Memorial University of Newfoundland

Department of Physics

Final Examination, December 2004
Course: PHYS 3750
Date of Examination: December 10, 2004
Time of Examination: 9:00 - 11:00

Number of pages: 8
Number of Students: 24
Number of hours: 2

No Examination aids other than calculators and data provided with this examination script are permitted.

ANSWER ALL QUESTIONS

1. Hydrogen atom

   (a) What is the spin-orbit interaction? How does it lead to the observed fine-structure splitting of the spectral lines of the hydrogen atom?

   (b) The $n = 3$ with $l = 2$ level of the hydrogen atom comprises ten states whose energies are equal (spin and m_l degeneracy) if the spin-orbit coupling is ignored and if no external magnetic field is applied. Draw a diagram that shows how the degenerated states split when one takes into account the spin-orbit coupling. For each level, indicate the corresponding j quantum number and the degeneracy of the level.

2. Probability Density

For a hydrogen atom in a state designated by the quantum number n and l, the probability of finding the electron at any location with radial coordinate between r and $r + dr$ is given by

$$P_{nl}(r)\ dr = R^*_{nl}(r)\ R_{nl}(r)\ 4\ \pi\ r^2\ dr\ .$$

Knowing that the radial part of the wavefunction for the hydrogen atom in the $n = 2$, $l = 1$ state is given by

$$R_{21} = A\ \frac{r}{\sqrt{6\ \pi\ a_o}}\ e^{-r/2a_o}$$

where A is a constant and a_o is the Bohr radius,

(a) find the value of A.

(b) Calculate the location at which the radial probability density P_{nl} is maximum.

(c) Explain why the expectation value $\langle r_{nl} \rangle$ of the position

$$\langle r_{nl} \rangle\ = n^2\ a_o \left\{ 1 + \frac{1}{2} \left[1 - \frac{l\ (l+1)}{n^2} \right] \right\}$$

does not necessarily correspond to the location at which the radial probability density P_{nl} is maximum.

3. Nuclear Potential

The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by a square well. Imagine one proton confined in a one-dimensional infinite square well of length R.

(a) Using the uncertainty principle, show how it is possible to estimate the energy of the ground state.

(b) Using the Schrödinger's equation or the interference of waves, show that the possible energy levels of the system are given by

$$E_n = \frac{\hbar^2 \, \pi^2 \, n^2}{2 \, m_p \, R^2}$$

(c) Find the wavelength of the photon which is required to excite the proton from $n = 1$ to $n = 3$.

(d) i. Do a sketch of the wavefunction and the probability density associated with the first excited state ($n = 2$). Use your sketch to justify why, in Quantum Mechanics, we cannot define the path followed by a particle.

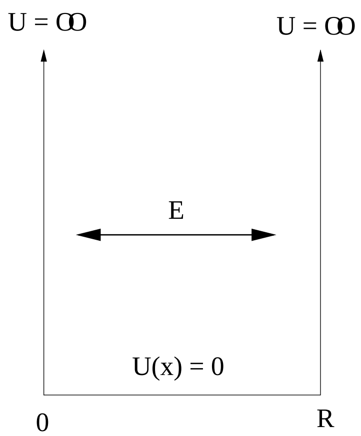

Figure 1: Nuclear Potential

4. Hydrogen Atom

   Consider the state with $n = 2$ and $l = 1$ in which the total wavefunction corresponds to the superposition of two wavefunctions with different m_l values,

$$\psi_{21} = A\left[\psi_{210} + \psi_{21-1}\right]$$

   (a) Calculate the expectation value of L_z.

   (b) Calculate the uncertainty on the value of L_z.

5. Hydrogen Atom

   Calculate the expectation value of the potential energy when the electron's wavefunction of an hydrogen atom is $\psi = \psi_{21-1}$. Use the potential

$$U(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

Formula Sheet

electron mass	=	m_e	=	9.11×10^{-31} kg	=	0.511 MeV/c^2
proton mass	=	m_p	=	1.673×10^{-27} kg	=	938.3 MeV/c^2
neutron mass	=	m_n	=	1.675×10^{-27} kg	=	939.6 MeV/c^2
Planck's constant	=	$\hbar$	=	1.06×10^{-34} J s		
Speed of light	=	c	=	3×10^8 m/s		
electron charge	=	e	=	1.602×10^{-19} C		
		ϵ_o	=	8.85×10^{-12} C^2/N $\cdot$ m^2		
Bohr magneton	=	μ_B	=	9.27×10^{-24} J/Tesla		
Conversion factor	=	1 eV	=	1.602×10^{-19} J		

Useful Integrals

$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$

$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{1\cdot3\cdot5\ldots(2n-1)}{2^{n+1}a^n}$

$\int_0^\infty x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}}$

$\int x \sin^2 ax\ dx = \frac{x^2}{4} - \frac{x \sin 2ax}{4a} - \frac{\cos 2ax}{8a^2}$

$\int x \cos^2 ax\ dx = \frac{x^2}{4} + \frac{x \sin 2ax}{4a} + \frac{\cos 2ax}{8a^2}$

$\int x^2 \sin^2 ax\ dx = \frac{x^3}{6} - \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin 2ax - \frac{x \cos 2ax}{4a^2}$

$\int x^2 \cos^2 ax\ dx = \frac{x^3}{6} + \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right) \sin 2ax + \frac{x \cos 2ax}{4a^2}$

