Solid State Physics I Examination

28th October 2015

This is a closed book exam. You are not allowed to bring books, notes etc. You can use a basic or scientific calculator, but no other electronic equipment having capabilities to display or pronounce the course content.

Do not forget to indicate your full name and student number on **each** sheet. Please write in a clear way!

Total points: 60.

This has exam has been drafted by J. Ye and verified by M. A. Loi

Date: 21/10/2015   Date: 21/10/2015
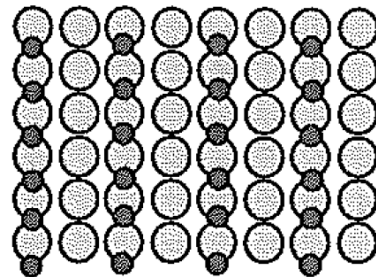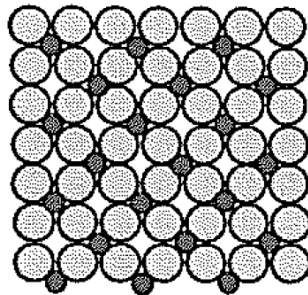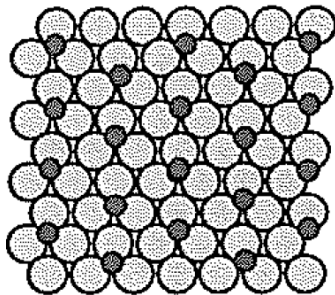
J. Ye   M. A. Loi

1) **Crystal structure (5 points).**

   a. Sketch the structure of ***body centered cubic***, ***face centered cubic*** and ***hexagonally close packed*** crystal. For each crystal structure, identify the basis vectors for the primitive cells.

   b. Indicate the planes with indices $(100), (110), (111), (300)$ and $(\bar{1}00)$ for simple cubic structure and show the atomic configuration in each plane.

   c. Find the primitive cell of the following 2D crystals:

Answer to question 1:

a.

BCC   FCC   HCP

b.

(100)   (110)   (111)

(300)   ($\bar{1}$00)

