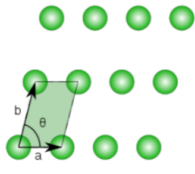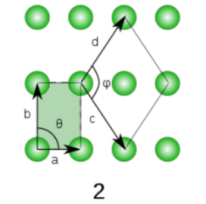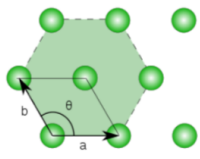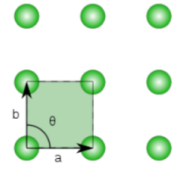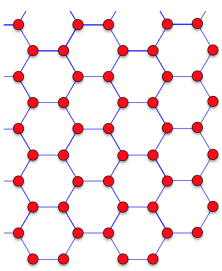## Solution Final Exam - Solid State Physics 1

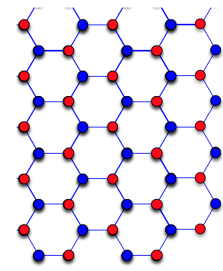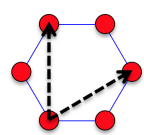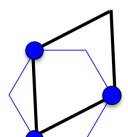**Question 1: Crystal structure (20+5 points)**

A.   *Crystal systems of carbon*
   1)   **(5p)**

$|a| \neq |b|, \theta \neq 90°$	$|a| \neq |b|, \theta = 90°$ $|c| = |d|, \varphi \neq 90°$	$|a| = |b|, \theta = 120°$	$|a| = |b|, \theta = 90°$
m	**o**	**h**	**t**

1 – oblique (monoclinic), 2 – rectangular (orthorhombic), 3 – centered rectangular (orthorhombic), 4 – hexagonal, and 5 – square (tetragonal).

   2)   **(2p)**

$|\vec{a}_1| = |\vec{a}_2| = \sqrt{3}a$, here a is the distance between the carbon atoms.

   3)   **(2p bonus)**
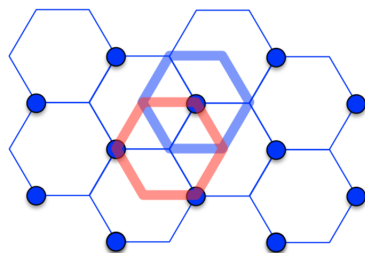
Refer to layer A (thin), the B layer (Blue thick) shift with $2(\mathbf{a}_1+\mathbf{a}_2)/3$, then the C layer (red thick) shift for $(\mathbf{a}_1+\mathbf{a}_2)/3$.

4) **(3p)** The key is how to make the proper curvature. For CNT, wrap up a graphene sheet and connect the handling of bonds at the edge, the surface normal is in a single plane for the whole surface. While for fullerene, the surface normal is not in a single plane, we need alternating pentagons and hexagons of carbon to realize this curvature.

Fullerene   Carbon Nanotube
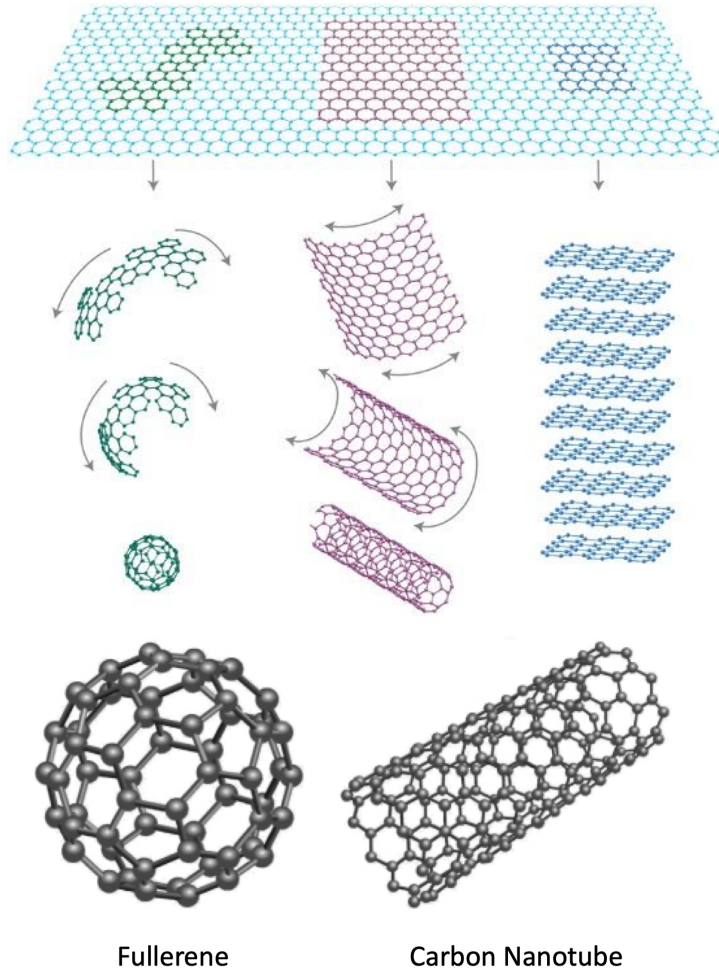
B.   *The crystal structure (left) of an antiferromagnetic compound MnO*

