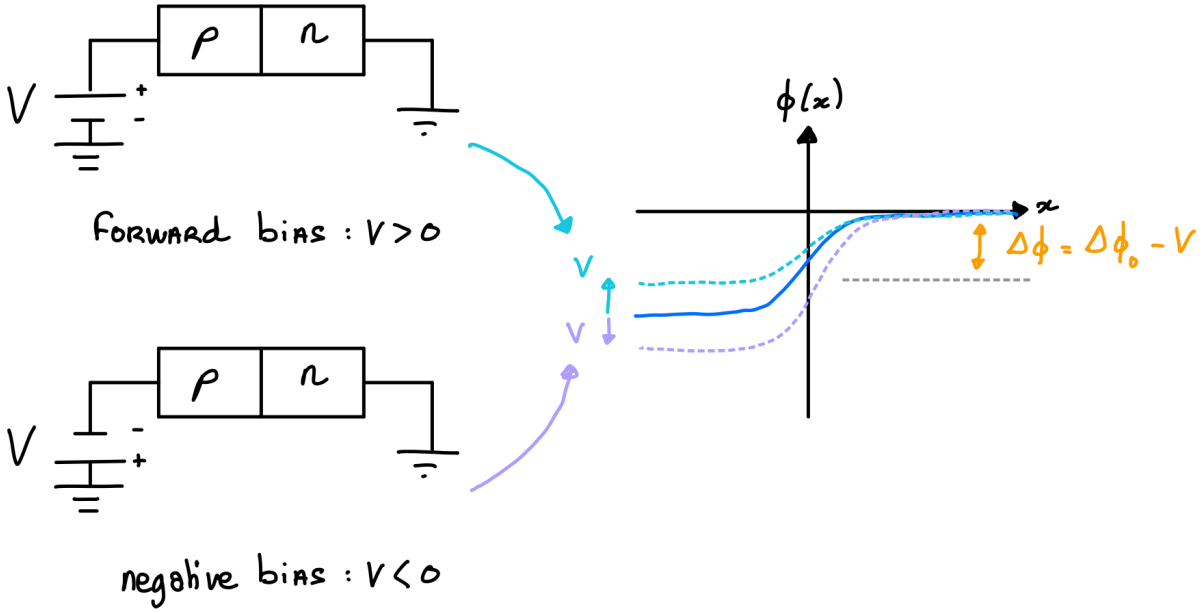
$$J_e^{\text{recombination}} \propto e^{-e\Delta\phi/k_BT}$$

at equilibrium,

$$J_e^{\text{generation}} = J_e^{\text{recombination}}$$

10 Rectification by an np-junction

We polarized the junction by applying a tension V, it is a non-equilibrium situation



$$d_{n,p}(V) = \left(\frac{(N_a/N_d)^{\pm 1}}{N_a + N_d} \frac{\epsilon \Delta\phi}{2\pi e} \right)^{1/2} = d_{n,p}(V=0) \left(1 - \frac{V}{\Delta\phi_0} \right)^{1/2}$$

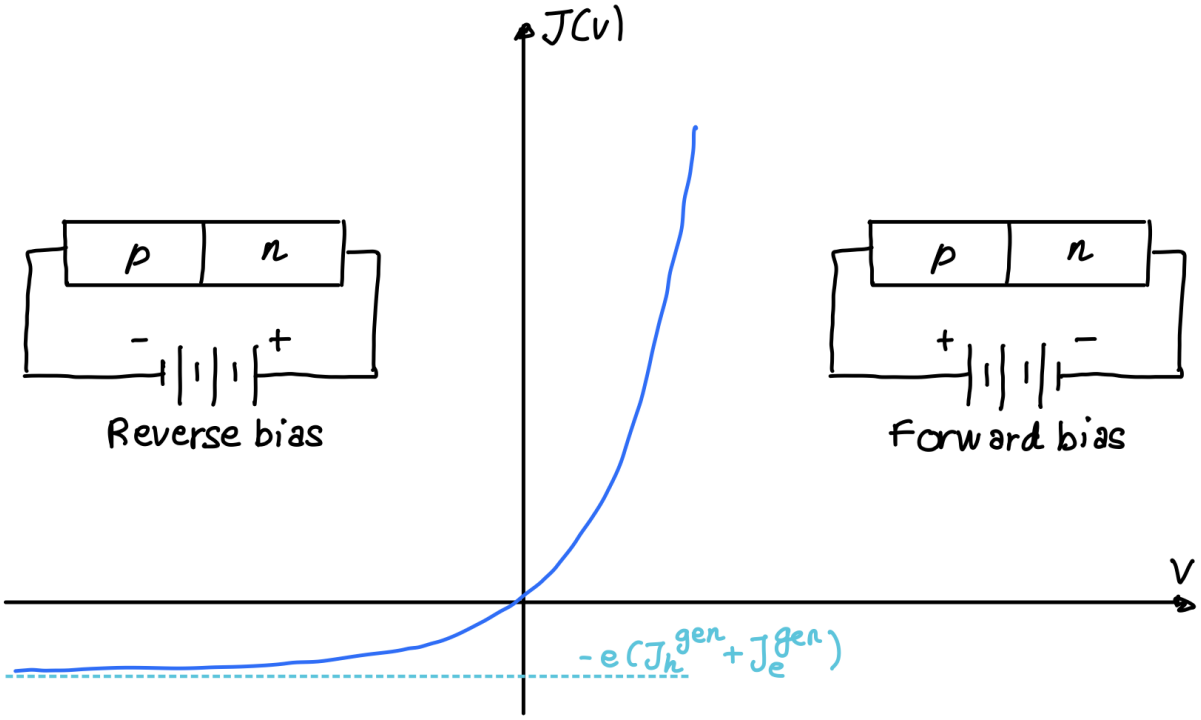
$$\begin{cases} V > 0, & d_n(V) < d_n(V=0), \quad d_p(V) < d_p(V=0) \\ V < 0, & d_n(V) > d_n(V=0), \quad d_p(V) > d_p(V=0) \end{cases}$$

$$J_e^{\text{recombination}} \propto e^{-e(\Delta\phi_0 - V)/k_B T}$$

$$J_e^{\text{recombination}}(V) = J_e^{\text{recombination}}(V=0) e^{eV/k_B T} = J_e^{\text{generation}} e^{eV/k_B T}$$

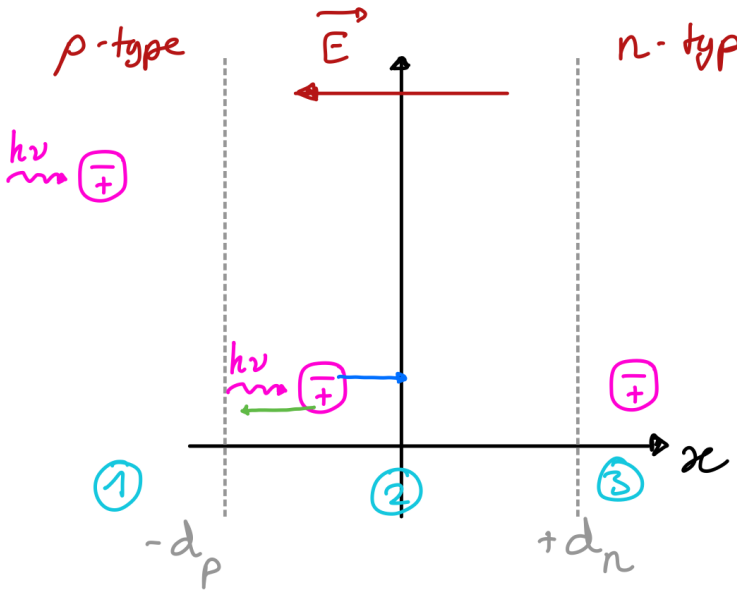
$$J_e^{p \to n} = J_e^{\text{generation}} - J_e^{\text{recombination}} = J_e^{\text{generation}} \left(1 - e^{eV/k_B T} \right)$$

$$\vec{J} = -e\vec{J}_e^{p \to n} + e\vec{J}_h^{p \to n} = e \left(J_h^{\text{generation}} + J_e^{\text{generation}} \right) \left(e^{eV/k_B T} - 1 \right)$$