(100)   (110)   (111)
($\bar{1}$00)
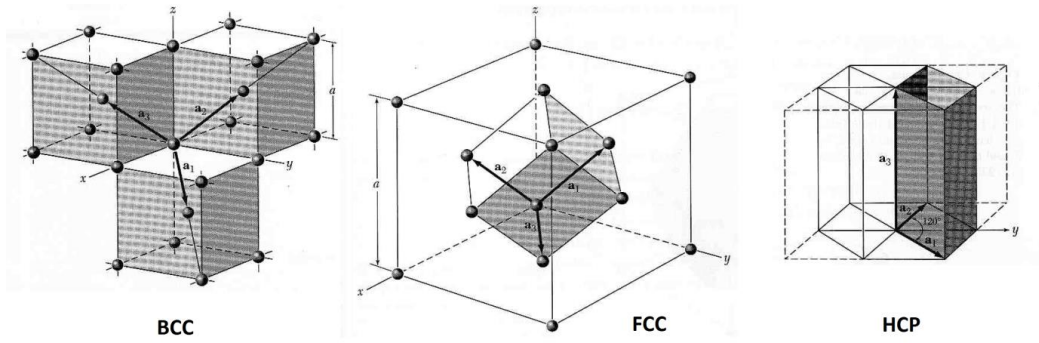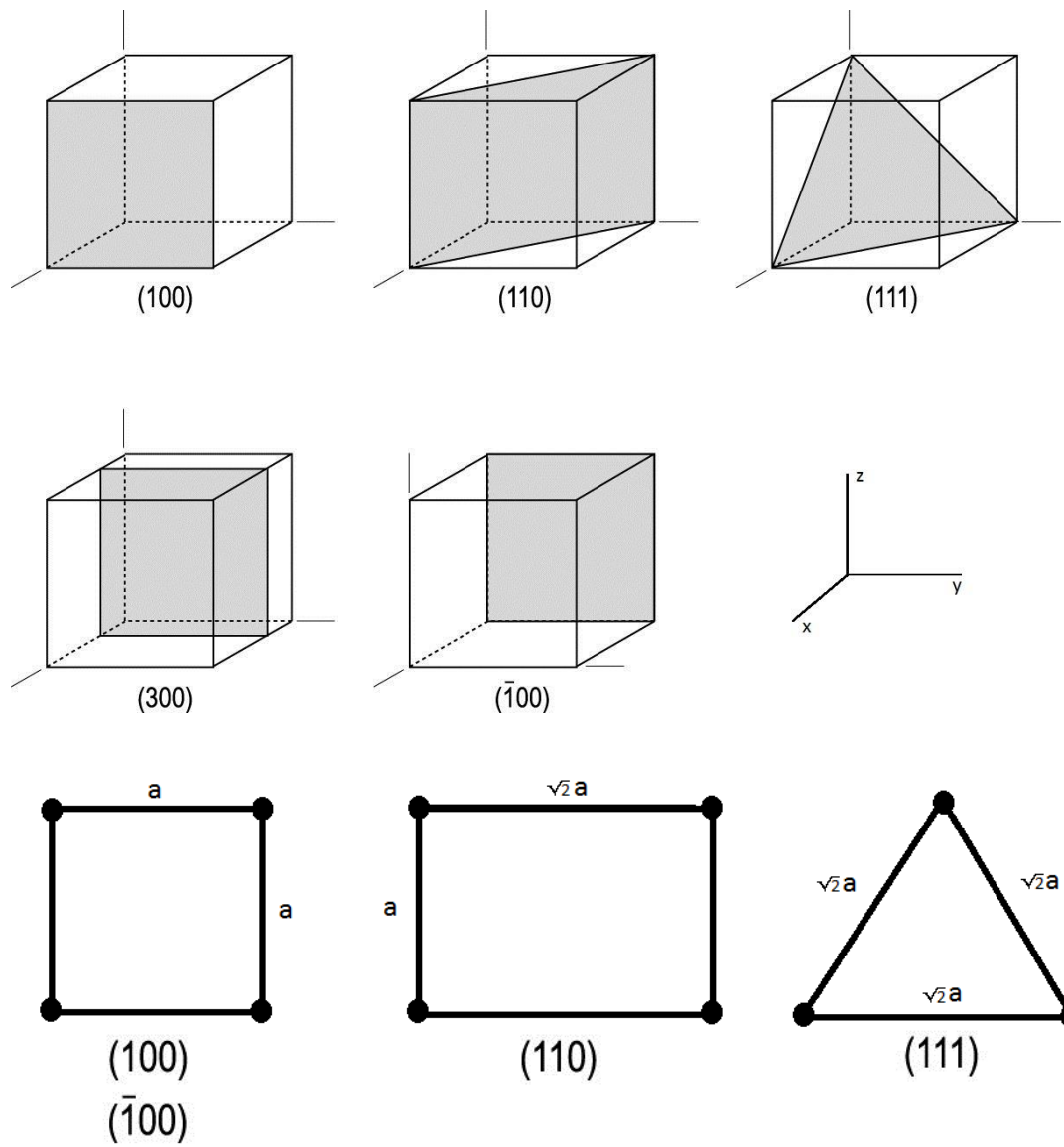
There are no atoms in (300) plane.

c.

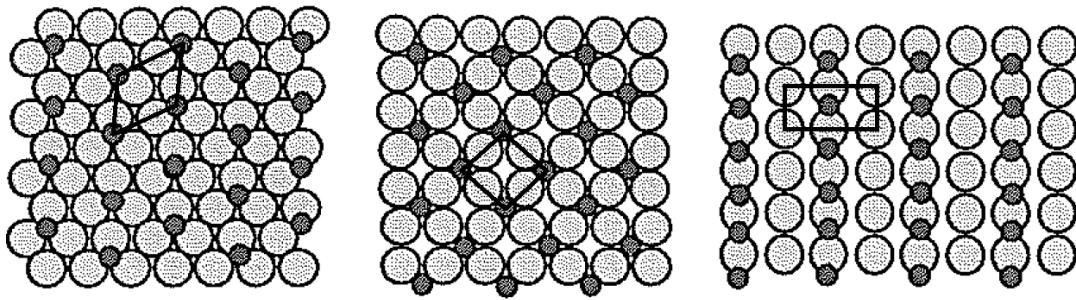2) **Wave diffraction and the reciprocal lattice (10 points)**.

