

Condensed Matter Physics I Notes

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1 Lecture 1

The free electron model. This assumes the valance electrons move in a uniform potential. The interactions between electrons and nuclei and other electrons are ignored. The electrons are treated quantum mechanically and Fermi Dirac statistics used.

We consider a wavefunction of the form

$$\psi = e^{i\vec{k} \cdot \vec{r}} \quad (1)$$

These have an energy of

$$E = \frac{\hbar^2 k^2}{2m} \quad (2)$$

We apply periodic boundary conditions, such that $\psi(x, y, z) = \psi(x + L, y, z)$. These give

$$k = \frac{2\pi}{L}(n_x + n_y + n_z) \quad (3)$$

where n_i are integers.

We also derive the density of states per unit volume. Consider the fermi-sphere, full of k values. We compute the number of states existent in a small shell. And then convert this to energy using the above $E(k)$ relation. Electrons are spin 1/2 fermions. We require 2 electrons per state.

$$g(E) = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}. \quad (4)$$

At 0 K we fill out to the fermi wave vector, k_F . We can define the integral from 0 to E_F of the density of states. This gives n . Converting E_F to k_F gives

$$n = \frac{k_F^3}{3\pi^2}. \quad (5)$$

There are limitations to the free electron model. It predicts a fermi sphere when it is in reality distorted. It also cannot explain band gaps, insulators or differences in conductivity. We turn to nearly free electron theory.

We do this firstly in terms of Bragg Diffraction. From some geometry we obtain that the phase difference between an incoming (unprimed) and outgoing (primed) wave scattering off a crystal element is

$$\exp(i(\vec{k} - \vec{k}') \cdot \vec{r}) \quad (6)$$

The amplitude of a wave scattered from a volume element is proportional to the local electron concentration $n(\vec{r})$ and the phase factor. The amplitude of the scattered wave in the direction \vec{k}' is given by

$$\int dV n(\vec{r}) \exp(i(\vec{k} - \vec{k}') \cdot \vec{r}) = \int dV n(\vec{r}) \exp(-i\Delta\vec{k} \cdot \vec{r}) = \sum_G \int dV n_G \exp(i(\vec{G} - \Delta\vec{k}) \cdot \vec{r}) \quad (7)$$

This is only non zero if we have the condition $G = \Delta\vec{k}$. In this case the scattering amplitude becomes

$$F = V n_G \quad (8)$$

The condition is called the Bragg condition. We can manipulate it mathematically:

$$\Delta \vec{k} = \vec{k}' - \vec{k} = \vec{G} \implies \vec{k}' = \vec{k} + \vec{G} \quad (9)$$

If we consider elastic scattering $|\vec{k}'| = |\vec{k}|$ the condition becomes:

$$|\vec{k}|^2 = (\vec{k} + \vec{G})^2. \quad (10)$$

Wavevectors which satisfy this are $\vec{k} = \pm \vec{G}/2$. If we consider these 2 wave vectors,

$$\psi^+ = 2 \cos(\vec{G} \cdot \vec{r}/2) \quad (11)$$

$$\psi^- = 2i \sin(\vec{G} \cdot \vec{r}/2) \quad (12)$$

we get 2 probability densities, one which has high intensity at the nuclei (position vector \vec{r}), $\psi(+)$, and another of which has a low intensity here ψ^- . ψ^+ has a lower energy. This heuristically explains the energy gap at the Brillouin Zone Boundary.

2 Lecture 2

Here we start with the nearly free electron model. This is valid for light elements only. We ignore electron electron repulsion and account for the ionic potential through a perturbation.

$$H = H_0 + V_{ion} \quad (13)$$

We consider normalized plane wave solutions and their associated energy.

$$\psi_k = \frac{\exp i \vec{k} \cdot \vec{r}}{L^{3/2}} \quad (14)$$

$$E_0(k) = \frac{\hbar^2 k^2}{2m} \quad (15)$$

We have, using second order non-degenerate perturbation theory that

$$E(k) = E_0(k) + \sum_{k' \neq k} \frac{|\langle k' | V_{ion} | k \rangle|^2}{E_0(k) - E_0(k')} \quad (16)$$

We note that $\langle k' | V_{ion} | k \rangle$ is the Fourier component. We derived above that this integral was only non-zero if $\Delta \vec{k} = \vec{G}$. This is a problem since the energy difference at 2 points which differ by G is zero. The denominator explodes. We hence require the use of degenerate perturbation theory. We describe the state by a linear combination of the 2 wave vectors:

$$|\psi\rangle = \alpha |k\rangle + \beta |k'\rangle \quad (17)$$

We solve for the energy gap through the matrix equation. We define $\langle k | V_{ion} | k \rangle = \langle k' | V_{ion} | k' \rangle = 0$. These energies are the same since they are degenerate states. Energy assignment is arbitrary.

$$H_{11} = \langle k | H_0 | k \rangle = E_0 \quad (18)$$

$$H_{22} = \langle k' | H_0 | k' \rangle = E_0 \quad (19)$$

$$H_{12} = \langle k | H_0 + V_{ion} | k' \rangle = \langle k | V_{ion} | k' \rangle = V_{-G} = V_G^* \quad (20)$$

$$H_{12} = \langle k | H_0 + V_{ion} | k' \rangle = \langle k' | V_{ion} | k \rangle = V_G \quad (21)$$

From the matrix equation we obtain

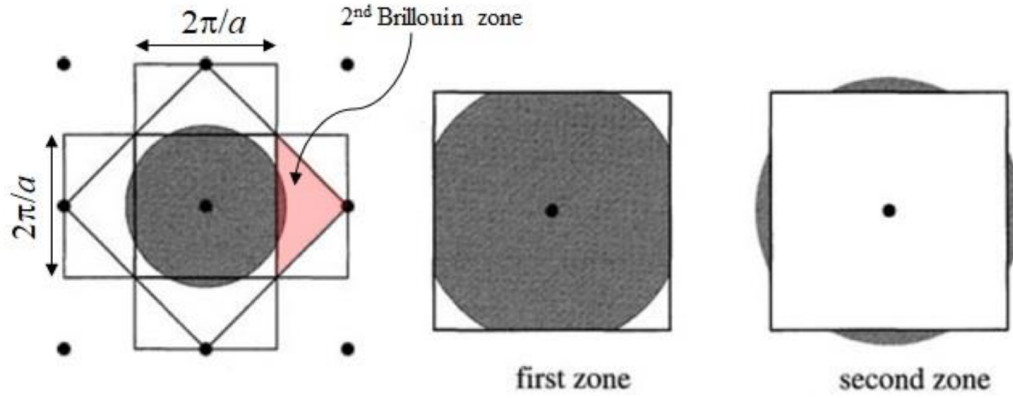


Figure 1: Group 2 metals conduct

$$E_{\pm} = E_0(k) \pm |V_G| \quad (22)$$

This implies that the energy split at the band gap is $2|V_G|$. We also obtain eigenstates where we have an equal contribution from each $\psi(+)$ and $\psi(-)$.

