# King's College London

UNIVERSITY OF LONDON



**M.Sci. EXAMINATION**

**CP/4477 Electronic properties of solids**

**Summer 2003**

**Time allowed: THREE Hours**

**Candidates must answer THREE questions.**
**No credit will be given for answering further questions.**

**The approximate mark for each part of a question is indicated in square brackets.**

**You must not use your own calculator for this paper.**
**Where necessary, a College calculator will have been supplied.**

**TURN OVER WHEN INSTRUCTED**

| | |
|---|---|
| Planck constant | $h = 6.626 \times 10^{-34}$ J s |
| Charge of a proton | $e = 1.602 \times 10^{-19}$ C |
| Rest mass of an electron | $m_0 = 9.109 \times 10^{-31}$ kg |
| Rest mass of a nucleon (proton or neutron) | $m_n = 1.674 \times 10^{-27}$ kg |
| Bohr magneton | $\mu_B = 9.274 \times 10^{-24}$ J T$^{-1}$ |
| Permeability of free space | $\mu_o = 4\pi \times 10^{-7}$ H m$^{-1}$ |
| Boltzmann constant | $k = 1.380 \times 10^{-23}$ J K$^{-1}$ |

## Answer THREE questions

1)

a) A monatomic metal crystallises in a body-centred cubic lattice, with lattice spacing $a$ along the cartesian axes. Taking one atom to be at the origin of the cartesian coordinate system, write down the coordinates of its 8 nearest neighbours.

[3 marks]

In the tight-binding approximation the energy $E(\mathbf{k})$ of an electron of wavevector $\mathbf{k} = k_x,\ k_y,\ k_z$ has the form

$$E(\mathbf{k}) = A + B \sum_j \exp\left(-i\mathbf{k}.\mathbf{r}_j\right)$$

when all the atoms are identical and only interactions between nearest-neighbours are considered. Here, $\mathbf{r}_j$ is the position of the $j^{\text{th}}$ atom relative to the central atom, $A = \langle\phi_1|H|\phi_1\rangle$ and $B = \langle\phi_1|H|\phi_2\rangle$; $\phi_1$ and $\phi_2$ are non-degenerate states localised at the origin and at one of the nearest neighbour sites respectively, and $H$ is the Hamiltonian.

b) Show that when this theory is applied to a body-centred cubic crystal with one atom at each lattice site, the electronic energy is

$$E = A + 8B\cos(k_x a/2)\cos(k_y a/2)\cos(k_z a/2).$$

[5 marks]

c) Show that surfaces with constant energy are spherical for small $\mathbf{k}$.

[4 marks]

d) The observed spread in energy of the allowed electronic states is 8.6 eV. What is the magnitude of $B$? State, with justification, whether you expect $B$ to be positive or negative.

[4 marks]

e) Using this value of $B$, calculate the effective mass component $m_{xx}$ at the point $k_x = \pi/(2a)$, $k_y = k_z = 0$ for a crystal with $a = 0.37$ nm.

[4 marks]

2) In free-electron theory, the density of electron states at energy $E$ is $g(E) = c\sqrt{E}$, where $c = 8\sqrt{2}\pi m_o^{3/2} V/h^3$, and $V$ is the volume occupied by the electrons.

a) For a gas containing $N$ electrons, derive an expression for the Fermi energy $E_F$ at 0 K. Show that the total energy $E_t$ of the electron gas at 0 K is $E_t = (3/5)NE_F$.

[5 marks]

b) Metallic potassium has a valency of one, a density of 862 kg m$^{-3}$ and an atomic weight of 39.1. Calculate the total energy $E_t$ of the electrons in one cubic metre of the metal at 0 K.

[3 marks]

c) The bulk modulus $B$ of a crystal is defined as the change in pressure $P$ required to produce a fractional change in volume $V$:

$$B = -V\left(\frac{\partial P}{\partial V}\right)_T ,$$

and $P$ can be related to $E_t$ by $PdV = -dE_t$. Calculate the value of $B$ at 0 K predicted by free-electron theory for metallic potassium. Compare your value with the experimental value of 3.0 GPa measured at room temperature.

[12 marks]



**SEE NEXT PAGE**

3)

a) Outline how one could make a 'quantum wire' of GaAs embedded inside a crystal of AlGaAs.

[2 marks]

b) In the longitudinal ($z$) direction in the wire, the energy of an electron is initially assumed to depend on the wavevector $k$ as $E = \hbar^2 k^2/2m$, and the wavefunctions of the electron are of the form $\psi(z) = \exp(ikz)/\sqrt{L}$, where $L$ is the length of the wire. Use cyclic boundary conditions to show that the separation of the allowed values of $k$ is $\Delta k = 2\pi/L$, and hence show that the density of electron states is

$$g(E) = \frac{2L}{h}\sqrt{\frac{m}{2E}}.$$

[5 marks]

c) Sketch plots of $E$ against $k$, and of $g(E)$ against $E$.