11 Some additional devices

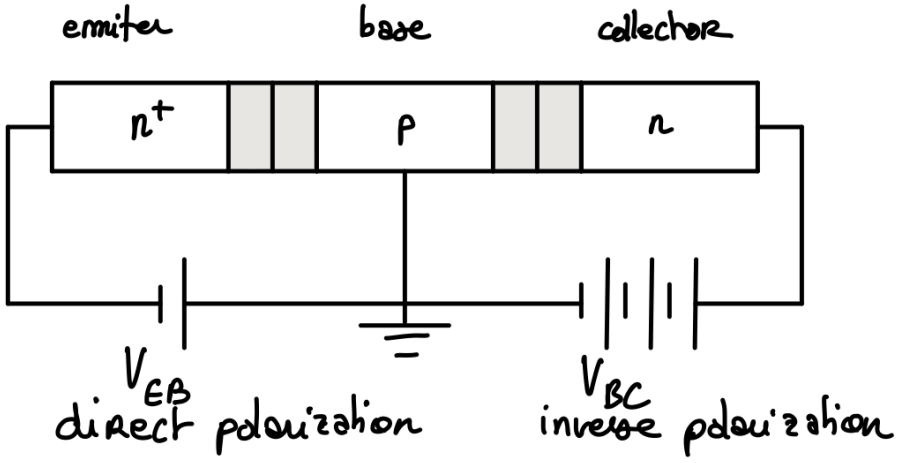
Solar cell, an illuminated *pn*-junction



In region 1 and 3 there is a diffusion photocurrent.

In region 2 there is a generation photocurrent

Bipolar transistors (Bardeen,Brattain, Shockley, 1947, Nobel Prize 1956)



Chapter 2

Magnetism

1 Recall of basic concepts

It all start with Maxwell equation,

$$\vec{\nabla} \cdot \vec{E} = 4\pi\rho \qquad \text{Coulomb}$$

$$\vec{\nabla} \cdot \vec{B} = 0 \qquad \text{Gauss}$$

$$\vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \qquad \text{Faraday}$$

$$\vec{\nabla} \times \vec{B} = \frac{4\pi}{c}\vec{J} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t} \qquad \text{Ampère}$$

in vacuum and with CGS units. The electric field $\vec{E}$ is in volt.cm^{-1}, the magnetic induction $\vec{B}$ in Gauss, the charge density in esu.cm^{-3} (where 1 esu is equal to 3.34×10^{-10} C) and the current density $\vec{J}$ in esu.s^{-1}.cm^{-2}.

We also have Lorentz's law:

$$\vec{F} = e\left(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}\right)$$

In a continuum media, the charge and the current has charges and currents induced by the fields, so we get,

$$\rho = \rho_f + \rho_{\text{ind}}$$

where ρ_f are the free charges and ρ_{ind} induced charge.

So we can define the electric displacement,

$$\vec{D} = \vec{E} + 4\pi\vec{P}$$

where $\vec{P}$ is the polarisation with $\vec{\nabla} \cdot \vec{P} = -\rho_{\text{ind}}$.

$$\vec{\nabla} \cdot \vec{E} = \vec{\nabla} \cdot (\vec{D} - 4\pi\vec{P}) = \vec{\nabla} \cdot \vec{D} + 4\pi\rho_{\text{ind}}$$

And so we get,

$$\boxed{\vec{\nabla} \cdot \vec{D} = 4\pi\rho_f}$$

$$\vec{P} = \chi_e \vec{E}$$

where χ_e is the electric susceptibility.

$$\vec{D} = (1 + 4\pi\chi_e)\vec{E} = \varepsilon\vec{E}$$

where ε is simply the dielectric constant and thus we get,

$$\vec{\nabla} \cdot \vec{E} = \frac{4\pi}{\varepsilon}\rho_f$$

$$\vec{J} = \vec{J}_f + \vec{J}_{\text{ind}}$$

And we can define the magnetic field,

$$\vec{H} = \vec{B} - 4\pi\vec{M}$$

with $\vec{M}$ the magnetisation,

$$\vec{\nabla} \times \vec{M} = \frac{1}{c}\left(\vec{J}_{\text{ind}} - \frac{\partial \vec{P}}{\partial t}\right)$$

$$\begin{aligned}\vec{\nabla} \times \vec{B} &= \frac{4\pi}{c}\left(\vec{J}_f + \vec{J}_{\text{ind}}\right) + \frac{1}{c}\frac{\partial \vec{E}}{\partial t} \\ &= \frac{4\pi}{c}\left(\vec{J}_f + c\vec{\nabla} \times \vec{M} + \frac{\partial \vec{P}}{\partial t}\right) + \frac{1}{c}\left(\frac{\partial \vec{D}}{\partial t} - 4\pi\frac{\partial \vec{P}}{\partial t}\right)\end{aligned}$$

So we get,

$$\boxed{\vec{\nabla} \times \vec{H} = \frac{4\pi}{c}\vec{J}_f + \frac{1}{c}\frac{\partial \vec{D}}{\partial t}}$$

$$\vec{M} = \chi_m \vec{H}$$

with χ_m the magnetic susceptibility.

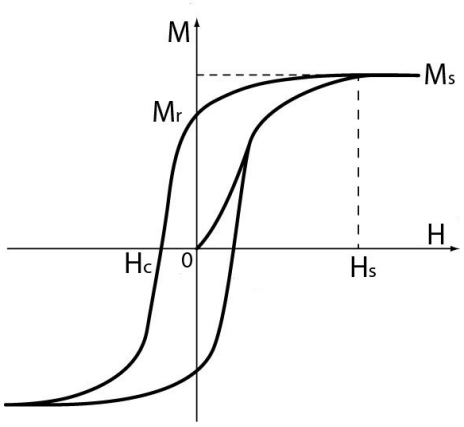
$$\vec{B} = \vec{H} + 4\pi\vec{M} = (1 + 4\pi\chi_m)\vec{H} = \mu\vec{H}$$

where μ is the magnetic permeability.

And so if we put all together the equations,

$$\begin{cases} \vec{\nabla} \cdot \vec{D} = 4\pi\rho_f \\ \vec{\nabla} \cdot \vec{B} = 0 \\ \vec{\nabla} \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t} \\ \vec{\nabla} \times \vec{H} = \frac{4\pi}{c}\vec{J}_f + \frac{1}{c}\frac{\partial \vec{D}}{\partial t} \end{cases}$$

- Paramagnetism
  This mean that $\mu > 1$, $\chi_m > 0$, $\mu - 1 \ll 1$ and $\vec{M}$ is parallel to $\vec{H}$.
- Diamagnetism
  $\mu < 1$, $\chi_m < 0$, $\mu - 1 \ll 1$ and $\vec{M}$ is parallel to $\vec{H}$.
- Ferromagnetism
  $\vec{B} = \vec{F}(\vec{H})$. F is not just a functon of $\vec{H}$, it depend on the magnetic history : hysteresis cycle.