    a. When a single crystal was irradiated by a X-ray beam with wavelength λ, derive the ***Bragg's law*** by considering scattering from neighboring crystal planes with separation d. Discuss the requirement on the wavelength λ of incident X-ray which causes diffraction.

    b. By considering the contribution of different atom inside a cell of Bravais lattice, discuss the ***structure factor*** and ***atomic form factor*** associated with electron cloud of jth atom $n_j(\boldsymbol{\rho})$, which is located inside the cell at $\boldsymbol{\rho} = \boldsymbol{r} - \boldsymbol{r}_j$, where $\boldsymbol{r}$ denote a Bravais lattice point.

    c. By analyzing the structure factor of NaCl, show the lattice planes ***h,k,l,*** from which diffraction peaks are expected. (hint: NaCl has two kinds of atoms in a cubic system, which can be considered as 4 Na at 000 FCC structure + 4 Cl at ½ ½ ½ FCC structure).

Na$^+$

Cl$^-$
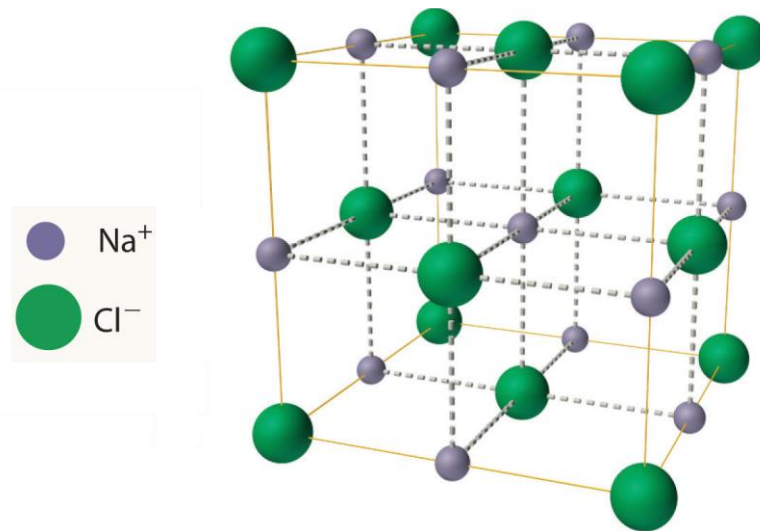
Answer to question 2:

a. A set of parallel atomic planes spaced d apart. X-rays are incident at an angle θ are reflected at successive layers of atoms. For any arbitrary angle θ emergent rays are not in phase. Diffraction (constructive interference) only occurs when the path difference of the ray AB+BC=2d sinθ is an integer number n of wavelength λ.
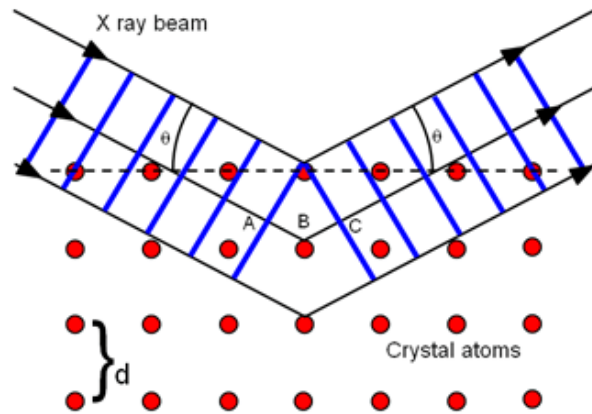
So that: $2dsin\theta = n\lambda$, where n – order of the diffraction, θ – Bragg angles. Bragg reflection occurs only for wavelength $\lambda \leq 2d$, θ=90° in extreme case. Otherwise the above relation cannot be satisfied.

