Problem Set 12

Problem 1: Use $[\widehat{x}_i, \widehat{p}_j] = i\hbar\delta_{ij}$ to verify that the angular momentum operators $\widehat{L}_i = \sum_{jk} \epsilon_{ijk}\widehat{x}_j\widehat{p}_k$ satisfy the commutation relations

$$[\widehat{L}_i, \widehat{L}_j] = i\hbar \sum_k \epsilon_{ijk}\widehat{L}_k, \qquad [\widehat{L}_i, \widehat{x}_j] = i\hbar \sum_k \epsilon_{ijk}\widehat{x}_k, \qquad [\widehat{L}_i, \widehat{p}_j] = i\hbar \sum_k \epsilon_{ijk}\widehat{p}_k.$$

Here $i, j, k \in \{1, 2, 3\}$ and sums run over these values. **Solution:** `Do` $[\widehat{L}_i, \widehat{x}_j]$ `first:`

$$\begin{aligned}
[\widehat{L}_i, \widehat{x}_j] &= \left[\sum_{k\ell} \epsilon_{ik\ell}\widehat{x}_k\widehat{p}_\ell\, ,\, \widehat{x}_j\right] = \sum_{k\ell} \epsilon_{ik\ell}[\widehat{x}_k\widehat{p}_\ell, \widehat{x}_j] \\
&= \sum_{k\ell} \epsilon_{ik\ell}\left([\widehat{x}_k, \widehat{x}_j]\widehat{p}_\ell + \widehat{x}_k[\widehat{p}_\ell, \widehat{x}_j]\right) = -i\hbar \sum_{k\ell} \epsilon_{ik\ell}\widehat{x}_k\delta_{j\ell} \\
&= -i\hbar \sum_k \epsilon_{ikj}\widehat{x}_k = +i\hbar \sum_k \epsilon_{ijk}\widehat{x}_k.
\end{aligned}$$

`In the second line I used the Leibniz property of the commutator, and in the last line I used the antisymmetry of the` ϵ `symbol. An almost identical calculation gives the` $[\widehat{L}_i, \widehat{p}_j]$ `commutator. Then`

$$\begin{aligned}
[\widehat{L}_i, \widehat{L}_j] &= \left[\widehat{L}_i\, ,\, \sum_{k\ell} \epsilon_{jk\ell}\widehat{x}_k\widehat{p}_\ell\right] = \sum_{k\ell} \epsilon_{jk\ell}\left([\widehat{L}_i, \widehat{x}_k]\widehat{p}_\ell + \widehat{x}_k[\widehat{L}_i, \widehat{p}_\ell]\right) \\
&= i\hbar \sum_{k\ell} \epsilon_{jk\ell}\left(\left(\sum_m \epsilon_{ikm}\widehat{x}_m\right)\widehat{p}_\ell + \widehat{x}_k\left(\sum_m \epsilon_{i\ell m}\widehat{p}_m\right)\right) \\
&= i\hbar \sum_{k\ell m} \left(\epsilon_{jk\ell}\epsilon_{ikm}\widehat{x}_m\widehat{p}_\ell + \epsilon_{jk\ell}\epsilon_{i\ell m}\widehat{x}_k\widehat{p}_m\right) \\
&= i\hbar \sum_{\ell m}\left(\sum_k \epsilon_{jk\ell}\epsilon_{ikm}\right)\widehat{x}_m\widehat{p}_\ell + i\hbar \sum_{km}\left(\sum_\ell \epsilon_{jk\ell}\epsilon_{mi\ell}\right)\widehat{x}_k\widehat{p}_m \\
&= i\hbar \sum_{\ell m}\left(\delta_{ji}\delta_{\ell m} - \delta_{jm}\delta_{\ell i}\right)\widehat{x}_m\widehat{p}_\ell + i\hbar \sum_{km}\left(\delta_{jm}\delta_{ki} - \delta_{ji}\delta_{km}\right)\widehat{x}_k\widehat{p}_m \\
&= i\hbar\left[\delta_{ji}\left(\sum_m \widehat{x}_m\widehat{p}_m\right) - \widehat{x}_j\widehat{p}_i + \widehat{x}_i\widehat{p}_j - \delta_{ji}\left(\sum_m \widehat{x}_m\widehat{p}_m\right)\right] = i\hbar\left(\widehat{x}_i\widehat{p}_j - \widehat{x}_j\widehat{p}_i\right) \\
&= i\hbar \sum_{\ell m}(\delta_{i\ell}\delta_{jm} - \delta_{j\ell}\delta_{im})\widehat{x}_\ell\widehat{p}_m = i\hbar \sum_{\ell m}\sum_k \epsilon_{ijk}\epsilon_{k\ell m}\widehat{x}_\ell\widehat{p}_m = i\hbar \sum_k \epsilon_{ijk}\widehat{L}_k.
\end{aligned}$$

