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Quantum Mechanics of Atoms, Statistical Mechanics, Solid State Physics, Semiconductivity

## Class Test 2

**60 min. (60 marks)**

1. (a) Derive the expression for the hydrogenic radial probability density

$$P(r)dr = r^2|R(r)|^2dr$$

using the normal expression for obtaining probabilities from wave functions. The hydrogenic wave function is

$$\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

and the volume element in spherical polar co-ordinates is

$$dV = r^2 \sin \theta dr d\theta d\phi. \tag{5}$$

- (b) Show that the most probable value for  $r$  for the 2p electronic state is  $4a_0$  (work from  $P(r)dr$ ) using the appropriate wavefunction in the attached table. (7)
- (c) How much more likely is a 1s electron in a hydrogen atom to be at a distance  $a_0$  from the nucleus than  $a_0/2$ . (8)

[20]

2. (a) The number of fermions in a fermi gas (for example, electrons in a metal) that have energies from  $\epsilon$  to  $\epsilon + d\epsilon$  is

$$\begin{aligned} n(\epsilon)d\epsilon &= g(\epsilon)f_{FD}(\epsilon)d\epsilon \\ &= \frac{8\sqrt{2}\pi L^3 m^{3/2}}{h^3} \frac{\sqrt{\epsilon}d\epsilon}{e^{(\epsilon-\epsilon_F)/kT} + 1} \end{aligned}$$

Consider  $N$  electrons in the low temperature limit where all the low-lying states are occupied. Show that the energy of the last filled state, known as the fermi energy, is given by

$$\epsilon_F = \frac{\hbar^2}{2m} \left( \frac{3N}{8\pi V} \right)^{2/3} . \quad (8)$$

- (b) The density of metallic zinc is  $7.13 \text{ g/cm}^3$  and the atomic mass of the zinc atom is  $65.4 \text{ u}$ . The Fermi energy in zinc metal is  $11.0 \text{ eV}$ . Work out the effective mass of a delocalised electron in Zinc metal. Express your answer in terms of the free electron mass. Why is there a difference ? (8)

[16]

3. (a) The velocity of an electron in a band is the group velocity of the wave packet  $v_g = \frac{d\omega}{dk}$ . The mass of the electron in the band is defined by Newton's 2nd Law of motion :-  $F = m^* \frac{dv}{dt} = \frac{dp}{dt} = \frac{d(\hbar k)}{dt}$ . Show then that the effective mass of the electron in a semiconductor is

$$m^* = \frac{\hbar^2}{\left( \frac{d^2 E}{dk^2} \right)} . \quad (8)$$

- (b) In an intrinsic semiconductor, the number of electrons in the conduction band and holes in the valence band is given by the following expressions, respectively

$$n_e = 2V \left( \frac{m_e^* kT}{2\pi \hbar^2} \right)^{3/2} e^{(\epsilon_F - \epsilon_g)/kT} \quad \text{and} \quad n_h = 2V \left( \frac{m_h^* kT}{2\pi \hbar^2} \right)^{3/2} e^{-\epsilon_F/kT} .$$

Show that the Fermi level will be approximately in the middle of the band gap. (8)

- (c) Using data for Gallium Arsenide,

$$\begin{aligned} m_e^* &= 0.072 m_e \\ m_h^* &= 0.4 m_e \\ \epsilon_g &= 1.0 \text{ eV}, \end{aligned}$$

verify that at room temperature, the Fermi-level is in the middle of the gap to within 7%. (8)

[24]

Total Marks

[60]

$n$	$l$	$m_l$	$\Phi(\phi)$	$\Theta(\theta)$	$R(r)$	$\psi(r, \theta, \phi)$
1	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{\sqrt{\pi}} \frac{e^{-r/a_0}}{a_0^{3/2}}$	$\frac{1}{\sqrt{\pi}} \frac{e^{-r/a_0}}{a_0^{3/2}}$
2	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{1}{2\sqrt{2}} \frac{a_0^{3/2}}{a_0^2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}} \frac{a_0^{3/2}}{a_0^2} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos \theta$	$\frac{1}{2\sqrt{6}} \frac{a_0^{3/2}}{a_0^2} e^{-r/2a_0}$	$\frac{1}{4\sqrt{2\pi}} \frac{a_0^{3/2}}{a_0^2} e^{-r/2a_0} \cos \theta$
2	1	$\pm 1$	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin \theta$	$\frac{1}{2\sqrt{6}} \frac{a_0^{3/2}}{a_0^2} e^{-r/2a_0}$	$\frac{1}{8\sqrt{\pi}} \frac{a_0^{3/2}}{a_0^2} e^{-r/2a_0} \sin \theta e^{\pm i\phi}$
3	0	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{1}{\sqrt{2}}$	$\frac{2}{81\sqrt{3}} \frac{a_0^{3/2}}{a_0^2} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$	$\frac{1}{81\sqrt{3\pi}} \frac{a_0^{3/2}}{a_0^2} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{6}}{2} \cos \theta$	$\frac{4}{81\sqrt{6}} \frac{a_0^{3/2}}{a_0^2} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{\sqrt{2}}{81\sqrt{\pi}} \frac{a_0^{3/2}}{a_0^2} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \cos \theta$
3	1	$\pm 1$	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{3}}{2} \sin \theta$	$\frac{4}{81\sqrt{6}} \frac{a_0^{3/2}}{a_0^2} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}} \frac{a_0^{3/2}}{a_0^2} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \sin \theta e^{\pm i\phi}$
3	2	0	$\frac{1}{\sqrt{2\pi}}$	$\frac{\sqrt{10}}{4} (3 \cos^2 \theta - 1)$	$\frac{4}{81\sqrt{30}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{6\pi}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0} (3 \cos^2 \theta - 1)$
3	2	$\pm 1$	$\frac{1}{\sqrt{2\pi}} e^{\pm i\phi}$	$\frac{\sqrt{15}}{2} \sin \theta \cos \theta$	$\frac{4}{81\sqrt{30}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0}$	$\frac{1}{81\sqrt{\pi}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0} \sin \theta \cos \theta e^{\pm i\phi}$
3	2	$\pm 2$	$\frac{1}{\sqrt{2\pi}} e^{\pm 2i\phi}$	$\frac{\sqrt{15}}{4} \sin^2 \theta$	$\frac{4}{81\sqrt{30}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0}$	$\frac{1}{162\sqrt{\pi}} \frac{a_0^{3/2}}{a_0^2} e^{-r/3a_0} \sin^2 \theta e^{\pm 2i\phi}$

\* The quantity  $a_0 = 4\pi\epsilon_0\hbar^2/m_e e^2 = 5.292 \times 10^{-11}$  m is equal to the radius of the innermost Bohr orbit.

Figure 1: Normalised wave functions of the hydrogen atom for  $n = 1, 2$  and  $3$ .