Quantum Mechanics

Solutions to the Problems in Homework Assignment 03

Fall, 2019

1. The Hamiltonian of a quantum system is given by $\hat{H} = \dfrac{\hat{\vec{p}}^2}{2m} + V(\vec{r})$ where $V(\vec{r})$ is the real-valued potential energy. The eigenvalue spectrum of $\hat{H}$ is discrete with the eigenequation of $\hat{H}$ given by $\hat{H}\psi_n(\vec{r}) = E_n\psi_n(\vec{r})$. Assume that $\psi_n(\vec{r})$'s are normalized.

   (a) Evaluate the commutators $[\hat{H}, x]$ and $[[\hat{H}, x], x]$.

   (b) Show that $\displaystyle\sum_{n'}(E_{n'} - E_n)\big|(\psi_{n'}, x\psi_n)\big|^2 = \frac{\hbar^2}{2m}$ using the result for the commutator $[[\hat{H}, x], x]$.

(a) Making use of the commutation relations $[x, \hat{p}_x] = i\hbar$, $[x, \hat{p}_y] = [x, \hat{p}_z] = 0$, we have

$$\begin{aligned}
[\hat{H}, x] &= \frac{1}{2m}[\hat{\vec{p}}^2, x] = \frac{1}{2m}[\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2, x] = \frac{1}{2m}[\hat{p}_x^2, x] \\
&= \frac{1}{2m}\big(\hat{p}_x[\hat{p}_x, x] + [\hat{p}_x, x]\hat{p}_x\big) \\
&= \frac{1}{2m}\big(-i\hbar\hat{p}_x - i\hbar\hat{p}_x\big) = -\frac{i\hbar}{m}\hat{p}_x.
\end{aligned}$$

For the commutator $[[\hat{H}, x], x]$, we have

$$[[\hat{H}, x], x] = -\frac{i\hbar}{m}[\hat{p}_x, x] = -\frac{i\hbar}{m}\cdot(-i\hbar) = -\frac{\hbar^2}{m}.$$

(b) Expanding the left hand side of the commutation relation $[[\hat{H}, x], x] = -\dfrac{\hbar^2}{m}$, we have

$$\hat{H}x^2 - 2x\hat{H}x + x^2\hat{H} = -\frac{\hbar^2}{m}.$$

Taking the average of the above equation in the eigenstate ψ_n of $\hat{H}$, we have

$$\big(\psi_n, (\hat{H}x^2 - 2x\hat{H}x + x^2\hat{H})\psi_n\big) = -\frac{\hbar^2}{m}(\psi_n, \psi_n) = -\frac{\hbar^2}{m}.$$

For $\big(\psi_n, \hat{H}x^2\psi_n\big)$, we have

$$\big(\psi_n, \hat{H}x^2\psi_n\big) = \big(\hat{H}\psi_n, x^2\psi_n\big) = \big(E_n\psi_n, x^2\psi_n\big) = E_n\big(\psi_n, x^2\psi_n\big).$$

For $\big(\psi_n, x^2\psi_n\big)$, making use of the property of the δ-function,

$$\int d^3r'\ \delta(\vec{r} - \vec{r}\,') = 1,$$

we have

$$\begin{aligned}
\big(\psi_n, x^2\psi_n\big) &= \int d^3r\ \psi_n^*(\vec{r})x^2\psi_n(\vec{r}) = \int d^3r \int d^3r'\ \psi_n^*(\vec{r})x^2\psi_n(\vec{r})\delta(\vec{r} - \vec{r}\,') \\
&= \int d^3r \int d^3r'\ \psi_n^*(\vec{r})xx'\psi_n(\vec{r}\,')\delta(\vec{r} - \vec{r}\,').
\end{aligned}$$

