PHYS851 Quantum Mechanics I, Fall 2009
HOMEWORK ASSIGNMENT 12

Topics Covered: Motion in a central potential, spherical harmonic oscillator, hydrogen atom, orbital electric and magnetic dipole moments

1. [20 pts] A particle of mass M and charge q is constrained to move in a circle of radius r_0 in the $x-y$ plane.

   (a) If no forces other than the forces of constraint act on the particle, what are the energy levels and corresponding wavefunctions?

   If the particle is forced to remain in the x-y plane, then it can only have angular momentum along the z-axis, so that $\vec{L} = L_z\vec{e}_z$ and $L^2 = L_z^2$.
   The kinetic energy can be found two ways:

   Method 1: Using our knowledge of angular momentum. We start by choosing ϕ as our coordinate

$$H = \frac{L^2}{2I} = \frac{L_z^2}{2Mr_0^2} \tag{1}$$

   so that the eigenstates are eigenstates of $L_z \to -i\hbar$
   $partial_\phi$, from which we see know that the energy levels are then $E_m = \frac{\hbar^2 m^2}{2Mr_0^2}$, where $m = 0, \pm1, \pm2, \pm3 \ldots ...$, and the wavefunctions are $\langle\phi|m\rangle = \frac{1}{\sqrt{2\pi}}e^{im\phi}$.

   Method 2: Solution from first principles. We start by choosing s as our coordinate, where s is the distance measured along the circle. The classical Lagrangian is then

$$\mathcal{L} = \frac{M\dot{s}^2}{2} \tag{2}$$

   the canonical momentum is $p_s = \partial_s L = M\dot{s}$. The Hamiltonian is then

$$H = p\dot{s} - \mathcal{L} = \frac{p_s^2}{2M} \tag{3}$$

   promoting s and p_s to operators, we must have $[S, P_s] = i\hbar$, so that in coordinate representation, we can take $S \to s$, and $P_s \to -i\hbar\partial_s$, which gives

$$H = -\frac{\hbar^2}{2M}\partial_s^2 \tag{4}$$

   the energy eigenvalue equation is then

$$-\frac{\hbar^2}{2M}\partial_s^2\psi(s) = E\psi(s) \tag{5}$$

   or equivalently

$$\partial_s^2\psi(s) = -\frac{2ME}{\hbar^2}\psi(s) \tag{6}$$

This has solutions of the form:

$$\psi(s) \propto e^{\pm i \frac{\sqrt{2ME}}{\hbar} s} \tag{7}$$

single-valuedness requires

$$\psi(s + 2\pi r_0) = \psi(s) \tag{8}$$

which means

$$\frac{\sqrt{2ME}}{\hbar} 2\pi r_0 = 2\pi m \tag{9}$$

where m is any integer. This gives

$$E = \frac{\hbar^2 m^2}{2Mr_0^2} \tag{10}$$

so that

$$\psi_m(s) = \frac{e^{ims/r_0}}{\sqrt{2\pi r_0}} \tag{11}$$

Both methods agree because $s = r_0\phi$.

(b) A uniform, weak magnetic field of amplitude B_0 is applied along the z-axis. What are the new energy eigenvalues and corresponding wavefunctions?

Using the angular momentum method, we now need to add the term $-\frac{qB_0}{2M} L_z$ to the Hamiltonian to account for the orbital magnetic dipole moment, which gives

$$H = \frac{L_z^2}{2Mr_0^2} - \frac{qB_0}{2M} L_z \tag{12}$$

so that the eigenstates are still L_z eigenstates, $\psi_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}$, where $m = 0, \pm 1, \pm 2, \ldots$, but the degeneracy is lifted so that

$$E_m = \frac{\hbar^2 m^2}{2Mr_0^2} - \frac{qB_0\hbar}{2M} m \tag{13}$$

(c) Instead of a weak magnetic field along the z-axis, a uniform electric field of magnitude E_0 is applied along the x-axis. Find an approximation for the low-lying energy levels that is valid in the limit $qr_0E_0 \gg \hbar^2/Mr_0^2$.
Hint: try expanding around the potential about a stable equilibrium point.

