Exam on “Solid State Physics”

WBPH068-05.2023-2024.1

Content: 13 pages (including this cover page)

Friday 25 Jan 2024; 15:00 - 17:00

ANSWERSHEET

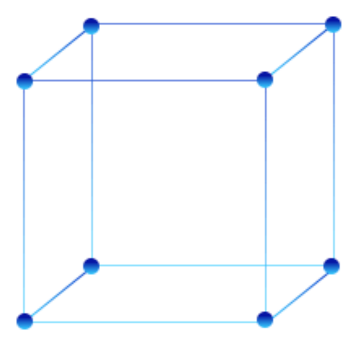
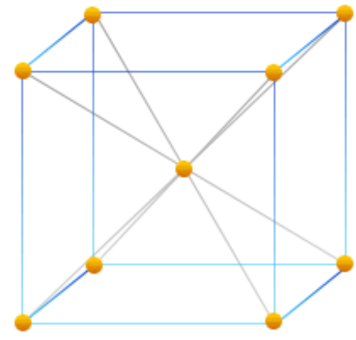
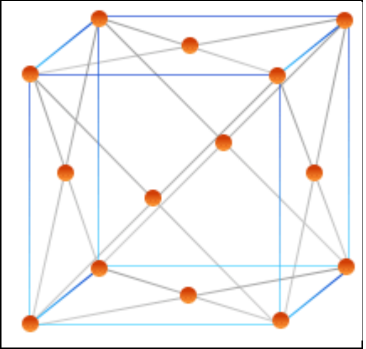
Question 1: Crystal structure and X-ray scattering

1) (10p) For the crystal types in the cubic system, considering a conventional cubic cell of lattice constant a, draw the simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) lattices. What are the respective sizes of their primitive cells?

~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~

For a conventional cell with side a, an SC crystal contains 1, a BCC crystal contains 2, and FCC contains 4 Bravais lattice sites. Therefore, if we regard, the size of the simple cubic cell as a^3, then the BCC size is $\frac{a^3}{2}$, and the FCC size is $\frac{a^3}{4}$.

Alternatively, we can determine the Bravais lattice vectors of SC, BCC, and FCC and reach the same conclusion.

Simple cubic	Base centered cubic	Face centered cubic
		
$\begin{cases} \vec{a}_1 = (100)a \\ \vec{a}_2 = (010)a \\ \vec{a}_3 = (001)a \end{cases}$	$\begin{cases} \vec{a}_1 = (\frac{1}{2}\,\frac{1}{2} - \frac{1}{2})a \\ \vec{a}_2 = (-\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})a \\ \vec{a}_3 = (\frac{1}{2} - \frac{1}{2}\,\frac{1}{2})a \end{cases}$	$\begin{cases} \vec{a}_1 = \left(0\,\frac{1}{2}\,\frac{1}{2}\right)a \\ \vec{a}_2 = \left(\frac{1}{2}\,0\,\frac{1}{2}\right)a \\ \vec{a}_3 = \left(\frac{1}{2}\,\frac{1}{2}\,0\right)a \end{cases}$
$V_p = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ $= a^3$	$V_p = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ $= \vec{a}_1 \cdot \left(\frac{1}{2}\,\frac{1}{2}\,0\right)a^2$ $= \frac{a^3}{2}$	$V_p = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ $= \vec{a}_1 \cdot \left(-\frac{1}{4}\,\frac{1}{4}\,\frac{1}{4}\right)a^2$ $= \frac{a^3}{4}$

2) (6p) When observing fruit arrangements below in an Asian market, you might notice that fruits, such as oranges, are often stacked in tetrahedrons to attract customers. For orange piles formed by close packing, determine the type of packing (AB or ABC) and the crystal structure. Assuming uniform sizes for each orange, calculate the volume fraction of the packing.
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~~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~~

Only two ways to assemble a closing packing of identical spheres (oranges): ABC/ABC and AB/AB, which led to two Bravais lattices, FCC and HCP, respectively.

The exact packing shown in the figure is ABC/ABC, hence FCC structure, with the resultant crystal having cubic features (the peak is a corner of a cube, *cf.* page 25 of lecture_1_Crystal Structure, note, the ridges are along the (1,1,0), (0,1,1), and (0,1,1) directions, therefore the second layer contains 3 oranges, third layer 6 oranges).

On the other hand, the HCP packing will give hexagonal crystal features.