Making use of the completeness relation of $\{\psi_n\}$,

$$\sum_{n'}\psi_{n'}^*(\vec{r}\,')\psi_{n'}(\vec{r}) = \delta(\vec{r} - \vec{r}\,'),$$

we have

$$\begin{aligned}\big(\psi_n, x^2\psi_n\big) &= \sum_{n'}\int d^3r \int d^3r'\ \psi_n^*(\vec{r})xx'\psi_n(\vec{r}\,')\psi_{n'}^*(\vec{r}\,')\psi_{n'}(\vec{r}) \\ &= \sum_{n'}\bigg[\int d^3r\ \psi_n^*(\vec{r})x\psi_{n'}(\vec{r})\bigg]\bigg[\int d^3r'\ \psi_{n'}^*(\vec{r}\,')x'\psi_n(\vec{r}\,')\bigg] \\ &= \sum_{n'}\big(\psi_n, x\psi_{n'}\big)\big(\psi_{n'}, x\psi_n\big) = \sum_{n'}\big(x\psi_n, \psi_{n'}\big)\big(\psi_{n'}, x\psi_n\big) \\ &= \sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2.\end{aligned}$$

We thus have

$$\big(\psi_n, \hat{H}x^2\psi_n\big) = E_n\sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2.$$

For $\big(\psi_n, x\hat{H}x\psi_n\big)$, we have

$$\begin{aligned}\big(\psi_n, x\hat{H}x\psi_n\big) &= \int d^3r\ \psi_n^*(\vec{r})x\hat{H}x\psi_n(\vec{r}) = \int d^3r\int d^3r'\ \psi_n^*(\vec{r})x\hat{H}\delta(\vec{r}-\vec{r}\,')x\psi_n(\vec{r}) \\ &= \int d^3r\int d^3r'\ \psi_n^*(\vec{r})x\hat{H}\delta(\vec{r}-\vec{r}\,')x'\psi_n(\vec{r}\,') \\ &= \sum_{n'}\int d^3r\int d^3r'\ \psi_n^*(\vec{r})x\hat{H}\psi_{n'}^*(\vec{r}\,')\psi_{n'}(\vec{r})x'\psi_n(\vec{r}\,') \\ &= \sum_{n'}\int d^3r\int d^3r'\ \psi_n^*(\vec{r})x\psi_{n'}^*(\vec{r}\,')\hat{H}\psi_{n'}(\vec{r})x'\psi_n(\vec{r}\,') \\ &= \sum_{n'}\int d^3r\int d^3r'\ \psi_n^*(\vec{r})x\psi_{n'}^*(\vec{r}\,')E_{n'}\psi_{n'}(\vec{r})x'\psi_n(\vec{r}\,') \\ &= \sum_{n'}E_{n'}\bigg[\int d^3r\ \psi_n^*(\vec{r})x\psi_{n'}(\vec{r})\bigg]\bigg[\int d^3r'\ \psi_{n'}^*(\vec{r}\,')x'\psi_n(\vec{r}\,')\bigg] \\ &= \sum_{n'}E_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2.\end{aligned}$$

For $\big(\psi_n, x^2\hat{H}\psi_n\big)$, we have

$$\big(\psi_n, x^2\hat{H}\psi_n\big) = \big(\psi_n, x^2E_n\psi_n\big) = E_n\big(\psi_n, x^2\psi_n\big).$$

Making use of the above-obtained result

$$\big(\psi_n, x^2\psi_n\big) = \sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2,$$

we have

$$\big(\psi_n, x^2\hat{H}\psi_n\big) = E_n\sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2.$$

Collecting the above-obtained results yields

$$\begin{aligned}\big(\psi_n, (\hat{H}x^2 - 2x\hat{H}x + x^2\hat{H})\psi_n\big) &= E_n\sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2 - 2\sum_{n'}E_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2 + E_n\sum_{n'}\big|\big(\psi_{n'}, x\psi_n\big)\big|^2 \\ &= -2\sum_{n'}\big(E_{n'} - E_n\big)\big|\big(\psi_{n'}, x\psi_n\big)\big|^2.\end{aligned}$$

From

$$\big(\psi_n, (\hat{H}x^2 - 2x\hat{H}x + x^2\hat{H})\psi_n\big) = -\frac{\hbar^2}{m},$$

we obtain

$$\sum_{n'}(E_{n'}-E_n)\big|\big(\psi_{n'},x\psi_n\big)\big|^2=\frac{\hbar^2}{2m}$$

which is the desired result.