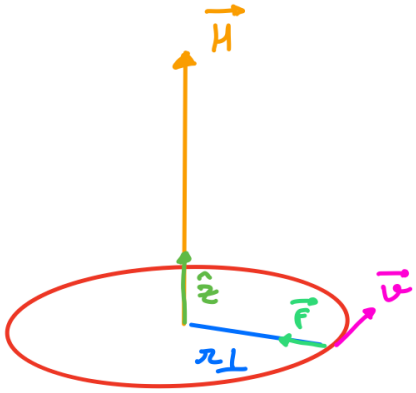


2 Diamagnetism

We can define diamagnetism as the currents that screen the applied field (Lorentz law)

2.1 Langevin approach

Langevin idea is a classical treatment of electrons under a magnetic field.



$$\vec{F}_L = -\frac{e}{c}\vec{v} \times \vec{B} \simeq -\frac{e}{c}\vec{v} \times \vec{H}$$

We have $\vec{B} \simeq \vec{H}$ because $|\chi_m| \ll 1$. Using $w = v/r_\perp$,

$$\vec{F}_L = -\frac{e}{c} w r_\perp H \hat{e}_r = -m r_\perp w^2 \hat{e}_r$$

$$w_{\text{cyclotron}} = \frac{eH}{mc}$$

Larmor's theorem is telling us that the motion of an electron around the nucleus in a magnetic field $\vec{B}$ is, to first order in $\vec{B}$, the same as without $\vec{B}$, superposed to a precession of frequency $w_{\text{Larmor}} = eB/2mc$.

Magnetic moment associated with an electric orbit,

$$\vec{\mu} = \frac{1}{2c}\int \mathrm{d}^3 r \vec{r} \times \vec{J}(r) = -\frac{e}{2mc}\vec{L} = -\frac{e r_\perp^2 w}{2c}\hat{z} = -\frac{e^2 H r_\perp^2}{4mc^2}\hat{z}$$

$$\vec{J}(r) = -\frac{ev}{2\pi r_\perp}\delta(z)\delta(\rho - r_\perp)\vec{e}_\varphi$$

$$I = \int_S \mathrm{d}\vec{S} \cdot \vec{J}(r) = \frac{ev}{2\pi r_\perp}$$

In one atom,

$$r_\perp^2 \longrightarrow \langle r_\perp^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle = \frac{2}{3}\langle r^2 \rangle$$

So we get the magnetic moment induced per atom,

$$\vec{\mu}_{\text{in}} = -\frac{e^2 H}{6mc^2} \sum_{\text{electrons}} \langle r_i^2 \rangle$$

Magnetization per unit volume

$$\vec{M} = \frac{N}{V}\vec{\mu}_{\text{in}} = -\frac{ne^2}{6mc^2}\vec{H} \sum_{\text{electrons}} \langle r_i^2 \rangle$$

And then we get Larmor susceptibility

$$\chi_m = \frac{M}{H} = -\frac{ne^2}{6mc^2} \sum_{\text{electrons}} \langle r_i^2 \rangle$$

This term is always present. It dominates in the case of insulators with atomic shells completed (Noble gases, alkaline ions Li^+, ions F^-). Otherwise other effects dominate.

2.2 Quantum treatment of diamagnetism

$$\vec{p}_i \longrightarrow \vec{p}_i + \frac{e}{c}\vec{A}(\vec{r})$$

For an uniform field $\vec{H}$ we can take the symmetric gauge

$$\vec{A} = -\frac{1}{2}\vec{r} \times \vec{H} \qquad \vec{H} = \vec{\nabla} \times \vec{A} \qquad \vec{\nabla} \cdot \vec{A} = 0$$

$$\mathcal{H} = \frac{1}{2m} \sum_i \left(\vec{p}_i - \frac{e}{2c}\vec{r}_i \times \vec{H} \right)^2 + \sum_i V(r_i) + g_0 \frac{\mu_B}{\hbar} H \sum S_i^z$$

$$\mu_B = \frac{e\hbar}{2mc} = 0.927 \times 10^{-20} \text{ erg.Gauss}^{-1} \qquad g_0 \simeq 2$$

$$\mathcal{H} = \sum_i \left(\frac{p_i^2}{2m} + V(r_i) \right) + \frac{\mu_B}{\hbar}\vec{L} \cdot \vec{H} + \frac{e^2}{8mc^2} H^2 \sum_i (x_i^2 + y_i^2) + g_0 \frac{\mu_B}{\hbar}\vec{S} \cdot \vec{H}$$

Using

$$\vec{L} = \sum_i \vec{L}_i \qquad\qquad \vec{S} = \sum_i \vec{S}_i$$

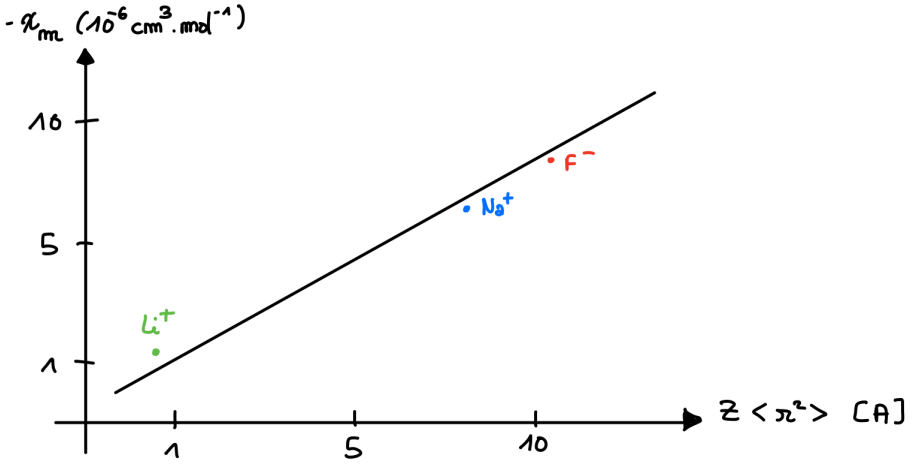
If $|\vec{H}|$ is small, perturbation theory yields

$$\Delta E_m = \frac{\mu_B}{\hbar}\vec{H} \cdot \langle n| \vec{L} + g_0 \vec{S} |n\rangle + \left(\frac{\mu_B}{\hbar}\right)^2 \sum_{n' \neq n} \frac{|\langle n| \vec{H} \cdot (\vec{L} + g_0 \vec{S}) |n'\rangle|^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2} H^2 \langle n| \sum_i (x_i^2 + y_i^2) |n\rangle$$

The linear term is dominant except when it vanishes (when all shells are filled). For low temperatures, only the ground state is populated,

$$M = -\frac{\partial E_0}{\partial H} = -\frac{N}{V}\frac{e^2 H}{6mc^2} \langle 0| \sum_i r_i^2 |0\rangle$$

Which is the same as the previous derivation.



3 Paramagnetism

We can divide in two cases,

1. Insulators having atoms/ions with partially filled shells.
2. Metals : Pauli's paramagnetism.

In the first case, we have a magnetic moment $\vec{\mu}$ (Hund's rules).

SCHEMA

Potential energy,

$$E_{\text{pot}} = -\vec{\mu} \cdot \vec{B} = -\mu B \cos\theta$$

$$\vec{\mu} = -\frac{\mu_B}{\hbar}\left(\vec{L} + g_0\vec{S}\right) = -\frac{\mu_B}{\hbar}g(L,S,J)\vec{J}$$

This equality is made using Weigner-Eckart's theorem. For $g_0 = 2$, we have Landé resulsts in

$$g(L,S,J) = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2(J+1)}$$

3.1 Classical treatment

Average orientation at thermodynamical equilibrium

$$\langle\cos\theta\rangle = \frac{\int \cos\theta e^{\mu H\cos\theta/k_BT}\mathrm{d}\Omega}{\int e^{\mu H\cos\theta/k_BT}\mathrm{d}\Omega}$$

We can rewrite $\mathrm{d}\Omega = \mathrm{d}\varphi\sin\theta\mathrm{d}\theta$.

$$\frac{\int \cos\theta e^{\mu H\cos\theta/k_BT}\mathrm{d}\Omega}{\int e^{\mu H\cos\theta/k_BT}\mathrm{d}\Omega} = \frac{\int_0^\pi \mathrm{d}\theta\cos\theta\sin\theta e^{\mu H\cos\theta/k_BT}}{\int_0^\pi \mathrm{d}\theta\sin\theta e^{\mu H\cos\theta/k_BT}} = \frac{\int_{-1}^{+1}\mathrm{d}z z e^{\mu H z/k_BT}}{\int_{-1}^{+1}\mathrm{d}z e^{\mu H z/k_BT}} = \coth\left(\frac{\mu H}{k_BT}\right) - \frac{k_BT}{\mu H} = \mathcal{L}\left(\frac{\mu H}{k_BT}\right)$$

where $\mathcal{L}(x) = \coth(x) - 1/x$ is Langevin's function.