Nevertheless, no matter whether you answer FCC or HCP, you should reach the same filling factor of 0.74 (this is intentional).

3) (10p) Explain (qualitatively is sufficient) the evolution of *x*-ray diffraction lines in the cubic system shown below. Why do the diffraction lines decrease as the complexity of the basis increases (or symmetry reduces)? The structure factor is given by $S_G = \sum_j f_j \exp\left(-i\vec{G}\cdot\vec{r}_j\right)$, where f_j represents the atomic scattering factor and the sum is taken over all atoms in the unit cell.

~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~

Sufficient Answer

With the increase in number of atoms in the basis, we can see the decrease of x-ray diffraction peaks. This can be understood in the following way, taking SC as a model system, the SC structure has no basis atom, therefore Laue spots come from all h, k, l with integer increments of 1, $h = 1, 2, 3, \cdots$, $k = 1, 2, 3, \cdots$, $l = 1, 2, 3, \cdots$ *etc.*

Therefore, while the SC has a complete $h^2 + k^2 + l^2$, $h = 1, 2, 3, \cdots$, $k = 1, 2, 3, \cdots$, $l = 1, 2, 3, \cdots$, the other structure with multiple atoms per basis is restricted by $S_G = \sum_j f_j \exp(i\vec{G} \cdot \vec{r}_j)$, where $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$, where $\vec{r}_j$ denote the position of jth atom in the basis.

The more basis atom appears, the more terms will be added to S_G. Therefore, we expect less $h^2 + k^2 + l^2$ values for x-ray lines, when we go down from the top, since for SC cell, the basis atoms are SC (1), BCC (2), FCC (4), and Diamond (8).

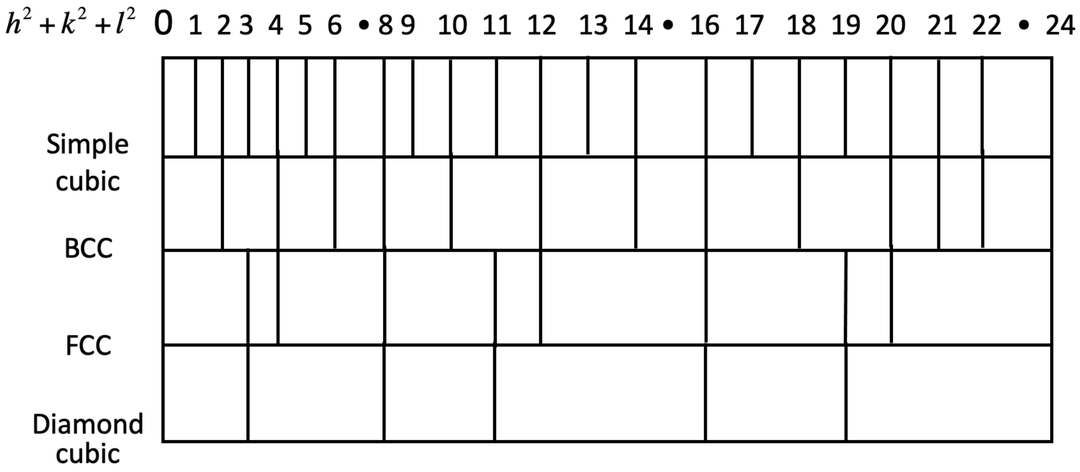
Full answer (complete as a reference, but not recommended)

We can consider the members of the cubic system as a cubic lattice with a corresponding basis. Thus, in an SC lattice has a basis consisting of one atom at the vertex of the cube; a BCC lattice – is a basis of two atoms: one at the vertex and the other at the body center; an FCC lattice - as a simple cubic with a basis of four atoms: one at the vertex and three on the faces of the cube; and Diamond - as two FCC, displaced by a quarter of the diagonal of the cube from each other. If we consider the elemental materials (f_i is the same for all atoms in a basis), then the corresponding structure factors and thus plane visibility are the following:

	SC	BCC	FCC	Diamond
Positions of atoms in the basis	(000)	(000), $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$.	(000), $\left(\frac{1}{2}\frac{1}{2}0\right)$, $\left(\frac{1}{2}0\frac{1}{2}\right)$, $\left(0\frac{1}{2}\frac{1}{2}\right)$.	(000), $\left(\frac{1}{2}\frac{1}{2}0\right)$, $\left(\frac{1}{2}0\frac{1}{2}\right)$, $\left(0\frac{1}{2}\frac{1}{2}\right)$, $\left(\frac{1}{4}\frac{1}{4}\frac{1}{4}\right)$, $\left(\frac{3}{4}\frac{3}{4}\frac{1}{4}\right)$, $\left(\frac{3}{4}\frac{1}{4}\frac{3}{4}\right)$, $\left(\frac{1}{4}\frac{3}{4}\frac{3}{4}\right)$.
Structural factor S_G.	$S_G = f$	$f(1 + e^{-i\pi(h+k+l)})$	$f(1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)})$	$f\left(1 + e^{-i\pi\frac{(h+k+l)}{2}}\right)(1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)})$
Visibility of Laue spots	All possible h, k, l (100) (110) (111) …	$h + k + l$ even (110) (200) (211) …	h, k, l same kind of parity (111) (200) (220) …	$h + k + l = 4n;\ 2n + 1$ (210) (220) (311) …
Position $h^2 + k^2 + l^2$	1 2 3 …	2 4 6 …	3 4 8 …	3 8 11 …

Taking the simplest example, consider the difference between the Simple Cubic (SC) and Body-Centered Cubic (BCC) structures. In the SC structure, we observe peaks corresponding to $x-$ray diffraction from crystalline planes, where constructive interference occurs. However, in the BCC structure, there exists a plane precisely positioned between the planes of the SC structure. This arrangement leads to reflected light lagging behind the incident light by $\lambda/2$, causing destructive interference.

Expanding on this reasoning, one can infer that as the complexity of the lattice structure increases or symmetry reduces (from SC to BCC to FCC to diamond), interference effects become more intricate. This extra complexity of having more than one basis atom results in missing diffraction lines. The reduced intensity reflects the increased complexity and diminished regularity of the lattice arrangement.



Question 2: Phonons and thermal properties.

Consider a linear chain of N atoms, all with mass M and force constant C.

1) (10p) Calculate and sketch the dispersion relation in the first Brillouin zone for the lattice vibration of the chain, where the interatomic distance is a.

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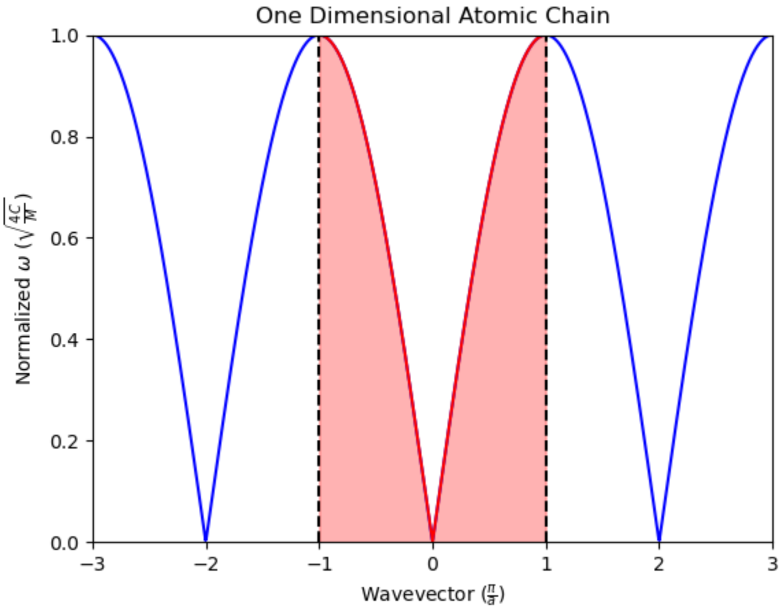
$M\ddot{u}_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) = C(u_{s+1} + u_{s-1} - 2u_s)$,

Use the general solution: $u_s = u_0 \exp(iska - i\omega t)$.

$u_{s\pm1} = u_s \exp(\pm ika)$,

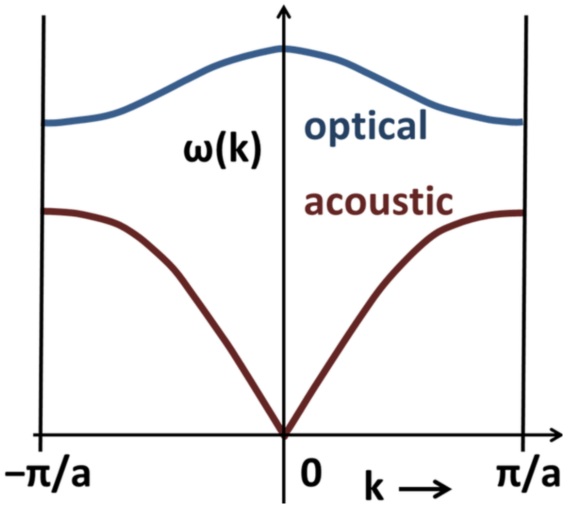
Then, we can solve $\omega(k) = \sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$.