1)   **(3p)** The Bravais lattice is face-centered cubic, where the length of the lattice vectors |a1| = |a2| = |a3| = a, and the angles between them are 90 degrees.

2) **(2p)**

The conventional and primitive unit cell for a FCC cubic crystal of lattice constant a are shown.

The primitive unit vectors are designated by $\vec{a}_1, \vec{a}_2, \vec{a}_3$ as shown in the figure.

Conventional FCC unit cell   Primitive FCC unit cell

$$\vec{a}_1 = \frac{a}{2}(\hat{i}+\hat{j}); \quad \vec{a}_2 = \frac{a}{2}(\hat{j}+\hat{k});$$

$$\vec{a}_3 = \frac{a}{2}(\hat{k}+\hat{i})$$
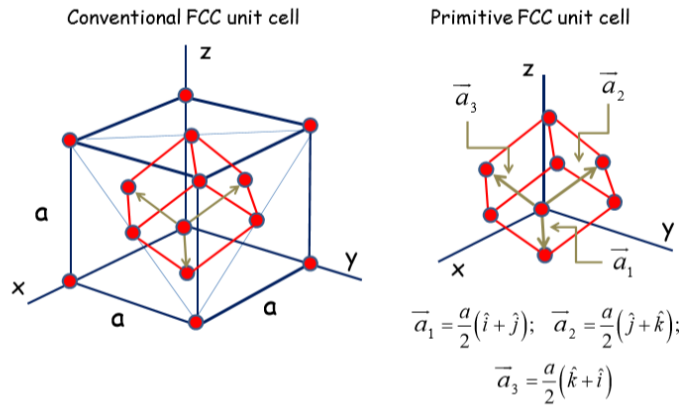
So the volume of the primitive cell is $1/4a^3$.

3) **(2p)** The lattices are two interlocked FCC lattices with each FCC lattice having 4 atoms in the basis. This totals 8 atoms in the unit cell and therefore 8 atoms in the basis.

4) **(3p bonus)**

The structure of MnO is exactly the same as that of NaCl, for which we have:

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 $\left[f_{Na} + f_{Cl}e^{2\pi i\left(\frac{h}{2}+\frac{k}{2}+\frac{l}{2}\right)}\right]$

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

5

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

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

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

5) **(3p)**

The magnetic unit cell is FCC with lattice vectors of length 2a. This means that the volume of the magnetic FCC unit cell is $8a^3$. The primitive cell for FCC has 1/4th of the volume of the conventional cell (as in 2)), so the volume of the magnetic primitive cell is $2a^3$.

Question 2: Phonons and thermal properties (20 points).

1) **(6p)**

2) The expression for the potential for generic positions r_n of the masses is:

$$U = Na\left(\frac{1}{r_{n,n+1}} - \frac{b}{\sqrt{r_{n,n+1}}}\right)$$

At zero temperature all atoms are at their equilibrium positions $r_n = R_0 n$ and all the forces equilibrated. Suppose the temperature is slightly increased, such that at very first moment only atom at position n moved out his equilibrium position $r_n = R_0 n + x_n$. This atom will experience force:

$$F = F_{n-1} + F_{n+1} = -2cx_n.$$

Here F_{n-1} and F_{n+1} are forces from nearest neighbors and c is elastic constant, which we are calculating. In harmonic approximation the forces are equal and point at the same direction. Further:

$$F_{n-1} = -\frac{\partial}{\partial x_n}V(R_0 + x_n)$$

$$F_{n+1} = -\frac{\partial}{\partial x_n}V(R_0 - x_n),$$

But it's important to write the expressions of V(R$_o$ + x$_n$) and V(R$_o$ − x$_n$) in Taylor series expansion.

