Introduction to Solid State Physics - NTU/Grad. Inst. Appl. Phys. – 博士資格考試 – Feb. 2014

[**Total points 120**]

1. [**10 pts**] What are Bragg and Von Laue formulations of x-ray diffraction by a crystal? Demonstrate the equivalence of the Bragg and Von Laue formulations.

2. [**2+2+2+2+2 = 10 pts**] (a) What is the structure factor in the x-ray diffraction from crystals? Calculate the structure factors for (b) simple cubic, (c) bcc, (d) fcc, and (e) diamond. Tabulate reflections which are possibly present in these lattices.

3. [**2+2+2+2+2+3+2 = 15 pts**] A fundamental concept in the description of any crystalline solid is that of Bravais lattice, which specifies the periodic array in which the repeated units of the crystal are arranged.

   (a) What is a Bravais lattice? Define one.

   (b) How many distinctive two-dimensional lattice types, and what are they (and draw them)?

   (c) How many distinctive three-dimensional lattice types, and what are they (and draw them)?

   (d) What is a primitive cell?

   (e) Which one of the Bravais lattice is the primitive cell of bcc lattice? Calculate the angle and the lattice constant(s).

   (f) What are the volume (conventional cell), lattice points per conventional cell, volume of primitive cell, lattice points per unit cell, number of nearest neighbors, nearest-neighbor distance, and packing fraction of a face-centered cubic lattice?

   (g) Prove that in a cubic crystal a direction [*hkl*] is perpendicular to a plane (*hkl*) having the same indices. What is the distance between each successive plane?

4. [**2 pts**] Crystal structures have been studied through diffraction of photons, neutrons, and electrons. Please describe the studies as much as you know and the differences among the three types of diffraction.

5. [**3 pts**] What are the principal types of crystalline binding? Give at least one example of material systems to each type.

6. [**10 pts**] Lennard-Jones potential is a simple model to estimate the total energy of an inert gas crystal and has the form $U_{tot} = 2N\varepsilon[\sum_j' \left(\frac{\sigma}{p_{ij}R}\right)^{12} - \sum_j' \left(\frac{\sigma}{p_{ij}R}\right)^{6}]$. (a) Please give an explanation to the meaning (what causes each of these terms...) of the first and second terms in the Lennard-Jones potential. (**3 pts**) (b) For fcc structure, we know $\sum_j' p_{ij}{}^{-12} \approx 12.132\,, \sum_j' p_{ij}{}^{-6} \approx 14.454$. Please calculate the equilibrium nearest-neighbor distance (**2 pts**) and the cohesive energy (**3 pts**) for inert gas crystal in fcc structure (Ne, Ar, Kr, Xe). You will discover that in this simple model the equilibrium nearest-neighbor distance and cohesive energy is the same for these four inert

gases. (c) From (b), we know that in this model the cohesive energy should be all the same. Please explain why the observed boiling points (melting points) of these four inert gases are different (**2 pts**).

	Neon	Argon	Krypton	Xenon
Boiling point (K)	27.3	87.4	121.5	166.6
Melting point (K)	24.7	83.6	115.8	161.7

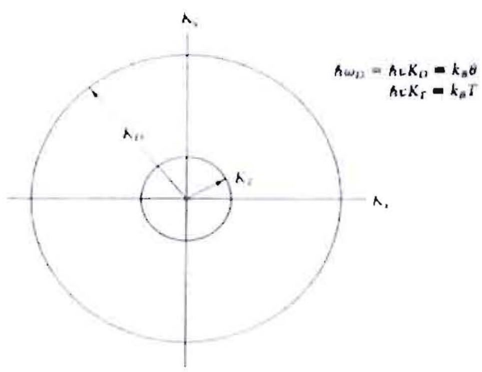
7. [**15 pts**] At temperature much below the Debye temperature and the Fermi temperature, the heat capacity can be written as the sum of the electronic and phonon contributions as

$$C/T = \gamma + AT^2$$

(a) Explain the failure of the classical Drude Model and the success of the Sommerfeld theory to give the correct expression for the electronic heat capacity. (5 points)

(b) Derive the T-linear dependence of the electronic heat capacity term using a qualitative approach based on the Fermi Dirac distribution function for the free electron gas. (5 points)

(c) Derive the ***Debye T^3 –law*** for the phonon heat capacity term by using a qualitative approach for the allowed excited phonon modes in the ***K*** – space. (5 points)



8. [**30 pts**] In the free electron gas model, the electron transport follows the so called the Ohm's law.

