Final Exam - Solid State Physics 1

Wednesday, 23rd of January 2019, 9:00-12:00

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 the course content.

Each sub-question is independently solvable. Work on the easy questions first and earn the bonus points as your last step!

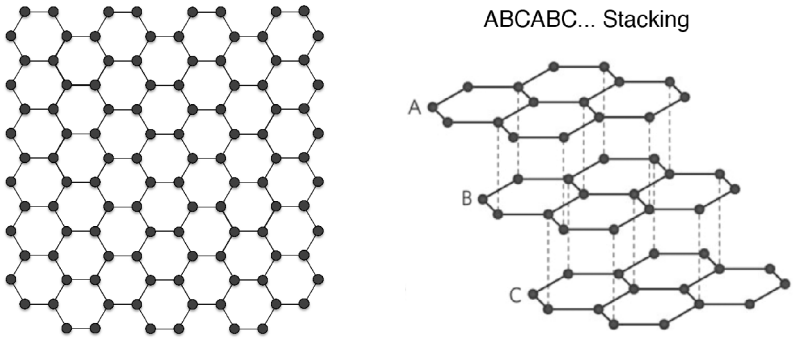
Don't forget to write your **full name** and **student number** on **each** sheet that contains your answer.

The exam has 5 questions with a total of 100 points plus 10 bonus points.

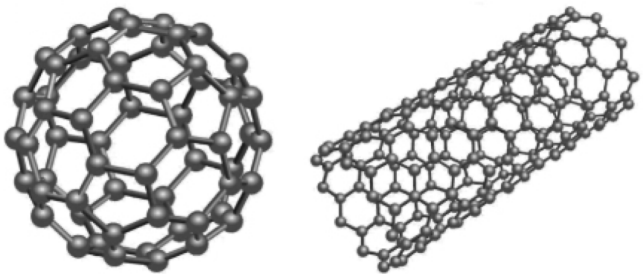
----------The Start of Questions----------

Question 1: Crystal structure (20+5 points)

A. Crystal systems of carbon

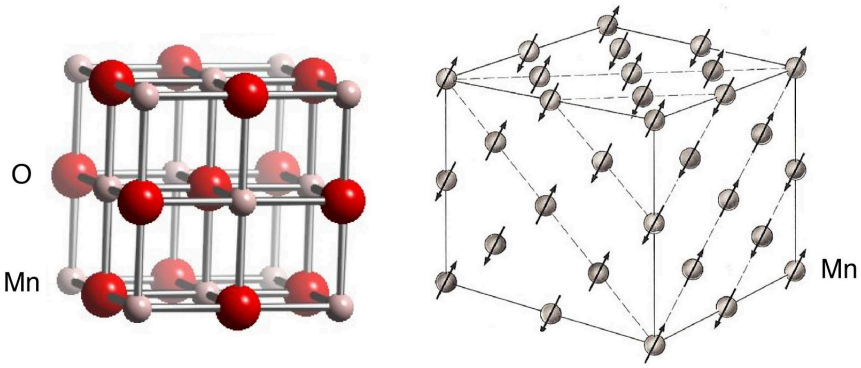


1) (**5p**) Draw all possible two-dimensional (2D) Bravais lattices. For each case, specify the relationship between two lattice vectors: $\boldsymbol{a}$, $\boldsymbol{b}$, and the angle θ between them.
2) (**2p**) As shown in the left panel above, if the bond length between carbon atoms is a, find the 2D Bravais lattice of the graphene (*i.e*. the length of lattice vectors evaluated in a and the angle θ in degree between the vectors).
3) (**2p bonus**) Graphite is a 3D single crystal of carbon. There are two naturally existing structures that can be constructed by stacking 2D graphene sheets in ABAB... or ABCABC... order. Briefly explain how to construct the ABC structure by shifting the layers while stacking them. (*i.e*. specify the direction and length of each shift).
4) (**3p**) From a 2D graphene sheet, briefly explain how to construct other allotropes of carbon for the 1D (carbon nanotubes), and 0D (fullerenes) systems.