$$2c = \frac{\partial}{\partial x_n}F\bigg|_{x_n=0} = \frac{\partial}{\partial x_n}(F_{n-1} + F_{n+1})\bigg|_{x_n=0} = \frac{ab^6}{2^6}.$$
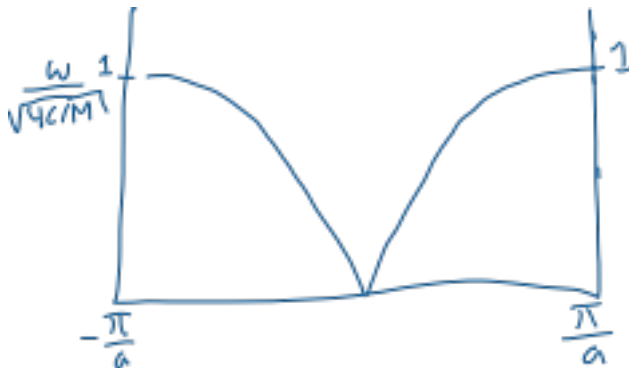
Thus $c = \dfrac{ab^6}{2^7}.$

The equation of motion is

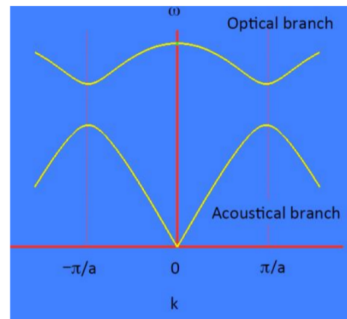$$M\ddot{x}_n = c(x_{n-1} + x_{n+1} - 2x_n),$$

where c is the force constant derived above.

2) **(2p)**

3)   (**3p**)

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

In case of diatomic 1D chain periodicity is doubled. Lattice constant increases from a to $2a$, this leads to reduced size of 1st BZ from $\frac{2\pi}{a}$ to $\frac{\pi}{a}$. Part of dispersion relation that belong to $\left[-\frac{\pi}{a}, -\frac{\pi}{2a}\right]$ and $\left[\frac{\pi}{2a}, \frac{\pi}{a}\right]$ becomes 2nd BZ. By applying zone folding we can obtain optical

(**2p**) If we think about a 1D chain, 3D vibration, we will have $3n$-3 optical mode, and 3 acoustic modes. For 1D chain 1D vibration, we will have n-1 optical mode and 1 acoustic mode, both answers are fine.

4)   (**4p**)
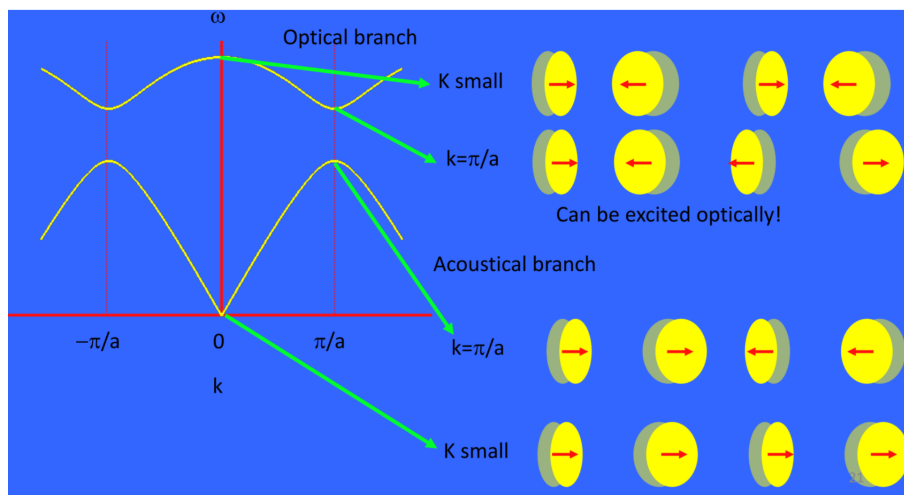
5)   (**3p**)

