33-756 Homework 3

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1. Representations of SO(3)

In class, we talked about the fact that there are matrix as well as functional representations of a Lie group—that is, the operators can be matrices or differential operators. A good way to understand the difference is to consider our friend SO(3). Suppose we have a representation $|l, m\rangle$. At this point, this is an abstract vector in a Hilbert space. Now consider the action of a rotation $R(\hat{\mathbf{n}}, \delta)$ on this state:

$$|l'm'\rangle = R(\hat{\mathbf{n}}, \delta) |lm\rangle .$$

(a) Prove that $l = l'$.

$$\begin{aligned}
|l'm'\rangle &= R |lm\rangle \\
L^2 |l'm'\rangle &= L^2 R |lm\rangle \\
&= R L^2 |lm\rangle \\
\hbar^2 l'(l'+1) |l'm'\rangle &= R \left(\hbar^2 l(l+1)\right) |lm\rangle \\
&\implies l'(l'+1) = l(l+1) \\
&\implies l' = \pm l
\end{aligned}$$

but we define $l \geq 0$, so $l' = l$. We can do the second step because L^2 commutes with rotations since $R \propto e^{-\imath \hat{\mathbf{n}} \cdot \hat{\mathbf{L}} \delta/\hbar}$.

(b) We may therefore write R as a matrix ${D^l}_{m,m'}$. These are called the Wigner D-matrices. We can derive these matrices in one of two ways depending on whether we are considering a representation on the space of functions or on matrices. Consider the state $l = 1$, $m = 0$. Perform an infinitesimal rotation around the x axis by an amount ϵ by using the 3 by 3 representation of the generator L_x. This example is a matrix representation.

$$R(\hat{\mathbf{x}}, \epsilon) \approx I - \frac{\imath}{\hbar} L_x \epsilon$$

We can find the matrix elements of L_x starting with the matrix elements of $L_\pm$:

$$\langle lm' | L_\pm | lm \rangle = \hbar \delta_{m',m+1} \sqrt{(l \mp 1)(l \pm m + 1)}$$

and $L_x = \frac{1}{2}(L_+ + L_-)$ so

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

so

$$R(\hat{\mathbf{x}}, \epsilon) = \begin{pmatrix} 1 & -\frac{\imath\epsilon}{\sqrt{2}} & 0 \\ -\frac{\imath\epsilon}{\sqrt{2}} & 1 & -\frac{\imath\epsilon}{\sqrt{2}} \\ 0 & -\frac{\imath\epsilon}{\sqrt{2}} & 1 \end{pmatrix}$$

Therefore,

$$R(\hat{\mathbf{x}}, \epsilon) |1,0\rangle = \begin{pmatrix} 1 & -\frac{\imath\epsilon}{\sqrt{2}} & 0 \\ -\frac{\imath\epsilon}{\sqrt{2}} & 1 & -\frac{\imath\epsilon}{\sqrt{2}} \\ 0 & -\frac{\imath\epsilon}{\sqrt{2}} & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -\frac{\imath\epsilon}{\sqrt{2}} \\ 1 \\ -\frac{\imath\epsilon}{\sqrt{2}} \end{pmatrix} = -\frac{\imath\epsilon}{\sqrt{2}} |1,-1\rangle + |1,0\rangle - \frac{\imath\epsilon}{\sqrt{2}} |1,+1\rangle$$

(c) Now consider the representation on the space of functions $\langle\theta,\varphi|l,m\rangle$. We know the eigenstates of L^2 and L_z are just $Y_l^m(\theta,\varphi) = \langle\theta,\varphi|l,m\rangle$. Perform the same infinitesimal rotation as in the previous problem only now in function space and show that the resulting linear combination of m's is the same as in the previous problem.