SCHEMA

There is two regimes.

Regime 1 is when $\mu H \ll k_BT$,

$$\mathcal{L}(x) = \frac{x}{3} + \mathcal{O}(x^3)$$

$$\langle\vec{\mu}\rangle = \mu\langle\cos\theta\rangle = \frac{\mu^2 H}{3k_BT}$$

The susceptibility,

$$\chi_m = n\frac{\langle\vec{\mu}\rangle}{H} = \frac{n\mu^2}{3k_BT} = \frac{C}{T}$$

Which is Curie's law with C Curie's constant.

Regime 2 is when $\mu B \gg k_BT$, on this regime, $\mathcal{L}(x) \to 1$, saturation.

$$M_{\text{saturation}} = n\mu$$

Value's estimations,

$$\mu \sim \mu_B = \frac{e\hbar}{2mc} = 0.6\times10^{-8}\ \text{eV.Gauss}^{-1}$$

At room temperature, meaning $T = 300$ K, we thus get $k_BT \simeq 26$ meV.

For $B = 1$ T$= 10^4$ Gauss, we thus have $\mu_B = 60$ meV which is greater than k_BT.

3.2 Quantum treatment

$$\hat{J}^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle \qquad \hat{J}_z |j,m\rangle = \hbar m |j,m\rangle$$

with $m = -j, -j+1, \cdots, j-1, j$, there is $2j+1$ levels.

$$E_{\text{pot}} = -\vec{\mu} \cdot \vec{B} = \mu_B g m B$$

$$\vec{\mu} = -\frac{\mu_B}{\hbar}(\vec{L} + g\vec{S}) = -\frac{\mu_B}{\hbar} g(L,S,J)\vec{J}$$

$$\begin{aligned} Z = e^{-\beta F} &= \sum_{m=-j}^{j} e^{-\beta \mu_B g m H} \\ &= e^{\beta \mu_B g J H} \sum_{m'=0}^{2j} e^{-\beta \mu_B g m' H} \\ &= e^{\beta \mu_B g J H} \left(\frac{1 - e^{-\beta \mu_B g (2j+1) H}}{1 - e^{-\beta \mu_B g H}} \right) \\ &= \frac{e^{\beta \mu_B g H (j+1/2)} - e^{-\beta \mu_B g H (j+1/2)}}{e^{\beta \mu_B g H/2} - e^{-\beta \mu_B g H/2}} \\ &= \frac{\sinh((j+1/2) g B \mu_B H)}{\sinh(B g \mu_B H/2)} \end{aligned}$$

Remark : with $|\alpha| < 1$,

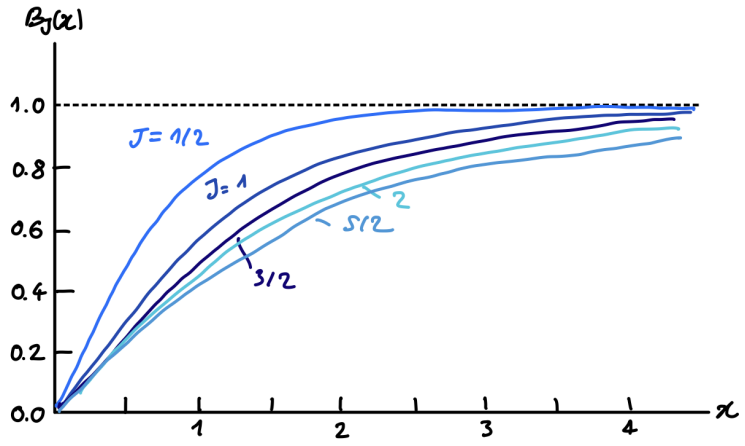
$$\sum_{i=0}^{N} \alpha^n = \frac{1 - \alpha^{N+1}}{1 - \alpha}$$

We know the expression of the magnetization of N ions in a volume V,

$$M = -\frac{N}{V}\frac{\partial F}{\partial H} = \frac{n}{\beta}\left(\frac{\partial \ln Z}{\partial H}\right) = n \mu_B g J B_J \left(\frac{\mu_B g J H}{k_B T}\right)$$

where the Brillouin function $B_J(x)$ is defined by

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



For $J \gg 1$ we recover the Langevin function with $\mu = \mu_B g J$. The small x region is the high-temperature regime : $\mu_B H \ll k_B T$,

$$\coth y \simeq \frac{1}{y}$$

for $y \ll 1$. And so we get

$$B_J(x) \simeq \frac{J+1}{3J} x$$

And thus,

$$M \simeq n\mu_B g \frac{J+1}{3} \frac{\mu_B g J H}{k_B T} = n \frac{(g\mu_B)^2}{3} \frac{J(J+1)}{k_B T} H$$

And if we calculate the magnetic susceptibility,

$$\chi_m = \frac{\partial M}{\partial H} = n \frac{(g\mu_B)^2}{3} \frac{J(J+1)}{k_B T} \sim \frac{1}{T}$$

Which is Curie's law.

The second regime is for larger x, meaning $\mu_B H \gg k_B T$, we have saturation :

$$M = n\mu_B g J = n\mu$$

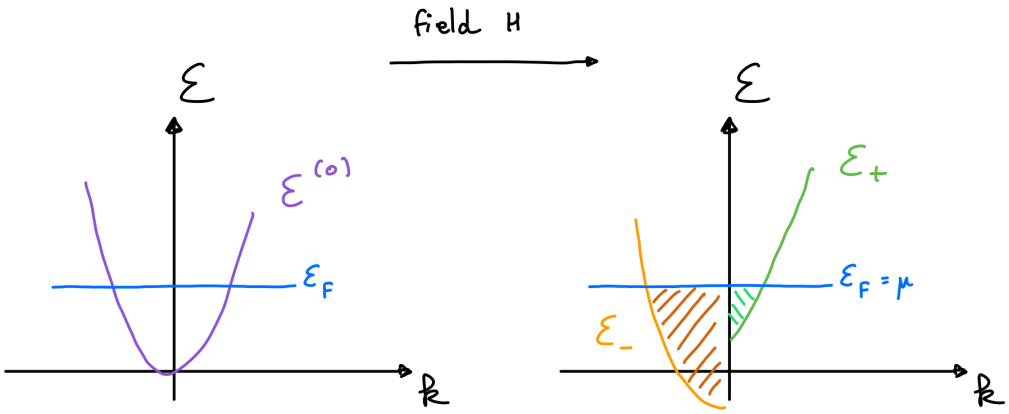
3.3 Pauli's paramagnetism (metals)

A metal is an electron gas. An electron gas has some features, each electron carry a spin $s = 1/2$, we know that they are non-localized, they are correlated by Pauli's exclusion principle. We define $n_\pm$ the number of electrons per unit volume with spin parallel $(+)$ or antiparallel $(-)$ to the applied field H.The magnetization density will be

$$M = -\mu_B (n_+ - n_-)$$

Electron's energy is its kinetic energy plus the Zeeman energy : if the electrons interact with the field only through their magnetic moments, then the only effect of the field is to shift the energy of each electronic level by $\pm\mu_B H$,

$$\mathcal{E}_\pm = \frac{\hbar^2 k^2}{2m} \pm \mu_B H = \mathcal{E}^{(0)} \pm \mu_B H$$