2. The Hamiltonian $\hat{H}(\lambda)$ of a quantum system depends on the real parameter λ, which leads to the λ-dependence of the eigenvalues and eigenfunctions of $\hat{H}(\lambda)$. The eigenequation of $\hat{H}(\lambda)$ reads $\hat{H}(\lambda)\psi_n(\lambda)=E_n(\lambda)\psi_n(\lambda)$. The eigenvalue spectrum of $\hat{H}(\lambda)$ is assumed to be discrete. Here the variable $\vec{r}$ in real space is suppressed. The eigenfunctions $\psi_n(\lambda)$'s are normalized.

   (a) Show that $E_n(\lambda)=\big(\psi_n(\lambda),\hat{H}(\lambda)\psi_n(\lambda)\big)$.

   (b) Derive the Hellmann-Feynman theorem $\dfrac{\partial E_n(\lambda)}{\partial\lambda}=\left(\psi_n(\lambda),\dfrac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)$.

(a) Making the scalar product of $\psi_n(\lambda)$ with $\hat{H}(\lambda)\psi_n(\lambda)=E_n(\lambda)\psi_n(\lambda)$, we have

$$\big(\psi_n(\lambda),\hat{H}(\lambda)\psi_n(\lambda)\big)=\big(\psi_n(\lambda),E_n(\lambda)\psi_n(\lambda)\big)=E_n(\lambda)\big(\psi_n(\lambda),\psi_n(\lambda)\big)=E_n(\lambda).$$

Thus,

$$E_n(\lambda)=\big(\psi_n(\lambda),\hat{H}\psi_n(\lambda)\big).$$

(b) Taking the partial derivative of $E_n(\lambda)$ with respective to λ yields

$$\frac{\partial E_n(\lambda)}{\partial\lambda}=\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},\hat{H}(\lambda)\psi_n(\lambda)\right)+\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+\left(\psi_n(\lambda),\hat{H}(\lambda)\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right).$$

Utilizing $\hat{H}(\lambda)\psi_n(\lambda)=E_n(\lambda)\psi_n(\lambda)$, we have

$$\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},\hat{H}(\lambda)\psi_n(\lambda)\right)=\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},E_n(\lambda)\psi_n(\lambda)\right)=E_n(\lambda)\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},\psi_n(\lambda)\right).$$

Utilizing $\hat{H}^\dagger(\lambda)=\hat{H}(\lambda)$, $\hat{H}(\lambda)\psi_n(\lambda)=E_n(\lambda)\psi_n(\lambda)$, and $E_n^*(\lambda)=E_n(\lambda)$, we have

$$\left(\psi_n(\lambda),\hat{H}(\lambda)\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right)=\left(\hat{H}(\lambda)\psi_n(\lambda),\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right)=\left(E_n(\lambda)\psi_n(\lambda),\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right)=E_n(\lambda)\left(\psi_n(\lambda),\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right).$$

The partial derivative of $E_n(\lambda)$ with respective to λ is then given by

$$\begin{aligned}
\frac{\partial E_n(\lambda)}{\partial\lambda}&=E_n(\lambda)\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},\psi_n(\lambda)\right)+\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+E_n(\lambda)\left(\psi_n(\lambda),\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right)\\
&=\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+E_n(\lambda)\left[\left(\frac{\partial\psi_n(\lambda)}{\partial\lambda},\psi_n(\lambda)\right)+\left(\psi_n(\lambda),\frac{\partial\psi_n(\lambda)}{\partial\lambda}\right)\right]\\
&=\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+E_n(\lambda)\frac{\partial\big(\psi_n(\lambda),\psi_n(\lambda)\big)}{\partial\lambda}\\
&=\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+E_n(\lambda)\frac{\partial 1}{\partial\lambda}\\
&=\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right)+E_n(\lambda)\cdot 0\\
&=\left(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)\right).
\end{aligned}$$

3. It is known that the eigenfunction of the position operator $\hat{\vec{r}}$ corresponding to the eigenvalue $\vec{r}\,'$ is given by $\psi_{\vec{r}'}(\vec{r}) = \delta(\vec{r} - \vec{r}\,')$ in real space.

