University of the Witwatersrand
Physics IIE (Engineering) : PHYS284 - 2006
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The H-atom, Statistical Mechanics, Semiconductivity

Class Test 2 — 60 + 10 min. (60 marks)

1. (a) Consider the radial wave equation for the hydrogenic atom:-

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2mr^2}{\hbar^2}\left[\frac{Ze^2}{4\pi\epsilon_0 r}+E-\frac{\hbar^2 l(l+1)}{2mr^2}\right]=0$$

Identify three types of energies for the terms collected in square brackets. (3)

(b) Hence explain that the magnitude of the orbital angular momentum is given by

$$|\mathbf{L}|=\sqrt{l(l+1)}\hbar$$

(4)

(c) Unsöld's theorem states that for any value of the orbital quantum number l, the probability densities summed over all possible values of m_l are angle independent. Verify this for $l = 2$ by showing

$$\Sigma_{m_l=-l}^{+l}|\Theta_{l,m_l}|^2|\Phi_{m_l}|^2 = const$$

using the attached table in figure 1 below of the normalised wave functions for the hydrogen atom. (6)

(d) What is the physical meaning of this mathematical fact. (2)

(e) Which group of the periodic table contains elements demonstrating Unsöld's theorem. (2)

(f) How does the mathematical form of the probability density illuminate the properties of these elements ? (2)

(g) Show that the 2s electron has a greater probability than the 2p electron to be between the nucleus and one Bohr radius in a hydrogen atom. (6)

[25]

2. (a) Starting with the wave-functions for two identical non-interacting quantum particles, show that the probability for two fermions to occupy the same quantum state is zero and the probability for two bosons to occupy the same quantum state is enhanced. (6)

(b) Use this result to state and explain the relative pressure exerted by similar gases of classical molecules, bosons and fermions for the same temperature. (4)

(c) Sketch the Fermi-Dirac distribution

$$f_{FD}(\epsilon) = \frac{1}{e^{(\epsilon - \epsilon_F)/kT} + 1}$$

at 0K, low but finite temperature and at a high temperature. (4)

(c) Show that if the average occupancy of a state of energy $\epsilon_F + \Delta\epsilon$ is f_1 at any temperature, then the average occupancy of a state of energy $\epsilon_F - \Delta\epsilon$ is $1 - f_1$. (6)

[20]

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

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

(5)

(b) Make a statement with justification concerning the relationship of the

i. charge,
ii. energy,
iii. effective mass,
iv. and momentum

of the hole state in the valence band with respect to the electron state. (4)

(c) In a one-dimensional lattice, the energy of an electron in the valence band as a function of its wave number, k, may be approximated by,

$$E = E_0(a^2k^2 - \frac{a^4}{2\pi^2}k^4)$$

where E_0 is a positive constant, and a is the lattice spacing. What is the effective mass an electron at the top of the band ?
(Express your answer in terms of E_0, a and $\hbar$). (6)

[15]

Total Marks [60]

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

*The quantity $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 5.292 \times 10^{-11}$ 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.