Homework 6, Quantum Mechanics 501, Rutgers

December 16, 2016

1) Using the matrix elements of the operator L_x in the subspace for $l = 1$ derived in the previous homework, show that the matrix for arbitrary rotations around the x-axis is given by

$$D_{mm'}(\theta) = \exp(-i\theta L_x/\hbar) = \begin{pmatrix} \frac{1}{2}\cos\theta + \frac{1}{2} & -\frac{i}{\sqrt{2}}\sin\theta & \frac{1}{2}\cos\theta - \frac{1}{2} \\ -\frac{i}{\sqrt{2}}\sin\theta & \cos\theta & -\frac{i}{\sqrt{2}}\sin\theta \\ \frac{1}{2}\cos\theta - \frac{1}{2} & -\frac{i}{\sqrt{2}}\sin\theta & \frac{1}{2}\cos\theta + \frac{1}{2} \end{pmatrix} \tag{1}$$

Ans.: One can diagonalize 3×3 matrix of the operator L_x, and derive the matrix of rotation. The alternative derivation relies on the Taylor series of the exponent. One can notice that

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

and

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}^3 = \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

hence the Taylor series

$$D_{mm'}(\theta) = \exp(-i\theta L_x/\hbar) = \exp\left(\frac{-i\theta}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\right) = \sum_n \frac{1}{n!}\left(\frac{-i\theta}{\sqrt{2}}\right)^n \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}^n \tag{2}$$

gives

$$D_{mm'}(\theta) = 1 + \sum_{n=1,3,\ldots} \frac{1}{n!}\left(\frac{-i\theta}{\sqrt{2}}\right)^n \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} 2^{(n-1)/2} + \sum_{n=2,4,\ldots} \frac{1}{n!}\left(\frac{-i\theta}{\sqrt{2}}\right)^n \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} 2^{(n-1)/2}$$

$$D_{mm'}(\theta) = \begin{pmatrix} 1/2 & 0 & -1/2 \\ 0 & 0 & 0 \\ -1/2 & 0 & 1/2 \end{pmatrix} + \frac{1}{\sqrt{2}}(-i\sin\theta)\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \frac{1}{2}\cos\theta\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \tag{3}$$

which is equivalent to the given matrix above.

Show that applying this matrix for the case of $\theta = \pi$ on the eigenfunction $|l = 1, m = 1\rangle$ gives the same result as rotating explicitly the function $Y_{1,1}(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi}$ by 180-degrees around the x-axis.

Ans.: The rotation by 180 degrees is

$$D(\pi) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{4}$$

hence rotating $(1, 0, 0)$ gives $(0, 0, -1)$.

The unrotated function corresponding to $(1, 0, 0)$ is $Y_{1,1}(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} = -\sqrt{\frac{3}{8\pi}}(x+iy)$ and the rotated, corresponding to $(0, 0, -1)$ is $-Y_{1,-1}(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi} = -\sqrt{\frac{3}{8\pi}}(x - iy)$

Rotation around x axis by 180 degrees amounts to $y \to -y$ and $z \to -z$. Indeed this transforms $Y_{1,1}$ into $-Y_{1,-1}$.

2) 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

$$\psi_{1,0,0}(r) = \frac{Z^{3/2}}{\sqrt{\pi a_0^3}} e^{-Zr/a_0} \tag{5}$$

Once the atomic number is changed, the ground state becomes

$$\overline{\psi}_{1,0,0}(r) = \frac{(Z+1)^{3/2}}{\sqrt{\pi a_0^3}} e^{-(Z+1)r/a_0} \tag{6}$$

and the first excited state becomes

$$\overline{\psi}_{2,0,0}(r) = \frac{(Z+1)^{3/2}}{\sqrt{32\pi a_0^3}} (2 - \frac{Z+1}{a_0} r) e^{-(Z+1)r/(2a_0)} \tag{7}$$

The probabilities are $P_1 = \langle \overline{\psi}_{1,0,0} | \psi_{1,0,0} \rangle^2$ and $P_2 = \langle \overline{\psi}_{2,0,0} | \psi_{1,0,0} \rangle^2$

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

3) 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

$$V(r) = -\frac{\hbar^2 g^2}{2\mu}\delta(r-a) \tag{8}$$

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 $u_l(r)$ in spherical coordinates using potential $V(r)$.

Ans.: Schroedinger equation reads

$$-u'' - g^2\delta(r-a)u + \frac{l(l+1)}{r^2}u = -\kappa^2 u \tag{9}$$

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 ($r > a$)?