`In the fifth line I used the identity` $\sum_\ell \epsilon_{jk\ell}\epsilon_{mi\ell} = \delta_{jm}\delta_{ki} - \delta_{ji}\delta_{km}$ `that was introduced in class, and then I used it again in the sixth line.`

Problem 2: A diatomic molecule made of two atoms of masses m_1 and m_2 with energy spectrum as in equation (9.111) of the text makes a purely rotational transition from an $\ell = \ell_0$ state to an $\ell = \ell_0 - 1$ state, emitting a photon of frequency ω_0 (so of energy $\hbar\omega_0$). What is the interatomic distance of the two atoms in this molecule in terms of m_1, m_2, ℓ_0, and ω_0? **Solution:** The energy spectrum given in equation (9.111) is

$$E_{n,\ell} = \left(n + \frac{1}{2}\right)\hbar\omega + \ell(\ell+1)\frac{\hbar^2}{2I},$$

where $n, \ell \in \{0, 1, 2, \ldots\}$ and I is the moment of inertia of the diatomic molecule. Thus, if d is the interatomic distance of the two atoms in the molecule, we have

$$I = \mu d^2, \qquad \text{where} \qquad \mu := \frac{m_1 m_2}{m_1 + m_2}.$$

A purely rotational transition is one in which the n quantum number does not change. So from the energy spectrum, the energy of the emitted photon is

$$\hbar\omega_0 = E_\gamma = E_{n,\ell_0} - E_{n,\ell_0-1} = [\ell_0(\ell_0+1) - (\ell_0-1)\ell_0]\,\frac{\hbar^2}{2I} = 2\ell_0\frac{\hbar^2}{\mu d^2}.$$

Solving for d gives

$$d = \sqrt{\frac{2\ell_0\hbar}{\mu\omega_0}}.$$

Problem 3: Consider a particle in a state with wave function $\psi = N(x+y+2z)e^{-\alpha r}$ where N is the normalization factor. Show, by rewriting the $Y_1^{\pm 1,0}$ functions in terms of x, y, z, and r, that

$$Y_{1,\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\frac{x \pm iy}{r}, \qquad\qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\frac{z}{r}. \tag{1}$$

Using this, find the probabilities $\mathcal{P}(L_z = ?)$ of measuring the the possible values of L_z for a particle in the state ψ given above. **Solution:** From from the text we have that

$$Y_{1,\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}, \qquad\qquad Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta.$$

In spherical coordinates $x \pm iy = r\sin\theta\, e^{\pm i\phi}$, and $z = r\cos\theta$, giving (1). Therefore

$$\begin{aligned}
\psi &= N(x+y+2z)e^{-\alpha r} \\
&= N\left\{\left(\frac{1-i}{2}\right)\left(\frac{x+iy}{r}\right) + \left(\frac{1+i}{2}\right)\left(\frac{x-iy}{r}\right) + 2\frac{z}{r}\right\} re^{-\alpha r} \\
&= N\left\{-\left(\frac{1-i}{2}\right)\left(\frac{8\pi}{3}\right)^{1/2} Y_1^1 + \left(\frac{1+i}{2}\right)\left(\frac{8\pi}{3}\right)^{1/2} Y_1^{-1} + 2\left(\frac{4\pi}{3}\right)^{1/2} Y_1^0\right\} re^{-\alpha r} \\
&= \mathcal{N}(r)\left\{-\frac{1-i}{\sqrt{2}}Y_1^1 + \frac{1+i}{\sqrt{2}}Y_1^{-1} + 2Y_1^0\right\},
\end{aligned}$$

