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Problem 1. The Hamiltonian of a quantum system is given by $\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\vec{r})$ 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 $\psi_n(\vec{r})$ are normalized.
(a) Evaluate the commutators $[\hat{H}, x]$ and $[[\hat{H}, x], x]$.
(b) Show that $\sum_{n'}(E_{n'} - E_n)|(\psi_{n'}, x\psi_n)|^2 = \frac{\hbar^2}{2m}$ using the result for the commutator $[[\hat{H}, x], x]$.

Solution:
(a)

$$\begin{aligned}
[\hat{H}, x]\psi =& \hat{H}x\psi - x\hat{H}\psi \\
=&[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})](x\psi) - x[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})]\psi \\
=& -\frac{\hbar^2}{2m}(\psi\nabla^2 x + 2\nabla x \cdot \nabla\psi + x\nabla^2\psi) + V(\vec{r})x\psi + \frac{\hbar^2}{2m}x\nabla^2\psi - xV(\vec{r})\psi \\
=& -\frac{\hbar^2}{m}\nabla\psi
\end{aligned} \tag{1}$$

$$\Longrightarrow [\hat{H}, x] = -\frac{\hbar^2}{m}\nabla \tag{2}$$

$$\begin{aligned}
[[\hat{H}, x], x]\psi =& [-\frac{\hbar^2}{m}\nabla, x]\psi \\
=& -\frac{\hbar^2}{m}\nabla(x\psi) + x\frac{\hbar^2}{m}\nabla\psi \\
=& -\frac{\hbar^2}{m}\psi\nabla x - \frac{\hbar^2}{m}x\nabla\psi + x\frac{\hbar^2}{m}\nabla\psi \\
=& -\frac{\hbar^2}{m}\psi
\end{aligned} \tag{3}$$

$$\Longrightarrow [[\hat{H}, x], x] = -\frac{\hbar^2}{m} \tag{4}$$

(b)

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

On the one hand,

$$\begin{aligned}(\psi_{n'}, x\hat{H}x\psi_n) - E_n(\psi_n, x^2\psi_n) =&(\psi_{n'}, x\hat{H}x\psi_n) - (E_n\psi_n, x^2\psi_n)\\ =&(\psi_{n'}, x\hat{H}x\psi_n) - (\hat{H}\psi_n, x^2\psi_n)\\ =&(\psi_{n'}, x\hat{H}x\psi_n) - (\psi_n, \hat{H}x^2\psi_n)\\ =&(\psi_{n'}, (x\hat{H}x - \hat{H}x^2\psi_n)\\ =&(\psi_{n'}, -[\hat{H}, x]x\psi_n) \end{aligned} \tag{5}$$

On the other hand,

$$\begin{aligned}(\psi_{n'}, x\hat{H}x\psi_n) - E_n(\psi_n, x^2\psi_n) =&(\psi_{n'}, x\hat{H}x\psi_n) - (\psi_n, x^2E_n\psi_n)\\ =&(\psi_{n'}, x\hat{H}x\psi_n) - (\psi_n, x^2\hat{H}\psi_n)\\ =&(\psi_{n'}, (x\hat{H}x - x^2\hat{H}\psi_n)\\ =&(\psi_{n'}, x[\hat{H}, x]\psi_n) \end{aligned} \tag{6}$$

Therefore,

$$\sum_{n'}(E_{n'} - E_n)|(\psi_{n'}, x\psi_n)|^2 = \frac{1}{2}[(\psi_{n'}, x[\hat{H}, x]\psi_n) + (\psi_{n'}, -[\hat{H}, x]x\psi_n)] \tag{7}$$

$$\begin{aligned}=&\frac{1}{2}(\psi_{n'}, (x[\hat{H}, x] - [\hat{H}, x]x)\psi_n)\\ =&\frac{1}{2}(\psi_{n'}, -[[\hat{H}, x], x]\psi_n)\\ =&\frac{\hbar^2}{2m}\end{aligned} \tag{8}$$

□

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

Solution: (a)

$$\begin{aligned}(\psi_n(\lambda), \hat{H}(\lambda)(\lambda)\psi_n(\lambda)) =& \int d^3r\psi_n^*(\lambda)\hat{H}\psi_n(\lambda)\\ =& \int d^3r\psi_n^*(\lambda)E_n(\lambda)\psi_n(\lambda)\\ =&E_n(\lambda)\int d^3r\psi_n^*(\lambda)\psi_n(\lambda)\\ =&E_n(\lambda)\end{aligned} \tag{9}$$