It is sufficient to plot $\omega(k)$ for $k \subset \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$.



2) (10p) Sketch the dispersion relationship if the mass or force constant changes, *i.e.*, if the monoatomic chain becomes a diatomic chain. How does the $\omega(k)$ relationship evolve with respect to the answer in question 1?

~~~~~~~~~~~~~~~~~~~~~~~~ Answer ~~~~~~~~~~~~~~~~~~~~~~~~



In a diatomic chain, there are two types of atoms alternately arranged along the chain, forming a repeating unit cell. Each type of atom interacts differently with its neighboring atoms, leading to a more complex interaction potential. The presence of the two different masses or force constants results in the formation of two branches: one for the acoustic phonons (low-frequency, long-wavelength modes) and one for the optical phonons (high-frequency, short-wavelength modes). The presence of bandgaps in the dispersion relation indicates ranges of frequencies where certain types of phonons cannot propagate through the material.

3) (6p) Suppose the pairwise potential between the 1D monoatomic chain is the so-called Lennard–Jones potential, $V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$. Estimate the lattice constant a, binding energy E, and force constant C.

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$$V'(r) = 4\epsilon\left[\frac{6}{\sigma}\left(\frac{\sigma}{r}\right)^{7} - \frac{12}{\sigma}\left(\frac{\sigma}{r}\right)^{13}\right]$$

The equilibrium position a can be found when

$$V'(a) = 4\epsilon\left[\frac{6}{\sigma}\left(\frac{\sigma}{a}\right)^{7} - \frac{12}{\sigma}\left(\frac{\sigma}{a}\right)^{13}\right] = 0$$

Therefore,

$$\left(\frac{\sigma}{a}\right)^{7} = 2\left(\frac{\sigma}{a}\right)^{13} \rightarrow 2\left(\frac{\sigma}{a}\right)^{6} = 1 \rightarrow a = 2^{\frac{1}{6}}\sigma.$$

At $a = 2^{\frac{1}{6}}\sigma$, $E = V(a) = -\epsilon$.

For the force constant, we use Taylor expansion at a, obtained above,

$$F(r) = -V'(r) = -\frac{dV(r)}{dr} = -4\epsilon\left[\frac{6}{\sigma}\left(\frac{\sigma}{r}\right)^{7} - \frac{12}{\sigma}\left(\frac{\sigma}{r}\right)^{13}\right]$$

Then the linear restoring force is the first term in the Taylor expansion around a, Let the small deviation from a as δ,

$$F(a+\delta) = F(a) + F'(a)\delta + \frac{1}{2!}F''(a)\delta^2 + \cdots$$

For the small deviation, we neglect the square term $\propto \delta^2$, and $F(a) = 0$,

$$\because F'(r) = -V''(r) = -4\epsilon\left[\frac{156}{\sigma^2}\left(\frac{\sigma}{r}\right)^{14} - \frac{42}{\sigma^2}\left(\frac{\sigma}{r}\right)^{8}\right],$$

$\therefore$ at $r = a = 2^{\frac{1}{6}}\sigma$

$$V''(a) = 4\epsilon\left[\frac{156}{\sigma^2}2^{-\frac{14}{6}} - \frac{42}{\sigma^2}2^{-\frac{8}{6}}\right] = -\frac{4\epsilon}{\sigma^2}\left(2^{-\frac{4}{3}}\right)[78 - 42] = \left(\frac{72}{\sqrt[3]{2}}\right)\frac{\epsilon}{\sigma^2}.$$