   (a) Find the eigenfunction $\varphi_{\vec{r}'}(\vec{p})$ of $\hat{\vec{r}}$ corresponding to the eigenvalue $\vec{r}\,'$ in momentum space through the Fourier transformation $\varphi_{\vec{r}'}(\vec{p}) = \dfrac{1}{(2\pi\hbar)^{3/2}} \displaystyle\int d^3r \; \psi_{\vec{r}'}(\vec{r}) e^{-i\vec{p}\cdot\vec{r}/\hbar}$.

   (b) The eigenequation of $\hat{\vec{r}}$ in momentum space reads $\hat{\vec{r}}\varphi_{\vec{r}'}(\vec{p}) = \vec{r}\,'\varphi_{\vec{r}'}(\vec{p})$. Using the above-obtained expression of $\varphi_{\vec{r}'}(\vec{p})$, deduce the expression of $\hat{\vec{r}}$ in momentum space. Does the obtained expression of $\hat{\vec{r}}$ in momentum space satisfy the fundamental commutation relations $[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$ with $\alpha, \beta = x, y, z$ in momentum space?

(a) The eigenfunction $\varphi_{\vec{r}'}(\vec{p})$ of $\hat{\vec{r}}$ corresponding to the eigenvalue $\vec{r}\,'$ in momentum space is given by

$$\varphi_{\vec{r}'}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r \; \psi_{\vec{r}'}(\vec{r}) e^{-i\vec{p}\cdot\vec{r}/\hbar} = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r \; \delta(\vec{r} - \vec{r}\,') e^{-i\vec{p}\cdot\vec{r}/\hbar} = \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}.$$

(b) Inserting $\varphi_{\vec{r}'}(\vec{p}) = \dfrac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}$ into the eigenequation of $\hat{\vec{r}}$ in momentum space, $\hat{\vec{r}}\varphi_{\vec{r}'}(\vec{p}) = \vec{r}\,'\varphi_{\vec{r}'}(\vec{p})$, we have

$$\frac{1}{(2\pi\hbar)^{3/2}} \hat{\vec{r}} e^{-i\vec{p}\cdot\vec{r}\,'/\hbar} = \frac{1}{(2\pi\hbar)^{3/2}} \vec{r}\,' e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}.$$

From the above equation, we see that the representation of $\hat{\vec{r}}$ in momentum space must be given by

$$\hat{\vec{r}} = i\hbar\vec{\nabla}_{\vec{p}}.$$

The component operators of $\hat{\vec{r}}$ in momentum space are given by

$$\hat{x} = i\hbar\frac{\partial}{\partial p_x}, \; \hat{y} = i\hbar\frac{\partial}{\partial p_y}, \; \hat{z} = i\hbar\frac{\partial}{\partial p_z}.$$

That is,

$$\hat{r}_\alpha = i\hbar\frac{\partial}{\partial p_\alpha}, \; \alpha = x, y, z.$$

We now evaluate the commutator $[\hat{r}_\alpha, \hat{p}_\beta]$. Let it act on an arbitray wave function $\varphi(\vec{p})$ in momentum space. We have

$$\begin{aligned}
[\hat{r}_\alpha, \hat{p}_\beta]\varphi(\vec{p}) &= [\hat{r}_\alpha, p_\beta]\varphi(\vec{p}) = \hat{r}_\alpha p_\beta\varphi(\vec{p}) - p_\beta\hat{r}_\alpha\varphi(\vec{p}) \\
&= i\hbar\frac{\partial}{\partial p_\alpha}\big[\, p_\beta\varphi(\vec{p})\,\big] - i\hbar p_\beta\frac{\partial\varphi(\vec{p})}{\partial p_\alpha} \\
&= i\hbar\varphi(\vec{p})\delta_{\alpha\beta} + i\hbar p_\beta\frac{\partial\varphi(\vec{p})}{\partial p_\alpha} - i\hbar p_\beta\frac{\partial\varphi(\vec{p})}{\partial p_\alpha} \\
&= i\hbar\varphi(\vec{p})\delta_{\alpha\beta}.
\end{aligned}$$

Because $\varphi(\vec{p})$ is arbitrary, we have

$$[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}.$$

Therefore, the obtained expression of $\hat{\vec{r}}$ in momentum space satisfies the fundamental commutation relations $[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$ with $\alpha, \beta = x, y, z$ in momentum space.