where $\mathcal{N}(r) \equiv N(4\pi/3)^{1/2} re^{-\alpha r}$. Therefore

$$|\psi\rangle = |\mathcal{N}\rangle \otimes \left(\sum_{m=-1}^{1} c_m |1,m\rangle\right), \qquad \text{with} \qquad c_{\pm 1} := (i \mp 1)/\sqrt{2}, \qquad c_0 := 2.$$

Here $|\mathcal{N}\rangle$ is a radial Hilbert space state with wavefunction $\mathcal{N}(r) = \langle r|\mathcal{N}\rangle$, and $|\ell, m\rangle$ are the usual $\widehat{L}^2$, $\widehat{L}_z$ angular momentum eigenstates.

The possible values of L_z that can be obtained are its eigenvalues, $m\hbar$. By the axioms of QM, $\texttt{Prob}(\widehat{L}_z = m\hbar) = \langle\psi|\widehat{P}_{L_z=m\hbar}|\psi\rangle$ where the projection operator on the $m\hbar$ eigenspace is

$$\widehat{P}_{L_z=m\hbar} = \sum_\ell \int_0^\infty r^2 dr\, |r\rangle|\ell, m\rangle\, \langle r|\langle \ell, m|,$$

so

$$\begin{aligned}
\texttt{Prob}(L_z = m]\hbar) &= \sum_\ell \int_0^\infty r^2 dr\, |\langle r; \ell, m|\psi\rangle|^2 \\
&= \sum_\ell \int_0^\infty r^2 dr\, |\langle r|\mathcal{N}\rangle|^2 \left| \sum_{m'} c_{m'} \langle \ell, m|1, m'\rangle \right|^2 \\
&= \left(\int_0^\infty r^2 dr\, \langle \mathcal{N}|r\rangle\langle r|\mathcal{N}\rangle \right) \cdot \sum_\ell \left| \sum_{m'} c_{m'} \delta_{\ell,1}\delta_{m,m'} \right|^2 \\
&= \langle\mathcal{N}|\mathcal{N}\rangle \cdot |c_m|^2,
\end{aligned}$$

where in the second line I inserted the expression for $|\psi\rangle$ we found above, in the third line I used the orthonormality of the $|\ell, m\rangle$ states, and in the last line I used the $\int_0^\infty r^2 rd|r\rangle\langle r| = 1$ completeness relation. The condition that $|\psi\rangle$ is normalized implies

$$1 = \langle\psi|\psi\rangle = \sum_{\ell,m} \int_0^\infty r^2 dr\, |\langle r; \ell, m|\psi\rangle|^2 = \langle\mathcal{N}|\mathcal{N}\rangle \cdot \left(\sum_m |c_m|^2 \right),$$

where in the second step I used a completeness relation, and the third step is exactly the same calculation as was done above. Combining the two calculations thus gives that

$$\texttt{Prob}(L_z = m\hbar) = \frac{|c_m|^2}{\sum_{m'} |c_{m'}|^2}.$$

So

$$\begin{aligned}
\text{Prob}(L_z = 0) = \frac{|2|^2}{|2|^2 + \left|\frac{1+i}{\sqrt{2}}\right|^2 + \left|\frac{1-i}{\sqrt{2}}\right|^2} &= \frac{4}{4+1+1} &= \frac{2}{3}, \\
\text{Prob}(L_z = \hbar) = \frac{\left|\frac{1-i}{\sqrt{2}}\right|^2}{|2|^2 + \left|\frac{1+i}{\sqrt{2}}\right|^2 + \left|\frac{1-i}{\sqrt{2}}\right|^2} &= \frac{1}{4+1+1} &= \frac{1}{6}, \\
\text{Prob}(L_z = -\hbar) = \frac{\left|\frac{1+i}{\sqrt{2}}\right|^2}{|2|^2 + \left|\frac{1+i}{\sqrt{2}}\right|^2 + \left|\frac{1-i}{\sqrt{2}}\right|^2} &= \frac{1}{4+1+1} &= \frac{1}{6}.
\end{aligned}$$