Without H,

$$g_\pm(\mathcal{E}) = \frac{1}{2} g^{(0)}(\mathcal{E})$$

With H,

$$\begin{cases} g_+(\mathcal{E}) = \frac{1}{2} g^{(0)}(\mathcal{E} - \mu_B H) \\ g_-(\mathcal{E}) = \frac{1}{2} g^{(0)}(\mathcal{E} + \mu_B H) \end{cases}$$

The number of electrons per unit volume ofeach spin species is given by

$$n_\pm = \int \mathrm{d}\mathcal{E}\, g_\pm(\mathcal{E}) f(\mathcal{E})$$

where f is the Fermi function

$$f(\mathcal{E}) = \frac{1}{e^{\beta(\mathcal{E}-\mu)} + 1}$$

$\mu_B H \ll \mathcal{E}_F$, it holds even for $H \sim 1$ T.

$$g_\pm(\mathcal{E}) = \frac{1}{2} g^{(0)}(\mathcal{E} \mp \mu_B H) \simeq \frac{1}{2} g^{(0)}(\mathcal{E}) \mp \frac{1}{2} \mu_B H g'(\mathcal{E})$$

$$n_\pm = \frac{1}{2} \int g^{(0)}(\mathcal{E}) f(\epsilon) \mathrm{d}\epsilon \mp \frac{1}{2} \mu_B H \int g'(\mathcal{E}) f(\mathcal{E}) \mathrm{d}\mathcal{E}$$

$$M = \mu_B^2 H \int \mathrm{d}\mathcal{E} g'(\mathcal{E}) f(\mathcal{E}) = -\mu_B^2 H \int \mathrm{d}\mathcal{E} g(\mathcal{E}) f'(\mathcal{E})$$

for a degenerate electron gas, $f'(\mathcal{E} \simeq -\delta(\mathcal{E} - \mathcal{E}_F)$,

$$M = \mu_B^2 H g^{(0)}(\mathcal{E}_F)$$

Pauli susceptibility,

$$\chi^{\text{Pauli}} = \mu_B^2 g^{(0)}(\mathcal{E}_F) = \mu_B \frac{m k_F}{\hbar^2 \pi^2} = \left(\frac{\alpha}{2\pi}\right)^2 (a_0 k_F)$$

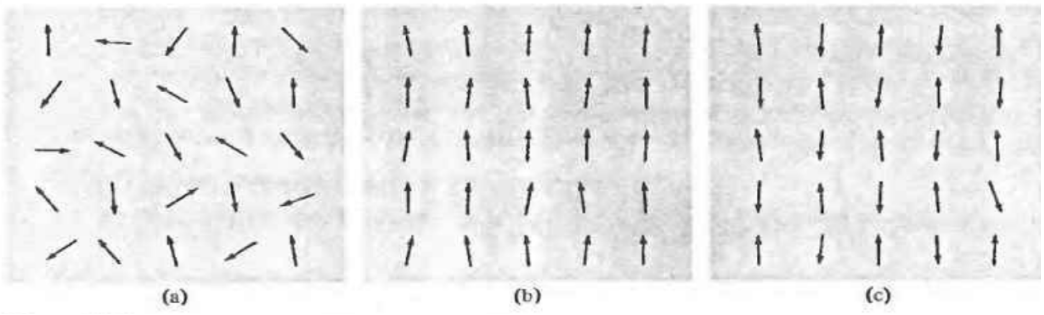
with $\alpha = e^2/\hbar c = 1/137$ the fine structure constant and $a_0 = \hbar^2/mc^2 = 0.52$ Å, the Bohr radius. χ^{Pauli} is relatively independent on temperature. It is much weaker than the Curie susceptibility of ions.

3.4 Diamagnetism of conduction electrons (Landau)

$$\chi^{\text{Landau}} = -\frac{1}{3}\chi^{\text{Pauli}} \longrightarrow \chi^{\text{total}} = \frac{2}{3}\chi^{\text{Pauli}}$$

4 Magnetic interactions

Without pre-existing magnetic moment (diamagnetism). With pre-existing magnetic moment (paramagnetism both localized and itinerant). Without interactions



In the left case, the magnetic moments are not oriented without external field : thermal fluctuations. In the middle case, it is with interactions that favor parallel spins (ferromagnetic coupling).

Before explaining bow magnetic interactions can arise from purely electrostatic couplings, we estimate the direct dipolar interaction energy of two magnetic dipoles $\vec{m}_1$ and $\vec{m}_2$, separated by $\vec{r}$:

$$U = \frac{1}{r^3}[\vec{m}_1 \cdot \vec{m}_2 - 3(\vec{m}_1 \cdot \hat{r})(\vec{m}_2 \cdot \hat{r})]$$

Atomic magnetic dipole moments have a magnitude $m_1 \approx m_2 \approx g\mu_B \approx e\hbar/mc$. Hence the size of U (ignoring its angular dependence) will be

$$U \approx \frac{(g\mu_B)^2}{r^3} \approx \left(\frac{e^2}{\hbar c}\right)\left(\frac{a_0}{r}\right)^3 \frac{e^2}{a_0} \approx \frac{1}{(137)^2}\left(\frac{a_0}{r}\right)^3 \text{ Ry}$$

In a magnetic solid, moments are typically about 2 Åapart, and hence U is no more than 10^{-4} eV. This is minute compared with electrostatic energy differences between atomic states, which are typically a fraction of an electron volt.

4.1 Exchange interaction

To illustrate how the Pauli principle can lead to magnetic effects even when there are no spin-dependent terms in the Hamiltonian, we consider a two-electron system with, a spin-independent Hamiltonian.

Because H does not depend on spin, the general stationary state Ψ will be the product of a purely orbital stationary state whose wave function $\psi(\vec{r}_1, \vec{r}_2)$ satisfies the orbital Schrödinger equation,

$$H\psi = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2)\psi + V(\vec{r}_1, \vec{r}_2)\psi = E\psi$$

with any linear combination of the four spin states

$$|\uparrow\uparrow\rangle\,, \qquad |\uparrow\downarrow\rangle\,, \qquad |\downarrow\uparrow\rangle\,, \qquad |\downarrow\downarrow\rangle\,.$$

We can choose these linear combinations to have definite values of the total spin S, and its component S_z along an axis. The appropriate linear combinations can be tabulated as follows

State	S	S_z	type
$\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle - \lvert\downarrow\uparrow\rangle)$	0	0	singlet
$\lvert\uparrow\uparrow\rangle$	1	1	triplet
$\frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\rangle + \lvert\downarrow\uparrow\rangle)$	1	0	triplet
$\lvert\downarrow\downarrow\rangle$	1	-1	triplet

The difference in energy for the Coulomb interaction (that do not depend on spin),

$$\Delta E \sim e^2 \int \mathrm{d}r_1 \int \mathrm{d}r_2 \frac{\psi^*(r_1, r_2)\psi(r_1, r_2)}{|r_1 - r_2|}$$

If ψ is symmetric, then ΔE is large, but, if ψ is antisymmetric, ΔE is smaller. So the orbital part want to be antisymmetric.

$$\Delta E^{\text{singlet, triplet}} = J - \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)I$$

4.1.1 Effective Hamiltonians

$$H_{\text{eff}} = \frac{p^2}{2m^*} = -\frac{\hbar^2}{2m^*}\nabla^2$$

where m^* is the effective mass. Heisenberg Hamiltonian,

$$H^{\text{spin}} = -2\sum_{\langle ij \rangle} \frac{I_{ij}^{(\text{exchange})}}{\hbar^2} \vec{S}_i \cdot \vec{S}_j$$

$I_{ij}^{(\text{exchange})}$ is the exchange constant, $\langle ij \rangle$ are the nearest neighbors.