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 $kr \to i\kappa r$ in the argument of the solution.

The solutions are thus

$$u(r) = A\; r\; j_l(i\kappa r) + B\; r\; n_l(i\kappa r) \tag{10}$$

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

$$j_l(x) \approx \frac{1}{x}\sin(x - l\pi/2) \tag{11}$$

$$n_l(x) \approx -\frac{1}{x}\cos(x - l\pi/2) \tag{12}$$

For imaginary argumen ix, these functions are

$$j_l(ix) \approx \begin{cases} \frac{\sinh(x)}{x}(-1)^{l/2} & l = 0, 2, 4, ... \\ -i\frac{\cosh(x)}{x}(-1)^{(l+1)/2} & l = 1, 3, 5, ... \end{cases} \tag{13}$$

$$n_l(ix) \approx \begin{cases} i\frac{\cosh(x)}{x}(-1)^{l/2} & l = 0, 2, 4, ... \\ \frac{\sinh(x)}{x}(-1)^{(l+1)/2} & l = 1, 3, 5, ... \end{cases} \tag{14}$$

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

$$h_l(ix) = n_l(ix) - ij_l(ix) \propto \frac{e^{-x}}{x} \tag{15}$$

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

$$h_l(ix) \approx \begin{cases} i(-1)^{l/2}\frac{e^{-x}}{x} & l = 0, 2, 4, ... \\ (-1)^{(l-1)/2}\frac{e^{-x}}{x} & l = 1, 3, 5, ... \end{cases} \tag{16}$$

Hence, the solution is

$$u_l(r) = \begin{cases} A\, r\, j_l(i\kappa r) & r < a \\ B\, r\, h_l(i\kappa r) & r > a \end{cases} \tag{17}$$

c) Integrating around the point $r = a$, determine the discontinuity condition, and hence equation for the eigenstates.
Ans.: The integration of the Schroedinger equation gives

$$u'(a^+) - u'(a^-) = -g^2 u(a) \tag{18}$$

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

$$Aaj_l(i\kappa a) = Bah_l(i\kappa a) \tag{19}$$

and ii) the discontinuity of the Schroedinger equation gives

$$Ba\kappa h_l'(i\kappa a) - Aa\kappa j_l'(i\kappa a) = -g^2 Aaj_l(i\kappa a) \tag{20}$$

The two equations can be combined together into the following condition

$$\frac{j_l'(i\kappa a)}{j_l(i\kappa a)} - \frac{h_l'(i\kappa a)}{h_l(i\kappa a)} = \frac{g^2 a}{\kappa a} \tag{21}$$

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

$$j_0(x) = \frac{\sinh(x)}{x} \tag{22}$$

$$h_0(x) = i\frac{e^{-x}}{x} \tag{23}$$

hence the above condition gives

$$\frac{2}{1 - e^{-2x}} = \frac{g^2 a}{x} \tag{24}$$

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

$$E = -\frac{\hbar^2}{2\mu a^2}(0.796812)^2 \tag{25}$$

4) A beam of composite 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 α 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

$$|S_x = +1\rangle = \frac{1}{2}|1,1\rangle + \frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{2}|1,-1\rangle \tag{26}$$

$$|S_x = -1\rangle = \frac{1}{2}|1,1\rangle - \frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{2}|1,-1\rangle \tag{27}$$

$$|S_x = 0\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle) \tag{28}$$

   The probabilities are then

$$P(+1) = |\langle S_x = +1|1,1\rangle|^2 = 1/4 \tag{29}$$

$$P(-1) = |\langle S_x = -1|1,1\rangle|^2 = 1/4 \tag{30}$$

$$P(0) = |\langle S_x = 0|1,1\rangle|^2 = 1/2 \tag{31}$$

   (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 operatore 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

$$|L_x = +1\rangle = \frac{1}{2}|1,1\rangle + \frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{2}|1,-1\rangle \tag{32}$$

$$|L_x = -1\rangle = \frac{1}{2}|1,1\rangle - \frac{1}{\sqrt{2}}|1,0\rangle + \frac{1}{2}|1,-1\rangle \tag{33}$$

$$|L_x = 0\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle) \tag{34}$$

and use standard expressions for the spherical harmonics, to obtain

$$\langle \mathbf{r} | L_x = \pm 1 \rangle = \sqrt{\frac{3}{8\pi}} (\pm \frac{z}{r} - i\frac{y}{r}) \tag{35}$$

$$\langle \mathbf{r} | L_x = 0 \rangle = -\sqrt{\frac{3}{4\pi}} \frac{x}{r} \tag{36}$$