Particularly, we write the equation for x_n,

$$m\ddot{x}_n = -k_1 (x_n - x_{n+1}) - k_1 (x_n - x_{n-1}) - k_2 (x_n - x_{n+2}) - k_2 (x_n - x_{n-2}).$$

Now using the normal mode equation

$$x_n = A\, e^{iqna - i\omega t},$$

we have

$$-m\,\omega^2\, x_n = -\left[k_1 (1 - e^{iqa}) + k_1 (1 - e^{-iqa}) + k_2 (1 - e^{2iqa}) + k_2 (1 - e^{-2iqa}) \right] x_n,$$

which yields

$$m\,\omega^2 = 4\,k_1 \sin\left(\frac{qa}{2}\right) + 4\,k_2 \sin(qa).$$

Question 3: Free electrons in an intermetallic compound (20+3 points)

1)   **(5p)**

For the Drude's model; Under an electric field E, the equation of motion for electrons is
$$m_e \frac{d\vec{v}}{dt} = -e\,\vec{E}$$
By integrating over time from t=0, we get the velocity at time t;
$$\vec{v}(t) = -e\,\vec{E}\,t/m_e$$
Considering the average time τ in between the collisions (momentum relaxation time), the drift velocity for electrons can be derived as:
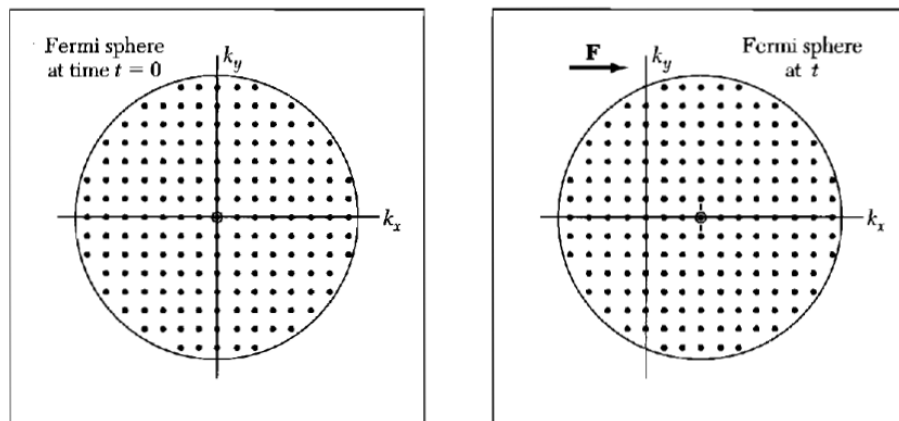$$\vec{v} = -e\,\vec{E}\,\tau/m_e$$
If we consider a charge flow through a metallic bar, the total number of electrons passing through it in unit of time is equal to $n\underline{v}A$ and the created charge current would be $-en\underline{v}A$. The current density is $J = -en\underline{v}$.

By replacing the average velocity, the current density is; $\vec{j} = ne^2 \frac{\tau}{m_e}\vec{E}$

That is Ohm's law with having conductivity as $\sigma = ne^2 \frac{\tau}{m_e}$.

2)   **(4p)**

Change of momentum of the electron can be shown as the shift of the Fermi sphere in k-space:The main difference between Drude and Sommerfeld model is that the Drude model is classical and provides the description in real space, however, the Sommerfeld model considers quantum theory and describes the behavior of electrons in k-space.

3) **(5p)**

The density of states k states $\frac{N}{L^3} = \frac{1}{a^3}$ and the number of valence electrons per atom is 1; $z = 1$.

$$4) \quad \sigma = \frac{nehk}{mE}$$

$$5) \quad \varepsilon = \frac{\hbar^2 k^2}{2m}$$

$$6) \quad \sigma = \frac{eh\,(2m\varepsilon)^{1/2}}{a^3 m\hbar\,E}$$

The discrepancy between the conductivity calculated using Drude's model and the one measured comes from the fact that the Drude model considers the classical free electron gas without interaction with the lattice. As it is mentioned, different ratios of the atoms do not change the lattice constant or the total valence electrons. So what causes the change in the measured resistivity is the crystal structure which is not considered in the Drude's model.