We can obtain a further equation where we attempt to calculate the energy splitting at a small distance δ from each of the Brillouin zone boundary wavevectors. In 1D we consider the wave vectors $k = \frac{\pi}{a} - \delta$ and $k' = -\frac{\pi}{a} - \delta$. We still solve the problem with degenerate perturbation theory. The diagonal elements become more complicated. You substitute each wave vector into the expression for energy. The off diagonal elements don't change. A Taylor expansion is used on the solution of the characteristic equation.

Now, band filling and electrical conductivity. First in one dimension. If we have N atoms in the solid, there are $2N$ states available per Brillouin Zone, due to spin (consider the length of the first BZB and the length taken up by 1 atom). Consider Lithium with $3N$ electrons. It takes up the first BZ and half of the second. It is therefore a conductor. Now consider Helium with $4N$ electrons. It fills the first and second BZ and is an insulator. This isn't always accurate, it predicts divalent metals as insulators.

We study the situation in 2D for a more accurate picture. Consider the competing effects in Figure (1).

- Small band gap: it is energetically favorable to jump the band gap and fill states of a smaller k (less kinetic energy).
- Large band gap: it is energetically favorable not to jump the band gap and to fill states of larger k (higher kinetic energy).

3 Lecture 3

Bloch's Theory offers an exact solution to the Schrödinger equation for a periodic potential. It makes no assumption regarding the interaction strength and works for strong electron-nuclear interaction.

The theory also explains why the electron mean free path, $\lambda = v_F \tau$, is $\sim 10 \text{ \AA}$, which is several times larger than the interatomic spacing $\sim 1-2 \text{ \AA}$.

3.1 Bloch's Theorem: implications of the Algebra

Bloch's Theorem assumes the wavefunction takes the form:

$$\psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{G}}(\vec{k}) \exp(i(\vec{k} + \vec{G}) \cdot \vec{r}) = \left(\sum_{\vec{G}} C_{\vec{G}}(\vec{k}) \exp(i\vec{G} \cdot \vec{r}) \right) \exp(i\vec{k} \cdot \vec{r}) = u(\vec{r}) \exp(i\vec{k} \cdot \vec{r}) \quad (23)$$

Note that $u(\vec{r})$ is a periodic function, since for any lattice translation vector \vec{T} we have $u(\vec{r} + \vec{T}) = u(\vec{r})$.

The solution implies that the electron wavefunction in a crystal is a plane wave whose amplitude is modulated by a periodic potential. The electron wavefunctions can therefore travel freely despite the presence of nuclei.

3.2 Bloch waves and Band structure

The solution to the characteristic Bloch Equation (found through requiring Equation (23) satisfies the Schrödinger Equation) can be approximated. Each reciprocal lattice vector \vec{G} has a characteristic equation. Each equation contains an infinite sum over \vec{G}' :

$$\left(\frac{\hbar^2}{2m} |\vec{k} + \vec{G}|^2 - E \right) C_{\vec{G}} + \sum_{\vec{G}'} C_{\vec{G}'} V_{\vec{G} - \vec{G}'} \quad (24)$$

It is assumed that the potential only depends on a finite number of reciprocal lattice vectors (say N). Fourier Components of V_G for other reciprocal lattice vectors will be zero.

Each (finite) equation in \vec{G} can be written in matrix form, and the energy required for non trivial solutions solved for through the characteristic equation.

The equation gives an N order polynomial in the energy E . Hence, for any given wave vector, there are N energies. This can be understood through the periodicity of the crystal. There is nothing to distinguish $\vec{k} = \vec{G}$ from $\vec{k} = 0$, copies of the $E - k$ distribution curve must be made at each reciprocal lattice point. Extrapolating the additional curves into the first Brillouin Zone accounts for the other energy solutions.

The extended zone scheme can be folded into the First BZ to give the reduced zone scheme.

4 Lecture 4

4.1 Effective Mass of Electrons

In a crystal we have a periodic potential. If we apply external force to the crystal, the electron moves as though this external force AND the force from the periodic potential is acting. Hence $F_{ext} \neq ma$. We introduce effective mass m^* which rectifies this issue:

$$F_{ext} = m^* a \quad (25)$$

m^* is defined with respect to the direction of motion:

$$m_{ij}^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k_i \partial k_j} \right)^{-1} \quad (26)$$

4.2 Magnetic Dipoles and Magnetic Moments

The magnetic moment of a current loop is defined:

$$\mu = IA \quad (27)$$

For an electron with total angular momentum \vec{J} (spin and orbital) we have:

$$\mu = -g_J \gamma \vec{J} \quad (28)$$

For the orbital angular momentum (\vec{l}) in particular, we have:

$$\mu = -\gamma \vec{l} \quad (29)$$

$$\gamma = \frac{e}{2m_e} \quad (30)$$

The Bohr magneton is the smallest unit of the magnetic moment, since the smallest unit of angular momentum is \hbar :

$$\mu_B = \frac{e\hbar}{2m_e} = \gamma\hbar \quad (31)$$

4.3 Magnetic Field Definitions

In vacuum:

$$\vec{B} = \mu_0 \vec{H}, \quad (32)$$

and in material:

$$\vec{B} = \mu_0(\vec{H} + \vec{M}). \quad (33)$$

Here, B is magnetic field measured in Tesla, H is magnetic field strength (A/m) and M is magnetization (A/m).

Magnetic susceptibility is defined

$$\chi = M/H \quad (34)$$

The energy of a magnetic dipole moment in a magnetic field is

$$E = -\vec{\mu} \cdot \vec{B} \quad (35)$$

Magnetization is therefore also defined

$$M = -\frac{dE_{vol}}{dB} \quad (36)$$

and is used for magnetic materials which are **weak**. If $\chi > 0$ the material is paramagnetic and if $\chi < 0$ the material is diamagnetic. χ is not typically used to quantify strength for (anti)ferromagnetic materials.