(b)

$$\begin{aligned}
&\frac{\partial E_n(\lambda)}{\partial\lambda}\\
=&\frac{\partial}{\partial\lambda}[\int d^3r\psi_n^*(\lambda)\hat{H}(\lambda)\psi_n(\lambda)]\\
=&\int d^3r\frac{\partial}{\partial\lambda}[\psi_n^*(\lambda)]E_n(\lambda)\psi_n(\lambda)+\int d^3r\psi_n^*(\lambda)[\frac{\partial}{\partial\lambda}\hat{H}(\lambda)]\psi_n(\lambda)+\int d^3r\psi_n^*(\lambda)E_n[\frac{\partial}{\partial\lambda}]\psi_n(\lambda)\\
=&E_n(\lambda)[\int d^3r\psi_n(\lambda)\frac{\partial}{\partial\lambda}\psi_n^*(\lambda)+\psi_n^*(\lambda)\frac{\partial}{\partial\lambda}\psi_n(\lambda)]+\int d^3r\psi_n^*(\lambda)\frac{\partial}{\partial\lambda}\hat{H}(\lambda)\psi_n(\lambda)\\
=&E_n(\lambda)\frac{\partial}{\partial\lambda}\int d^3r\psi_n(\lambda)\psi_n^*(\lambda)+\int d^3r\psi_n^*(\lambda)\frac{\partial}{\partial\lambda}\hat{H}(\lambda)\psi_n(\lambda)\\
=&E_n(\lambda)\frac{\partial}{\partial\lambda}1+\int d^3r\psi_n^*(\lambda)\frac{\partial}{\partial\lambda}\hat{H}(\lambda)\psi_n(\lambda)\\
=&\int d^3r\psi_n^*(\lambda)\frac{\partial}{\partial\lambda}\hat{H}(\lambda)\psi_n(\lambda)\\
=&(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda))
\end{aligned}\tag{10}$$

□

Problem 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 $\varphi_{\vec{r}'}(\vec{p})=\frac{1}{(2\pi\hbar)^{3/2}}\int d^3r\psi_{\vec{r}'}(\vec{r})e^{-i\vec{p}\cdot\vec{r}/\hbar}$.
(b) The eigenequation of $\vec{r}$ 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 the momentum space?

Solution:
(a) The eigenfunction of $\hat{\vec{r}}$

$$\begin{aligned}
\varphi_{\vec{r}'}(\vec{p})=&\frac{1}{(2\pi\hbar)^{3/2}}\int d^3r\psi_{\vec{r}'}(\vec{r})e^{-i\vec{p}\cdot\vec{r}/\hbar}\\
=&\frac{1}{(2\pi\hbar)^{3/2}}\int d^3r\delta(\vec{r}-\vec{r}')e^{-i\vec{p}\cdot\vec{r}/\hbar}\\
=&\frac{1}{(2\pi\hbar)^{3/2}}e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}
\end{aligned}\tag{11}$$

(b) The expression of $\hat{\vec{r}}$ in momentum space

$$\hat{\vec{r}}\varphi_{\vec{r}'}(\vec{p})=\vec{r}'\varphi_{\vec{r}'}(\vec{p})\tag{12}$$

$$\Longrightarrow\hat{\vec{r}}\frac{1}{(2\pi\hbar)^{3/2}}e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}=\frac{\vec{r}'}{(2\pi\hbar)^{3/2}}e^{-i\vec{p}\cdot\vec{r}\,'/\hbar}\tag{13}$$

$$\Longrightarrow\hat{\vec{r}}=i\hbar\nabla_{\vec{p}}\tag{14}$$

$$\begin{aligned}[\hat{r}_x,\hat{p}_x]\psi =&[i\hbar\frac{\partial}{\partial p_x},p_x]\psi\\ =&i\hbar\frac{\partial}{\partial p_x}(p_x\psi)-i\hbar p_x\frac{\partial}{\partial p_x}\psi\\ =&i\hbar\psi+i\hbar p_x\frac{\partial}{\partial p_x}\psi-i\hbar p_x\frac{\partial}{\partial p_x}\psi\\ =&i\hbar\psi \qquad (15)\\ \Longrightarrow&[\hat{r}_x,\hat{p}_x]=i\hbar \qquad (16)\end{aligned}$$

$$\begin{aligned}[\hat{r}_x,\hat{p}_y]\psi =&[i\hbar\frac{\partial}{\partial p_x},p_y]\psi\\ =&[i\hbar\frac{\partial}{\partial p_x},p_y]\psi\\ =&i\hbar\frac{\partial}{\partial p_x}(p_y\psi)-i\hbar p_y\frac{\partial}{\partial p_x}\psi\\ =&0 \qquad (17)\\ \Longrightarrow&[\hat{r}_x,\hat{p}_y]=0 \qquad (18)\end{aligned}$$