7) **(6p)**

The stoichiometry is determined by calculating the number of atoms of each metal per unit cell;
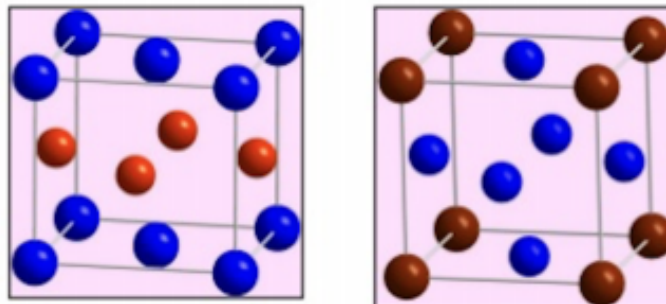
(a)   (b)

(a) Left structure is "AB"

$\quad$ Atom A $\Rightarrow 8\times1/8+2\times1/2 = 2$

$\quad$ Atom B $\Rightarrow 4\times1/2=2$

(b) The right structure is "A₃B"

$\quad$ Atom A $\Rightarrow 6\times1/2=3$

$\quad$ Atom B $\Rightarrow 8\times1/8=1$

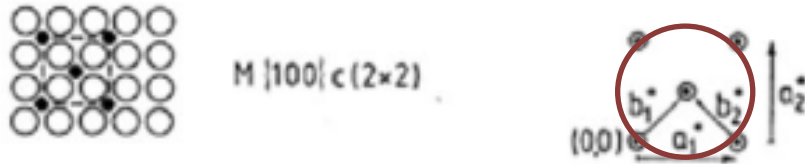$K_x = (2\pi/L)n_x,\ \ K_y= (2\pi/L)n_y$

Total number of electrons $\ NZ = \left(\frac{L}{2\pi}\right)^2 \times 2\pi\,K_F{}^2$

$$K_F = \left(2\left(\frac{N}{L^2}\right)Z\pi\right)^{\frac{1}{2}}$$

$\frac{N}{L^2} = \frac{1}{a^2}$ and the number of valence electrons per atom is 1, there are 2 atoms as

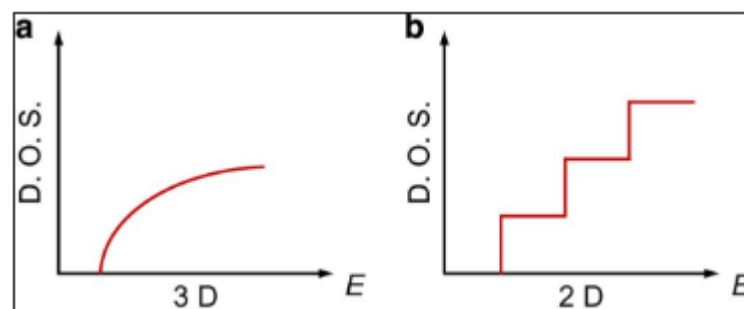basis so we consider $Z = 2$. Therefore; $K_F = \left(\frac{4}{a^2}\pi\right)^{\frac{1}{2}} = 3.54/a$

$$D(E)dE=2D(k)dk= \left(\frac{L}{2\pi}\right)^2 \times 4\pi k dk$$

Considering dispersion relation for the free electron gas; $E=\hbar^2 k^2/2m$

$$D(E)= \left(\frac{L}{2\pi}\right)^2 \times 4\pi k \; dk/dE= \left(\frac{L}{2\pi}\right)^2 \times 4\pi k \times (m/\hbar^2 k)= \left(\frac{L}{2\pi}\right)^2 \times 4\pi m/\hbar^2.$$

8) **(3p bonus)**

As we know the density of states in a 2D and 3D system is the following;

By growth, the system has gradual evolution in the density of states profile which starts with quantized states and smooths to 3D sqrt(E) dependence.

Question 4: Carrier doing in a semiconductor (20+2 points)

1) **(3p)**

We consider the band structure of Si and presence of 4 levels in the valence band. The fact that the diamond crystal structure of Si has 2 basis means that the number of valence electrons per unit is 8. These 8 electrons occupy all the available states in the valence band, while the conduction band remains empty. Check the 4 available dispersions along the WΓ, WL, direction (other directions have degenerated dispersion). As a result, the Fermi energy has to locate in the gap of the semiconductor.