4.4 Magnetism is Quantum Mechanical

Bohr-van Leeuwen Theorem states: Classical physics predicts zero magnetism at thermal equilibrium. This is justified through the following: consider placing an electron in a magnetic field. Using the Lorentz force:

$$\vec{F} = -e(\vec{v} \times \vec{B}) \quad (37)$$

Hence, the force is perpendicular to the velocity (and displacement), since $dW = \vec{F} \cdot d\vec{s}$, the work done on it is zero. Classically, if no work is done a system should not change in energy and thus not become magnetized.

We can further explore the motion of an electron in a magnetic field. Given

$$\vec{\tau} = \vec{\mu} \times \vec{B} \quad (38)$$

and that

$$\vec{\tau} = \frac{d\vec{l}}{dt} = -\frac{1}{\gamma} \frac{d\vec{\mu}}{dt} \implies \frac{d\vec{\mu}}{dt} = -\gamma(\vec{\mu} \times \vec{B}) \quad (39)$$

The motion is of Larmor precession. Because the angle between the B field and the moment doesn't change, the potential energy of the system doesn't change.

However, we know materials have an energy response to magnetic fields, hence magnetism is Quantum Mechanical in origin.

5 Lecture 5

5.1 Larmor Precession & Precession Frequency

We can show through solving Equation (37) explicitly that the magnetic moment components in Larmor Precession take the form:

$$\mu_x(t) = \mu \sin(\theta) \cos(\omega t) \quad (40)$$

$$\mu_y(t) = \mu \sin(\theta) \sin(\omega t) \quad (41)$$

$$\mu_z(t) = \mu \cos(\theta) \quad (42)$$

Where it is assumed the B field points in the z direction. The precessional frequency is given by

$$\omega = \gamma B = \frac{eB}{2m} \quad (43)$$

5.2 Langevin Theory of Diamagnetism (Classical)

The classical explanation of diamagnetism (an increase in the energy of a subsystem when subject to magnetic field) is through Larmor Precession. It was thought that the **precession** generated a magnetic field which opposed the external B field.

The equation for the magnetic moment or magnetization generated due to precession can be derived through classical arguments. Here, we use the precession frequency to express a time period, and thus obtain current. We then derive susceptibility by assuming that the magnetization was **weak**. This gave:

$$B \approx \mu_0 H \quad (44)$$

$$\chi \approx \frac{M\mu_0}{B} = -\frac{ne^2\mu_0 Z \langle r^2 \rangle}{6m} \quad (45)$$

The most important part here is that the **diamagnetic susceptibility is independent of temperature**. Note that we rectify the idea that the bulk system has zero magnetism by considering "partial orbits".

5.3 Quantum Hamiltonian in a Magnetic Field

The Hamiltonian for a charged particle in a magnetic field (neglecting the spin orbit interaction) is

$$\hat{H} = \frac{(\vec{p} + e\vec{A})^2}{2m} + V + g_s \gamma \vec{B} \cdot \vec{s}. \quad (46)$$

We can set the gauge to be symmetric:

$$\vec{A}(\vec{r}) = (\vec{B} \times \vec{r})/2 \quad (47)$$

we obtain:

$$\hat{H} = \left(\frac{\vec{p}^2}{2m} + V \right) + \gamma \vec{B} \cdot (\vec{l} + g_s \vec{s}) + \frac{e^2}{8m} (\vec{B} \times \vec{r})^2 \quad (48)$$

The first term is standard, the second is the paramagnetic term and the third is the diamagnetic term (it is always present, though sometimes overpowered by the paramagnetic term).

The expected energy shift due to the diamagnetic term is calculated through standard QM. The B field is always assumed along z . The expectation for x^2 and y^2 are assumed equal to $\langle r^2 \rangle / 3$. Magnetism is derived through $-\frac{dE}{dB}$ and susceptibility equal to that derived in classical magnetism.

5.4 Anisotropy in Materials with Delocalized Electrons

In materials like benzene and graphite, delocalized electrons increase $\langle r^2 \rangle$ which implies stronger diamagnetism.

The susceptibility is also anisotropic. Note that in the derivation of χ quantum mechanically, we assumed that \vec{B} and \vec{r} were perpendicular. However if they are parallel the values of χ is minimized.

6 Lecture 6

6.1 Quantum Mechanical Angular Momentum

In QM, only the total magnitude and one component of the angular momentum (usually the z one) can be known simultaneously. We have for a generalized angular momentum \vec{J} , given usually by the QM sum of the spin and orbital angular momentum:

$$|\vec{J}| = \sqrt{j(j+1)}\hbar \quad (49)$$

$$j_z = m_j\hbar : |m_j| \leq j \quad (50)$$

We can then derive the energy of a magnetic dipole moment with angular momentum \vec{J} in a magnetic field pointing in the z direction as

$$\vec{\mu}_j = -g_j\gamma\vec{J} \implies E = -\vec{\mu}_j \cdot \vec{B} = -\mu_{j_z}B = g_j\gamma J_z B = g_j\gamma\hbar m_j B = g_j\mu_B m_j B \quad (51)$$

6.2 Spin Orbit Coupling

Spin orbit coupling arises due to proton orbiting about the electron in the electron's frame of reference. The energy of an electron now has dependence on the total angular momentum \vec{J} . The spin orbit interaction energy is given by

$$\Delta E = -\vec{\mu}_s \cdot \vec{B} = \frac{1}{2mc^2r} \frac{dV}{dr} \vec{s} \cdot \vec{l} \quad (52)$$

where $\vec{s} \cdot \vec{l}$ is

$$\vec{s} \cdot \vec{l} = \frac{\hbar^2}{2} [j(j+1) - s(s+1) - l(l+1)] \quad (53)$$

This leads to energy level splitting, the interaction is much greater for heavy atoms with large $V(r)$ terms. Energy splittings are of the order 10^{-4} eV, much smaller than the eV separation of atomic energy levels.