Similarly, we have

$$[\hat{r}_y,\hat{p}_y]=[\hat{r}_z,\hat{p}_z]=i\hbar \qquad (19)$$

$$[\hat{r}_y,\hat{p}_z]=[\hat{r}_z,\hat{p}_x]=0 \qquad (20)$$

Therefore, the obtained expression of $\hat{\vec{r}}$ in momentum space satisfy the fundamental commutation relations

$$[\hat{r}_\alpha,\hat{p}_\beta]=i\hbar\delta_{\alpha\beta} \qquad (21)$$

with $\alpha,\beta=x,y,z$ in the momentum space. □

Problem 4. The Hamiltonian of a quantum system is given by $\hat{H}=\frac{\hat{\vec{p}}^2}{2m}+\hat{V}(\vec{r})$ where $\hat{V}(\vec{r})$ 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 $(\psi_n,\frac{\hat{\vec{p}}^2}{2m}\psi_n)=\frac{1}{2}(\psi_n,\vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n)$; also write as $\langle T\rangle=\frac{1}{2}\langle\vec{r}\cdot\vec{\nabla}V(\vec{r})\rangle_n$ with $\hat{T}=\frac{\hat{\vec{p}}^2}{2m}$ the kinetic energy operator.

Solution:
(a) Hamiltonian in real space

$$\hat{H}=\frac{\hat{\vec{p}}^2}{2m}+\hat{V}(\vec{r})=-\frac{\hbar^2}{2m}\nabla^2+\hat{V}(\vec{r}) \qquad (22)$$

$$\Longrightarrow\frac{\partial\hat{H}}{\partial\hbar}=-\frac{\hbar}{m}\nabla^2 \qquad (23)$$

The Hellmann-Feynman theorem in real space

$$\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)) \tag{24}$$

$$\Longrightarrow\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),-\frac{\hbar}{m}\nabla^2\psi_n(\lambda)) \tag{25}$$

$$(\text{or}\quad\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\frac{2}{\hbar}\frac{\hat{\vec{p}}^2}{2m}\psi_n(\lambda))) \tag{26}$$

(b) Hamiltonian in momentum space

$$\hat{H}=\frac{\hat{\vec{p}}^2}{2m}+\hat{V}(\vec{r}) \tag{27}$$

$$\Longrightarrow\frac{\partial\hat{H}}{\partial\hbar}=\nabla V(\vec{r})\cdot\frac{\partial\hat{\vec{r}}}{\partial\hbar}=\nabla V(\vec{r})\cdot\frac{\partial i\hbar\nabla_{\vec{p}}}{\partial\hbar}=\nabla V(\vec{r})\cdot i\nabla_{\vec{p}} \tag{28}$$

The Hellmann-Feynman theorem in momentum space

$$\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\frac{\partial\hat{H}(\lambda)}{\partial\lambda}\psi_n(\lambda)) \tag{29}$$

$$\Longrightarrow\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\nabla V(\vec{r})\cdot i\nabla_{\vec{p}}\psi_n(\lambda)) \tag{30}$$

$$(\text{or}\quad\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\frac{\vec{r}}{\hbar}\cdot\nabla V(\vec{r})\psi_n(\lambda))) \tag{31}$$

(c) Using the results obtained in the previous two parts

$$\frac{\partial E_n(\lambda)}{\partial\lambda}=(\psi_n(\lambda),\frac{2}{\hbar}\frac{\hat{\vec{p}}^2}{2m}\psi_n(\lambda)))=(\psi_n(\lambda),\frac{\vec{r}}{\hbar}\cdot\nabla V(\vec{r})\psi_n(\lambda))) \tag{32}$$

$$\Longrightarrow(\psi_n,\frac{\hat{\vec{p}}^2}{2m}\psi_n)=\frac{1}{2}(\psi_n,\vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n) \tag{33}$$