b. **Structure factor** is a scattering amplitude of a single cell. The structure factor is a particularly useful tool in the interpretation of interference patterns obtained in X-ray, electron and neutron diffraction experiments. It is given by

$$S_G = \sum_j f_j exp(-iG \cdot r_j),$$

where $f_j = \int dV n_j(\rho) exp(-iG \cdot \rho)$ integrated over all space, $\rho = r - r_j$.

f_j is an **atomic form factor** and is a measure of the scattering amplitude of a wave by an isolated atom (or molecule like in case of crystalline fullerene). The atomic form factor depends on atom, bond and angle, thus is different for each basis atom. The common feature of all form factors is that they involve a Fourier transform of a spatial density distribution $n_j(\rho)$ of the scattering object from real space to momentum space.

c. For NaCl you can also think of the structure as simple FCC and the atom is replaced by pair of atoms (1Na+1Cl) with the new structure factor $\left[f_{Na} + f_{Cl}e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)} \right]$

$$F_{hkl} = \left[1 + e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+0\right)} + e^{2\pi i\left(\frac{h}{2}+0+\frac{l}{2}\right)} + e^{2\pi i\left(0+\frac{k}{2}+\frac{l}{2}\right)} \right] \times \left[f_{Na} + f_{Cl}e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)} \right]$$

$$- F_{hkl} = 0 \times \left[f_{Na} + f_{Cl} e^{2\pi i \left(\frac{h}{2} + \frac{k}{2} + \frac{l}{2} \right)} \right] \text{ when } h, \, k, \, l \text{ mixed} \rightarrow |F_{hkl}|^2 = 0$$

$$- F_{hkl} = 4 \times [f_{Na} + f_{Cl}] \text{ when } h, \, k, \, l \text{ all even} \rightarrow |F_{hkl}|^2 = 16(f_{Na} + f_{Cl})^2$$

$$- F_{hkl} = 4 \times [f_{Na} - f_{Cl}] \text{ when } h, \, k, \, l \text{ all odd} \rightarrow |F_{hkl}|^2 = 16(f_{Na} - f_{Cl})^2$$

3) Phonons, Crystal vibrations and thermal properties (15 points).

Consider the normal modes of a linear monoatomic chain, in which the force constant between nearest-neighbor atoms is C. Let the mass of each atom equal to M, which is separated by nearest-neighbor separation, a.

a. Find the dispersion relationship $\omega(K)$ of this linear chain.

b. Sketch in the dispersion relation and indicate the first Brillouin zone.

c. Show that the density of vibrational modes of the system is $D(\omega) = \dfrac{2N}{\pi}\dfrac{1}{\sqrt{\omega_m^2 - \omega^2}}$, where
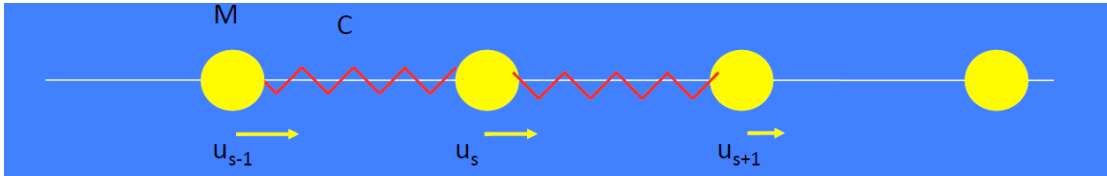
ω_m is a maximum frequency and N is a total amount of atoms.

d. What would happen to the dispersion relation $\omega(K)$ in the case of diatomic chain?

e. Find the heat capacity of monoatomic chain in the linear regime $\omega = vk$ at low temperature when $\hbar\omega \gg kT$.