Fullerene Carbon Nanotube

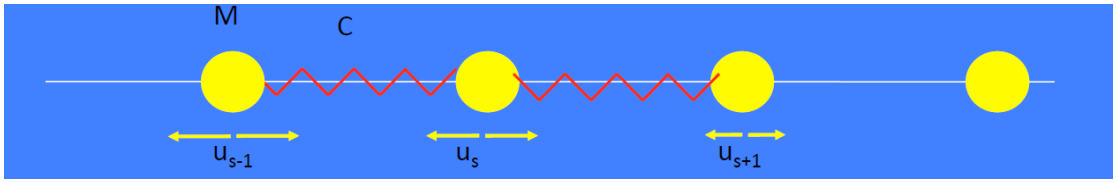
B. The crystal structure (left) of an antiferromagnetic compound MnO shown below can be identified by *X*-ray scattering. On the other hand, by magnetic neutron scattering, the antiferromagnetic ordering of Mn^{2+} ions can also be identified showing opposite magnetization between alternative planes in [111] directions.



1) (**3p**) From the crystal structure (left), determine the Bravais lattice vectors using a cartesian coordinate and the lattice constant *a* between the Mn^{2+} ions.
2) (**2p**) Calculate the volume of the primitive cell in terms of *a*.
3) (**2p**) If we describe the crystal structure determined in question (1) as simple cubic plus a basis, determine the total number of atoms in the basis.
4) (**3p bonus**) Calculate the phase factor by summing up $f_i e^{i\phi_i}$ from the i^{th} atom in the basis and determine the scattering intensity by using f_{Mn} and f_{O}, which are the scattering intensities from the individual Mn^{2+} and O^{2-} ions.
5) (**3p**) Compared with *X*-ray scattering, the neutron scattering is sensitive to the magnetic structure of the crystal (right panel). Determine the magnetic Bravias lattice by finding the underlying periodicity of the "magnetic environment" of each Mn^{2+} ion. Calculate the volume of the magnetic primitive cell.

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

As shown below, consider a linear chain of *N* atoms all with mass *M*.



1) **(6p)** If The potential energy between two neighboring masses at a distance r is: $V(r) = a(\frac{1}{r} - \frac{b}{\sqrt{r}})$

and the interactions in the chain only extend to the nearest neighbors, calculate the equilibrium distance R_0 and determine the equilibrium energy for the whole system (hint: be aware of the *double-counting* of atoms). Determine the force constant C between nearest-neighbor atoms, calculate the normal mode of this linear monoatomic chain.

2) **(2p)** Sketch the dispersion relation in the first Brillouin zone.

3) **(3p)** Sketch the dispersion relation in the first Brillouin zone if either the force constant or mass of the atoms changes so that the mono-atomic chain becomes a di-atomic chain. How will the $\omega(k)$ relationship evolve?

4) **(2p)** If the number of atoms in the basis increases from 2 to n, describe any change to the dispersion relationship $\omega(k)$.

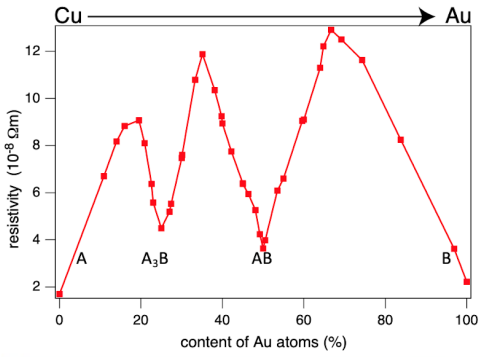
5) **(4p)** In the di-atomic chain, briefly discuss the motion of atoms in the chain for the vibrational states at $k = 0$ and for k at the edge of first Brillouin zone. (hint: consider the motion of basis itself and atoms inside the basis).

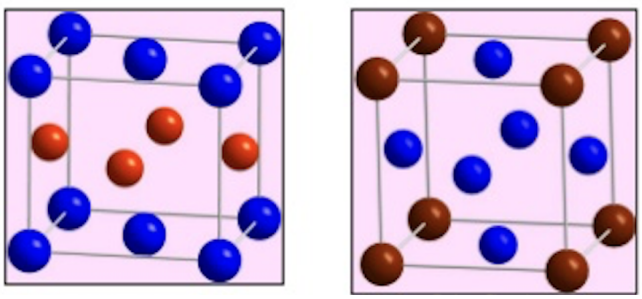
6) **(3p)** If the force constant for the i^{th} atom is C_i and the interaction between the atoms extends to the second nearest neighbors, show that the phonon dispersion becomes:

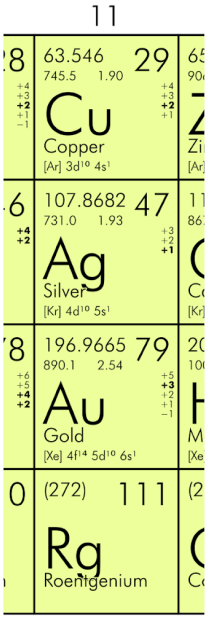
$$\omega^2 = \frac{4}{m}(C_1 sin^2(ka/2) + C_2 sin^2(ka))$$

$$(cos(x) = \frac{e^x + e^{-x}}{2},\ cos^2 x + sin^2 x = 1,\ cos 2x = cos^2 x - sin^2 x)$$

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







Many metals can form intermetallic compounds with a continuously variable ratio. The simplest example, called binary alloy, can be represented by the crystal formed by mixing gold (Au) and copper (Cu). The electrical resistivity versus the ratio has been measured showing minimums in two specific stoichiometry (meaning the ratio between Au and Cu).

1) (**5p**) View the electrons as free classical particles, the electrical transport can be described by the Drude's model. Show that the Ohm's law is valid in Drude's model.
(here *e* is the elemental charge, *n* is the carrier density, and the total scattering time follows $\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3}$, where the τ_1, τ_2, and τ_3... are the scattering time scale for mechanism 1, 2, and 3...).

2) (**4p**) In the Sommerfeld's model, the Ohm's law can be derived by using the same τ. Sketch the change of momentum of the electrons due to the τ. What is the main difference in discussing the Ohm's law in Drude's model and Sommerfeld's model?

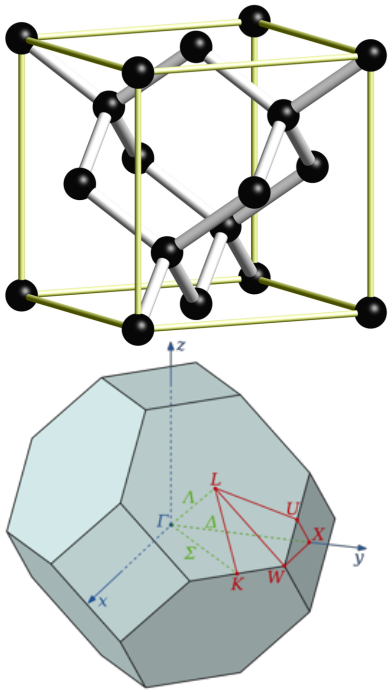
3) (**5p**) If we assume the distance *a* between atoms remains the same for all different ratios and the elements in group 11 give only 1 valence electron. Calculated the conductivity using Drude's model. Explain the discrepancy between the conductivity calculated using Drude's mode and the measured resistivity.

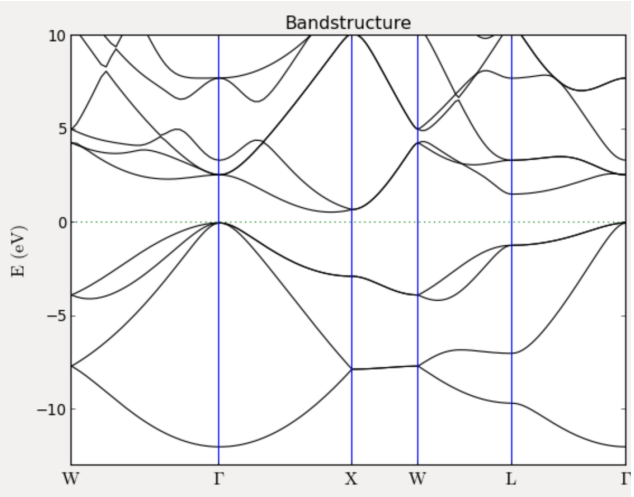
4) (**6p**) Identify the stoichiometry (the ratio of Au/Cu) for the two crystal structures shown above. If you can make a very thin AuCu film of one atom thick by isolating any {100} plane with 1:1 ratio from the two crystals above, calculate and sketch the 2D density of states by considering the quantization due to confinement along the *z*-axis. Draw the Fermi surface of your mono-atomic thick AuCu film.
(for the simplest case you can treat the confinement as if they are from the infinitely high potentials)

5) (**3p bonus**) Briefly discuss the gradual evolution of band structure from 2D to 3D when we grow the film from atomically thin to bulk.

