Homework 5, Quantum Mechanics 501, Rutgers

December 3, 2015

1) A hydrogen-like atom with atomic number \( Z \) is in its ground state when, due to nuclear processes (operating at a time scale much shorter than the characteristic time scale of the \( H \) atom), its nucleus is modified to have the atomic number increased by one unit, i.e. to \( Z + 1 \). The electronic state of the atom does not change during this process. What is the probability of finding the atom in the new ground state at a later time? Answer the same question for the new first excited state.

**Ans.:** The hydrogen ground state wave function is

\[
\psi_{1,0,0}(r) = \frac{Z^{3/2}}{\sqrt{\pi a_0^3}} e^{-Zr/a_0}
\]  

Once the atomic number is changed, the ground state becomes

\[
\psi_{1,0,0}(r) = \frac{(Z + 1)^{3/2}}{\sqrt{\pi a_0^3}} e^{-(Z+1)r/a_0}
\]  

and the first excited state becomes

\[
\psi_{2,0,0}(r) = \frac{(Z + 1)^{3/2}}{\sqrt{32\pi a_0^3}} (2 - \frac{Z + 1}{a_0}r)e^{-(Z+1)r/(2a_0)}
\]

The probabilities are \( P_1 = \langle \psi_{1,0,0} | \psi_{1,0,0} \rangle^2 \) and \( P_2 = \langle \psi_{2,0,0} | \psi_{1,0,0} \rangle^2 \)

The evaluation of the radial integrals gives \( P_1 = \frac{(Z(Z+1))^3}{(Z+\frac{1}{2})^6} \) and \( P_2 = \frac{2^{11}}{3^8} \frac{(Z(Z+1))^3}{(Z+\frac{1}{2})^8} \).

6) Consider the delta-shell potential model, which is a very simple model of the force experienced by a neutron interacting with a nucleus. In this model, the force experienced by neutron has the form

\[
V(r) = -\frac{\hbar^2 g^2}{2\mu}\delta(r - a)
\]

Here \( r \) is written in spherical coordinates.

Investigate the existence of bound states in the case of negative energy.
a) Write down the Schroedinger equation for \( u(r) \) in spherical coordinates using potential \( V(r) \).

\textbf{Ans.:} Schroedinger equation reads

\[
-u'' - g^2 \delta(r - a)u + \frac{l(l + 1)}{r^2} u = -\kappa^2 u
\]  

where

\[\kappa = \sqrt{-\frac{2\mu E}{\hbar^2}}.\]

b) What are solutions for free particles (\( V = 0 \))? Which solution can be used for interior part (\( r < a \)) and which for exterior part (\( r > a \))?

\textbf{Ans.:} The solution for free particles was given in class, namely spherical bessel and spherical neuman functions. However, these functions are solutions for \( E > 0 \). Here we need bound states, which can be obtained by changing \( kr \rightarrow i\kappa r \) in the argument of the solution.

The solutions are thus

\[u(r) = A r j_l(i\kappa r) + B r n_l(i\kappa r)\]  

For small \( r \), only \( j_l(x) \) are well behaved. For large \( r \) we need solution that falls off. The following large \( x \gg 1 \) expansion of spherical bessel and neuman functions was given in class

\[
j_l(x) \approx \frac{1}{x} \sin(x - l\pi/2) \] 

\[
n_l(x) \approx -\frac{1}{x} \cos(x - l\pi/2) \] 

For imaginary argument \( ix \), these functions are

\[
j_l(ix) \approx \begin{cases} \frac{\sinh(x)}{x} (-1)^{l/2} & l = 0, 2, 4, \ldots \\ -\frac{i\cosh(x)}{x} (-1)^{(l+1)/2} & l = 1, 3, 5, \ldots \end{cases} \] 

\[
n_l(ix) \approx \begin{cases} \frac{i\cosh(x)}{x} (-1)^{l/2} & l = 0, 2, 4, \ldots \\ \frac{\sinh(x)}{x} (-1)^{(l+1)/2} & l = 1, 3, 5, \ldots \end{cases} \] 

The following combination of bessel and neuman function falls off in infinity

\[h_l(ix) = n_l(ix) - ij_l(ix) \propto e^{-x} \] 

This function is also called spherical Henkel function. One can check explicitly

\[
h_l(ix) \approx \begin{cases} i(-1)^{l/2}e^{x/2} & l = 0, 2, 4, \ldots \\ (-1)^{(l-1)/2}e^{-x} & l = 1, 3, 5, \ldots \end{cases} \] 

Hence, the solution is

\[u_l(r) = \begin{cases} Ar j_l(i\kappa r) & r < a \\ Br h_l(i\kappa r) & r > a \end{cases} \]
c) Integrating around the point $r = a$, determine the discontinuity condition, and hence equation for the eigenstates.