In the Y_{lm} basis, we can write the L_x operator as

$$L_x = -\imath\hbar \left[-\sin(\varphi)\frac{\partial}{\partial\theta} - \cot(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi} \right]$$

so that

$$R(\hat{\mathbf{x}}, \epsilon) = 1 + \epsilon\cos(\varphi)\frac{\partial}{\partial\theta} + \epsilon\cos(\theta)\cos(\varphi)\frac{\partial}{\partial\varphi}$$

The $|1,0\rangle$ state can be written as

$$Y_{10}(\theta,\varphi) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta)$$

so

$$\begin{aligned} R(\hat{\mathbf{x}}, \epsilon) Y_{10}(\theta,\varphi) &= \left(1 + \epsilon\cos(\varphi)\frac{\partial}{\partial\theta}\right) \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta) \\ &= \frac{1}{2}\sqrt{\frac{3}{\pi}} \left(\cos(\theta) - \epsilon \underbrace{\cos(\varphi)}_{\frac{e^{\imath\varphi}+e^{-\imath\varphi}}{2}} \sin(\theta) \right) = Y_{10} - \frac{\imath\epsilon}{\sqrt{2}}(Y_{1,-1} + Y_{1,+1}) \end{aligned}$$

2. Spherical and Cartesian Bases

When we consider the 3 dimensional (defining) representation of SO(3), we can think of the states either as Cartesian basis vectors or as spherical basis vectors $|l=1,m=1\rangle$, $|l=1,m=-1\rangle$, and $|l=1,m=0\rangle$. Calculate the relation between the Cartesian basis vectors $|\hat{\mathbf{x}}\rangle$, $|\hat{\mathbf{y}}\rangle$, and $|\hat{\mathbf{z}}\rangle$. First determine which of the three spherical vectors corresponds to $|\hat{\mathbf{z}}\rangle$ using the fact that this vector is invariant under rotations around the z axis. Then determine the relation between the x and y basis vectors in terms of the spherical basis vectors by using the fact that they are invariant under rotations around the x and y axes respectively. Next, consider a general vector $A_x\hat{\mathbf{x}} + A_y\hat{\mathbf{y}} + A_z\hat{\mathbf{z}}$ and write the components in the spherical basis in terms of A_x, A_y, and A_z.

We can first attribute $|\hat{\mathbf{z}}\rangle = |1,0\rangle$ since $L_z |lm\rangle = \hbar m |lm\rangle$. If we were to act an infinitesimal rotation on this vector, we would find that $\left(I - \frac{\imath}{\hbar}\epsilon L_z\right)|10\rangle = (|10\rangle + 0\,|10\rangle) = |10\rangle$. However, the other vectors will give a factor of ± 1 from the eigenvalue of L_z, which means they are not invariant under this rotation. The other two basis vectors are invariant under rotations about the other two axes, but since we are in the L_z basis, it will be convenient to use linear combinations of $L_\pm$. We can act L_x on a general vector and see what conditions are required for that product to go to 0, since $R(\hat{\mathbf{x}}) \propto I - \frac{\imath}{\hbar}L_z$.

$$\begin{aligned}
L_x\left(a\,|1,-1\rangle + b\,|1,0\rangle + c\,|1,+1\rangle\right) &= \frac{1}{2}\left(L_+ + L_-\right)\left(a\,|1,-1\rangle + b\,|1,0\rangle + c\,|1,+1\rangle\right)\\
&= \frac{\hbar\sqrt{2}}{2}\left(a\,|1,0\rangle + b\,|1,+1\rangle + b\,|1,-1\rangle + c\,|1,0\rangle\right)\\
&= 0
\end{aligned}$$

so $b = 0$ and $a = -c$. Therefore,

$$\hat{\mathbf{x}} = \frac{1}{\sqrt{2}}\left(|1,-1\rangle - |1,+1\rangle\right)$$