□

Problem 5. The ladder operators of the orbital angular momentum are defined by $\hat{L}_\pm=\hat{L}_x+i\hat{L}_y$.
(a) Derive the expression of $\hat{L}_\pm$ in the spherical coordinate system.
(b) Show that $\hat{L}_\pm Y_{lm}(\theta,\phi)=\hbar\sqrt{l(l+1)-m(m\pm1)}Y_{l,m\pm1}(\theta,\phi)$.
(c) Show that

$$\cos\theta Y_{lm}=\left[\frac{(l+m)(l-m)}{(2l-1)(2l+1)}\right]^{1/2}Y_{l-1,m}+\left[\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]Y_{l+1,m},$$

$$\sin\theta e^{\pm i\phi}Y_{lm}=\pm\left[\frac{(l\mp m)(l\mp m-1)}{(2l-1)(2l+1)}\right]^{1/2}Y_{l-1,m\pm1}\mp\left[\frac{(l\pm m+2)(l\pm m+1)}{(2l+1)(2l+3)}\right]^{1/2}Y_{l+1,m\pm1}$$

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Solution: (a)

$$\begin{aligned}
\frac{\partial}{\partial x} =&\frac{\partial r}{\partial x}\frac{\partial}{\partial r}+\frac{\partial\cos\theta}{\partial x}\frac{\partial}{\partial\cos\theta}+\frac{\partial\tan\phi}{\partial x}\frac{\partial}{\partial\tan\phi}\\
=&\frac{x}{r}\frac{\partial}{\partial r}+\frac{-xz}{r^3}\frac{-1}{\sin\theta}\frac{\partial}{\partial\theta}-\frac{y}{x^2}\cos^2\phi\frac{\partial}{\partial\phi}\\
=&\sin\theta\cos\phi\frac{\partial}{\partial r}+\frac{1}{r}\sin\theta\cos\phi\cos\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}-\frac{1}{r}\frac{\sin\theta\sin\phi}{\sin^2\theta\cos^2\phi}\cos^2\phi\frac{\partial}{\partial\phi}\\
=&\sin\theta\cos\phi\frac{\partial}{\partial r}+\frac{1}{r}\cos\phi\cos\theta\frac{\partial}{\partial\theta}-\frac{1}{r}\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi}
\end{aligned}\tag{34}$$

$$\begin{aligned}
\frac{\partial}{\partial y} =&\frac{\partial r}{\partial y}\frac{\partial}{\partial r}+\frac{\partial\cos\theta}{\partial y}\frac{\partial}{\partial\cos\theta}+\frac{\partial\tan\phi}{\partial y}\frac{\partial}{\partial\tan\phi}\\
=&\frac{y}{r}\frac{\partial}{\partial r}+\frac{-yz}{r^3}\frac{-1}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{x}\cos^2\phi\frac{\partial}{\partial\phi}\\
=&\sin\theta\sin\phi\frac{\partial}{\partial r}+\frac{1}{r}\sin\theta\sin\phi\cos\theta\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}+\frac{1}{r}\frac{1}{\sin\theta\cos\phi}\cos^2\phi\frac{\partial}{\partial\phi}\\
=&\sin\theta\sin\phi\frac{\partial}{\partial r}+\frac{1}{r}\sin\phi\cos\theta\frac{\partial}{\partial\theta}+\frac{1}{r}\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi}
\end{aligned}\tag{35}$$

$$\begin{aligned}
\frac{\partial}{\partial z} =&\frac{\partial r}{\partial z}\frac{\partial}{\partial r}+\frac{\partial\cos\theta}{\partial z}\frac{\partial}{\partial\cos\theta}+\frac{\partial\tan\phi}{\partial z}\frac{\partial}{\partial\tan\phi}\\
=&\frac{z}{r}\frac{\partial}{\partial r}+\left(\frac{1}{r}-\frac{z^2}{r^3}\right)\frac{-1}{\sin\theta}\frac{\partial}{\partial\theta}\\
=&\cos\theta\frac{\partial}{\partial r}+\frac{1}{r}(1-\cos^2\theta)\frac{-1}{\sin\theta}\frac{\partial}{\theta}\\
=&\cos\theta\frac{\partial}{\partial r}-\frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}
\end{aligned}\tag{36}$$