$\left(\int_0^\infty x^2 e^{-x} dx = \Gamma(3) = 2! \right)$

Answers to question 3:

a. Consider 1D chain as shown on the picture:

We assume that the force on ion s caused by displacement of ion $s + p$ is proportional to the difference $u_{s+p} - u_s$ of their displacement. Let's consider only nearest-neighbor interactions with $p = \pm 1$. The total force on s from ions $s \pm 1$:

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$$

The equation of motion of an ion s is

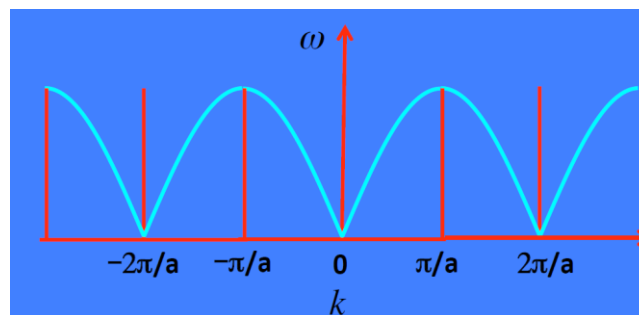$$M\frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

Where M is the mass of ion, C is the force constant. Since the equation is the same at each s, the solution must have the same form at each s differing only by a phase factor: $u_s(t) = u \cdot e^{ikas} \cdot e^{-i\omega t}$.

$$-\omega^2 M = C\left[e^{ika} + e^{-ika} - 2\right]$$

By substitution $2coska = e^{ika} + e^{-ika}$ we can obtain

$$\omega^2 = \frac{2C}{M}(1 - coska) = \frac{4C}{M}sin^2\frac{ka}{2} \Rightarrow \omega(k) = \sqrt{\frac{4C}{M}}\left|sin\frac{ka}{2}\right|$$

b. Than dispersion relation is:

c. if the total length of the chain is L, than the allowed values of k are

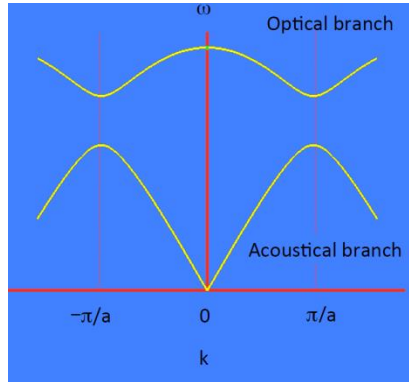$$-\frac{\pi}{a} < k = n\frac{2\pi}{L} \le \frac{\pi}{a}$$

The maximum frequency is then $\omega_{max} = 2\left(\frac{C}{M}\right)^{\frac{1}{2}}$

The number of states in the interval dk is $D(k)dk = dk \cdot \frac{L}{2\pi}$, so the number of states in the

interval $d\omega$ is $D(\omega)d\omega = 2D(k) \cdot \frac{dk}{d\omega}d\omega$, which gives the DOS

$$D(\omega) = \frac{2L}{a\pi}\frac{1}{\omega_{max}\left|\cos\frac{ka}{2}\right|} = \frac{2N}{\pi} \cdot \frac{1}{\sqrt{\omega_{max}^2 - \omega^2}}$$

d. In the case of diatomic chain we should expect a formation of optical phonon branch. Dispersion relation would have a gap at zone boundary.

e. In the linear regime (low ω) DOS can be calculated as in **c** by taking into an account

$\omega = vk$. $D(\omega) = \frac{L}{\pi v}$. Heat capacity is $C = \frac{dU}{dT}$, where U is the total energy of system:

$$U = \int_0^{\omega_{max}} D(\omega)\frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}d\omega$$

Taking into an account that $\hbar\omega \gg kT$ and DOS we can find

$$U = \frac{L}{\pi v}\int_0^{\omega_{max}} \hbar\omega \cdot e^{-\frac{\hbar\omega}{k_B T}}d\omega$$

Than heat capacity is

$$C = \frac{L}{\pi v}\int_0^{\omega_{max}} \hbar\omega \cdot \frac{d}{dT}\left(e^{-\frac{\hbar\omega}{k_B T}}\right)d\omega = \frac{L}{\pi v}\int_0^{\omega_{max}} \hbar\omega \cdot \frac{\hbar\omega}{k_B T^2} \cdot e^{-\frac{\hbar\omega}{k_B T}}d\omega$$

