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Student ID No:..... Questions : 4

UNIVERSITY OF TASMANIA

EXAMINATIONS FOR DEGREES AND DIPLOMAS

October-November 2021

KYA322 STATISTICAL PHYSICS AND SOLID STATE PHYSICS

First and Only Paper

Ordinary Examination

Examiner: Dr. Andrew McCulloch

Time Allowed: Two (2) hours

Reading Time: Fifteen (15) minutes

Instructions:

Answer THREE (3) questions. Begin each question in your answer book on a new page.

All questions have equal value of 20 marks, but parts within a question may be weighted differently as indicated.

1. This question focuses on the physics of solids without considering the microscopic structure.

(a) What is the Einstein model of a solid? List both the successes and the shortcomings of the model.

[2 marks]

(b) State the assumptions of the Debye model of heat capacity for a solid.

[2 marks]

(c) Einstein obtained an expression for the expectation value of the energy of a single oscillator at frequency ω

$$\langle E \rangle = \hbar\omega \left(n_{\mathrm{B}}(\beta\hbar\omega) + \frac{1}{2} \right)$$

Consider a three-dimensional solid as modelled using the framework of Debye.

(i) Write an expression for the total energy in the system for oscillators with frequencies $\omega(\mathbf{k})$

[1 mark]

(ii) What is the density of states $g(\omega)$? Justify the validity of the expression

$$E = \int_0^{\omega_{\text{cutoff}}} \mathrm{d}\omega \; g(\omega) \; \hbar\omega \; \left[n_{\mathrm{B}}(\beta\hbar\omega(\mathbf{k})) + 1/2 \right]$$

[2 marks]

(iii) Assuming linear dispersion, what is the density of states $g(\omega)$ in the above expression?

[3 marks]

Continued...

(iv) The cutoff frequency can be evaluated by ensuring there are the correct number of modes in the system. If there are N oscillators, what should be the total number of oscillators? Justify your response.

[2 marks]

(v) Compute the cutoff frequency cutoff

[3 marks]

(d) A triumph of Debye's theory was the explanation of the cubic dependence on temperature for the heat capacity at low temperature. Briefly explain why this behaviour occurs.

[3 marks]

(e) Careful observation of the heat capacity for metals at very low temperatures shows deviation from this cubic behaviour. Provide a brief explanation for this discrepancy.

[2 marks]

Continued...

2. This question focuses on incorporating microscopic structure into the physics of solids in one dimension.

(a) Consider a one-dimensional diatomic chain, where the spring constants between neighbouring atoms are identical and equal to κ, but neighbouring masses are different, alternating between m_1 and m_2.

You are going to derive the dispersion relation for this system.

(i) Sketch the system as described above, ensuring to mark the unit cell length a on the diagram

[2 marks]

(ii) Denoting the position of the n^{th} particle of mass m_1 as x_n and the position of the n^{th} particle of mass m_2 as y_n, show that the equations of motion for the system are

$$m_1\ddot{\delta x}_n = -\kappa(\delta x_n - \delta y_{n-1}) - \kappa(\delta x_n - \delta y_n)$$
$$m_2\ddot{\delta y}_n = -\kappa(\delta y_n - \delta x_n) - \kappa(\delta y_n - \delta x_{n+1})$$

[2 marks]

(iii) Solve that above set of equations for the normal modes of the system to show that

$$\omega^2 = \frac{\kappa}{m_1 m_2}\left(m_1 + m_2 \pm \sqrt{(m_1+m_2)^2 - 2m_1 m_2 \cos(ka)}\right)$$

[6 marks]

(iv) Find the sound velocity for the acoustic branch around $k = 0$

[3 marks]

Continued...

(b) We now alter our one-dimensional diatomic chain to a triatomic chain. How many optical modes and how many acoustic modes would you expect?

[1 mark]

(c) The one-dimensional chain provides an excellent model for understanding the properties of solids in one dimension. With explicit reference to covalent bonding as modelled through the linear combination of atomic orbitals, explain why it that we can use a harmonic potential to well describe the interatomic potential.

[6 marks]

Continued...

3. This question focuses on the describing the geometry of, and the scattering from, solids.

(a) A triangular lattice has primitive lattice vectors $\mathbf{a_1} = a\hat{\mathbf{x}}$ and $\mathbf{a_2} = (a/2)\hat{\mathbf{x}} + (a\sqrt{3}/2)\hat{\mathbf{y}}$.