Next, for $L_y = \frac{1}{2\imath}(L_+ - L_-)$,

$$\begin{aligned}
L_y\left(a\,|1,-1\rangle + b\,|1,0\rangle + c\,|1,+1\rangle\right) &= \frac{1}{2\imath}\left(L_+ - L_-\right)\left(a\,|1,-1\rangle + b\,|1,0\rangle + c\,|1,+1\rangle\right)\\
&= \frac{\hbar\sqrt{2}}{2\imath}\left(a\,|1,0\rangle + b\,|1,+1\rangle - b\,|1,-1\rangle - c\,|1,0\rangle\right)\\
&= 0
\end{aligned}$$

so $b = 0$ and $a = c$. Therefore,

$$\hat{\mathbf{y}} = \frac{1}{\sqrt{2}}\left(|1,-1\rangle + |1,+1\rangle\right)$$

Now let's consider a general vector $A_x\hat{\mathbf{x}} + A_y\hat{\mathbf{y}} + A_z\hat{\mathbf{z}}$ and transform it into the spherical basis:

$$\begin{aligned}
A_x\hat{\mathbf{x}} + A_y\hat{\mathbf{y}} + A_z\hat{\mathbf{z}} &= A_x\left(|1,-1\rangle - |1,+1\rangle\right) + A_y\left(|1,-1\rangle + |1,+1\rangle\right) + A_z\,|1,0\rangle\\
&= \left(A_x + A_y\right)|1,-1\rangle + \left(A_y - A_x\right)|1,+1\rangle + A_z\,|1,0\rangle
\end{aligned}$$

3. Basis in Functional Space

We can think of $Y_{1m}(\theta,\varphi)$ as $\langle\hat{\mathbf{n}}(\theta,\varphi)|1,m\rangle$ where $\hat{\mathbf{n}}$ is a Cartesian unit vector in the direction (θ,φ). Choose values for θ and φ that place $\hat{\mathbf{n}}$ along the three axes, and compare the resulting projection for each m to the result you got from the previous problem.

We can imagine a general scalar which is the functional projection of a vector in spherical coordinates:

$$A_{-1}Y_{1,-1}(\theta,\varphi) + A_0Y_{1,0}(\theta,\varphi) + A_{+1}Y_{1,+1}(\theta,\varphi)$$

Along the $\hat{\mathbf{z}}$ axis, $\theta = 0$ and $\varphi = 0$, so the $Y_{1,-1}$ and $Y_{1,+1}$ spherical harmonics will cancel out:

$$Y_{1,-1}(0,0) = Y_{1,+1}(0,0) = 0$$

so $\langle\hat{\mathbf{z}}|l,m\rangle = A_0Y_{1,0}$, where $A_0 = 1$ for normalization.
Along $\hat{\mathbf{x}}$, $\theta = \frac{\pi}{2}$ and $\varphi = 0$ so $Y_{1,0} = 0$ and $A_{-1} = -A_{+1}$ since

$$Y_{1,-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} = -Y_{1,+1}$$

Again, for normalization, this means that $\langle \hat{\mathbf{x}}|l,m\rangle = \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,+1}\right)$.
Finally, along the $\hat{\mathbf{y}}$ axis, $\theta = \frac{\pi}{2}$ and $\varphi = \frac{\pi}{2}$. Now, $A_{-1} = A_{+1}$ since

$$Y_{1,-1} = -\frac{1}{2}\imath\sqrt{\frac{3}{2\pi}} = Y_{1,+1}$$

so $\langle \hat{\mathbf{y}}|l,m\rangle = \frac{1}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,+1}\right)$, which agrees with the result in the previous problem.

4. The Runge-Lenz Vector

Show that the Runge-Lenz vector is a Hermitian operator, and show that it commutes with the Hamiltonian.

