Memorial University of Newfoundland

Department of Physics

Final Examination, December 2003
Course: PHYS 3750
Date of Examination: December 16, 2003
Time of Examination: 9:00 - 11:00

Number of pages: 7
Number of Students: 11
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) When the spin-orbit interaction is taken into account, it is sometimes said that m_l and m_s are no longer "good quantum numbers". Explain why this terminology is appropriate. What are the good quantum numbers for the one-electron atom when the spin-orbit interaction is taken into account?

   (c) Consider the $n = 2$ state of the hydrogen atom, enumerate the possible values of j.

   (d) For the $n = 2$ state of the hydrogen atom, in a first time, draw a diagram that shows how degenerated states split when one takes into account the spin-orbit coupling. In a second time, show how these levels are further splitted when a small external magnetic field is applied. In each case, clearly identify the different levels using the appropriate quantum numbers and also indicate the degeneracy of the different states.

2. The Rigid Rotator

A particle of mass μ is fixed at one end of a rigid rod of negligible mass and length R. The other end of the rod, located at the origin, is attached to a bearing so that the particle can only rotate in the $x-y$ plane. This two dimensional "rigid rotor" is illustrated in Fig. 1.

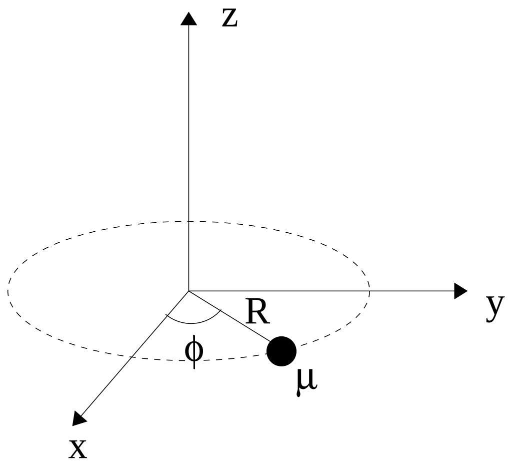

Figure 1: A rigid rotator moving in the $x-y$ plane

(a) Write a classical expression for the total energy of the system. Write your expression in terms of the angular momentum L of the particle and the moment of inertia, $I = \mu R^2$. (Hint: Set the potential energy $U(r)$ equal to zero and neglect the rod since it has a negligible mass.)

(b) Since the motion of the particle is limited to the $x-y$ plane, the angular momentum is pointing in the z-direction, we must have

$$L = L_z \ .$$

By introducing the appropriate operators into the previous energy equation, show how we can easily obtain the time-independent Schrödinger's equation

$$-\frac{\hbar}{2\ I}\frac{d^2\Psi(\phi)}{d\phi^2} = E\ \Psi(\phi)$$

where $I = \mu\ R^2$ is the moment of inertia, and $\Psi(\phi)$ is the wave function written in terms of the angular coordinate ϕ.

(c) Show that a particular solution to the time-independent Schrödinger's equation for the rigid rotator is

$$\Psi(\phi) = e^{im\phi}$$

and find the relation between m and the total energy E.

(d) Apply the boundary condition in order to obtain the allowed values of the quantum number m.

(e) Normalize the wave function $\Psi(\phi) = A\ e^{im\phi}$.

(f) Calculate the expectation value of the angular momentum L_z.

(g) What is the uncertainty on the value of the angular momentum L_z?

3. 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

$$R_{21} = A\ r\ e^{-r/2a_o}$$

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) calculate the expectation value $\langle r \rangle$ for that state and show that it is equal to

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

(d) Explain why the expectation value $\langle r \rangle$ is not equal to the location at which the radial probability density P_{nl} is maximum.

4. Two-dimensional rectangular box

A particle is confined in a two-dimensional rectangular box such that

$$\begin{aligned} U(x,y) &= 0 \qquad && 0 \le x \le a,\ \ 0 \le y \le b \\ &= \infty && \text{elsewhere} \end{aligned}$$

(a) Using the time-independent Schrödinger's equation in two dimension

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

Show that the general wavefunction

$$\Psi(x,y) = A\ \sin(k_x\ x)\ \sin(k_y\ y)$$

is a solution of the Schrödinger's equation for a particle in a two-dimensional box.

(b) Using the boundary conditions, find the possible values for k_x and k_y. Introduce, two quantum numbers (n_x, n_y) to distinguish the different solutions.

(c) Write the energy of the different levels as a function of the quantum numbers n_x and n_y.

(d) Make a diagram showing the first 10 energy levels for $b = a$. For each level, indicate the energy relative to the ground state energy, the quantum numbers associated to that state, and the degeneracy of that state.

(e) Again, for $b = a$, what would be the wavelength of the photon that is emitted for a transition between the fifth excited state and the ground state?

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

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

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

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

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

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

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

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

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

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

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

with the total wavefunction given by

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

One-Electron Atoms:

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

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

These wavefunctions are orthogonal and normalized, hence

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

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

Magnetic Properties

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

orbital magnetic moment $\quad \vec{\mu}_L = -g_l\ \mu_B\ \frac{\vec{L}}{\hbar}$

intrinsic magnetic moment $\quad \vec{\mu}_S = -g_s\ \mu_B\ \frac{\vec{S}}{\hbar}$

Total magnetic moment $\quad \vec{\mu} = \vec{\mu}_L + \vec{\mu}_S$

Total angular momentum $\quad \vec{J} = \vec{L} + \vec{S}$

g-factors

orbital $\quad g_l = 1$

electron spin $\quad g_s = 2$

OPERATORS

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

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

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