And $\therefore$ $F(a+\delta) = -\left(\frac{72}{\sqrt[3]{2}}\right)\frac{\epsilon}{\sigma^2}\delta.$

$$c = \left(\frac{72}{\sqrt[3]{2}}\right)\frac{\epsilon}{\sigma^2}.$$

Question 3: Free electrons in metals

1) (10p) Consider a 1D free electron gas formed in a mono-valent metal with a lattice constant a and a total length L. Calculate the Fermi energy E_F and the electron density of states $D(E)$ (hint: be aware of double counting in the states).

~~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~~

1D free electron gas has discrete energy states, quantized according to boundary conditions as: $E_n = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2$, where $n = 1,2,3,\cdots$.

The Fermi energy – is the maximum energy, which electrons can have in a metal at zero temperature. Due to the Pauli exclusion principle, each nth energy level can be occupied only by 2 electrons. Which makes the maximum energy level to be occupied:

$$E_n = \frac{\hbar^2}{2m}(\frac{2\pi n}{L})^2.$$

The density of states can be obtained using the formula:

$$g(\varepsilon)L = G(\varepsilon) = \frac{dN}{d\varepsilon} = 2\frac{d}{dk}\left(\frac{2k}{\frac{2\pi}{L}}\right)\left(\frac{d\kappa}{d\varepsilon}\right) = \left(\frac{2L}{\pi}\right)\left(\frac{m}{\hbar^2 k}\right) = \frac{L}{\pi}\left(\sqrt{\frac{2m}{\hbar^2}}\right)\varepsilon^{-\frac{1}{2}}.$$

2) (6p) If the transport of electrons is characterized by the Drude model, demonstrate that assuming a single parameter τ, the mean scattering time is sufficient to describe Ohm's law.

~~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~~

In the Drude model of electrical conduction in metals, electrons are treated as classical particles moving through a lattice of fixed ions. The model assumes that electrons collide with the lattice ions, experiencing scattering events that randomize their motion. In the Drude model, the equation of motion for an electron in an electric field E is given by $m\left(\frac{d}{dt} + \frac{1}{\tau}\right) = -eE$. Where τ is the mean free time between collisions (mean scattering time). The current density can be expressed as $J = -ne\langle v\rangle$, where n is the density of electrons. From the equation of motion, we have $\langle v\rangle = \frac{-e\tau}{m}E$. Substituting this expression into the current density formula,

we get $J = \frac{ne^2\tau}{m}E$ is the equation that resembles Ohm's law, $J = \sigma E$, where σ is the conductivity. In the Drude model, the conductivity is given by $\sigma = \frac{ne^2\tau}{m}$.

Note, we see that assuming a single parameter τ, the mean scattering time, is sufficient to describe Ohm's law in the Drude model. The mean scattering time characterizes the average time between collisions experienced by electrons in the metal, and it governs the overall conductivity of the material.