For **problems 4-7**, consider a rigid rotator immersed in a uniform magnetic field in the z direction, with the hamiltonian

$$\widehat{H} = \frac{1}{2I}\widehat{L}^2 + \omega_0 \widehat{L}_z$$

where I and ω_0 are given positive constants. Suppose the wave function of the rotator at time $t = 0$ is given by

$$\langle \theta, \phi | \psi(0) \rangle = \sqrt{\frac{3}{4\pi}} \sin\theta \, \sin\phi. \qquad (2)$$

Problem 4: What values of L_z will be obtained if a measurement is carried out at time $t = 0$, and with what probability will these values occur? **Solution:** `Writing` $\sin\phi = (2i)^{-1} e^{i\phi} - (2i)^{-1} e^{-i\phi}$, `and comparing` (2) `to expressions for` $Y_{\ell=1,m=\pm 1} = \langle \theta, \phi | \ell, m \rangle$ `we see that`

$$|\psi(0)\rangle = \frac{i}{\sqrt{2}} \left(|1,1\rangle + |1,-1\rangle \right).$$

`Therefore, similarly as in the last problem, we can only have` $L_z = \pm\hbar$ `with equal probabilities`

$$\texttt{Prob}(L_z = \pm\hbar) = |\langle 1, \pm 1 | \psi(0) \rangle|^2 = \left| \frac{i}{\sqrt{2}} \right|^2 = \frac{1}{2}.$$

Problem 5: If a measurement of $\widehat{L}_x$ is carried out at time $t = 0$, what results can be obtained and with what probabilities? **Solution:** `Since the state is in the` $\ell = 1$ `eigenspace of` $\widehat{L}^2$, `the` $\widehat{L}_x$ `eigenvalues can only be` 0, `or` $\pm\hbar$ `ie, just the same as` $\widehat{L}_z$. `Recall from earlier in the course that in the` L_z `eigenbasis ordered as` $\{|1,1\rangle, |1,0\rangle, |1,-1\rangle\}$, `the matrix elements of` $\widehat{L}_z$ `and` $\widehat{L}_x$ `are`

$$\widehat{L}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad \widehat{L}_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

`(See, eg, equation (3.28) of the text, or problem set 4.) From this matrix expression for` $\widehat{L}_x$ `it is easy to find the normalized eigenvectors`

$$|L_x{=}\hbar\rangle \leftrightarrow \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \qquad |L_x{=}0\rangle \leftrightarrow \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \qquad |L_x{=}-\hbar\rangle \leftrightarrow \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}.$$

`Thus`

$$\texttt{Prob}(L_x{=}\hbar) = |\langle L_x{=}\hbar | \psi \rangle|^2 = \left| \tfrac{1}{2} \begin{pmatrix} 1 & \sqrt{2} & 1 \end{pmatrix} \ \tfrac{i}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{8}(2+2) = \frac{1}{2},$$

$$\texttt{Prob}(L_x{=}0) = |\langle L_x{=}0 | \psi \rangle|^2 = \left| \tfrac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & -1 \end{pmatrix} \ \tfrac{i}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \right|^2 = 0,$$

$$\texttt{Prob}(L_x{=}-\hbar) = |\langle L_x{=}-\hbar | \psi \rangle|^2 = \left| \tfrac{1}{2} \begin{pmatrix} 1 & -\sqrt{2} & 1 \end{pmatrix} \ \tfrac{i}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{8}(2+2) = \frac{1}{2}.$$