By substituting $x = \dfrac{\hbar\omega}{k_B T}$ we can estimate

$$C = \frac{Lk_B^2 T}{\pi v \hbar} \int_0^\infty x^2 e^{-x} dx = 2\frac{Lk_B^2 T}{\pi v \hbar}$$

4) Electrons. Free electron Fermi gas (20 points)

a. Consider a free electron gas with N electrons of identical mass m in a box with volume L^3. Calculate E_F and the electron density of states $D(E)$.

b. What will happen to $D(E)$ when the free electron gas is confined by infinite high potential well $V(i)$ of width d where $i = x, y, z$, for proper confinement in x, y, z direction to form a quantum well (2D), wire (1D), or dot (0D). Calculate and sketch evolution of the relationship from 3D to 0D case.

c. Discuss the degeneracy (without considering the degeneracy in spin) of the first 1-4 energy levels when reduced dimensionality in 2D, 1D and 0D system introduces energy quantization by restricting electron movement from a plane wave into a standing wave.

d. Consider now a 1D chain with electron density $n = N/L$, N where L is a chain length. Derive ground state energy U_0 at $T = 0$ K for the 1D electron gas.
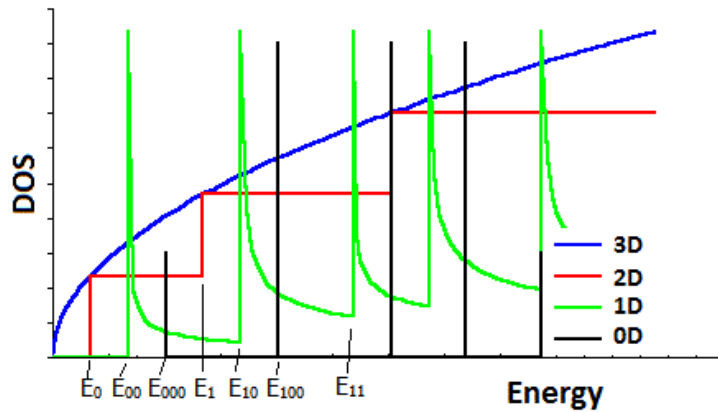
Answers to question 4:

a. and **b.** in 3D $E_F = \frac{\hbar^2 k_F^2}{2m}$, k_F defined by $N = 2\left(\frac{L}{2\pi}\right)^3 \frac{4}{3}\pi k_F^3 \Rightarrow k_F = \left(\frac{3N\pi^2}{L^3}\right)^{\frac{1}{3}} \Rightarrow$

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3N\pi^2}{L^3}\right)^{\frac{2}{3}}$$

Dimension of the system	Energy of the system	DOS
3D	$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$	$D(E) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}(E)^{\frac{1}{2}}$
2D	$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right) + E_{n_z}$	$D(E) = \frac{L^2 m}{\pi\hbar^2}(E)^0$
1D	$E = \frac{\hbar^2}{2m}\left(k_x^2\right) + E_{n_y} + E_{n_z}$	$D(E) = \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}(E)^{-\frac{1}{2}}$
0D	$E = E_{n_x} + E_{n_y} + E_{n_z}$	$D(E) = 2\delta(E)$

Corresponding sketch of DOS:

Than the degeneracy of energy levels in this case can be represented by the following table

2D		1D			0D			
n_x	Degeneracy	n_x	n_y	Degeneracy	n_x	n_y	n_z	Degeneracy
1	1	1	1	1	1	1	1	1
2	1	1	2	2	1	1	2	3
3	1	2	2	1	1	2	2	3
4	1	1	3	2	1	1	3	3
5	1	2	3	2	2	2	2	1
6	1	1	4	2	1	2	3	6

c. $U_0 = \int_0^{E_F} E \cdot D(E)dE = \int_0^{E_F} \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}(E)^{\frac{1}{2}}dE = \frac{2L}{3\pi}\left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}}E_F^{\frac{3}{2}}$