Here we need to add the electric monopole energy. The electrostatic potential of a uniform E-field along $\vec{e}_x$ is $\phi(\vec{r}) = -E_0 x$, so that the potential energy is $U = -qE_0 x$. The full Hamiltonian of the particle is then given by

$$H = \frac{L_z^2}{2Mr_0^2} - qE_0 r_0 \cos(\phi) \tag{14}$$

The stable equilibrium point is at $\phi = 0$. Expanding to second-order about the equilibrium then gives

$$H = -\frac{\hbar^2}{2Mr_0^2}\partial_\phi^2 - qE_0 r_0 + \frac{qE_0 r_0}{2}\phi^2 \tag{15}$$

This is just a harmonic oscillator Hamiltonian, with $M_{eff} = Mr_0^2$, and $\omega = \sqrt{\frac{qE_0}{2Mr_0}}$, so that the energy levels are

$$E_n = -qE_0 r_0 + \hbar\sqrt{\frac{qE_0}{2Mr_0}}\left(n + \frac{1}{2}\right) \tag{16}$$

where $n = 0, 1, 2, \ldots$. This approximation must be valid only when the level spacing is small compared to the depth of the cos potential, so that

$$\hbar\sqrt{\frac{qE_0}{2Mr_0}} \ll qE_0 r_0 \tag{17}$$

which is equivalent to

$$\frac{\hbar^2}{2Mr_0^2} \ll qE_0 r_0 \tag{18}$$

2. [10 pts] Write out the fully-normalized hydrogen wavefunctions for all of the 3p orbitals. Expand out any special functions in terms of elementary functions. You can look these up in a book or on-line, but keep in mind that you will be penalized if your expression is not properly normalized.

We have

$$\psi_{n,\ell,m}(r,\theta,\phi) = \sqrt{\frac{8(n-\ell-1)!}{2n(a_0 n)^3(n+\ell)!}}e^{-r/a_0 n}\left(\frac{2r}{a_0 n}\right)^{\ell} L_{n-\ell-1}^{(2\ell+1)}\left(\frac{2r}{a_0 n}\right) Y_\ell^m(\theta,\phi) \tag{19}$$

Using Mathematica, I then get for $n = 3$ and $\ell = 1$,

$$\psi_{3,1,1}(r,\theta,\phi) = \frac{1}{81 a_0^{7/2}\sqrt{\pi}} e^{-r/3a_0}(6a_0 - r) r \sin\theta e^{i\phi} \tag{20}$$

$$\psi_{3,1,0}(r,\theta,\phi) = \frac{\sqrt{2}}{81 a_0^{7/2}\sqrt{\pi}} e^{-r/3a_0}(6a_0 - r) r \cos\theta \tag{21}$$

$$\psi_{3,1,-1}(r,\theta,\phi) = \frac{1}{81 a_0^{7/2}\sqrt{\pi}} e^{-r/3a_0}(6a_0 - r) r \sin\theta e^{-i\phi} \tag{22}$$

Normalization checks out:

Untitled-1 1

In[823]:=

```
Clear[ψ, n, l, m, r, θ, ϕ, a]
```

In[863]:=

$$\psi[n\_, l\_, m\_, r\_, \theta\_, \phi\_] := \sqrt{\frac{8\,(n-l-1)\,!}{2\,n\,(a\,n)^3\,(n+l)\,!}}\;\text{Exp}\left[\frac{-r}{a\,n}\right] \left(\frac{2\,r}{a\,n}\right)^l \text{LaguerreL}\left[n-l-1,\,2\,l+1,\,\frac{2\,r}{a\,n}\right] \text{SphericalHarmonicY}[l,\,m,\,\theta,\,\phi]$$

In[864]:=

```
ψ311 = FullSimplify[ψ[3, 1, 1, r, θ, ϕ]]
```

Out[864]=

$$\frac{\sqrt{\frac{1}{a^3}}\;e^{-\frac{r}{3a}+i\phi}\;r\,(-6\,a+r)\;\text{Sin}[\theta]}{81\,a^2\sqrt{\pi}}$$