4. The Hamiltonian of a quantum system is given by $\hat{H} = \dfrac{\hat{\vec{p}}^{\,2}}{2m} + \hat{V}(\hat{\vec{r}})$ where $\hat{V}(\hat{\vec{r}})$ is the Hermitian potential energy operator. The eigenequation of $\hat{H}$ reads $\hat{H}\psi_n = E_n\psi_n$. Assume that the eigenvalue spectrum of $\hat{H}$ is discrete and that ψ_n's are normalized. Take $\hbar$ to be the parameter in the Hellmann-Feynman theorem.

(a) Apply the Hellmann-Feynman theorem in real space.

(b) Apply the Hellmann-Feynman theorem in momentum space.

(c) Using the results obtained in the previous two parts, derive the virial theorem $\left(\psi_n, \frac{\hat{\vec{p}}^2}{2m}\psi_n\right) = \frac{1}{2}\big(\psi_n, \vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n\big)$; also written as $\big\langle \hat{T}\big\rangle_n = \frac{1}{2}\big\langle \vec{r}\cdot\vec{\nabla}V(\vec{r})\big\rangle_n$ with $\hat{T} = \frac{\hat{\vec{p}}^2}{2m}$ the kinetic energy operator.

(a) In real space, the Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}).$$

The partial derivative of $\hat{H}$ with respect to $\hbar$ is given by

$$\frac{\partial \hat{H}}{\partial \hbar} = -\frac{\hbar}{m}\nabla^2.$$

Applying the Hellmann-Feynman theorem in real space, we obtain

$$\frac{\partial E_n}{\partial \hbar} = \left(\psi_n, \frac{\partial \hat{H}}{\partial \hbar}\psi_n\right) = \left(\psi_n, -\frac{\hbar}{m}\nabla^2\psi_n\right) = \frac{2}{\hbar}\left(\psi_n, \frac{\hat{\vec{p}}^2}{2m}\psi_n\right).$$

(b) In momentum space, the Hamiltonian is given by

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(i\hbar\vec{\nabla}_{\vec{p}}).$$

The partial derivative of $\hat{H}$ with respect to $\hbar$ is given by

$$\frac{\partial \hat{H}}{\partial \hbar} = \frac{1}{\hbar}\big[\vec{r}\cdot\vec{\nabla}V(\vec{r})\big]_{\vec{r}\to i\hbar\vec{\nabla}_{\vec{p}}}.$$

Let $\varphi_n(\vec{p})$ be the eigenfunction corresponding to E_n in momentum space. Applying the Hellmann-Feynman theorem in momentum space, we obtain

$$\frac{\partial E_n}{\partial \hbar} = \left(\varphi_n, \frac{\partial \hat{H}}{\partial \hbar}\varphi_n\right) = \frac{1}{\hbar}\left(\varphi_n, \big[\vec{r}\cdot\vec{\nabla}V(\vec{r})\big]_{\vec{r}\to i\hbar\vec{\nabla}_{\vec{p}}}\varphi_n\right).$$

The average on the right hand side can be also evaluated in real space. We have

$$\frac{\partial E_n}{\partial \hbar} = \frac{1}{\hbar}\big(\psi_n, \vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n\big).$$

(c) From the above two results obtained respectively from applying the Hellmann-Feynman theorem in real and momentum spaces, we have

$$\left(\psi_n, \frac{\hat{\vec{p}}^2}{2m}\psi_n\right) = \frac{1}{2}\big(\psi_n, \vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n\big).$$