6.3 Multi-electron atoms & LS coupling

In atoms we want to minimize energy. The energy has 2 contributions, that from the Coulomb interaction and that from Spin Orbit Coupling. In **light** atoms it is assumed the **Coulomb** interaction dominates. This energy is minimized first in **LS Coupling**. To achieve this the following are maximized individually (in this order):

- The spin angular momentum. Parallel spins minimize the coulomb repulsion since the spatial wavefunction is required to be antisymmetric.

- The orbital angular momentum. Electrons must move in the same direction of orbit.

Only after this do we choose the value of J which minimizes the spin orbit energy. This is $|L - S|$ if the band is less than half full and $|L + S|$ if the band is more than half full.

6.4 Magnetism in Multi-electron Atoms

It can be shown that the paramagnetic part of the Hamiltonian in Equation (46) after the energy splitting due to spin orbit coupling is included is:

$$\gamma g_j \vec{B} \cdot \vec{J} \quad (54)$$

where

$$g_j = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \quad (55)$$

Atom with full shells and $S = L = J = 0$ do not have a contributing paramagnetic term and are diamagnetic materials. Atoms with incomplete shells are paramagnetic.

7 Lecture 7

7.1 Langevin Theory of Paramagnetism (Classical Approach)

A material with no long range magnetic order is classified as paramagnetic. The average magnetic dipole moment and hence magnetization and susceptibility can be calculated through Maxwell Boltzmann Statistics. It is assumed that each dipole is randomly oriented and independent of the next.

Note that the angular density of states is proportional to the area of the sphere ($2\pi \sin(\theta)$). The proportionality constant to give the number of states cancels. For the expectation of ratio of magnetization to saturation magnetization (where all dipoles are aligned) is:

$$L(y) = \frac{\mu_z}{\mu} = \frac{M}{M_s} = \coth(y) - \frac{1}{y} \quad (56)$$

$L(y)$ is called the Langevin function and y is:

$$y = \frac{\mu B}{k_B T} \quad (57)$$

In the limit of weak field (small y), $\coth(y) = \frac{y}{3} + \frac{1}{y}$ and $L(y)$ becomes:

$$\frac{\mu_z}{\mu} = \frac{M}{M_s} = \frac{\mu B}{3k_B T} \quad (58)$$

Since the material is only weakly paramagnetic we can approximate

$$\chi \approx \frac{M \mu_0}{B} = \frac{n \mu_0 \mu^2}{3k_B T} \propto \frac{1}{T} \quad (59)$$

This is called Curie's Law.

7.2 Quantum Paramagnetism

To analyze paramagnetism quantum mechanically we discretize the j_z into $2j + 1$ values. We use classical Maxwell Boltzmann Statistics to calculate the expectation of the magnetic moment. The expectation value of the magnetic moment for $J = 1/2$ is:

$$\langle \mu_z \rangle = \mu_B \tanh\left(\frac{\mu_B B}{k_B T}\right) \quad (60)$$

Again, in the weak field limit we obtain $\tanh(y) \approx y$ and hence

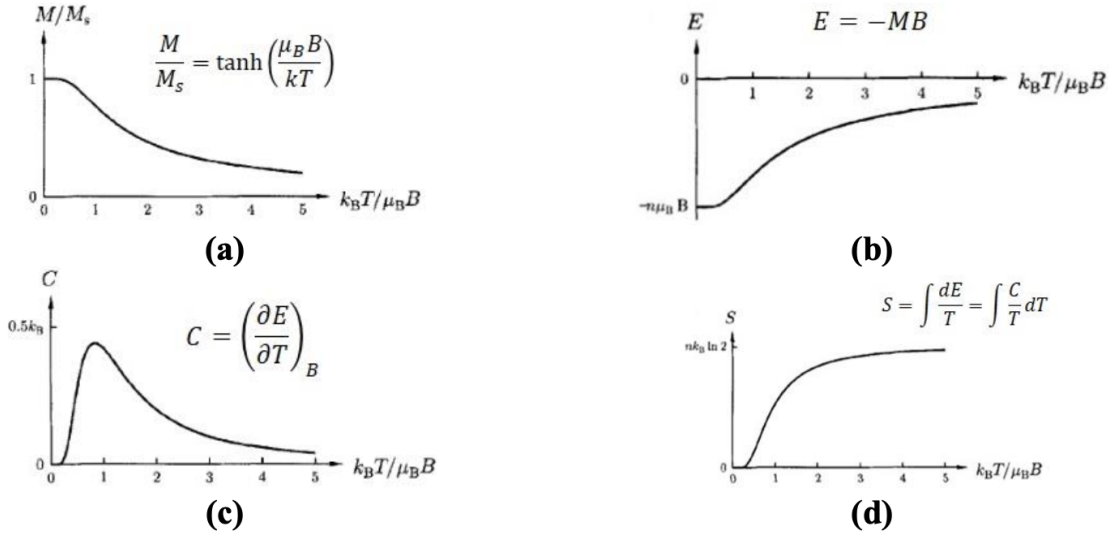


Figure 2: Thermodynamics properties of $J=1/2$ paramagnetic solid.

$$\frac{\mu_z}{\mu_B} = \frac{M}{M_s} = \frac{\mu_B B}{k_B T} \implies \chi = \frac{n\mu_0\mu_B^2}{k_B T} \quad (61)$$

Note the missing factor of 3 on the denominator when compared to the classical case. We again obtain the Curie law stated above, with the exact value of χ being a factor of 3 larger.

We can derive for the general case of $2j+1$ m_j values and obtain the **Brillouin function**. As $J \rightarrow \infty$ the magnetization approaches that predicted by Langevin Theory. This function has trigonometric dependence in $y = \frac{gJ\mu_B JB}{k_B T}$. To visualize M for a given y , find where the 2 curves intersect.

7.3 Thermodynamic Properties of Paramagnetic Solids

There are 4 key thermodynamic properties predicted of a $J = 1/2$ paramagnetic system. They are depicted in Figure (2):

- Magnetization. The magnetization increases toward M_s as temperature decreases or magnetic field increases. Graph (a).
- Energy. It is a mirror image of the magnetization. $E = -\vec{M} \cdot \vec{B}$. Graph (b).
- Heat Capacity. The derivative of the energy curve with respect to temperature while held at a constant magnetic field. Shows a **Schottky anomaly**. The moments are aligned due to low temperatures to the left of the peak and a small change in temperature changes the magnetization and hence energy dramatically. The moments are as disordered as they can be far past the right of the peak, hence the heat capacity drops to zero. Graph (c).
- Entropy. This is given as $S = \int \frac{C}{T} dT$. It's value increases with T and saturates at high temperatures. Graph (d).