In[865]:=

```
ψ310 = FullSimplify[ψ[3, 1, 0, r, θ, ϕ]]
```

Out[865]=

$$\frac{\sqrt{\frac{1}{a^3}}\;e^{-\frac{r}{3a}}\sqrt{\frac{2}{\pi}}\;(6\,a-r)\;r\,\text{Cos}[\theta]}{81\,a^2}$$

In[866]:=

```
ψ31m1 = FullSimplify[ψ[3, 1, -1, r, θ, ϕ]]
```

Out[866]=

$$\frac{\sqrt{\frac{1}{a^3}}\;e^{-\frac{r}{3a}-i\phi}\;(6\,a-r)\;r\,\text{Sin}[\theta]}{81\,a^2\sqrt{\pi}}$$

In[870]:=

```
Integrate[Conjugate[ψ311] ψ311 r² Sin[θ],
 {ϕ, 0, 2 π}, {θ, 0, π}, {r, 0, ∞}, Assumptions → a > 0]
```

Out[870]=

```
1
```

In[871]:=

```
Integrate[Conjugate[ψ310] ψ310 r² Sin[θ],
 {ϕ, 0, 2 π}, {θ, 0, π}, {r, 0, ∞}, Assumptions → a > 0]
```

Out[871]=

```
1
```

3. [20 pts] Numerically compute the matrix elements of the z-component of the orbital electric and magnetic dipole moments for the $|200\rangle \to |100\rangle$, $|210\rangle \to |100\rangle$, and $|211\rangle \to |100\rangle$ transitions in hydrogen. Be sure to show your work.

For the electric dipole moments, we need to compute $e\langle i|Z|f\rangle = e\langle i|R\cos\Theta|f\rangle$. The selection rules are $m_f = m_i$ and $L_f = L_i \pm 1$. Of these three transitions, only $|210\rangle \to |100\rangle$ satisfies these selection rules. Using the wavefunction from 12.2, and mathematica, and taking $a_0 = 5.20 \times 10^{-10}$m and $e = -1.6 \times 10^{-19}$C, we find

$$\langle 200|eZ|100\rangle = 0 \quad (23)$$

$$\langle 210|eZ|100\rangle = \int_0^\infty dr\, r^2 \int_0^\pi d\theta\, \cos\theta \int_0^\pi d\phi\, \psi^*_{2,1,0}(r,\theta,\phi) r\cos\theta \psi_{1,0,0}(r,\theta,\phi)$$

$$= 6.305 \times 10^{-29}\text{Cm} \quad (24)$$

$$\langle 211|eZ|100\rangle = 0 \quad (25)$$

For the magnetic dipole moments, we need $\mu = \frac{e}{2m_e}L_z$, so the selection rule is $m_i = m_f$. The dipole moment is then $\mu = \frac{e\hbar}{2m_e}m_\ell$. This gives zero for all transitions. Note that when spin is included, there will can be non-zero magnetic dipole transitions between these levels.

4. [15 pts] Based on the classical relation $E = T + V$, where E is the total energy, T is the kinetic energy, and V is the potential energy, what is the probability that the velocity of the relative coordinate exceeds the speed of light for a hydrogen atom in the 1s state? What about the 2s state? Based on these answers, which of the two energy levels would you expect to have a larger relativistic correction?

Using $H = T + V$ and $T = \frac{1}{2}mv^2$, we find

$$v = \sqrt{\frac{2}{m}(E - V)}$$

so for the hydrogen system with principle quantum number n this gives

$$v^2(r) = \frac{2}{m}\left[-\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2} + \frac{e^2}{4\pi\epsilon_0 r}\right]$$

Setting this equal to c^2 and solving for r_c gives

$$r_c(n) = \frac{ma_0^2 n^2 e^2}{2\pi\epsilon_0(m^2 a_0^2 c^2 n^2 + \hbar^2)}$$

with the parameters (from Google) $m = 9.10 \times 10^{-31}$kg, $a_0 = 5.29 \times 10^{-11}$m, $e = 1.60 \times 10^{-19}$C, $\epsilon_0 = 8.85 \times 10^{-12}\text{C}^2\text{N}^{-1}\text{m}^{-2}$, $c = 3.00 \times 10^8\text{ms}^{-1}$, and $\hbar = 1.05 \times 10^{-34}$Js, we find:

For $n = 1$: $r_c(1) = 5.62 \times 10^{-15}$m

For $n = 2$: $r_c(2) = 5.62 \times 10^{-15}$m

So we see that dependence on n is very weak.