Making use of $\hat{T} = \frac{\hat{\vec{p}}^2}{2m}$ and the angular brackets for averages, we can put the above equation into the following form

$$\big\langle \hat{T}\big\rangle_n = \frac{1}{2}\big\langle \vec{r}\cdot\vec{\nabla}V(\vec{r})\big\rangle_n.$$

Multiplying the factor of 2 on both sides of the above equation, we can reduce the vertical space occupied by the equation

$$2\big\langle \hat{T}\big\rangle_n = \big\langle \vec{r}\cdot\vec{\nabla}V(\vec{r})\big\rangle_n$$

which is the mathematical expression of the virial theorem.

5. The ladder operators of the orbital angular momentum are defined by $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$.

   (a) Derive the expressions of $\hat{L}_\pm$ in the spherical coordinate system.

   (b) Show that $\hat{L}_\pm Y_{\ell m}(\theta,\phi) = \hbar\sqrt{\ell(\ell+1) - m(m\pm 1)}\, Y_{\ell,m\pm 1}(\theta,\phi)$.

   (c) Show that

$$\cos\theta Y_{\ell m} = \left[\frac{(\ell+m)(\ell-m)}{(2\ell-1)(2\ell+1)}\right]^{1/2} Y_{\ell-1,m} + \left[\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}\right]^{1/2} Y_{\ell+1,m},$$
$$\sin\theta e^{\pm i\phi} Y_{\ell m} = \pm\left[\frac{(\ell\mp m)(\ell\mp m-1)}{(2\ell-1)(2\ell+1)}\right]^{1/2} Y_{\ell-1,m\pm 1} \mp \left[\frac{(\ell\pm m+2)(\ell\pm m+1)}{(2\ell+1)(2\ell+3)}\right]^{1/2} Y_{\ell+1,m\pm 1}.$$

(a) In the spherical coordinate system, the expressions of $\hat{L}_x$ and $\hat{L}_y$ are given by

$$\hat{L}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right),$$
$$\hat{L}_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right).$$

Making use of the expressions of $\hat{L}_x$ and $\hat{L}_y$, we find that the expression for $\hat{L}_+$ is given by

$$\begin{aligned}\hat{L}_+ &= \hat{L}_x + i\hat{L}_y \\ &= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) - \hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \\ &= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\end{aligned}$$

and that the expression for $\hat{L}_-$ is given by

$$\begin{aligned}\hat{L}_- &= \hat{L}_x - i\hat{L}_y \\ &= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) + \hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \\ &= \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right).\end{aligned}$$

(b) The expression of the spherical harmonic functions in terms of the associated Legendre polynomials is given by

$$Y_{\ell m}(\theta,\phi) = (-1)^m\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)e^{im\phi}.$$

Applying $\hat{L}_+$ to $Y_{\ell m}(\theta,\phi)$, we have

$$\hat{L}_+ Y_{\ell m}(\theta,\phi) = (-1)^m\hbar\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\left[\frac{dP_\ell^m(\cos\theta)}{d\theta} - m\cot\theta P_\ell^m(\cos\theta)\right]e^{i(m+1)\phi}.$$

In terms of $x = \cos\theta$, the derivative of $P_\ell^m(\cos\theta)$ with respect to θ can be written as

$$\frac{dP_\ell^m(\cos\theta)}{d\theta} = -\sqrt{1-x^2}\,\frac{dP_\ell^m(x)}{dx}.$$