5)   Fermi surfaces (10 points)

  a. Explain what is the Fermi surface?

  b. In a 3D metal, what will happen at the Fermi level by applying an external magnetic field B? Sketch the change of density of states. Calculate the magnetization M due to the spin paramagnetic response as a function of density of state $D(E_F)$ and μ_B.

  c. If the same 3D metal was cooled to low temperature and exhibit a superconducting transition. Sketch the change of density of state after entering the superconducting state. Discuss two characteristic macroscopic phenomena associated with the superconducting state. Under an increasing external magnet field, discuss or sketch the change of B field inside type I and II superconductor.

  d. For the case of a two-dimensional square lattice (with lattice constant a) draw a diagram of the reciprocal lattice showing the Fermi surfaces for atoms with one, two, three and four valence electrons. To do that you might need to calculate k_F. Map the Fermi surface for the case of four electrons per atom into the first Brillouin zone.

Answers to question 5:

a. The Fermi surface is the surface of constant energy E_F in $\boldsymbol{k}$ space. The Fermi surface separates the unfilled orbitals from the filled orbitals, at absolute zero. The electrical properties of the metal are determined by the volume and shape of the Fermi surface, because the current is due to changes in the occupancy of states near the Fermi surface.

b. Spin up electrons (parallel to field) are shifted opposite to spin down electrons (antiparralel to B field), and the energy shift is determined by Zeeman energy $\Delta E = \pm \mu_B B$. Such a shift cause a net magnetization of a metal, since the total amount of aligned spins is larger than the amount of antiparallel spins.

$$M = \mu_B(N_\uparrow - N_\downarrow) = \mu_B \frac{1}{2} D(E_F) 2\mu_B B$$

This is a way to measure the density of states.
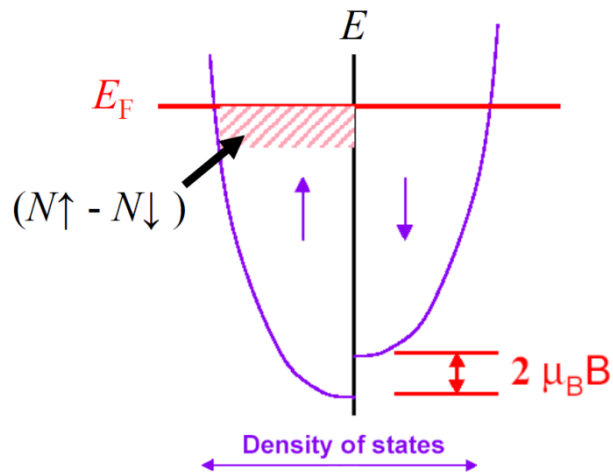
c. In 3D case, formation of a gap $(\Delta \sim k_B T_c)$ in the DOS of superconductor $D(E_F)$, in the vicinity of Fermi level E_F.
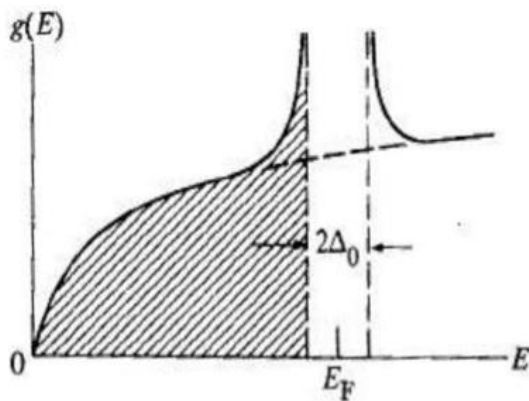

After the suerpconduting transtion, the characteristic macroscopic phenomena are zero resistivity and Meissner effect.

For I Type superconductors can act as a perfect diamagnets in external magnetic field below a critical field H_c which is correlated with $\rho \to 0$. For type II superconductor, perfect diamagnetic only below H_{c1} where $\rho \to 0$ is correlated with a higher critial field H_{c2} indicating that even in the zero resistance state $\rho \to 0$, inside the supercondutor $B \neq 0$.