3) (8p) At low temperatures far below the Debye and Fermi temperatures (T_D and T_F, respectively), repeated measurements of specific heat in a 3D metal

consistently show a linear relationship between $\frac{c}{T}$ and T^2. Find the contributions to the specific heat from electrons and phonons from the measurement result shown below.

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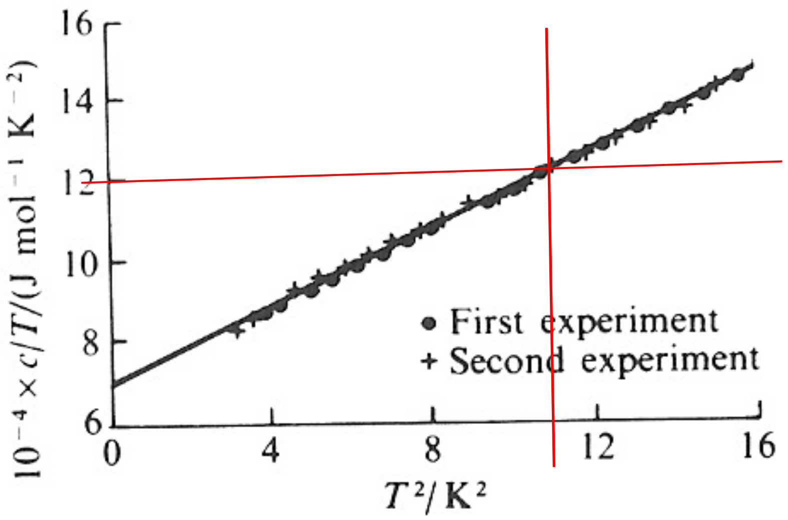


At low temperatures far below the Debye and Fermi temperatures, the specific heat may be written as the sum of electron and phonon contributions:

$C = \gamma T + AT^3$, hence, $\frac{C}{T} = \gamma + AT^2$.

When $\frac{C}{T}$ is plotted versus T^2, the intercept with y-axis is the γ, the electronic contribution.

The slope is the coefficient A, for phononic contributions.

Thus, $\gamma = 7 \times 10^{-4} \frac{\text{J}}{\text{mol}\cdot\text{K}^2}$ and $A = \frac{12}{11} \approx 1.1 \frac{\text{J}}{\text{mol}\cdot\text{K}^4}$.

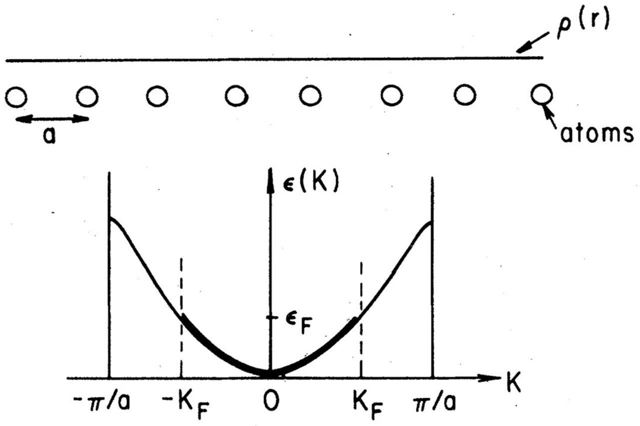
4) (Bonus 5p) In 1955, R. Peierls showed that a one-dimensional electron gas of a mono-valent chain, subject to a crystal lattice, is not stable at low temperatures. It forms a new state, called the charge density wave (CDW) state. Explain the consequence of forming such a state (in the $E(k)$ relationship shown below). And argue why this state is preferred.

∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼ *Answer* ∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼∼

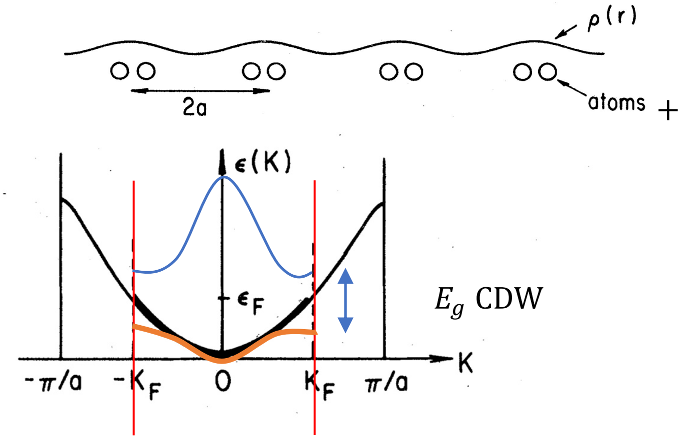
If we consider a monovalent metal providing one electron per primitive cell, the band is initially half-filled. Following a simple derivation (same as Q3.1), $N_z = \frac{2V_k}{V_{s.s}} = \frac{2\cdot 2k_F}{\frac{2\pi}{L}} = \frac{2k_F L}{\pi}$, where $L = Na, Z = 1$. Therefore, $k_F = \frac{\pi N Z}{2Na} = \frac{\pi}{2\alpha}$.

As the electrons close to the zone edge, $k = k_{BZ}$ undergo Bragg diffraction, resulting in a gap opening at $k = k_{BZ}$. Therefore, the energy gaps introduced by the CDW state can lead to the formation of an insulator. Namely, before the CDW transition, the system is a metal with half half-filled band. After the CDW transition, it has a filled band, therefore, the system becomes an insulator.

Pictorially, the process can be shown as,
Before CDW transition

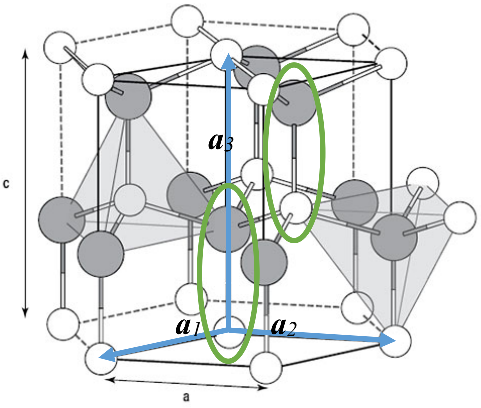


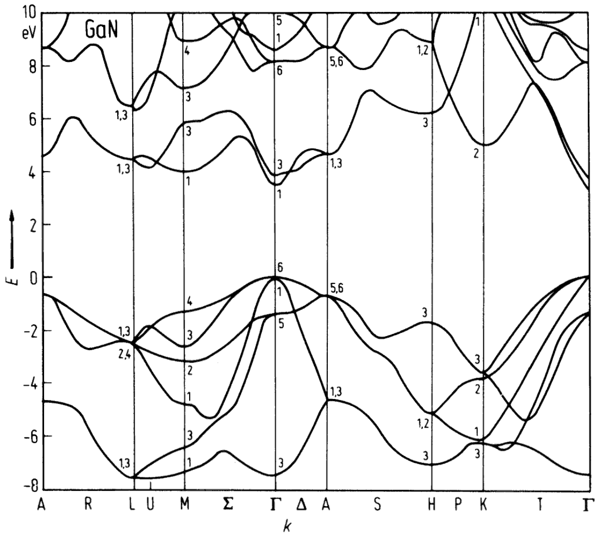
After CDW transition



Question 4: Semiconductor and superconductor

1) (10p) GaN (Ga is gray) is a crucial wide-bandgap semiconductor used in white-colored LEDs. The discoverers were awarded the Nobel Prize in Physics in 2014. GaN crystallizes in the Wurtzite-type structure (below), which is the other main family of semiconductors besides the Zinc-blend structure.