7.4 Adiabatic Cooling

The process for adiabatic cooling is shown in Figure (3). It is as follows:

- Initial cooling to a temperature T_i in zero field.
- Isothermal magnetization (entropy decrease at constant T).

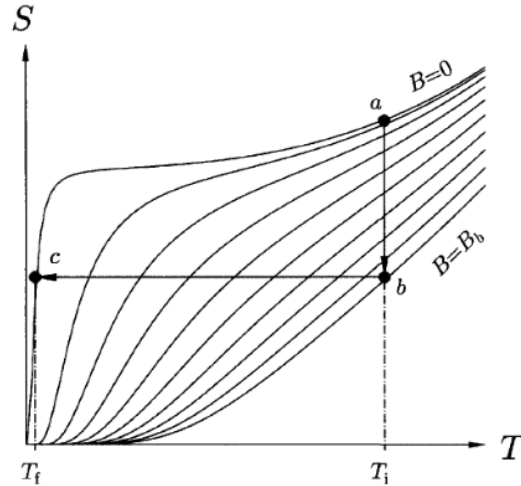


Figure 3: Adiabatic cooling

- Adiabatic demagnetization (field turned off without heat exchange). Spin disorder increases entropy, hence to maintain a fixed S , the lattice cools down.

8 Lecture 8

We now move to studying **ferromagnetism** and **anti-ferromagnetism**. These materials show long range magnetic order.

8.1 Pauli Exclusion Principle and Symmetry

Electrons are indistinguishable fermions. Their total wavefunction must be antisymmetric:

- If the spin wavefunction is anti-symmetric (called the singlet state), then the spatial wavefunction must be symmetric.
- If the spin wavefunction is symmetric (called the triplet state), then the spatial wavefunction must be anti-symmetric.

8.2 Exchange Interaction

The symmetries of the wavefunction dictate the coulomb repulsion energy. This is quantified through the **exchange interaction**. This adds an additional term to the magnetic Hamiltonian. The sum is just over all electrons:

$$\hat{H}_{mag} = \sum_{i,j} -J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_i \gamma g_J \vec{B} \cdot \vec{J}_i + \frac{e^2}{8m} (\vec{B} \times \vec{r})^2 \quad (62)$$

Looking to the sign of J_{ij} :

- Positive: parallel spins, hence the triplet state are favored. E.g. in a single atom in Hund's rule. **Ferromagnetic materials are defined through a positive J_{ij}** , they hence show long range alignment of spins.
- Negative: anti-parallel spins and hence the singlet state are favored. E.g. if spatial wavefunctions symmetric in covalent bonding.

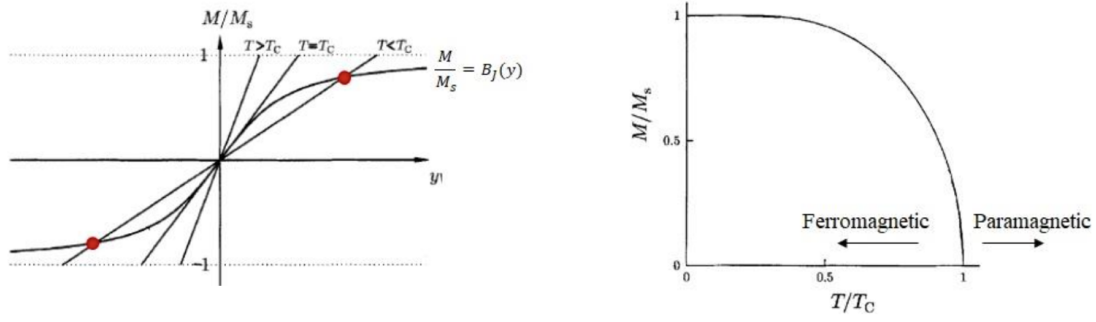


Figure 4: The temperature dependence of spontaneous magnetization

8.3 Weiss Theory of Ferromagnetism

In the Weiss Theory of Ferromagnetism, a molecular field, B_{mf} is defined:

$$\vec{B}_{mf} = \frac{1}{\gamma g_J} \sum_{i,j} -J_{i,j} \vec{S}_j = \lambda \vec{M} \quad (63)$$

The magnetic Hamiltonian in the $L = 0$ state, where we assume the diamagnetic contribution is negligible becomes:

$$\hat{H}_{mag} = \sum_i \gamma g_J \vec{S}_i \cdot (\vec{B} + \vec{B}_{mf}) \quad (64)$$

8.4 Spontaneous Magnetization and the Critical Temperature

To solve for the magnetization, we use the paramagnetic result, replacing \vec{B} with $\vec{B} + \vec{B}_{mf}$. We obtain:

$$\frac{M}{M_s} = B_J(y) \quad (65)$$

where B_J is the Brillouin Function and y now takes the form:

$$y = \frac{g_J \mu_B J}{k_B T} (B + \lambda M) \quad (66)$$

Consider a case with no external \vec{B} field and gradually increase the temperature (decrease y): see Figure (5). Above the critical temperature T_c we have non-zero spontaneous magnetization, and above it we do not and the material has undergone a second order phase transition to a paramagnet. T_c is called the Curie Temperature.

8.5 Magnetic Susceptibility of the Paramagnetic Phase

Above T_c we can quantify a χ . Again we assume a small B field, approximate B_J using a Taylor expansion and quantify $\chi = \frac{M \mu_0}{B}$ to obtain the Curie Weiss law:

$$\chi \propto \frac{1}{T - T_c} \quad (67)$$

9 Lecture 9

9.1 Magneto-crystalline Anisotropy

In metals, some electron orbital are subject to greater coulomb repulsion than others and thus become distorted, this distortion (called orbital quenching) gives an $L = 0$ sate along certain axis. The

reduction from the expected angular momentum to zero gives rise to different magnetization properties in different directions.

Many ferromagnetic materials therefore have an 'easy axis of magnetization'. There is an energy penalty to magnetize in any direction which is not 'easy'.

For hexagonal crystals, made from Basal Planes, the energy penalty per unit volume when magnetizing at an angle θ to the easy axis is:

$$E = K_1 \sin^2(\theta) + K_2 \sin^4(\theta) \quad (68)$$

K_1 and K_2 constants.