Type II supercondutor is a perfect diamgnet when $H < H_{c1}$. When $H_{c1} < H < H_{c2}$, magentic field penerate the vortex core.

- ## Type I superconductor
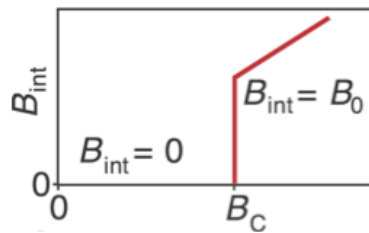
- ## Type II superconductor
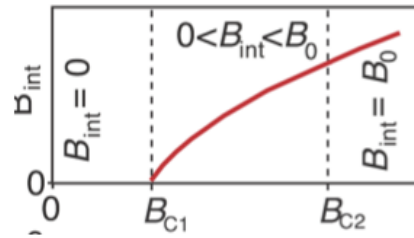
d. At first, let's find a radius of Fermi sphere in 2D system with N atoms and Z valence electrons:

$$2 \left(\frac{L}{2\pi} \right)^2 \pi k_F^2 = NZ$$

$$k_F = \left(\frac{2\pi NZ}{L^2} \right)^{\frac{1}{2}} = \left(\frac{2\pi Z}{a^2} \right)^{\frac{1}{2}} = \frac{\pi}{a} \cdot \left(\frac{2Z}{\pi} \right)^{\frac{1}{2}}$$
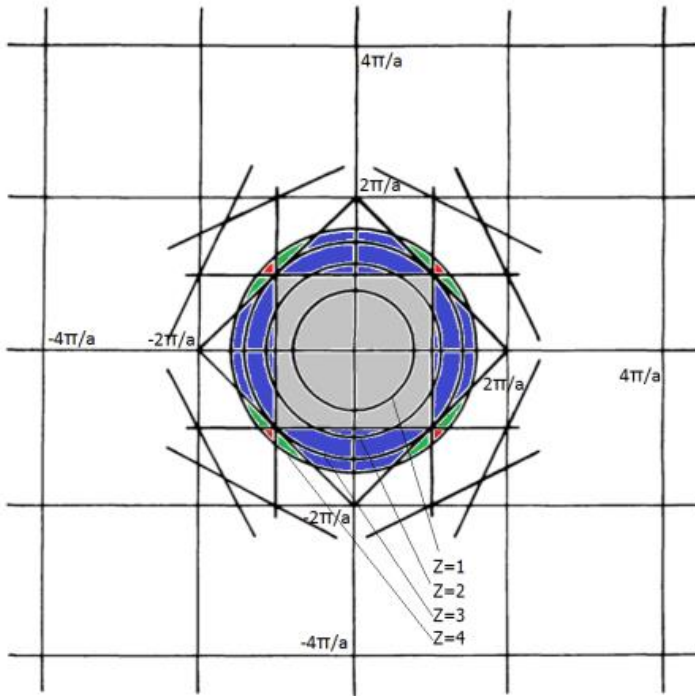
So, the radius of Fermi sphere in case of one, two, three and four valence electrons are:

$$k_1 = \frac{\pi}{a} \cdot \left(\frac{2}{\pi} \right)^{\frac{1}{2}} \approx 0.79 \frac{\pi}{a}$$

$$k_2 = \frac{\pi}{a} \cdot \left(\frac{4}{\pi} \right)^{\frac{1}{2}} \approx 1.13 \frac{\pi}{a}$$

$$k_3 = \frac{\pi}{a} \cdot \left(\frac{6}{\pi} \right)^{\frac{1}{2}} \approx 1.38 \frac{\pi}{a}$$

$$k_4 = \frac{\pi}{a} \cdot \left(\frac{8}{\pi} \right)^{\frac{1}{2}} \approx 1.59 \frac{\pi}{a}$$

Fermi surface diagrams for four electrons per atom mapped into first Brillouin zone (contribution from each BZ is mentioned below):