Magnetic anisotropy : preferred orientation axis (due to the crystal lattice)

Ising model,

$$H^{\text{Ising}} = -\sum_{\langle ij \rangle} I_{ij} S_i^z S_j^z$$

5 Molecular field (mean field), Pierre Weiss 1907

$$\begin{aligned} H^{\text{spin}} &= -2\sum_{\langle ij \rangle} \frac{I}{\hbar^2} \vec{S}_i \cdot \vec{S}_j \\ &= -\frac{2I}{\hbar^2} \sum_i \vec{S}_i \sum_{j \in \text{nn}} \vec{S}_j \\ &\approx -\frac{I}{\hbar^2} \sum_i \vec{S}_i z \langle \vec{S} \rangle \\ &= -\frac{I}{\hbar^2} z \left(\frac{\hbar}{g\mu_B} \right)^2 \langle \vec{\mu} \rangle \cdot \sum_i \vec{\mu}_i \end{aligned}$$

with z the coordination number and

$$\vec{\mu} = \frac{g\mu_B}{\hbar} \vec{S} \qquad\qquad \vec{M} = n\langle \vec{\mu} \rangle$$

We can write a new field,

$$\vec{B}_m = \frac{zI}{ng^2\mu_B^2}\vec{M} = \gamma\vec{M}$$

with the molecular field constant

$$\gamma = \frac{zI}{ng^2\mu_B^2}$$

$$M = \vec{M}\cdot\vec{z} = n\mu_B gJB_J\left(\frac{\mu_B gJ}{k_B T}\left(H+\gamma M\right)\right)$$

For $J = 1/2$,

$$B_J(x) = \tanh(x)$$

We make the external field $H = 0$ and thus, $x = \beta\mu_B\gamma M$

$$M = n\mu_B\tanh(x) = \frac{x}{\beta\mu_B\gamma} \to \frac{x}{\beta\alpha} = \tanh(x) \qquad \alpha = zI$$

$x = 0$ is always a solution,

$$\beta\alpha < 1 \to T > T_c = \frac{\alpha}{k_B}$$

This is the paramagnetic phase.

$$\beta\alpha > 1 \to T < T_c = \frac{\alpha}{k_B}$$

Two extra solutions, this is the ferromagnetic phase.

$$\beta\alpha = 1 \to T = T_c = \frac{\alpha}{k_B}$$

Phase transition.

Let's make an expansion for $T \simeq T_c$, thus $x_0 \ll 1$,

$$\frac{x}{\beta\alpha} = \tanh(x) \simeq x - \frac{x^3}{3}$$

For $x \neq 0$,

$$x_0^2 = 3\left(1-\frac{1}{\beta\alpha}\right) = 3\left(1-\frac{T}{T_c}\right) = \frac{3}{T_c}(T_c - T) \qquad T < T_c$$

Thus,

$$M \propto (T_c - T)^{\beta}, \qquad \beta = 1/2$$

where β is a critical exponent and M is an order parameter.

If now we take $H \neq 0$ but very small,

$$\frac{M}{n\mu_B} = \frac{x}{\beta\alpha} = \tanh(x + aH) \simeq (x + aH) - \frac{1}{3}(x + aH)^3$$

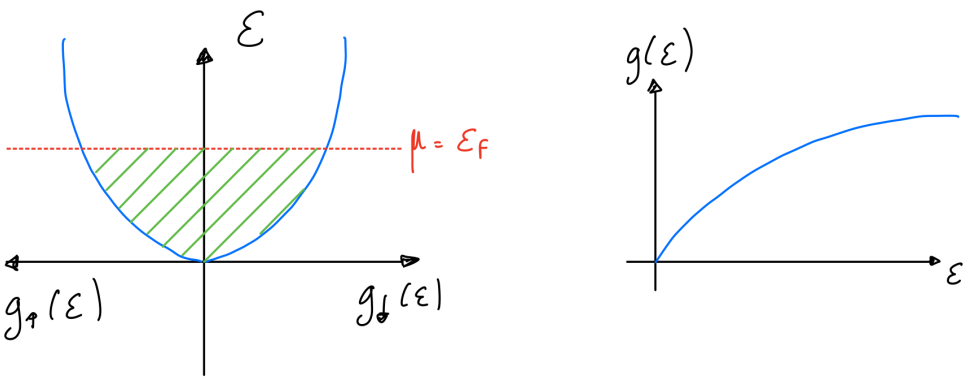
$$x\left(\frac{1}{\beta\alpha} - 1\right) = aH$$

$$x = \frac{\mu_B \gamma M}{k_B T} = \frac{aH}{1/\beta\alpha - 1} - \frac{aHT_c}{T - T_c}$$

$$\chi_m \sim \frac{1}{T - T_c}$$

Curie-Weiss law

6 Stoner - Wohlfarth model for itinerant ferromagnetism



Without interactions,

$$g_{\uparrow\downarrow}(\epsilon) = \frac{1}{2} g^{(0)}(\epsilon)$$

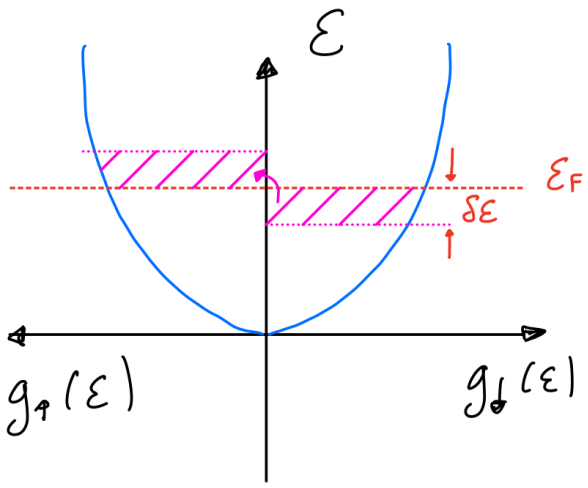
At $T = 0$ and $H = 0$,

$$n_{\uparrow} = n_{\downarrow}$$

With exchange interactions, there is two effects (which compete),

i) Exchange energy, that favors parallel spins,

ii) The single-particle energy favors an alternate in the occupation.



$$\delta n = \frac{1}{2} g^{(0)}(\epsilon_F)\delta\epsilon$$

$$\delta E_b = \delta n \delta\epsilon = \frac{\delta n^2}{g^{(0)}(\epsilon_F)/2} = \left(\frac{M}{\mu_B}\right)^2 \frac{1}{2g^{(0)}(\epsilon_F)} \qquad M = \mu_B(n_\uparrow - n_\downarrow) = 2\mu_B \delta n$$

$$\delta E_m = -\frac{I}{2}\left(\frac{M}{\mu_B}\right)^2$$

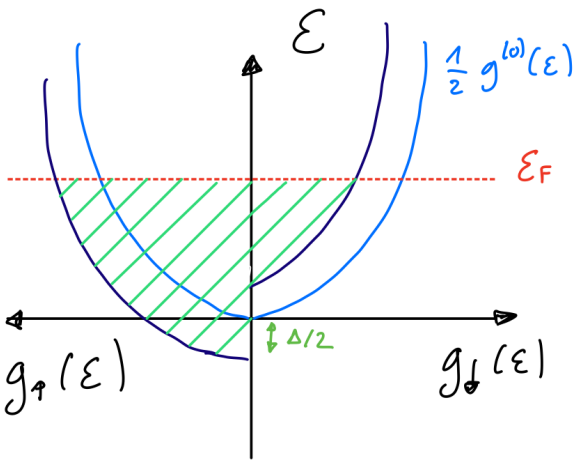
$$\delta E = \delta E_b + \delta E_m = \left(\frac{M}{\mu_B}\right)^2 \frac{1}{2g^{(0)}(\epsilon_F)} \left(1 - I g^{(0)}(\epsilon_F)\right)$$

if $\delta E > 0$, the paramagnetic state is stable, otherwise, if $\delta E < 0$ the paramgnetic state is unstable.

Stoner criterion, if $I g^{(0)}(\epsilon_F) > 1$ we have ferromagnetism.