2) **(4p)**

Energy and momentum conservation in the optical absorption of Si:

In Si the lowest energy transition possible is a "indirect non-vertical" transition – weak !!! – must involve phonon to conserve momentum

$$\hbar\omega_{photon} = E_g + \hbar\omega_{phonon}$$

Lowest en
empty ba

ct transition"

tical transition"

Highest er
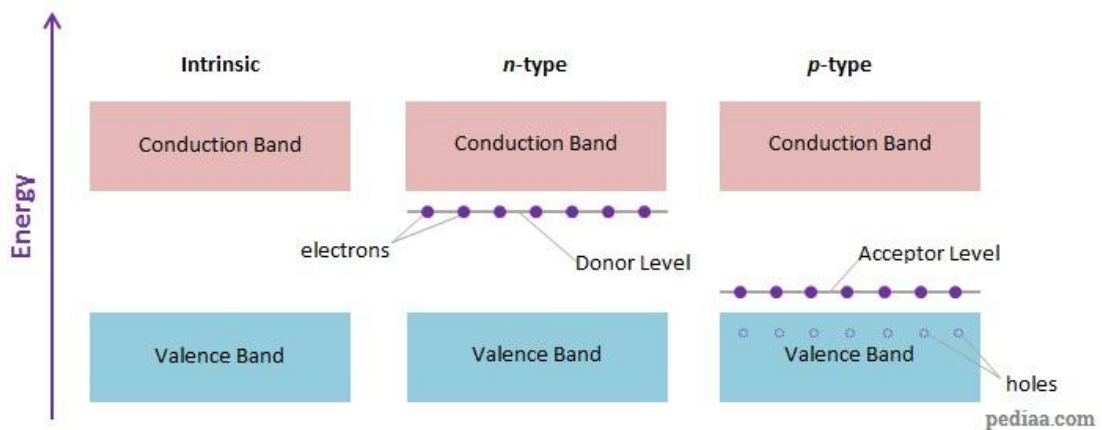filled ba

final state: $k_c \neq 0$

X = (2,0,0) π/a   0   L = (1,1,1) π/a

$$(\text{inital state}) \ k_{photon} = (\text{final state}) \ k_c + K \cong 0$$

Weak absorption and emission

Si

Absorption

1.1 eV

photon energy
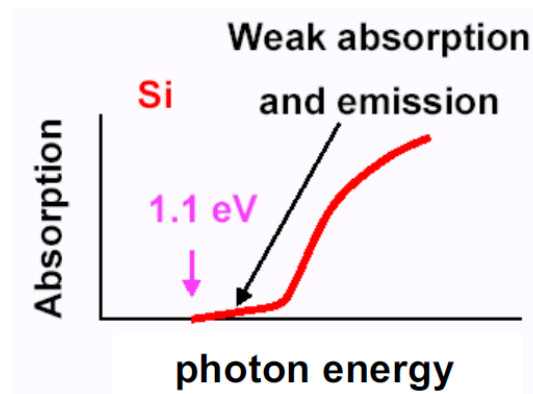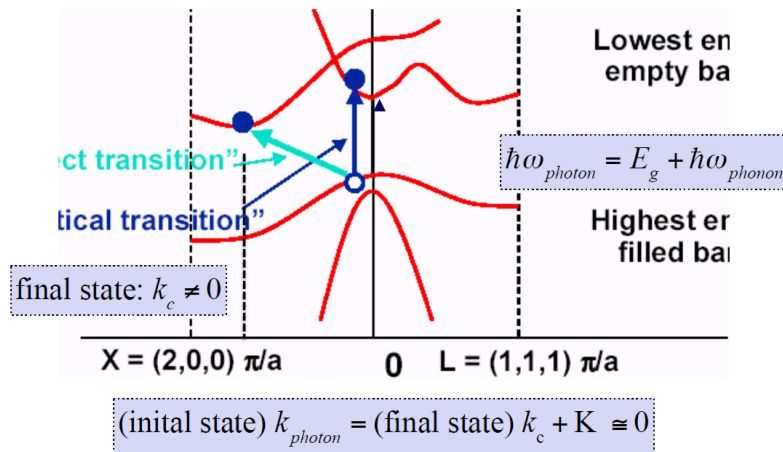
3)   **(2p)**

$Z = 3$, acceptor, and $Z = 5$, donor, And the impurity levels with respect to the valence and conduction bands;

