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SUMMER EXAMINATIONS 2000

B.Sc. (Honours) Experimental Physics

EP417: Solid State Physics – Paper 3

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Time allowed: TWO hours
Answer THREE questions.

Q.1 Consider the case of a crystalline material with a simple cubic structure with orthogonal basic vectors a, b, c in the x, y, z directions, respectively. Derive formulae for the basic vectors (A, B, C) of the reciprocal lattice for this material in terms of a, b, c, and show that the reciprocal lattice is also simple cubic.

Explain how one may treat the alkali halide crystals as having a simple cubic lattice with a basis of eight atoms.

X-ray scattering from a simple cubic lattice obeys the Laue equation,

$$\Delta k = G_{hkl}$$

where G_{hkl} is the general reciprocal lattice vector: $G_{hkl} = hA + kB + lC$. Explain why X-ray scattering from alkali halide crystals does not occur for some $h\ k\ l$ values. The situation is even more restrictive for KBr. Explain why this is so.

Q.2 Explain how a classical analysis of the molar heat capacity of solids leads to the Dulong and Petit law.

A quantum analysis of lattice vibrations leads to the concept of phonons, the quantum state of the lattice being described by the product state

$$|n\rangle = |n_1\rangle.|n_2\rangle.|n_3\rangle.|n_4\rangle.... = |n_1, n_2, n_3, n_4,...\rangle ,$$

where n_i gives the number of phonons in mode i.

The atomic displacement operator for the atom at the origin is given by

$$u = \sum_k \sqrt{\frac{\hbar}{2mN\omega_k}}\, e_k\,(a_k + a_k^+)$$

where the a_k and a_k^+ operators have the property

$$a_k\,|n_k\rangle = \sqrt{n_k}\;|n_k - 1\rangle, \qquad a_k^+\,|n_k\rangle = \sqrt{(n_k + 1)}\;|n_k + 1\rangle$$

and the Hamiltonian describing the energy, E, of the vibrating lattice of N atoms is

$$H = \sum_k \frac{\hbar\omega}{2}(a_k^+ a_k + a_k a_k^+)$$

Using the Debye density of vibrational modes, explain how one calculates $\langle u\rangle$, $\langle u^2\rangle$, and $\langle E\rangle$ for the lattice when in thermal equilibrium at temperature T. From this derive a formula for the molar heat capacity. Sketch its variation with temperature, and show that it agrees with the Dulong and Petit law at high temperatures.

Q.3 The simplest model for non-interacting electrons in a solid (the Fermi Gas model) ignores the periodic nature of the electronic potential energy. Show that for this model the electron eigenstates can be represented as travelling waves: $\exp(i\mathbf{k}\cdot\mathbf{r} - i\omega t)$ with energy $\hbar^2\mathbf{k}^2/2m$, and the $\mathbf{k}$ values are given by $\mathbf{k} = \frac{2\pi}{L}(n_1\hat{\mathbf{x}} + n_2\hat{\mathbf{y}} + n_3\hat{\mathbf{z}})$, where n_1, n_2, n_3 are integers, and the solid is in the form of a cube of side L. We saw in class that when the periodic nature of the potential is taken into account, the electronic energy levels are grouped into bands with forbidden regions ("gaps") between the bands. Do you have any *physical* picture to explain the occurrence of these gaps at the Brillouin zone boundaries?

What form of statistical treatment is used to describe the equilibrium distribution of electrons among these states? Explain the concept of the Fermi level, and indicate the position of the Fermi level within these band states for the case of (i) a metal, and (ii) a pure semiconductor.

In what manner does the process of electrical conduction in pure semiconductors differ from that in metals?

Q.4 Using the classical Langevin theory, derive an expression for the magnetisation, M, of a paramagnetic material as a function of temperature and of magnetic field. Indicate what changes would have to be made to develop this into a quantum theory?

Estimate a typical value for the magnetic moment of an atom (in SI units). Over what range of temperatures would we expect the Langevin theory to predict a simple linear dependence of magnetisation on field, for fields less that 1 tesla?

Explain, very briefly and with a minimum of mathematical detail, why the conduction electrons in a metal make only a weak contribution to the magnetisation of the metal.

Q.5 Answer *each* of the following.

(a) Discuss the dependence of the photoluminescence process in semiconducting materials on the nature of the bandgap.

(b) Show, on general symmetry principles, that the wavefunction for an electron in a periodic potential has the Bloch form: $\psi(\mathbf{r}) = \exp(i\mathbf{k}.\mathbf{r})\,u_{\mathbf{k}}(\mathbf{r})$, where $u_{\mathbf{k}}(\mathbf{r})$ is a periodic function with the periodicity of the potential. Indicate the values which $\mathbf{k}$ can have. Assume that the solid is in the form of a rectangular prism and that the wavefunctions obey periodic boundary conditions.

Values of some physical constants:

$\hbar = 1.0544 \times 10^{-34}$ J s
$e = 1.602 \times 10^{-19}$ C
m (mass of electron) $= 0.91 \times 10^{-30}$ kg
$c = 3 \times 10^{8}$ m s^{-1}
$k = 1.38 \times 10^{-23}$ J K^{-1}