**Ans.:** The integration of the Schrödinger equation gives

\[ u'(a^+) - u'(a^-) = -g^2 u(a) \]  

(14)

We have two boundary conditions: i) continuity at $r = a$ gives

\[ A_aj_l(i\kappa a) = B_ah_l(i\kappa a) \]  

(15)

and ii) the discontinuity of the Schrödinger equation gives

\[ B_ah_l'(i\kappa a) - A_aj_l'(i\kappa a) = -g^2 A_aj_l(i\kappa a) \]  

(16)

The two equations can be combined together into the following condition

\[ \frac{j_l'(i\kappa a)}{j_l(i\kappa a)} - \frac{h_l'(i\kappa a)}{h_l(i\kappa a)} = \frac{g^2 a}{\kappa a} \]  

(17)

d) Assuming that $g^2 a = 2$, solve (possibly numerically) for bound state energy at $l = 0$.

**Ans.:** For $l = 0$

\[ j_0(x) = \frac{\sinh(x)}{x} \]  

(18)

\[ h_0(x) = i\frac{e^{-x}}{x} \]  

(19)

hence the above condition gives

\[ \frac{2}{1 - e^{-2x}} = \frac{g^2 a}{x} \]  

(20)

We are hence looking for the solution of

\[ x = 1 - e^{-2x} \]

for which numerical solution is $\kappa a = 0.796812$. The bound state energy hence is

\[ E = -\frac{\hbar^2}{2\mu a^2}(0.796812)^2 \]  

(21)

3) A beam of particles is subject to a simultaneous measurement of the spin operators $S^2$, and $S_z$. The measurement gives pairs of values $s = m_s = 0$ and $s = 1, m_s = 1$ with probabilities 3/4 and 1/4 respectively.
(a) Reconstruct the state of the beam immediately before the measurement.

**Answ.** Before the measurements, the wave function must have been

\[ |\psi\rangle = \frac{\sqrt{3}}{2} |0,0\rangle + e^{i\alpha} \frac{1}{2} |1,1\rangle \]

where \( \alpha \) is any real number.

(b) The particles in the beam with \( s = 1, m_s = 1 \) are separated out and subjected to a measurement of \( S_x \). What are the possible outcomes and their probabilities?

**Answ.** Possible outcomes are eigenvalues of \( S_x \) operator for \( s = 1 \) particles. To compute probabilities, we need eigenvectors of operator \( S_x \) (in the \( s = 1 \) sector).

The eigenvectors are

\[ |S_x = +1\rangle = \frac{1}{2} |1,1\rangle + \frac{1}{\sqrt{2}} |1,0\rangle + \frac{1}{2} |1, -1\rangle \]  
\[ |S_x = -1\rangle = \frac{1}{2} |1,1\rangle - \frac{1}{\sqrt{2}} |1,0\rangle + \frac{1}{2} |1, -1\rangle \]  
\[ |S_x = 0\rangle = \frac{1}{\sqrt{2}} (|1,1\rangle - |1, -1\rangle) \]

The probabilities are then

\[ P(+1) = | \langle S_x = +1 | 1,1 \rangle |^2 = 1/4 \]  
\[ P(-1) = | \langle S_x = -1 | 1,1 \rangle |^2 = 1/4 \]  
\[ P(0) = | \langle S_x = 0 | 1,1 \rangle |^2 = 1/2 \]

(c) For the purpose of understanding the symmetry of the wave function, it is convenient to replace spin operators with corresponding orbital angular momentum operators, i.e., \( S_x \to L_x \) and \( S^2 \to L^2 \). Write down the spatial wave functions of the states that arise from the second measurement if the operator was orbital angular momentum operator \( L_x \). Give the \( x, y, z \) dependence of such wave functions.

Hint: First figure out the decomposition of the measured states in terms of \( |l, m_l\rangle \) states. Using spherical harmonics, express the resulting wave function in real space.

**Answ.** We repeat the decomposition

\[ |L_x = +1\rangle = \frac{1}{2} |1,1\rangle + \frac{1}{\sqrt{2}} |1,0\rangle + \frac{1}{2} |1, -1\rangle \]  
\[ |L_x = -1\rangle = \frac{1}{2} |1,1\rangle - \frac{1}{\sqrt{2}} |1,0\rangle + \frac{1}{2} |1, -1\rangle \]  
\[ |L_x = 0\rangle = \frac{1}{\sqrt{2}} (|1,1\rangle - |1, -1\rangle) \]
and use standard expressions for the spherical harmonics, to obtain

\begin{align*}
(r|L_x = \pm 1) &= \sqrt{\frac{3}{8\pi}} \left( \pm \frac{z}{r} - \frac{iy}{r} \right) \\
(r|L_x = 0) &= -\sqrt{\frac{3}{4\pi}} \frac{x}{r}
\end{align*}

(31)  
(32)