Problem 6: What is $\langle\theta,\phi|\psi(t)\rangle$? **Solution:** Recall that $|\psi(t)\rangle = \sum_E e^{-iEt/\hbar}|E\rangle\langle E|\psi(0)\rangle$ where $|E\rangle$ are an orthonormal basis of energy eigenstates. Since

$$\widehat{H}|\ell,m\rangle = \left(\tfrac{1}{2I}\widehat{L}^2 + \omega_0\widehat{L}_z\right)|\ell,m\rangle = \left(\tfrac{\hbar^2}{2I}\ell(\ell+1) + \omega_0\hbar m\right)|\ell,m\rangle,$$

we see that the $|\ell,m\rangle$ form an energy eigenbasis with energy eigenvalues $E(\ell,m) = \left(\frac{\hbar^2}{2I}\ell(\ell+1) + \omega_0\hbar m\right)$. We then get

$$\begin{aligned}
|\psi(t)\rangle &= \sum_{\ell,m} e^{-iE(\ell,m)t/\hbar}|\ell,m\rangle\langle\ell,m|\psi(0)\rangle \\
&= \sum_{\ell,m} e^{-iE(\ell,m)t/\hbar}|\ell,m\rangle\frac{i}{\sqrt{2}}\langle\ell,m|\left(|1,1\rangle + |1,-1\rangle\right) \\
&= \frac{i}{\sqrt{2}}\left(e^{-iE(1,1)t/\hbar}|1,1\rangle + e^{-iE(1,-1)t/\hbar}|1,-1\rangle\right) \\
&= \frac{ie^{-i\hbar t/I}}{\sqrt{2}}\left(e^{-i\omega_0 t}|1,1\rangle + e^{i\omega_0 t}|1,-1\rangle\right),
\end{aligned}$$

where in the second line I put in the expression for $|\psi(0)\rangle$ we found above, in the third line I used the orthonormality of the angular momentum eigenstates, and in the fourth line I used the expression for the energy eigenvalues found above. Thus

$$\begin{aligned}
\langle\theta,\phi|\psi(t)\rangle &= \frac{ie^{-i\hbar t/I}}{\sqrt{2}}\left(e^{-i\omega_0 t}\langle\theta,\phi|1,1\rangle + e^{i\omega_0 t}\langle\theta,\phi|1,-1\rangle\right) \\
&= \frac{ie^{-i\hbar t/I}}{\sqrt{2}}\left(e^{-i\omega_0 t}Y_{1,1}(\theta,\phi) + e^{i\omega_0 t}Y_{1,-1}(\theta,\phi)\right) \\
&= -\frac{i\sqrt{3}}{4\sqrt{\pi}}e^{-i\hbar t/I}\left(e^{-i\omega_0 t}\sin\theta\, e^{i\phi} - e^{i\omega_0 t}\sin\theta\, e^{-i\phi}\right) \\
&= \sqrt{\frac{3}{4\pi}}e^{-i\hbar t/I}\sin\theta\,\sin(\phi-\omega_0 t),
\end{aligned}$$

where I used the expression for $Y_{1,\pm1}(\theta,\phi)$ in the third line.

Problem 7: What is $\langle L_x\rangle$ for this state at time t? **Solution:**

$$\begin{aligned}
\langle L_x\rangle = \langle\psi(t)|\widehat{L}_x|\psi(t)\rangle &= \left|\frac{ie^{-i\hbar t/I}}{\sqrt{2}}\right|^2\left(e^{+i\omega_0 t}\langle 1,1| + e^{-i\omega_0 t}\langle 1,-1|\right)\widehat{L}_x\left(e^{-i\omega_0 t}|1,1\rangle + e^{i\omega_0 t}|1,-1\rangle\right) \\
&= \frac{1}{2}\begin{pmatrix} e^{+i\omega_0 t} & 0 & e^{-i\omega_0 t}\end{pmatrix}\frac{\hbar}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}e^{-i\omega_0 t}\\0\\e^{i\omega_0 t}\end{pmatrix} = \frac{\hbar}{2\sqrt{2}}\begin{pmatrix}0 & e^{+i\omega_0 t}+e^{-i\omega_0 t} & 0\end{pmatrix}\begin{pmatrix}e^{-i\omega_0 t}\\0\\e^{i\omega_0 t}\end{pmatrix} \\
&= 0.
\end{aligned}$$

In the first line I put in the expression for $|\psi(t)\rangle$ found in the last problem. In the second line I used the vector/matrix expression for the states and operator as in **problem 5**.