Trigonometry Formulas

$\cos^2 \alpha = \frac{1}{2}(1 + \cos 2\alpha)$

$\sin^2 \alpha = \frac{1}{2}(1 - \cos 2\alpha)$

$\cos \alpha = \frac{e^{i\alpha} + e^{-i\alpha}}{2}$

$\sin \alpha = \frac{e^{i\alpha} - e^{-i\alpha}}{2i}$

Schrödinger's equation in one dimension

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x)}{\partial x^2} + U(x)\ \Psi(x) = E\ \Psi(x)$$

with the total wavefunction given by

$$\Psi_n(x,t) = \Psi_n(x)\ \Phi_n(t) = \Psi_n(x)\ e^{-iE_n t/\hbar}$$

Uncertainty Principle

$$\Delta x\ \Delta P_x \geq \frac{\hbar}{2}$$

<u>One-Electron Atoms</u>:

$$H\ \Psi_{n,l,m_l}(r,\theta,\phi) = E_n\ \Psi_{n,l,m_l}(r,\theta,\phi)$$

$$\Psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\ Y_{l,m_l}(\theta,\phi)$$

These wavefunctions are orthogonal and normalized, hence

Some Eigenfunctions for the One-Electron Atom

Numbers m_l	Eigenfunctions
0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\cos\theta$
±1	$\psi_{21\pm1} = \frac{1}{8\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Zr}{a_0}e^{-Zr/2a_0}\sin\theta\, e^{\pm i\varphi}$
0	$\psi_{300} = \frac{1}{81\sqrt{3\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(27-18\frac{Zr}{a_0}+2\frac{Z^2r^2}{a_0^2}\right)e^{-Zr/3a_0}$
0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0}e^{-Zr/3a_0}\cos\theta$
±1	$\psi_{31\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{Zr}{a_0}\right)\frac{Zr}{a_0}e^{-Zr/3a_0}\sin\theta\, e^{\pm i\varphi}$
0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}(3\cos^2\theta-1)$
±1	$\psi_{32\pm1} = \frac{1}{81\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}\sin\theta\cos\theta\, e^{\pm i\varphi}$
±2	$\psi_{32\pm2} = \frac{1}{162\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2}\frac{Z^2r^2}{a_0^2}e^{-Zr/3a_0}\sin^2\theta\, e^{\pm 2i\varphi}$

Figure 2: One-Electron Wavefunctions

$$\int_0^\infty \int_0^{2\pi} \int_0^{\pi} \Psi^*_{n_f,l_f,m_{lf}}(r,\theta,\phi)\ \Psi_{n_i,l_i,m_{li}}(r,\theta,\phi)\ r^2 \sin\theta\ d\theta\ d\phi\ dr = \delta_{n_f,n_i}\ \delta_{l_f,l_i}\ \delta_{m_{lf},m_{li}}$$

These wavefunctions are orthogonal and normalized, hence

$$\int_0^\infty \int_0^{2\pi} \int_0^\pi \Psi^*_{n_f,l_f,m_{lf}}(r,\theta,\phi)\ \Psi_{n_i,l_i,m_{li}}(r,\theta,\phi)\ r^2 \sin\theta\ d\theta\ d\phi\ dr = \delta_{n_f,n_i}\ \delta_{l_f,l_i}\ \delta_{m_{lf},m_{li}}$$

$$\begin{aligned}
E_n &= -\frac{\mu\ Z^2\ e^4}{(4\ \pi\ \epsilon_o)^2\ 2\ \hbar^2\ n^2} = -\frac{13.6\ Z^2}{n^2}\ eV \qquad n = 1,\ 2,\ 3,\ \cdots \\
a_o &= \frac{4\ \pi\ \epsilon_o\ \hbar^2}{\mu\ e^2} = 0.529\ \mathring{A} \qquad \text{Bohr'r radius} \\
L &= \sqrt{l(l+1)}\ \hbar, \qquad l = 0,\ \cdots\ ,\ n-1 \\
L_z &= m_l\ \hbar, \qquad m_l = -l,\ -l+1,\ \cdots\ ,\ l-1,\ l \\
\text{degeneracy} &= (2l+1)
\end{aligned}$$

<u>Magnetic Properties</u>

$$E_{mag} = -\vec{\mu}\cdot\vec{B}$$

orbital magnetic moment	$\vec{\mu}_L = -g_l\ \mu_B\ \frac{\vec{L}}{\hbar}$
intrinsic magnetic moment	$\vec{\mu}_S = -g_s\ \mu_B\ \frac{\vec{S}}{\hbar}$
Total magnetic moment	$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S$
Total angular momentum	$\vec{J} = \vec{L} + \vec{S}$

<u>g-factors</u>

orbital	$g_l = 1$
electron spin	$g_s = 2$

<u>Spin-Orbit Coupling</u>

$$\Delta E = \frac{1}{2m^2\ c^2}\frac{1}{r}\frac{dV(r)}{dr}\ \vec{\mathbf{S}}\cdot\vec{\mathbf{L}}$$

OPERATORS

$$
\begin{aligned}
P_x &= -i\hbar \, \frac{\partial}{\partial x} \\
E &= i\hbar \, \frac{\partial}{\partial t} \\
\Delta x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2}
\end{aligned}
$$

In spherical polar coordinates

$$
\begin{aligned}
L_x &= i\hbar \left(\sin\phi \, \frac{\partial}{\partial \theta} + \cot\theta \; \cos\phi \, \frac{\partial}{\partial \phi} \right) \\
L_y &= i\hbar \left(-\cos\phi \, \frac{\partial}{\partial \theta} + \cot\theta \; \sin\phi \, \frac{\partial}{\partial \phi} \right) \\
L_z &= -i\hbar \, \frac{\partial}{\partial \phi}
\end{aligned}
$$

Using that $L^2 = L_x^2 + L_y^2 + L_z^2$,

$$
L^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \, \frac{\partial}{\partial \theta} \left(\sin\theta \, \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \, \frac{\partial^2}{\partial \phi^2} \right]
$$