The probability to be within this radius, however, depends strongly on n. For $n = 1$, we have

$$P(r < r_c(1)) = \int_0^{r_c(1)} dr\, R_{10}^2(r) = 4\int_0^{r_c(1)/a_0} dx\, e^{-2x}x^2 = 8.00 \times 10^{-13}$$

for $n = 2$ we have

$$P(r < r_c(2)) = \int_0^{r_c(2)} dr\, R_{20}^2(r) = 2\int_0^{r_c(2)/a_0} dx\, e^{-2x}x^2(1 - x^2) = 4.00 \times 10^{-13}$$

Therefore we would expect the ground-state to have the larger relativistic correction.

5. [10 pts] Consider the Earth-Moon system as a gravitational analog to the hydrogen atom. What is the effective Bohr radius (give both the formula and the numerical value). Based on the classical energy and angular momentum, estimate the n and m quantum numbers for the relative motion (take the z-axis as perpendicular to the orbital plane).

The Bohr radius for Hydrogen is given by

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

From wikipedia I found $M_M = 7.35 \times 10^{22}$kg, $M_E = 5.97 \times 10^{24}$kg, $r_M = 3.84 \times 10^8$m, and $v_M = 1.022 \times 10^3 \text{ms}^{-1}$

To compute the Bohr radius for the moon, we just need to make the substitutions

$$m \to \mu = \frac{M_M M_E}{M_M + M_E} = \frac{7.35 \times 10^{22} \cdot 5.97 \times 10^{24}}{7.35 \times 10^{22} + 5.97 \times 10^{24}} = 7.2610^{22}\text{kg}$$

$$\frac{e^2}{4\pi\epsilon_0} \to GM_M M_E = (6.67 \times 10^{-11})(5.97 \times 10^{24})(7.35 \times 10^{22}) = 2.93 \times 10^{37}$$

This gives

$$a_M = \frac{\hbar^2}{GM_M^2 M_E} = 4.67 \times 10^{-129}\text{m}$$

The classical energy is

$$E = \frac{1}{2}\mu v_E^2 - \frac{GM_M M_E}{r_M} = -3.83 \times 10^{28}\text{J}$$

Solving

$$E = -\frac{\hbar^2}{2\mu a_M^2 n^2}$$

for n gives

$$n = \frac{\hbar}{\sqrt{-2\mu a_M^2 E}} = 2.77 \times 10^{68}$$

To calculate m, we take $L_z = \mu v_M r_M$ and us

$$m = \frac{L_z}{\hbar} = \frac{\mu v_M r_M}{\hbar} = 2.74 \times 10^{68}$$

Just for fun:
For a transition from n to $n-1$, the energy released is

$$\Delta E = -\frac{\hbar^2}{2\mu a_M^2}\left[\frac{1}{n^2} - \frac{1}{(n-1)^2}\right] = -\frac{\hbar^2}{2\mu a_M^2}\frac{(n-1)^2 - n^2}{n^2(n-1)^2} = \frac{\hbar^2}{2\mu a_M^2}\frac{2n-1}{n^2(n-1)^2} \approx \frac{\hbar^2}{2\mu a_M^2}\frac{2}{n^3}$$

This gives a numerical result of $\Delta E = 2.76 \times 10^{-40}$J. With $\lambda = 2\pi\hbar c/\Delta E$ we find $\lambda = 7.10 \times 10^{14}$m. Using 1lyr $= 9.46 \times 10^{15}$m we find that $\lambda = 0.075$ light years. The lunar month is 27.21 days, or 0.074 years. Coincidence?