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

Single crystal silicon has an indirect bandgap E_g = 1.12 eV. We assume equal effective hole and electron mass $m_e = m_h = m_0$, where m_0 is the rest mass of the electron. Impurity with a concentration of $N = 10^{18}$ cm^{-3} was doped. The impurity energy level of the dopant is E_d = 0.2 eV from the band edge (*i.e.* either to the top of the valence band or to the bottom of the conduction band).





1) (**3p**) Using the free electron model and band calculation above consider the diamond structure of Si (valence electron Z = 4), show that E_F will locate inside the energy gap.
2) (**4p**) Discuss the energy and momentum conservation in the optical absorption of Si. Sketch the optical absorption of Si as the function of the energy of the incident photons.
3) (**2p**) For the boron (Z = 3) and phosphorous (Z = 5) doping, Sketch the impurity level with respect to the valence and conduction band.
4) (**6p**) Show that the intrinsic conduction in this material is negligible at 300 K. The n and p are the carrier concentration of intrinsic conduction,

   $np = 4(\frac{k_B T}{2\pi\hbar^2})^3 (m_e m_h)^{3/2} e^{-\frac{E_g}{k_B T}}$, and for the impurity doping with donor N_d, the carrier density is $n = \sqrt{2}(\frac{m_e k_B T}{2\pi\hbar^2})^{3/4} \sqrt{N_d} e^{-\frac{E_d}{2k_B T}}$.

   k_B = 1.38×10^{-23} J/K, m_0 = 9.1×10^{-31} kg, $\hbar$ = 6.58×10^{-16} eVs = 1.05×10^{-34} Js
5) (**2p**) Express the effective mass from the dispersion relationship $E(k)$.
6) (**3p**) Calculate the conductivity σ of the material, given the carrier mobility μ = 100 cm^2/Vs.
7) (**2p bonus**) If the dispersion relationship is $E_c + \frac{\hbar^2 k^2}{2m_e}$ or $E_v - \frac{\hbar^2 k^2}{2m_h}$. Roughly

indicate the shape and location of the Fermi surface for B and P doping, respectively. (The location can be referred to the high symmetry points of Γ, X, W of the first Brillouin zone).

Question 5: Magnetism and superconductivity (20 points)

Hamiltonian of an atom under a magnetic field can be written as $H = H_0 + \mu_B(\mathbf{L} + g\mathbf{S}) \cdot \mathbf{B} + \frac{e^2}{8m_e}\sum_i(\mathbf{B} \times \mathbf{r}_i)^2$

, where the H_0 is the Hamiltonian without the magnetic field ***B*** and $g = 2$.

1) (**3p**) Which term in the Hamiltonian above corresponds to the diamagnetism and explain the microscopic origin of the universal existence of diamagnetism?
2) (**2p**) We want to choose one material from those listed below for shielding magnetic field from the earth (<10^{-4} Tesla). Which material from the list would be my best choice?

Note:
$\mathbf{B} = \mu_0(1 + \chi)\mathbf{H}$

	$\chi/10^{-6}$	$\chi_m/10^{-10}$ (m^3 mol^{-1})
water	−90	−16.0
benzene	−7.2	−6.4
NaCl	−13.9	−3.75
graphite (∥)	−260	−31
graphite (⊥)	−3.8	−4.6
Cu	−1.1	−0.078
Ag	−2.4	−0.25
$CuSO_4 \cdot 5H_2O$	176	192
$MnSO_4 \cdot 4H_2O$	2640	2.79×10^3
Al	22	2.2
Na	7.3	1.7

3) (**5p**) Considering the spin paramagnetism of electrons in metals, which term in the Hamiltonian should be considered? Sketch the change to the density of states when a bulk metal is subjected to a magnetic field ***B***? Mark the spin quantum number S_z and magnetic moment on the density of states.
4) (**2p**) When a magnetic field ***B*** is applied, calculate the magnetization ***M*** of N electrons, each has a moment $\boldsymbol{\mu}_B$.
5) (**2p**) What are the two hallmark physical properties that differentiate a superconductor from any other conductors?
6) (**4p**) When a superconductor is cooled below the superconducting transition temperature T_c, qualitatively describe the differences between a superconductor and a perfect conductor ($\rho = 0$) when both of them are placed in the magnetic field.

----------The End of Questions----------