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NATIONAL UNIVERSITY OF IRELAND
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SUMMER EXAMINATIONS 1999

B.Sc. (Honours) in
Experimental Physics and
Applied Mathematics & Physics

EP417: Solid State Physics – Paper 3

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Time Allowed: TWO hours	Answer THREE questions

Q.1 Give the general relationship between the fundamental translation vectors of the real lattice, **a**, **b**, **c**, and the fundamental vectors of the reciprocal lattice, **A**, **B**, **C**. Write down expressions for **a**, **b**, **c** for a body centred cubic (bcc) lattice and for a face centred cubic (fcc) lattice in terms of unit vectors along the orthogonal Cartesian axes. Show that the reciprocal lattice associated with a fcc real lattice is bcc.

Discuss the concept of Miller indices, and explain the relationship between Miller indices and the reciprocal lattice, in the case of a crystal lattice described by a cubic unit cell.

Q.2 Derive the Debye formula for the density of vibrational modes in a crystalline solid,

$$\rho(\omega) = 9N\omega^2/\omega_D^3$$

where ω_D is the Debye frequency. Indicate the approximations which are inherent in the model.

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 second quantised formula for the atomic displacement operator for the atom at the origin is

$$\mathbf{u} = \Sigma_k \sqrt{\hbar/(2mN\omega_k)}\, \mathbf{e}_k (a_k + a_k^+)$$

where the a_k and a_k^+ operators have the property

$$a_k |n_k\rangle = n_k^{1/2} |n_k - 1\rangle, \qquad a_k^+ |n_k\rangle = (n_k + 1)^{1/2} |n_k + 1\rangle ,$$

and where $\mathbf{e}_k$ is the unit polarisation vector.

Derive an expression for the mean square displacement of the atom, and discuss its variation with temperature. What expression for the mean square displacement of the atom would one expect from a classical analysis?

p.t.o.

Q.3 Describe, briefly, the Fermi gas model for conduction electrons in a solid, and derive an expression for the density of electron states as a function of energy. Derive an expression for the Fermi energy, E_F, the maximum energy of the electrons at T = 0 K.

Either
estimate the contribution of the conduction electrons to the molar heat capacity of a solid, and compare it with the molar heat capacity due to lattice vibrations,

or
derive a formula for the temperature-dependent magnetic susceptibility due to the conduction electrons in a metal.

NOTE: You may find the following relationship useful.

$$\int_0^\infty \frac{x^\ell}{e^{x-x_0}+1}dx \;=\; \frac{x_0^{\ell+1}}{\ell+1}\left(1+\frac{\pi^2\,\ell(\ell+1)}{6x_0^2}+\cdots\right)$$

when $x_0 >> 1$

Q.4 Show that the density of electrons in the conduction band in an intrinsic semiconducting material at low temperature is given by

$$n_i = 2\,(2\pi m_e kT / h^2)^{3/2} \exp[-(E_C - E_F) / kT]$$

where all the terms have their usual meanings. There is a corresponding formula for the density of holes in the valence band. Derive an expression for the position of the Fermi level, and show that at T = 0 K the Fermi level is midway in the bandgap.

Consider the case of extrinsic silicon ($E_{gap} \approx 1$ eV) with a donor density of 10^{22} m^{-3}. Discuss, briefly, how the position of the Fermi level (E_F) in this material varies with temperature between 0 K and 1000 K. What is the value of the Fermi energy at T = 0 K?

Q.5 Answer *three* of the following questions.

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

(b) Discuss, briefly, the concept of electrical conduction by "holes" in semiconductors.

(c) Discuss radiative electron-hole recombination transitions in direct and indirect bandgap materials.

(d) Discuss the Curie law behaviour of paramagnetic materials.

(e) Explain briefly why the materials which exhibit strong magnetic properties always contain transition metal atoms or rare earth atoms .