9.2 Anti-ferromagnetism and Weiss Theory

Anti-ferromagnetic order is such that neighboring spins are anti aligned. The exchange constant is therefore negative to minimize the coulomb interaction. Weiss Theory divides the lattice into 2 sub lattices, spin up (+) and down (-). The molecular field due to each sub lattice is defined:

$$\vec{B}_{mf} = -|\lambda|\vec{M}_{\mp} = |\lambda|\vec{M}_{\pm} \quad (69)$$

where we have changed the sign from that defined for ferromagnets (since J_{ij} has). Again, we adapt the magnetic Hamiltonian

$$\hat{H}_{mag} = \sum_i \gamma g_J \vec{S}_i \cdot (\vec{B} + \vec{B}_{mf}^{\mp}) = \sum_i \gamma g_J \vec{S}_i \cdot (\vec{B} - |\lambda|\vec{M}^{\mp}) \quad (70)$$

and use the result from paramagnetic materials:

$$\frac{M^{\pm}}{M_s} = B_J(y^{\pm}) \quad (71)$$

where B_J is the Brillouin Function and y now takes another form:

$$y^{\pm} = \frac{gJ\mu_B J}{k_B T} (B - |\lambda|M^{\mp}) \quad (72)$$

9.3 Above the Néel Temperature (T_N)

We can study the spontaneous magnetization of each **sub-lattice** at zero applied magnetic field. If we increase the temperature (and decrease y), we introduce disorder and at T_N create a paramagnet. This is called the Néel Temperature. We can find the susceptibility of an anti-ferromagnet turned paramagnet by approximating (70) under small y^{\pm} . Note that this is only valid at high temperatures and thus small M^{\mp} . We obtain:

$$\chi \propto \frac{1}{T + T_N} \quad (73)$$

9.4 Anti-ferromagnet susceptibility below T_N

χ depends on the direction in which the magnetic field is applied:

- Field Parallel to \vec{M} : At 0 K, the magnetic field cannot flip the anti aligned lattice and χ is zero. Higher temperatures tend to introduce disorder into the spin alignment. The magnetic field works to restore order to the sub-lattice it is aligned to.
- Field perpendicular to \vec{M} : A partial tilt in \vec{M} is obtained. A full tilt is prevented by the energy penalty due to magneto crystalline anisotropy.

The temperature dependence of each applied field is shown in Figure (5)

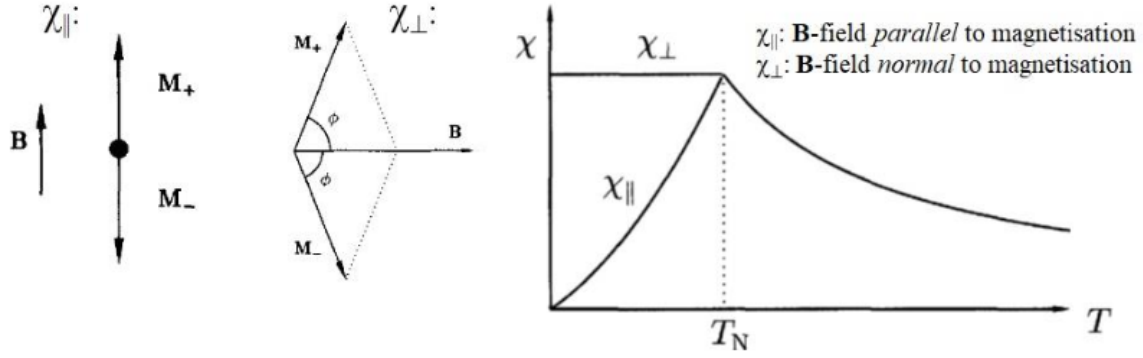


Figure 5: Anisotropic susceptibility of an anti ferromagnet

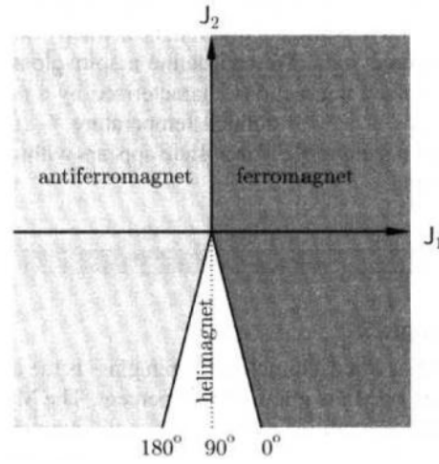


Figure 6: Helimagnetic stability

9.5 Helimagnetism

This is where the spin vector rotates by an angle θ between successive planes. We can determine the conditions which favor Helimagnetic ordering through:

$$E = -2NS^2(J_1 \cos(\theta) + J_2 \cos(2\theta)) \quad (74)$$

Here, N is the number of atoms in the plane and the factor of 2 is included to account for the fact that atoms at i interact with those both above and below their plane at $i \pm 1$ and $i \pm 2$.

We can extremize this by differentiating to obtain:

$$\cos(\theta) = -\frac{J_1}{4J_2} \quad (75)$$

The minimum energy is obtained when $J_2 < 0$ (second derivative test). The Helimagnetism stability region is shown in Figure (6)

10 Lecture 10

10.1 Low Temperature Magnetization in Ferromagnets

We can take the low temperature limit of the Weiss Theory of ferromagnetism. $y \rightarrow \infty$, and obtain that the magnetism is predicted to fall off exponentially. This is not what we see in experiment. It actually drops faster than predicted.

The Weiss model assumes that disorder is introduced by a full spin flip (which is a high energy process). There is an alternative mechanism for generating spin disorder which has a lower activation energy. This is the formation of **spin waves**.