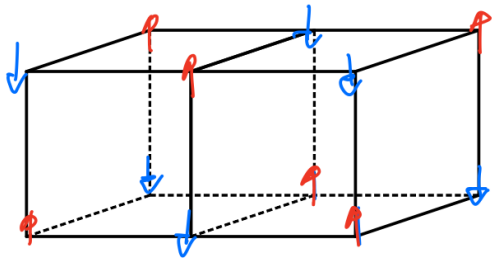
We need $g^{(0)}(\epsilon_F)$ large : d bands, I large : important overlap of the wavefunctions. These are typical of transition metals : Fe, Co, Ni.

Mott-Slater model : the effect of the exchange interaction is that of a uniform magnetic field H_m ($\propto M$)

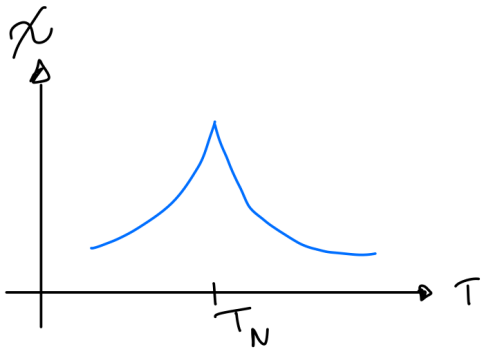


$$\Delta = \epsilon_{k\downarrow} - \epsilon_{k\uparrow} = MH_m$$

7 Antiferromagnetism and ferrimagnetism



$I > 0$ the anti alignment of spins is favored : there is two sub lattices A and B



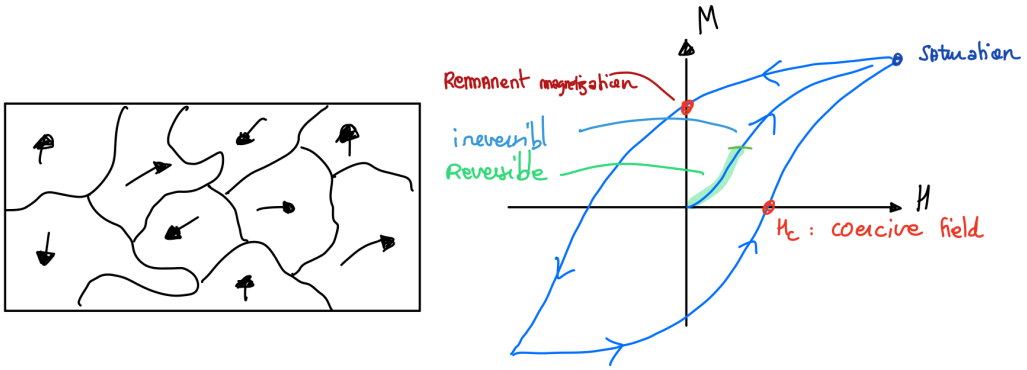
With T_N the Néel temperature below it, we have order, but $M_A = -M_B \neq 0$.

Ferrimagnetic order is when the two sublattices have different magnetization $M_A \neq -M_B$:

$$M = M_A + M_B \neq 0$$

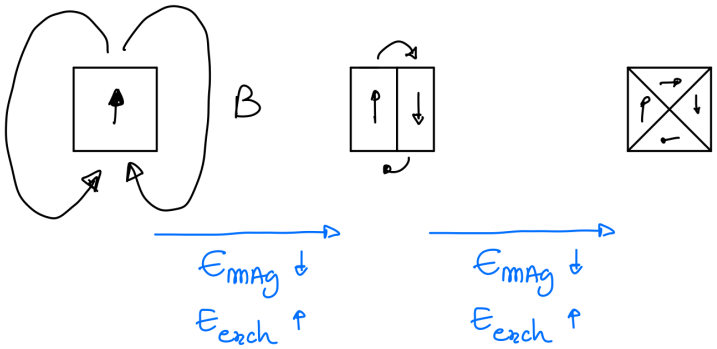
8 Magnetic domains

For Fe, $T_c > 1000°$ K,



Energy of the dipole interaction $1/r^3$. Exchange energy, stronger but falls exponentially with r. Magnetic energy,

$$E_{\text{mag}} = \frac{1}{2c} \int \vec{B}^2 \mathrm{d}r$$



Anisotropy energy is the tendency to have the magnetization along a favorable crystal axis.

Domain wall,

SCHEMA46

The abrupt change is penalized by the exchange energy. The very smooth change is penalized by the anisotropy energy. λ results from the balance in between the exchange and anisotropy energies.

Bloch domain wall : the rotation of the magnetization is in a plane perpendicular to the spins of the two domains

SCHEMA47

Chapter 3

Superconductivity

1 Phenomenology

SCHEMA48

H.K. Onnes 1911 (Leiden). Vanishing resistivity below 4.2 K for Hg. The phenomenon is found in many elements, alloys.

10^{-5} Ω limit in 1911.

SCHEMA49

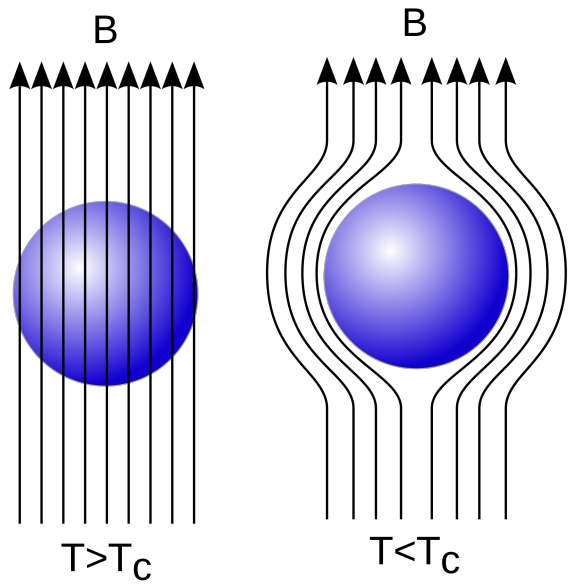
The specific heat has a discontinuity at $T = T_c$

SCHEMA50

$$C_n = C_{n_e} + C_{n_{\text{Phonons}}} = \gamma T + \beta T^3$$

$$C_s \sim e^{-A/k_B T}$$

Meissnes-Ochsenfeld effect (1933) ; perfect diamagnetism exclusion of the magnetic field below T_c



SCHEMA52

2 London equations (F. and H. London 1935)

Recall : electrodynamics in a normal metal

$$\vec{\nabla}\cdot\vec{E}=4\pi\rho \qquad \vec{\nabla}\times\vec{E}=-\frac{1}{c}\frac{\partial\vec{B}}{\partial t}$$

$$\vec{\nabla}\cdot\vec{B}=0 \qquad \vec{\nabla}\times\vec{B}=\frac{4\pi}{c}\vec{J}+\frac{1}{c}\frac{\partial\vec{E}}{\partial t}$$

$$\vec{J}=\sigma\vec{E} \qquad \sigma(\omega)=\frac{\sigma_0}{1-i\omega\tau} \qquad \sigma_0=\frac{ne^2\tau}{m}$$

We consider all temporal dependences $e^{-i\omega t}$, continuity equation,

$$\vec{\nabla}\cdot\vec{J}+\frac{\partial\rho}{\partial t}=0\longrightarrow\vec{\nabla}\cdot\vec{J}(\omega)=i\omega\rho(\omega)$$

$$\vec{\nabla}\cdot\vec{P}=-\rho=\frac{i}{\omega}\vec{\nabla}\cdot\vec{J}\longrightarrow\vec{P}=\frac{i}{\omega}\vec{J}$$

$$\vec{D}=\vec{E}+4\pi\vec{P}=\left(1+\frac{4\pi i}{\omega}\sigma\right)\vec{E}$$