Intrinsic	n-type	p-type
Conduction Band	Conduction Band	Conduction Band

electrons   Donor Level   Acceptor Level

| Valence Band | Valence Band | Valence Band |

holes

pediaa.com

4)   **(6p)**

In order to judge the negligibility of intrinsic conduction, we need to compare the density of the intrinsic charge carriers with the extrinsic one. The density of the intrinsic charge carriers;

$$n_i^2 = 4\left(\frac{K_B T}{2\pi \hbar^2}\right)^3 (m_e m_h)^{\frac{3}{2}} e^{-\frac{E_g}{K_B T}} = 4\left(\frac{1.38\times10^{-23}\times300}{2\pi\times(1.05\times10^{-34})^2}\right)^3 \left(9.1\times10^{-31}\right)^3 e^{-\frac{1.12}{25.84\times10^{-3}}} =$$

9.6 x 10^{31} m^{-3}

n_i= 9.8 x 10^{15} m$^{-3} \sim 10^{10}$ cm^{-3}

$$n = \sqrt{2}\left(\frac{m_e K_B T}{2\pi \hbar^2}\right)^{3/4} (N_d)^{\frac{1}{2}} e^{-\frac{E_d}{2K_B T}}$$

$$= \sqrt{2}\left(\frac{9.1\times10^{-31}\times1.38\times10^{-23}\times300}{2\pi\times(1.05\times10^{-34})^2}\right)^{3/4} \left(10^{18}\right)^{\frac{1}{2}} e^{-\frac{0.1}{25.84\times10^{-3}}} \sim 10^{17}\ cm^{-3}$$

$n \gg n_i$

5) **(2p)**

Effective mass: $\frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{d^2 E}{dk^2}\right)$

6) **(3p)**

$$\sigma = ne\mu_e + pe\mu_p \sim ne\mu_e = 10^{17}\times1.6\times10^{-19}\times100 = 1.6\frac{1}{\Omega.cm}$$

7) **(2p bonus)**

Considering the dispersion relations and the band structure of Silicon, we observe that the corresponding K values are Γ and X for $E_c + \frac{\hbar^2 k^2}{2m_e}$ and $E_v - \frac{\hbar^2 k^2}{2m_h}$, respectively. At these points, there will be Fermi surfaces associated that all are spheres because of the assumption of $m_e = m_h$, (which is our assumption for simplicity, for the real crystal, the Fermi surface is elliptical due to the different effective mass along different crystal directions.

**Question 5: Magnetism and superconductivity (20 points)**

1) **(3p)**

The third term, correlated to the electron motion in the shell as a whole around the atom.

2) **(2p)**

First all, we need to shield the magnetic field, therefore, the χ should be negative, so that the **B** will be smaller than μ_0**H**. From the list, Graphite has the largest χ with a negative value.

3) **(5p)**

The second term. A sketch is a plot below if field **B** is pointing up. Note the spin vector and spin quantum number S_z is antiparallel to the magnetic moment.
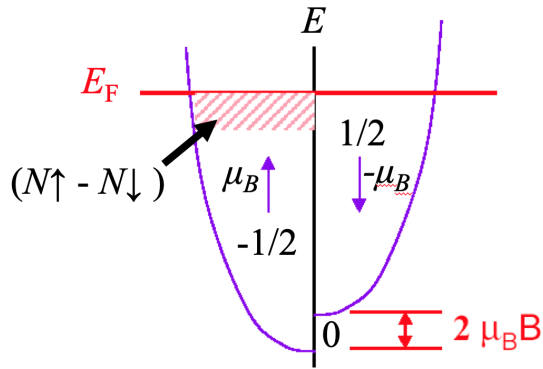
4) **(2p)**

   When a magnetic field **B** is applied, the magnetization **M** of N electrons, each has a moment **μ_B** is: $M = \mu_B(N\uparrow - N\downarrow) = \mu_B(1/2)D(E_F)2\mu_B B = \mu_B^2 D(E_F)B$

5) **(2p)**

   Zero resistance and Meissner effect (perfect diamagnetism)

6) **(4p)** The magnetic flux Φ inside a "perfect conductor": $\frac{d\Phi}{dt} = 0$, namely the flux cannot be changed. While for the superconductor $\Phi = 0$. Equivalently, it is also correct to show the point schematically.