(a) Derive the Ohm's law to express the electrical conductivity as

$J = \sigma E$, where $\boldsymbol{\sigma = ne^2\tau/m}$, and τ is the collision time. (3 points)

(b) The mobility is defined as the ratio of the drift velocity to the electrical field as $\mu = \upsilon/E$. Show that the electrical conductivity to be related to μ as $\boldsymbol{\sigma = ne\mu}$, and $\boldsymbol{\mu = e\tau/m}$ (3 points)

(c) The thermal conductivity ***K*** of a solid is defined with respect to the steady law of heat down a long rod with a temperature gradient ***dT/dx***, where j_U is equal to $-K\, dT/dx$, and j_U is the thermal energy transmitted across per unit area per unit time. Show that thermal conductivity is given as ***K = 1/3 C v l,*** where ***C*** is the heat capacity per unit volume, υ is the average particle velocity, and ***l*** is the mean free path between collisions. (5 points)

(d) Following the equation for total heat capacity in the problem 7, the explicit expression for γ ***is*** $\frac{1}{2}\pi^2 N k_B T/T_F$, where T_F is the Fermi temperature. Derive the electron thermal conductivity to be $K_{el} = (\pi^2 n\, k_B^2 T\tau)/3m$ (5 points)

(e) Taking the ratio of electron thermal conductivity to electrical conductivity, and derive the **Wiedemann –Franz Law, and the Lorentz number.** (4 points)

(f) Describe the thermoelectric effect, and give the definitions of thermopower, the Peltier coefficient, and the relationship between the two. (10 points)

9. [10 pts] (a)What is Bloch's Theorem? [5 points] (b)Prove it. (You may prove it from general quantum mechanical consideration or other considerations.) [Hint: 1. You may try to construct a translation operator of the wave function, and consider its commutation relation with Hamiltonian. 2. You can also follow the approach in Kittel book.]
10. [5 pts] In the free electron model, we cannot explain why there are insulators and semiconductors because we do not have the concept of energy gap at that time. Please compare the difference between free electron model and nearly free electron model, and explain the origin of the energy gap. (You don't need to give out a throughout calculation to prove the existence of energy gap.)
11. [10 pts] Kronig-Penney Model.

(a) For the delta-function potential and with P being far less than 1, find the lowest energy at k =0. [5 points] (b) For the same problem, find the first band gap at k=π/a. [5 points]

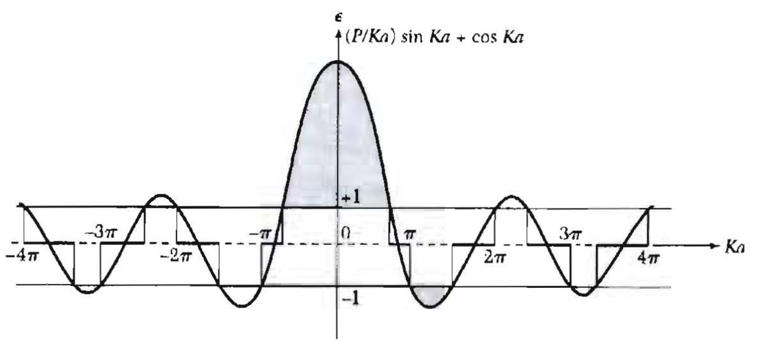


Figure 5 Plot of the function $(P/Ka)\sin Ka + \cos Ka$, for $P = 3\pi/2$. The allowed values of the energy ϵ are given by those ranges of $Ka = (2m\epsilon/\hbar^2)^{1/2}a$ for which the function lies between ± 1. For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.