And then the dielectric constant,

$$\epsilon(\omega) = 1 + \frac{4\pi i}{\omega}\sigma = 1 + \frac{4\pi i n e^2 \tau}{m\omega(1 - i\omega\tau)} \overset{\omega\tau \gg 1}{=} 1 - \frac{\omega_p^2}{\omega^2(1 + i/\omega\tau)}$$

With the plasma frequency,

$$\omega_p^2 = \frac{4\pi n e^2}{m}$$

$$\epsilon(\omega) \simeq 1 - \frac{\omega_p^2}{\omega^2}$$

$\omega \ll \omega_p \longrightarrow \epsilon < 0$, $\omega \gg \omega_p \longrightarrow \epsilon > 0$

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = -\vec{\nabla}^2 \vec{E} = \frac{i\omega}{c}\vec{\nabla} \times \vec{B} = \frac{i\omega}{c}\left(\frac{4\pi\sigma}{c} - \frac{i\omega}{c}\right)\vec{E}$$

$$\vec{\nabla}^2 \vec{E} = -\frac{\omega^2}{c^2}\left(1 + i\frac{4\pi\sigma}{\omega}\right)\vec{E} = -\frac{\omega^2}{c^2}\epsilon(\omega)\vec{E}$$

$\epsilon(\omega) > 0$, propagative solution ($\omega > \omega_p$). $\epsilon(\omega) < 0$, exponentially damped solutions ($\omega < \omega_p$).
Perfect conductor $\tau \to +\infty$

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau} \simeq \frac{i}{\omega\tau}\frac{n_s e^2 \tau}{m} = \frac{i}{\omega\Lambda}$$

$$\Lambda = \frac{m}{n_s e^2}$$

$$\vec{J} = \frac{i}{\omega\Lambda}\vec{E} \longrightarrow \dot{J} = -i\omega J = \frac{E}{\Lambda}$$

$$\vec{E} = \frac{\partial}{\partial t}(\Lambda \vec{J})$$

Which is the first London equation
Alternative derivation. Ballistic motion of electrons

$$m\dot{\vec{v}} = -e\vec{E} \longrightarrow \vec{J} = -en_s\vec{v}$$

$$\dot{\vec{J}} = -en_s\dot{\vec{v}} = \frac{e^2 n_s}{m}\vec{E} = \frac{1}{\Lambda}\vec{E}$$

$$\vec{\nabla}\times\vec{E} = \Lambda\frac{\partial}{\partial t}\vec{\nabla}\times\vec{J} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \longrightarrow \frac{\partial}{\partial t}(c\Lambda\vec{\nabla}\times\vec{J}+\vec{B}) = 0$$

In order to obtain the Meissner effect, we must impose that the integration constant vanishes, meaning that

$$\vec{B} = -c\vec{\nabla}\times(\Lambda\vec{J})$$

Which is the second London equation.

So, the London equations,

$$\boxed{\vec{E} = \frac{\partial}{\partial t}(\Lambda\vec{J})} \qquad \boxed{\vec{B} = -c\vec{\nabla}\times(\Lambda\vec{J})} \qquad \Lambda = \frac{m}{n_s e^2}$$

Ampere's law,

$$\vec{\nabla}\times\vec{B} = \frac{4\pi}{c}\vec{J}$$

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{B}) = -\vec{\nabla}^2 B = \frac{4\pi}{c}\vec{\nabla}\times\vec{J} = -\frac{4\pi}{c^2\Lambda}\vec{B}$$

Thus we get the differential equation,

$$\nabla^2 B = \frac{4\pi}{\Lambda c^2}B \qquad\qquad \nabla^2 J = \frac{4\pi}{\Lambda c^2}J$$

SCHEMA52

$$\frac{\partial B_x}{\partial z^2} = \frac{4\pi}{\Lambda c^2}B_x \longrightarrow B_x(z) = B_x^0\exp\Big(-\frac{z}{\lambda}\Big)$$

With

$$\lambda = \left(\frac{\Lambda c^2}{4\pi}\right)^{1/2} = \left(\frac{mc^2}{4\pi n_s e^2}\right)^{1/2}$$

the penetration depth ~ 260 Å.

$$\frac{\partial^2 J_y}{\partial z^2} = \frac{4\pi}{\Lambda c^2}J_y \longrightarrow J_y(z) = J_y^0\exp\Big(-\frac{z}{\lambda}\Big)$$

3 BCS Theory (Bardeen, Cooper, Schrieffer, 1957)

Isotope effect : T_c varies if we change the isotope, this means that electron-phonon coupling is relevant.

We have an attractive interaction between electrons close to the Fermi energy.

SCHEMA53

The first electron polarizes the lattice, and can attract a second electron : it is a retard interaction.

SCHEMA54

$v_{\mathrm{F}} \sim 10^8$ cm/s, $2\pi/\omega_{\mathrm{D}} \sim 10^{-13}$ s. The distance between the two electrons that attract themselves ~ 1000 Å.

In presence of a Fermi sea, the attractive interaction leads to Cooper pairs (a bound state).

SCHEMA55

The two electrons interact only among them, they are excluded from the Fermi

$$-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)\psi(r_1,r_2)+V(r_1,r_2)=E\psi(r_1,r_2)=(\epsilon+2\epsilon_{\mathrm{F}}^0)\psi(r_1,r_2)$$

TABLEAU

$$\psi(\vec{r_1},\vec{r_2})=\sum_k g(\vec{k})e^{i\vec{k}\cdot\vec{r}_1-i\vec{k}\cdot\vec{r}_2}\phi(r_1,r_2)\longrightarrow\sum_k g(\vec{k})\cos\Big(\vec{k}\cdot(\vec{r_1}-\vec{r_2})\Big)\phi_{\mathrm{singlet}}(r_1,r_2)$$

The spin part ϕ is a singlet, meaning a symmetric orbital wavefunction.

$$(\epsilon-2\epsilon_k)g(k)=\sum_{k'>k_{\mathrm{F}}}V_{kk'}g(k'),\qquad\qquad \epsilon_k=\frac{\hbar^2k^2}{2m}-\epsilon_{\mathrm{F}}^0$$

$$V_{kk'}=\frac{1}{\Omega}\int \mathrm{d}rV(r)e^{i(k'-k)\cdot\vec{r}}$$

Describes the scattering of a pair of electrons $(\vec{k},-\vec{k})$ to $(\vec{k'},-\vec{k'})$. The simplification (Cooper 1956),

$$V_{kk'}=\begin{cases}-V \text{ for } 0<\epsilon_k,\epsilon_{k'}<\hbar\omega_{\mathrm{D}}\\ 0 \text{ otherwise}\end{cases}$$

$$V(k)=-\frac{V}{\epsilon-2\epsilon_k}\sum_{k'>k_F}g(k')\longrightarrow\sum_{k>k_F}g(k)-\sum_{k>k_F}\frac{V}{\epsilon-2\epsilon_k}\sum_{k'>k_F}g(k')\longrightarrow\frac{1}{V}=\sum_{k>k_F}\frac{1}{2\epsilon_k-\epsilon}$$

$$\sum_{k>k_F} \frac{1}{2\epsilon_k - \epsilon} \simeq \frac{D(\epsilon_F^0)}{2} \int_0^{\hbar\omega_D} \frac{\mathrm{d}\epsilon_k}{2\epsilon_k - \epsilon} = \frac{D(\epsilon_F^0)}{4} \ln\left(\frac{2\hbar\omega_D - \epsilon}{-\epsilon}\right) = \frac{1}{V}$$

With $D(\epsilon_F^0)$ the density of states at the Fermi level per spin.

$$\epsilon = \frac{2\hbar\omega_D}{1 - \exp(4/VD(\epsilon_F^0))} \simeq -2\hbar\omega_D \exp\left(-\frac{4}{VD(\epsilon_F^0)}\right)$$

The $\simeq$ comes from weak coupling (in general $VD(\epsilon_F^0) < 0.6$). $\epsilon < 0$! it exists a bound state (with respect to ϵ_F). The theory is not analytic in V !