(i) Draw the lattice described by the above basis vectors (draw at least 3×3 lattice points)

[1 marks]

(ii) On the lattice above, draw both the primitive unit cell as defined by the primitive lattice vectors and the Wigner-Seitz cell

[2 marks]

(iii) Find the primitive lattice vectors of the reciprocal lattice

[3 marks]

(iv) What physical significance does the Wigner-Seitz cell of the reciprocal lattice hold?

[2 marks]

(b) What basis could be used in combination with the above lattice to return a honeycomb structure (that is, the structure of graphene)?

[2 marks]

(c) Now consider the structure of CsCl: a simple cubic with the basis Cs at [0,0,0] and Cl at [1/2, 1/2, 1/2]

(i) What kind of bonding would you expect for this structure?

[1 marks]

(ii) Compute the structure factor S for X-ray scattering from CsCl with a general set of Miller indices (hkl)

[3 marks]

Continued...

(d) Now consider the case of pure Cs, which has the same structure but with the chlorine atom replaced by a caesium atom (a simple cubic with the basis Cs at [0,0,0] and [1/2, 1/2, 1/2]).

(i) What kind of bonding would you expect for this structure?

[1 marks]

(ii) Using a previous result or otherwise, compute the structure factor S for X-ray scattering for pure Cs with a general set of Miller indices (hkl)

[1 marks]

(e) Consider the case of X-ray scattering from the planes defined by the Miller indices (220). What scattered intensity would one expect in the case of CsCl versus pure Cs?

[2 marks]

(f) The sample of CsCl was accidentally mislabelled, and it turns out that it is actually CsI, which has the identical structure except with Cl ($Z = 17$) replaced with I ($= 53$). Again, for diffraction from the planes defined by the Miller indices (220), what scattered intensity would expect from the CsI as compared to the CsCl? For reference, the atomic number of caesium is $Z = 55$.

[2 marks]

Continued...

4. This question focuses on band structure and its applications

(a) What is meant by the free electron model, the nearly-free electron model and the tight binding model? In what circumstances are the models appropriate?

[2 marks]

(b) Consider a square lattice of monovalent atoms in two dimensions.

(i) Roughly sketch the first Brillouin zone for the lattice (only the shape is important), and indicate the Fermi sea in the absence of a periodic potential

[1 mark]

(ii) Repeat the process above for both a weak and strong periodic potential

[2 marks]

(c) Barium ($Z = 56$) is a divalent atom, and the Fermi surface is shown below:

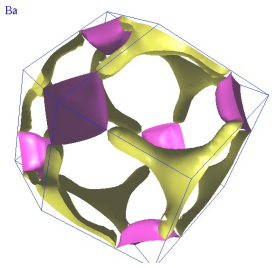

Figure 1: Fermi surface of barium

Explain the features of this surface, explicitly referencing the 2D analogues from the previous section, and what statements (if any) can be made about the conductivity and specific heat of barium based upon the Fermi surface alone?

[4 marks]

Continued...

(d) Consider a semiconductor quantum well: a material which is uniform $Al_xGa_{1-x}As$ with a thin layer of GaAs that is a material that has three regions. Recall that the energy eignestates of a quantum well have energies

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

.

We can model this system as a two-dimensional electron gas.

(i) Show that the density of states for a free electron gas is

$$g(E) = \frac{m}{\pi\hbar^2}\Theta(E)$$

where $\Theta(E)$ is the Heaviside step function

[3 marks]

(ii) Show that the density of states for electrons in the well is given by

$$g(E) = \frac{m_e^*}{\pi\hbar^2}\sum_{n>0}\Theta\left(E - E_c - \frac{\hbar^2\pi^2}{2m_e^*}\frac{n^2}{L^2}\right)$$

where E_c is the conduction band energy.

[2 marks]

(iii) What is the density of states for holes in this system?

[1 mark]

Continued...

(e) Now consider a "quantum wire": a one-dimensional block of GaAs in embedded in the $Al_xGa_{1-x}As$. The cross-section of the wire is an $L \times L$ square and the system is well described by a one-dimensional electron gas. Show the density of states for electrons is given by

$$g(E) = \frac{\sqrt{2m_e^*}}{\pi\hbar^2} \sum_{n_1,n_2>0} \left(E - E_c - \frac{\hbar^2\pi^2}{2m_e^*} \frac{n_1^2 + n_2^2}{L^2} \right)^{1/2} \Theta \left(E - E_c - \frac{\hbar^2\pi^2}{2m_e^*} \frac{n_1^2 + n_2^2}{L^2} \right)$$

[5 marks]

END OF QUESTIONS