Making use of the recursion relations

$$2mxP_\ell^m(x) = \sqrt{1-x^2}\left[P_\ell^{m+1}(x) + (\ell+m)(\ell-m+1)P_\ell^{m-1}(x)\right],$$
$$\sqrt{1-x^2}\frac{d}{dx}P_\ell^m(x) = \frac{1}{2}\left[P_\ell^{m+1}(x) - (\ell+m)(\ell-m+1)P_\ell^{m-1}(x)\right],$$

we have

$$\begin{aligned}
\hat{L}_+ Y_{\ell m}(\theta,\phi) &= (-1)^m \hbar \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} \left\{ -\frac{1}{2}\left[P_\ell^{m+1}(\cos\theta) - (\ell+m)(\ell-m+1)P_\ell^{m-1}(\cos\theta)\right] \right. \\
&\quad \left. - \frac{1}{2}\left[P_\ell^{m+1}(\cos\theta) + (\ell+m)(\ell-m+1)P_\ell^{m-1}(\cos\theta)\right] \right\} e^{i(m+1)\phi} \\
&= (-1)^{m+1}\hbar \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^{m+1}(\cos\theta) e^{i(m+1)\phi} \\
&= \hbar\sqrt{(\ell+m+1)(\ell-m)}\left[(-1)^{m+1}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m-1)!}{(\ell+m+1)!}}\, P_\ell^{m+1}(\cos\theta) e^{i(m+1)\phi} \right] \\
&= \hbar\sqrt{(\ell+m+1)(\ell-m)}\, Y_{\ell,m+1}(\theta,\phi) \\
&= \hbar\sqrt{\ell(\ell+1) - m(m+1)}\, Y_{\ell,m+1}(\theta,\phi).
\end{aligned}$$

Applying $\hat{L}_-$ to $Y_{\ell m}(\theta,\phi)$, we have

$$\begin{aligned}
\hat{L}_- Y_{\ell m}(\theta,\phi) &= (-1)^m \hbar \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} \left[-\frac{dP_\ell^m(\cos\theta)}{d\theta} - m\cot\theta P_\ell^m(\cos\theta)\right] e^{i(m-1)\phi} \\
&= (-1)^m \hbar \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} \left\{ \frac{1}{2}\left[P_\ell^{m+1}(\cos\theta) - (\ell+m)(\ell-m+1)P_\ell^{m-1}(\cos\theta)\right] \right. \\
&\quad \left. - \frac{1}{2}\left[P_\ell^{m+1}(\cos\theta) + (\ell+m)(\ell-m+1)P_\ell^{m-1}(\cos\theta)\right] \right\} e^{i(m-1)\phi} \\
&= (-1)^{m-1}\hbar \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, (\ell+m)(\ell-m+1) P_\ell^{m-1}(\cos\theta) e^{i(m-1)\phi} \\
&= \hbar\sqrt{(\ell+m)(\ell-m+1)}\left[(-1)^{m-1}\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m+1)!}{(\ell+m-1)!}}\, P_\ell^{m-1}(\cos\theta) e^{i(m-1)\phi} \right] \\
&= \hbar\sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell,m-1}(\theta,\phi) \\
&= \hbar\sqrt{\ell(\ell+1) - m(m-1)}\, Y_{\ell,m-1}(\theta,\phi).
\end{aligned}$$

(c) For $\cos\theta Y_{\ell m}(\theta,\phi)$, making use of the recursion relation

$$(\ell-m+1)P_{\ell+1}^m(x) = (2\ell+1)xP_\ell^m(x) - (\ell+m)P_{\ell-1}^m(x)$$

with $x = \cos\theta$, we have

$$\begin{aligned}
\cos\theta Y_{\ell m}(\theta,\phi) &= \frac{1}{2\ell+1}(-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}} \left[(\ell+m)P_{\ell-1}^m(\cos\theta) + (\ell-m+1)P_{\ell+1}^m(\cos\theta)\right] e^{im\phi} \\
&= (-1)^m \left[\sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell-1)(2\ell+1)}} \sqrt{\frac{(2\ell-1)}{4\pi}\frac{(\ell-m-1)!}{(\ell+m-1)!}} P_{\ell-1}^m(\cos\theta) \right. \\
&\quad \left. + \sqrt{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}} \sqrt{\frac{(2\ell+3)}{4\pi}\frac{(\ell-m+1)!}{(\ell+m+1)!}} P_{\ell+1}^m(\cos\theta) \right] e^{im\phi} \\
&= \sqrt{\frac{(\ell+m)(\ell-m)}{(2\ell-1)(2\ell+1)}}\, Y_{\ell-1,m}(\theta,\phi) + \sqrt{\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}\, Y_{\ell+1,m}(\theta,\phi).
\end{aligned}$$