   Determine the unit cell and basis of GaN from the crystal structure. Discuss the energy and momenta conservation in the optical absorption process of GaN.
   Sketch the optical absorption intensity versus photon energy, considering that the gap size of GaN is roughly 3.2 eV.





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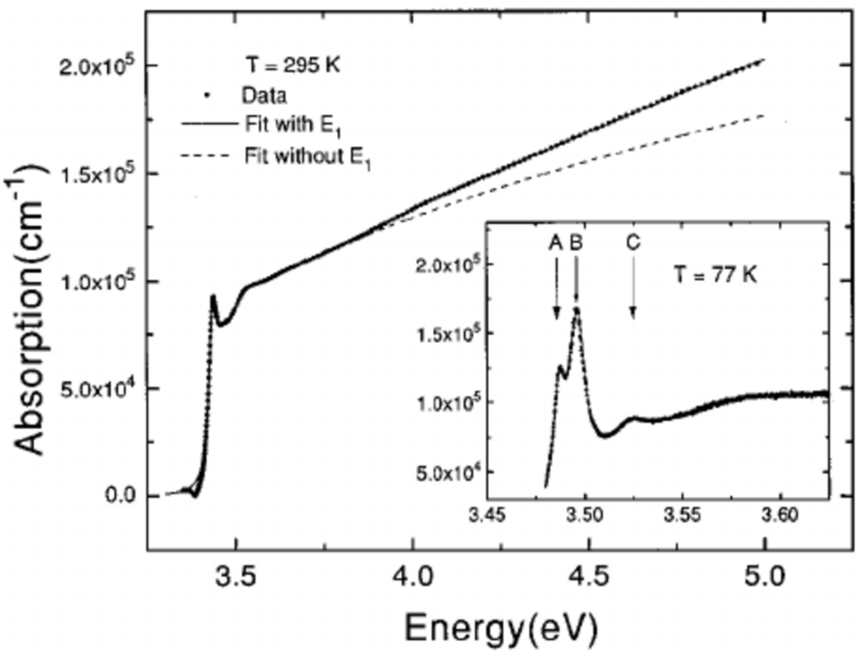

The Wurtzite structure belongs to the hexagonal lattice, composed of two interpenetrating HCP-like lattices of the same dimension. These identical lattices of Ga and N are further displaced along the $\vec{a}_3$ axis, with a distance equal to the Ga-N bond length. Therefore, the Wurtzite structure can be constructed by an HCP-like structure with a basis of two atoms. Since HCP is a hexagonal lattice with a 2-atom basis, the Wurtzite structure has four atoms per primitive cell.

The experimental absorption spectrum for GaN exhibits an abrupt upturn at the onset at 3.2 eV. The absorption spectrum is expected to resemble something close to the dashed line (without those peaks).
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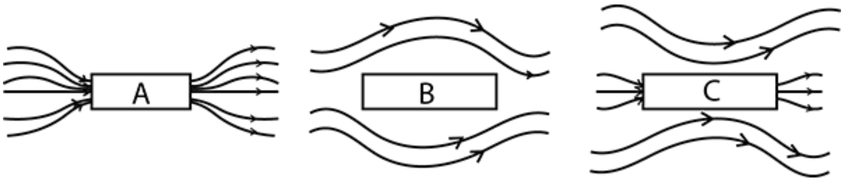
As GaN is a direct band gap material, the band diagram indicates that the transition occurs at the Γ point. The transition involves the momentum of final and initial states, $p_f = p_i \rightarrow p_e + p_h = p_{hp} = hk_c + hk_v \cong 0$.
The energy associated with the transition is $\delta E = E_g = E_c - E_v = 3.2$ eV.

Note, it's important to note that the experimental shape may differ from the classic square root due to excitonic peaks at the absorption edge (resulting from the formation of excitons). If your answer has a clear onset at 3.2 eV, it is more than sufficient.

2) (6p) Based on the change of magnetic field shown below, determine for cases A, B, and C which one is diamagnetic, paramagnetic, and ferromagnetic, respectively. Also, specify the magnitude and/or sign of χ in the magnetization.



~~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~~

Material A →ferromagnet, B → diamagnet, C → paramagnet.

Since $\vec{M} = \chi\vec{H}$, and $\vec{B} = \mu_0(\vec{H} + \vec{M}) = \mu_0(1 + \chi)\vec{H}$. Therefore, para- or diamagnetic is compared with vacuum, whether having the material A, B, or C can increase or decrease the magnetization compared with vacuum $\vec{B} = \mu_0\vec{H}$.

Therefore, $\chi > 0, \rightarrow$ Paramagnetism

$\chi < 0, \rightarrow$ Diamagnetism.

$\chi = \infty, \rightarrow$ Ferromagnetism

3) (8p) Consider a metal that demonstrates superconducting properties at a critical temperature T_c. What is the Hallmark change of physical properties that characterize the superconducting transition?

