Answer EVERY question from section A and TWO questions from section B.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.
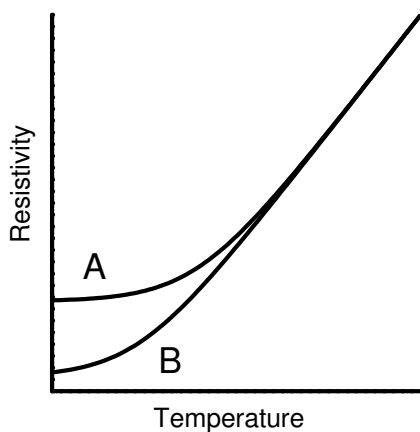
$$
\begin{array}{rclr}
\text{Mass of the electron} & m_e & = & 9.11 \times 10^{-31} \text{ kg} \\
\text{Charge on the electron} & e & = & -1.602 \times 10^{-19} \text{ C} \\
\text{Permittivity of free space} & \epsilon_0 & = & 8.854 \times 10^{-12} \text{ F m}^{-1} \\
\text{Boltzmann's constant} & k_B & = & 1.38 \times 10^{-23} \text{ J K}^{-1} \\
\text{Planck's constant}/2\pi & \hbar & = & 1.05 \times 10^{-34} \text{ J s} \\
\text{Speed of light} & c & = & 3 \times 10^8 \text{ m s}^{-1}
\end{array}
$$

SECTION A   [Part marks]

1. Sketch the general form of the "dispersion relation" expected for the phonons present in a one dimensional chain of indentical atoms connected together by identical springs. Label the axes and give typical values of the units.   [3]

   Indicate what changes are needed to describe the case of a (three-dimensional) cubic crystal, such as Gallium Arsenide, containing two equally spaced atoms of different mass per unit cell.   [4]

2. The graph above shows the resitivity measured as a function of temperature for two samples of Bismuth. Which part(s) of the curves can be explained by the presence of phonons in the sample?.   [4]

   Which of the two samples is likely to have the higher purity? Explain.   [3]

3. According to the "tight-binding" model for spherically symmetric wavefunctions, the energy ϵ_k of an electron of wavevector **k** is given by the expression,

$$\epsilon_k = -\alpha - \gamma \sum_m e^{-i\mathbf{k}\cdot\rho_m},$$

where the sum is over nearest neighbours in the crystal. What is the typical form of the integrals α and γ? **[4]**

Evaluate ϵ_k for a (two-dimensional) square lattice of atoms spaced a apart as a function of wavevector components k_x and k_y pointing parallel to the two edges of the square. **[3]**

4. A phosphorus (Z=15) atom substitutes for one of the silicon (Z=14) atoms in a crystalline block of silicon. Give two reasons why the wavefunction of the additional (fifteenth) electron extends much further than it does in a free phosphorus atom. **[4]**

Show with the aid of a suitable diagram where the energy of this extra electron lies with respect to the electronic levels of the silicon host.. **[3]**

5. Which two physical interactions are responsible for the cohesion in an ionic crystal? What determines the "ionic radius" of the ions? **[3]**

KF, RbF, KCl and RbCl all crystallise in the NaCl structure. If the lattice parameters of KF, RbF and KCl are $0.534nm, 0.564nm$ and $0.630nm$ respectively, what would you expect for the lattice parameter of RbCl? **[3]**

6. How can the presence of point defects be detected in an ionic crystal? **[2]**

If silver melts at $962°$C and contains an intrinsic relative concentration of 3×10^{-7} of lattice vacancies, estimate the energy required to remove an atom from the interior of the crystal lattice. **[4]**

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7. Metal-insulator transition in a 2D hexagonal lattice. Consider a two dimensional monoatomic crystal of atoms forming a hexagonal lattice with spacing a_0. Each atom contributes *two* electrons which may be considered initially to form a free-electron metal.

   (a) Draw aligned pictures of the real-space unit cell and its reciprocal lattice. Indicate the First Brillouin Zone (FBZ) on your diagram. **[6]**

   (b) Explain why the electrons are not allowed to be in the same quantum state and hence what region of reciprocal space is occupied by the filled electron states (at T=0). Label the "Fermi surface" on your diagram. For this purpose, you should assume the electrons are free and do not interact with the atom cores. **[6]**

   (c) Now consider turning on the interaction with the atom cores, which opens up a band gap ΔG at the FBZ boundary. Show on your diagram how this changes the shape of the Fermi surface. **[6]**

   (d) Estimate the minimum value of the band gap, ΔG_0, needed for the material to become insulating. Calculate the value of ΔG_0 in electron volts when $a_0 = 0.35nm$. **[12]**

8. Intrinsic carrier concentration in the conduction band of silicon. Silicon has a band gap of $1.1eV$ and and an average effective mass of $m^* = 0.3m_e$ for electrons in its conduction band.

   (a) Indicate how the energy band diagram for electrons in silicon differs from that of free electrons due to the "effective mass". **[6]**

   (b) Deduce an expression for the "density of states", the number of electron states per unit energy in the conduction band. **[6]**

   (c) Hence derive the following expression for the density of electrons in the conduction band,

   $$n = 2 \left(\frac{m^* k_B T}{2\pi\hbar^2} \right)^{3/2} e^{(\mu - E_C)/k_B T}$$

   where E_C is the energy of the conduction band edge. You will need to use the standard integral $\int_0^\infty \sqrt{x} e^{-x} dx = \frac{1}{2}\sqrt{\pi}$. What is the meaning assigned to the symbol μ that has been introduced? **[9]**

   (d) It can be said that the silicon becomes a conductor when its carrier concentration reaches $10^{20} m^{-3}$. Estimate the temperature at which this occurs for intrinsic (undoped) silicon, for which you can assume that μ lies at the middle of the band gap. **[9]**

9. According to the Deybe theory of the specific heat of a solid, the internal vibrational energy of a volume V of a solid containing N atoms is:

$$U = A(T) \int_0^{x_D} \frac{x^3 dx}{e^x - 1}$$

where $x = \hbar\omega/k_B T$ is the dimensionless form of the vibration frequency ω. This allows use of the standard integral:

$$\int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}.$$

(a) What assumptions are made in the Debye theory about the distribution of frequency modes as a function of their wavevector K? **[6]**

(b) Derive an expression for the (dimensionless) Debye cutoff frequency x_D in terms of the these assumptions. **[8]**

(c) By equating the *high-temperature* limit of the above expression to the classical result $U = 3Nk_B T$, deduce the unknown function $A(T)$. **[7]**

(d) Hence derive an expression for the *low-temperature* specific heat of a solid in the Debye theory. **[9]**

10. The first four peaks of the powder diffraction pattern, measured from a certain substance, are listed below. X-rays of wavelength $\lambda = 0.154nm$ were used.

Detector angle (2θ)	Relative intensity
20.7°	5
29.5°	81
36.3°	3
42.2°	52

(a) Why is diffraction only seen at these angles shown and not in between? State the law that connects the Bragg angle, θ, and the crystal lattice spacing. **[6]**

(b) Deduce the crystal symmetry and the lattice parameter from the observed angles. **[10]**

(c) At what 2θ angle would you expect the next peak to appear? **[6]**

(d) What information about the crystal structure can you deduce from the intensity information? **[8]**

END OF PAPER