[2 marks]

d) A weak interaction between each electron and the lattice is introduced, in the form of a potential

$$V(z) = \sum_K V_K \exp(iKz),$$

where $K$ is a reciprocal lattice vector. Justify the use of this form of the potential.

[3 marks]

e) Show that the interaction mainly affects states with wavevectors $k = K/2$, and obtain an expression for the size of the energy gaps that are generated by the potential.

[4 marks]

f) Sketch (without mathematical derivation) the new form of the plot of $E$ against $k$, and also of the density of states function $g(E)$ against $E$.

[4 marks]

4.) *Data for GaAs:*

| | |
|---|---|
| Energy gap | $E_g = 1.43$ eV |
| Relative permittivity | $\epsilon = 10.9$ |
| Effective mass of an electron | $m^\star = 0.072\, m_0$ |
| Lattice spacing along cartesian axes | $a_0 = 0.565$ nm |

a) A quantum well, 6 nm thick, of GaAs is sandwiched between thick layers of an AlGaAs alloy which is lattice-matched to GaAs. Assuming that a particle of mass $m$ in an infinitely deep potential well of width $d$ has energy levels

$$E = \frac{h^2}{8md^2} n^2, \quad n = 1, 2 \ldots,$$

calculate the energies of the electron states with $n = 1$ and $n = 2$ in the well.

[2 marks]

b) In the $x$, $y$ plane of the layer, an electron is assumed to have free-electron behaviour. Show that with cyclic boundary conditions the values of $k_x$ and $k_y$ are equispaced, with an interval $\Delta k_x = \Delta k_y = 2\pi/L$, where $L$ is the width of the layer in both the $x$ and $y$ directions.

[3 marks]

c) Show that in each of the quantum states the density of energy states resulting from the two-dimensional free motion is $m/(\pi\hbar^2)$ per unit area.

[4 marks]

d) The quantum layer is doped with $\sigma$ electrons per unit area, and the Fermi energy is measured as $E_F = 40$ meV above the $n = 1$ electron level. Calculate the value of $\sigma$.

[3 marks]

e) A magnetic field $B$ is applied perpendicular to the quantum layer of GaAs. Show that there are $N = eB/h$ states in each Landau level, and hence calculate the value of the magnetic field $B_9$ at which 9 Landau levels are completely filled.

[4 marks]

f) The transverse resistance is defined as $\rho_T = E/J$ where $E$ is the electric field created by the Hall effect and $J$ is the current flowing divided by the width $L$ of the layer. Calculate the value of $\rho_T$ for the quantum layer placed in the field $B_9$.

[4 marks]



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5.)

a) Consider a paramagnetic system with $n$ non-interacting magnetic moments per unit volume, each with total angular momentum $J$, magnetic quantum number $m_J$, and Landé factor $g$. Show that the average magnetic moment in a magnetic induction field $B$, at temperature $T$, may be written as

$$\langle\mu\rangle = \frac{\sum_{m_J} g\mu_B\, m_J\, \exp\left(g\mu_B\, m_J\, B/kT\right)}{\sum_{m_J} \exp\left(g\mu_B\, m_J\, B/kT\right)}.$$

[4 marks]

b) The expression above may also be written as

$$\langle\mu\rangle = g\mu_B\, J\, F(J,y),$$

where the Brillouin function $F(J,y)$ is

$$F(J,y) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}y\right) - \frac{1}{2J}\coth\left(\frac{y}{2J}\right)$$

and $y = (g\mu_B\, J\, B)/(kT)$.

Using the fact that in the limit $y \to 0$ $F(J,y) \to ay$, where $a = (J+1)/3J$, show that the magnetic susceptibility of this system may be written as

$$\chi = \frac{C}{T}$$

where

$$C = \frac{n\mu_0\, \mu_B^2\, g^2\, J(J+1)}{3k}.$$

[5 marks]

c) If the magnetic moments now interact with each other, the effective field acting on each ion may be written as $B = B_0 + \lambda M$, where $B_0$ is the external applied field, $M$ is the magnetisation per unit volume, and $\lambda$ is a molecular field constant.

Show that the metal becomes ferromagnetic in zero applied field below a temperature

$$T_C = \frac{n\lambda\, g^2\, \mu_B^2\, J(J+1)}{3k}.$$

[6 marks]

d) In the next order approximation for small $Y$, $F(J,y) = ay - by^3$, where $a$ is given above and $b$ is positive. Using the molecular field model for ferromagnetism, show that as $T$ approaches $T_C$ from below, the spontaneous magnetisation of a ferromagnet vanishes as $(T_C - T)^{1/2}$.

[5 marks]