10.2 Equation of Motion for a Spin Wave

We can produce a non-rigorous derivation of the equation of motion for spin waves. We consider a constant $J_{ij} = J_{ex}$ and that atoms only interact with their nearest neighbors.

$$\sum_{i,j} -J_{ij} \vec{S}_i \cdot \vec{S}_j = \sum_j -2J_{ex} \vec{S}_j \cdot \vec{S}_{j+1} \quad (76)$$

If we consider an atom at sight j , the energy contribution from its interaction with nearest neighbors is:

$$-2J_{ex} \vec{S}_j \cdot (\vec{S}_{j-1} + \vec{S}_{j+1}) \quad (77)$$

This is obtained from substituting $j-1, j$ into the sum above. The magnetic moment caused by an atom at position j is $\mu_j = -g_s \gamma S_j$. We can substitute this to obtain

$$-\vec{\mu}_j \cdot \frac{-2J_{ex}}{g_s \gamma} (\vec{S}_{j-1} + \vec{S}_{j+1}) \quad (78)$$

We can consider the right hand part of this equation to be an effective magnetic field (since $E = \vec{\mu} \cdot \vec{B}$). We can therefore derive a torque ($\vec{\tau}$) on the moment:

$$\vec{\tau} = \frac{d\vec{S}_j}{dt} = \vec{\mu}_j \times \vec{B}_{eff} \quad (79)$$

Following the math and adding in an extra factor of \hbar from QM we obtain:

$$\frac{d\vec{S}_j}{dt} = \frac{2J_{ex}}{\hbar} [\vec{S}_j \times (\vec{S}_{j-1} + \vec{S}_{j+1})] \quad (80)$$

Assuming that the spins are roughly parallel to the z axis (such that $S^z \approx S$ and computing the cross product gives us an equation for each component of S^i .

We can derive a dispersion relation for the spins (angular frequency vs momentum) through assuming wave-like solutions of the form:

$$S_j^i = A \exp i(qja - \omega t) \quad (81)$$

Substitution of these solutions into each equation implies there is a 90 degree phase difference between S^x and S^y , while $S^z \approx S$. The motion is therefore cyclical about the z axis.

The energy momentum relationship obtained from the above relationship is:

$$\hbar\omega = 4J_{ex}S(1 - \cos(qa)) \quad (82)$$

For a given q the spin wave can take 1 fixed energy. The energy is also quantized since the allowed wave vectors q are quantized by the discrete atomic lattice ($q = \hbar k$). The dispersion diagram is shown in Figure (7). Spin-waves are thought of as quasi-particles called magnons.

10.3 Quantum Mechanical Interpretation

Define $|0\rangle$ as the quantum mechanical state where all spins are aligned. Define $|j\rangle$ as that where the spin at site j is flipped. It can be shown that $|j\rangle$ is not an eigen-state of \hat{H}_{mag} . The excited state $|q\rangle$ that is an eigen-state of \hat{H}_{mag} is a superposition of spin flips spread over all N atoms:

$$|q\rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqja} |j\rangle \quad (83)$$

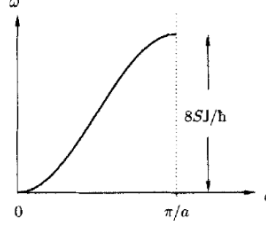


Figure 7: Magnon dispersion relation

Magnons with a long wavelength (i.e. small q), have a very small formation energy $\hbar\omega$. The change in angular momentum due to a single spin flip is 1, hence magnons are bosons.

11 Lecture 11

11.1 Bloch's $T^{3/2}$ Law for Ferromagnets

At low temperatures magnetization decreases from M_s according to:

$$\Delta M \propto T^{3/2} \quad (84)$$

This is due to the thermal excitation of magnons, where 1 magnon corresponds to 1 spin flip. We can derive ΔM from Bose-Einstein Statistics:

$$\Delta M \propto \int g_m(E) f_{BE}(E) dE \quad (85)$$

To derive the density of states at low temperatures we can take a small angle approximation on Equation (80). This shows the energy is proportional to q^2 . Furthermore, magnons are plane waves, where q satisfies the boundary conditions: $q = \frac{mL}{2\pi}$. We therefore take inspiration from the electron density of states and state it proportional to \sqrt{E} .

11.2 Demagnetising Fields and Domain Formation

From Maxwell's Equations:

$$\nabla \cdot \vec{B} = 0 \implies \nabla \cdot \vec{M} = -\nabla \cdot \vec{H} \quad (86)$$

A uniform magnetization creates a non-zero $\nabla \cdot \vec{M}$ at the free surfaces. A demagnetizing field \vec{H}_d must then be present. Now, recall $E = -\vec{\mu} \cdot \vec{B} = -\vec{M} \cdot \mu_0 \vec{H}_d$. This would increase the energy of the crystal (since the 2 are antiparallel).

To reduce the energy of magnetic materials, the ferromagnets split into magnetic domains. The optimal configuration minimizes the external magnetic field lines through aligning \vec{M} along the surfaces.

11.3 Domain Wall types

On crossing domain walls magnetic moments must change their orientation. This happens gradually over N atoms. The number of atoms the re-ordering happens over is determined by 2 opposing factors:

- Exchange Energy (alignment of spins).
- Anisotropic energy density (direction of easy axis of magnetization).

Two neighboring domain walls have antiparallel spins. The reordering of spins can either happen parallel to the domain wall (Bloch walls) or in a plane perpendicular to the domain wall (Néel walls), Figure (8).

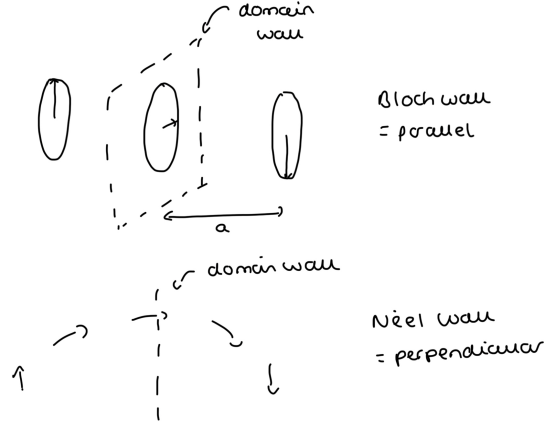


Figure 8: Magnetic Moment Re-ordering

11.4 Domain wall Energy and Width

Analyzing each of the competing factors:

- Exchange energy: Considering the exchange to act between nearest neighbors: $E_{nn} = -2J_{ex}\vec{S}_j \cdot \vec{S}_{j+1}$. If the spins were perfectly aligned: $E_{tot} = -2J_{ex}S^2N$. If the spins are aligned at some angle $\Delta\theta$: $E = -2J_{ex}NS^2\cos(\Delta\theta)$. Assuming $\Delta\theta$ is small and calculating an energy difference, we can obtain the energy per unit area. We assume each spin takes an area of $1/a^2$ and obtain:

$$\sigma_1 = \frac{J_{ex}(S\pi)^2}{Na^2} \quad (87)$$

Hence, a minimization in exchange energy occurs with a large N .