~~~~~~~~~~~~~~~~~~~~~~~~ *Answer* ~~~~~~~~~~~~~~~~~~~~~~~~

The hallmark change of physical properties that characterizes the superconducting transition is the abrupt onset of zero electrical resistance. Below a critical temperature T_c, superconductors exhibit:

1. Zero resistance: Electric current flows without resistance.
2. Perfect diamagnetism: superconductors expel magnetic fields from their interior, known as the Meissner effect.

We can also accept the following,
Critical magnetic field H_c: above which system loses superconductivity.
Critical current density J_c: above which system loses superconductivity.
Energy gap in the density of states: An energy gap in the density of states for electrons near the Fermi level, representing the energy needed to break apart Cooper pairs.

4) (Bonus 5p) In addition to the Hallmarks discussed in the above questions, further experimental details are presented below by measuring the heat capacity of a superconducting state (c_s) and normal state (c_n, orange). The normal state is obtained by applying a large magnetic field that destroys the superconducting state. What insights can we gain from the result regarding the formation of Cooper pairs by pairing two $s = \pm\frac{1}{2}$ electrons?

~~~~~~~~~~~~~~~~~~~~~~ Answer ~~~~~~~~~~~~~~~~~~~~~~

In the BCS theory of superconductors, all electrons form Cooper pairs, constituting the ground state of the system. To create a Cooper pair, we need two spin-half electrons to pair in a way that total $S = 0$.

In the BCS state, the superconductor exhibits a gap Δ at the Fermi level of the density of states (DOS). At $T = 0$, the Cooper pair cannot carry normal current and heat due to the absence of excited states caused by Δ. This is similar to an intrinsic semiconductor at $T = 0$ where $np = 0$. As the temperature increases from 0 to T_c, the system undergoes a process of excitations across the gap Δ to form normal electrons, analogous to the formation of intrinsic carriers in semiconductors at finite T. In a BCS superconductor, at $T = 0$, $n_{en} = 0$, all particles are n_{es}, where n_{en} and n_{es} representing the density of "normal electrons" and "Cooper pairs" respectively. Whereas, at $T = T_c, n_{es} = 0, n_{en} = n$, indicating the density of carriers in a normal metal.

Due to the difference in the excitation process,
For normal electrons, any temperature dependence, or Fermionic excitation is set by the Fermi-Dirac distribution for normal electron → $c_e \propto T$.
For BCS superconductor, Fermionic excitation over the gap $\Delta(T)$
Therefore, we expect a jump from c_n to c_s at T_c.

Owing to the small $\Delta(T)$, the excitation over the gap is much easier, resulting in $c_s > c_n$. On the other hand, when a sufficiently large magnetic field destroys the superconductivity gap $\Delta(T)$, the excitation through the gap disappears, and the heat capacity follows c_n even below T_c.