For $\sin\theta e^{i\phi} Y_{\ell m}(\theta,\phi)$, we have

$$\sin\theta e^{i\phi} Y_{\ell m}(\theta,\phi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, \sin\theta P_\ell^m(\cos\theta) e^{i(m+1)\phi}.$$

Making use of

$$\sqrt{1-x^2}P_\ell^m(x) = \frac{1}{2\ell+1}\left[-P_{\ell-1}^{m+1}(x) + P_{\ell+1}^{m+1}(x)\right]$$

with $x = \cos\theta$, we have

$$\begin{aligned}
\sin\theta e^{i\phi}Y_{\ell m}(\theta,\phi) &= (-1)^m\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{1}{2\ell+1}\left[-P_{\ell-1}^{m+1}(\cos\theta) + P_{\ell+1}^{m+1}(\cos\theta)\right]e^{i(m+1)\phi} \\
&= (-1)^{m+1}\sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}}\sqrt{\frac{(2\ell-1)}{4\pi}\frac{(\ell-m-2)!}{(\ell+m)!}}P_{\ell-1}^{m+1}(\cos\theta)e^{i(m+1)\phi} \\
&\quad - (-1)^{m+1}\sqrt{\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)}}\sqrt{\frac{(2\ell+3)}{4\pi}\frac{(\ell-m)!}{(\ell+m+2)!}}P_{\ell+1}^{m+1}(\cos\theta)e^{i(m+1)\phi} \\
&= \sqrt{\frac{(\ell-m)(\ell-m-1)}{(2\ell-1)(2\ell+1)}}Y_{\ell-1,m+1}(\theta,\phi) - \sqrt{\frac{(\ell+m+1)(\ell+m+2)}{(2\ell+1)(2\ell+3)}}Y_{\ell+1,m+1}(\theta,\phi).
\end{aligned}$$

For $\sin\theta e^{-i\phi}Y_{\ell m}(\theta,\phi)$, we have

$$\sin\theta e^{-i\phi}Y_{\ell m}(\theta,\phi) = (-1)^m\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,\sin\theta P_\ell^m(\cos\theta)e^{i(m-1)\phi}.$$

Making use of

$$\sqrt{1-x^2}P_\ell^m(x) = \frac{1}{2\ell+1}\left[(\ell+m-1)(\ell+m)P_{\ell-1}^{m-1}(x) - (\ell-m+2)(\ell-m+1)P_{\ell+1}^{m-1}(x)\right]$$

with $x = \cos\theta$, we have

$$\begin{aligned}
\sin\theta e^{-i\phi}Y_{\ell m}(\theta,\phi) &= (-1)^m\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\,\frac{1}{2\ell+1}\Big[(\ell+m-1)(\ell+m)P_{\ell-1}^{m-1}(x) \\
&\qquad -(\ell-m+1)(\ell-m+2)P_{\ell+1}^{m-1}(x)\Big]e^{i(m-1)\phi} \\
&= -(-1)^{m-1}\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell+1)}}\sqrt{\frac{(2\ell-1)}{4\pi}\frac{(\ell-m)!}{(\ell+m-2)!}}P_{\ell-1}^{m-1}(\cos\theta)e^{i(m-1)\phi} \\
&\quad + (-1)^{m-1}\sqrt{\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}\sqrt{\frac{(2\ell+3)}{4\pi}\frac{(\ell-m+2)!}{(\ell+m)!}}P_{\ell+1}^{m-1}(\cos\theta)e^{i(m-1)\phi} \\
&= -\sqrt{\frac{(\ell+m)(\ell+m-1)}{(2\ell-1)(2\ell+1)}}Y_{\ell-1,m-1}(\theta,\phi) + \sqrt{\frac{(\ell-m+2)(\ell-m+1)}{(2\ell+1)(2\ell+3)}}Y_{\ell+1,m-1}(\theta,\phi).
\end{aligned}$$