I'm assuming we are meant to check the commutation with the following Hamiltonian:

$$H = \frac{\vec{\mathbf{p}}^2}{2m} - \frac{e^2}{r}\vec{\mathbf{r}}$$

In general, for two Hermitian operators A and B, $(AB)^\dagger = B^\dagger A^\dagger$. The Runge-Lenz vector is defined as:

$$\vec{\mathbf{A}} = \frac{1}{2m}\left[\vec{\mathbf{p}} \times \vec{\mathbf{L}} - \vec{\mathbf{L}} \times \vec{\mathbf{p}}\right] - \frac{e^2}{r}\vec{\mathbf{r}}$$

or

$$A_i = \frac{1}{2m}\left[\epsilon_{ijk}p_jL_k - \epsilon_{ijk}L_jp_k\right] - \frac{e^2}{r}r_i = \frac{1}{m}$$

so

$$A_i^\dagger = \frac{1}{2m}\left[\epsilon_{ijk}L_k^\dagger p_j^\dagger + \epsilon_{ijk}p_k^\dagger L_j^\dagger\right] - \frac{e^2}{r}r_i^\dagger$$

All of these operators are Hermitian, so

$$A_i^\dagger = \frac{1}{2m}\left[\epsilon_{ijk}L_kp_j + \epsilon_{ijk}p_kL_j\right] - \frac{e^2}{r}r_i$$

Finally, $p_kL_j = L_jp_k + \imath\hbar\epsilon_{jkl}p_l$ and $L_kp_j = p_jL_k - \imath\hbar\epsilon_{jkl}p_l$ so switching the order of the L's and p's just creates terms that cancel:

$$A_i^\dagger = \frac{1}{2m}\left[\epsilon_{ijk}p_jL_k + \epsilon_{ijk}L_jp_k\right] - \frac{e^2}{r}r_i = A_i$$

so $\vec{\mathbf{A}}$ is Hermitian.
Next, I will show that this vector commutes with the Hamiltonian. First, I will take a slight detour.

$$[L_i, p_l] = [\epsilon_{ijk}r_jp_k, p_l] = \epsilon_{ijk}\left(r_j[p_k,p_l] + [r_j,p_l]p_k\right) = \epsilon_{ijk}\delta_{jl}\imath\hbar p_k = \epsilon_{ilk}\imath\hbar p_k$$

so

$$\left[L^2, \vec{\mathbf{p}}\right] \mapsto [L_iL_i, p_j] = [L_i,p_j]L_i + L_i[L_i,p_j] \mapsto \imath\hbar\left(\vec{\mathbf{p}} \times \vec{\mathbf{L}} - \vec{\mathbf{L}} \times \vec{\mathbf{p}}\right)$$

We can then write the RL vector in the following form:

$$\vec{\mathbf{A}} = \frac{1}{2m\imath\hbar}\left[L^2, \vec{\mathbf{p}}\right] - \frac{e^2}{r}\vec{\mathbf{r}}$$

Therefore,

$$\begin{aligned}
\left[\vec{\mathbf{A}}, H\right] &= \frac{1}{2m\imath\hbar}\left[\left[L^2,\vec{\mathbf{p}}\right], H\right] - e^2\left[\frac{\vec{\mathbf{r}}}{r}, H\right] \\
&= \frac{1}{2m\imath\hbar}\left(\left[[\vec{\mathbf{p}},H],L^2\right] + \left[\left[H,L^2\right],\vec{\mathbf{p}}\right]\right) - \frac{e^2}{2m}\left[\frac{\vec{\mathbf{r}}}{r}, \vec{\mathbf{p}}^2\right] \\
&= \frac{-e^2}{2m\imath\hbar}\left(\left[\left[\vec{\mathbf{p}}, \frac{\vec{\mathbf{r}}}{r}\right], L^2\right]\right) - \frac{e^2}{2m}\left[\frac{\vec{\mathbf{r}}}{r}, \vec{\mathbf{p}}^2\right]
\end{aligned}$$

since $\left[H, L^2\right] = 0$ because the Hamiltonian is spherically symmetric.

$$\left[p_i, \frac{r_j}{r}\right] = -\imath\hbar\left(\partial_i \frac{r_j}{r} - \frac{r_j}{r}\partial_i\right) = -\imath\hbar\left(\frac{\delta_{ij}}{r} - \frac{r_i r_j}{r^3} - \frac{r_j}{r}\partial_i\right)$$

I ran out of time to complete the other commutators, sorry.