- Anisotropic energy density: Recall that you pay an energy penalty when magnetizing along an axis which is not easy. The energy density introduced by this anisotropy is given by:

$$\Delta E = \sum_i K \sin^2(i\Delta\theta) \quad (88)$$

which can be expressed as an integral assuming $\Delta\theta$ small and N large:

$$E = \frac{1}{\Delta\theta} \int_0^\pi K \sin^2(\theta) d\theta = \frac{N}{\pi} \int_0^\pi K \sin^2(\theta) d\theta = \frac{NK}{2} \quad (89)$$

The energy per unit **area** (parallel to the domain wall) is then

$$\sigma_2 = \frac{NKa}{2} \quad (90)$$

Hence, the anisotropy contribution favors a small N .

We can sum the contributions, differentiate and minimize to obtain an equilibrium N :

$$N = \pi S \sqrt{\frac{2J_{ex}}{Ka^3}} \quad (91)$$

implying:

$$\sigma_T = \pi S \sqrt{\frac{2J_{ex}K}{a}} \quad (92)$$

Hence, we prefer a low anisotropy constant and a small exchange energy.

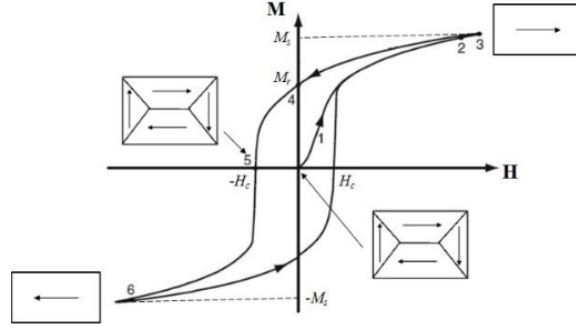


Figure 9: Hysteresis Loop

11.5 Magnetic Hysteresis

Hysteresis arises due to domain wall pinning cause by defects, Figure (9). We lose an energy equal to

$$E = \oint \vec{M} \cdot d\vec{B} \quad (93)$$

per magnetization cycle.

Soft magnets have small hysteresis loops and easy wall motion. Easy wall motion is allowed by wide domain walls, hence soft magnets have large J_{ex} and small K . Hard magnets have large hysteresis loops, which imply difficult domain wall motion. This is governed by narrow domain walls (a small J_{ex} and large K).

12 Lecture 12

Here we develop a band theory of magnetic materials. This models magnetism in metals arising from delocalize conduction electrons, unlike in an insulator where it comes from localized magnetic moments.

12.1 Pauli Paramagnetism

Considering the spin up, spin down density of states $g(E) \propto \sqrt{E}$. If we apply a magnetic field, the energy of the associated magnetic moments increases or decreases dependent on if they are anti-aligned or aligned:

$$\Delta E = \pm \mu_B B \quad (94)$$

All electrons must be below E_F must be occupied at zero Kelvin. Hence the anti-aligned moments are transferred to the aligned segment. This leads to a net magnetization:

$$M = \mu_B (\Delta n_{\downarrow} - \Delta n_{\uparrow}) \quad (95)$$

We can assume that it it only moments within $\mu_B B$ of E_F which change energy, hence:

$$M = g(E_F) \mu_B^2 B \quad (96)$$

From this, and the definition of the density of states we can derive the magnetic susceptibility, which is **independent of temperature**. This is unlike Curie's Law for isolated magnetic moments in paramagnetism.

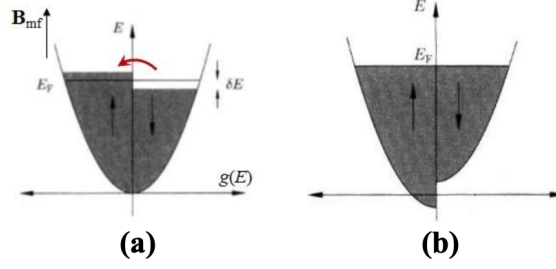


Figure 10: Spontaneous magnetization in metallic ferromagnets

12.2 Ferromagnetism in Metals

Recall Ferromagnetic materials have an internal molecular field B_{mf} , characterized by the exchange interaction. This internal field leads to the transfer of electrons from the anti-aligned band to the aligned band, leading to a spontaneous magnetization. See Figure (10) There are 2 competing effects which limit the transfer electrons:

- The increase in kinetic energy of the transferred electrons. We calculate this thorough:

$$\Delta KE = \left(\frac{1}{2} g(E_F) \delta E \right) \delta E \quad (97)$$

- The decrease in potential energy of these electrons, this can be calculated through

$$\Delta PE = - \int \vec{B} \cdot d\vec{M} = - \int \lambda M' dM' = - \frac{\lambda M^2}{2} \quad (98)$$

Using M from earlier:

$$\Delta PE = - \frac{1}{2} (\lambda \mu_B^2) [g(E_F) \delta E]^2 \quad (99)$$

The term $U = \lambda \mu_B^2$ is called the Coulomb energy.

The net exchange in energy for a metallic ferromagnet is therefore:

$$\Delta E = \frac{1}{2} g(E_F) (\delta E)^2 [1 - U g(E_F)] < 0 \quad (100)$$

giving the **Stoner Criterion**:

$$U g(E_F) > 1 \quad (101)$$

For effective ferromagnets we therefore require a large U or a large $g(E_F)$. The latter condition is most likely in transitions metals where the valance electrons are in d-orbitals: $g(E_{fd}) \gg g(E_{fs})$, Figure (11).

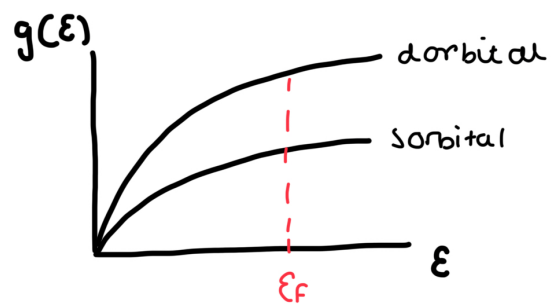


Figure 11: d and s orbital density of states