The ladder operator

$$\begin{aligned}
\hat{L}_\pm =&\hat{L}_x\pm i\hat{L}_y\\
=&\frac{\hbar}{i}\left[y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\pm i\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\right]\\
=&\hbar\left[\mp(x\pm iy)\frac{\partial}{\partial z}\pm z\left(\frac{\partial}{\partial x}\pm i\frac{\partial}{\partial y}\right)\right]\\
=&\hbar r\left[\mp\sin\theta e^{\pm i\phi}\frac{\partial}{\partial z}\pm\cos\theta\left(\frac{\partial}{\partial x}\pm i\frac{\partial}{\partial y}\right)\right]\\
=&\hbar\left[\mp\sin\theta e^{\pm i\phi}\left(r\cos\theta\frac{\partial}{\partial r}-\sin\theta\frac{\partial}{\partial\theta}\right)\right.\\
&\left.\pm\cos\theta\left(r\sin\theta e^{\pm i\phi}\frac{\partial}{\partial r}+\cos\theta e^{\pm i\phi}\frac{\partial}{\partial\theta}\pm\frac{ie^{\pm i\phi}}{\sin\theta}\frac{\partial}{\partial\phi}\right)\right]\\
=&\hbar e^{\pm i\phi}\left[\pm\sin^2\theta\frac{\partial}{\partial\theta}\pm\left(\cos^2\theta\frac{\partial}{\partial\theta}\pm\frac{i\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)\right]\\
=&\hbar e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)
\end{aligned}\tag{37}$$

(b)

$$\begin{aligned}
&\hat{L}_\pm Y_{lm}(\theta,\phi)\\
=&\hbar e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\phi}\right)(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi}\\
=&\hbar e^{\pm i\phi}(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left(\pm e^{im\phi}\frac{\partial}{\partial\theta}P_l^m(\cos\theta)+i\cot\theta P_l^m(\cos\theta)\frac{\partial}{\partial\phi}e^{im\phi}\right)\\
=&\hbar e^{\pm i\phi}(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left(\pm e^{im\phi}\frac{\partial}{\partial\theta}P_l^m(\cos\theta)-m\cot\theta P_l^m(\cos\theta)e^{im\phi}\right)\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left(\pm\frac{\partial}{\partial\theta}P_l^m(\cos\theta)-m\cot\theta P_l^m(\cos\theta)\right)e^{i(m\pm1)\phi}\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left(\pm\frac{\partial\cos\theta}{\partial\theta}\frac{\partial}{\partial\cos\theta}P_l^m(\cos\theta)-m\cot\theta P_l^m(\cos\theta)\right)e^{i(m\pm1)\phi}\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left(\mp\sin\theta\frac{\partial}{\partial\cos\theta}P_l^m(\cos\theta)-m\cot\theta P_l^m(\cos\theta)\right)e^{i(m\pm1)\phi}\\
&\text{(using the recursion formula }(2l+1)(1-x^2)\frac{dP_l^m(x)}{dx}=(l+1)(l+m)P_{l-1}^m(x)-l(l-m+1)P_{l+1}^m(x))\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\left\{\mp\frac{\sin\theta}{(2l+1)(1-\cos^2\theta)}[(l+1)(l+m)P_{l-1}^m(\cos\theta)\pm l(l-m+1)P_{l+1}^m(\cos\theta)]\right.\\
&\left.-m\cot\theta P_l^m(\cos\theta)\right\}e^{i(m\pm1)\phi}\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{1}{(2l+1)\sin\theta}[\mp(l+1)(l+m)P_{l-1}^m(\cos\theta)\pm l(l-m+1)P_{l+1}^m(\cos\theta)\\
&-m(2l+1)\cos\theta P_l^m(\cos\theta)]e^{i(m\pm1)\phi}\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{1}{(2l+1)\sin\theta}[\mp(l\pm m+1)(l+m)P_{l-1}^m(\cos\theta)\pm(l\mp m)(l-m+1)P_{l+1}^m(\cos\theta)\\
&+m(l+1-m)P_{l+1}^m(\cos\theta)-m(2l+1)\cos\theta P_l^m(\cos\theta)+m(l+m)P_{l-1}^m(\cos\theta)]e^{i(m\pm1)\phi}\\
&\text{(using the recursion formula }(l+1-m)P_{l+1}^m(x)-(2l+1)xP_l^m(x)+(l+m)P_{l-1}^m(x)=0)\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{e^{i(m\pm1)\phi}}{(2l+1)\sin\theta}[\mp(l\pm m+1)(l+m)P_{l-1}^m(\cos\theta)\pm(l\mp m)(l-m+1)P_{l+1}^m(\cos\theta)]
\end{aligned}\tag{38}$$

For raising operator, using the recursion formula $(2l+1)(1-x^2)^{\frac{1}{2}}P_l^m(x)=(l+m)(l+m-1)P_{l-1}^{m-1}(x)-$

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$(l-m+2)(l-m+1)P_{l+1}^{m-1}(x)$

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

For raising operator, using the recursion formula $(2l+1)(1-x^2)^{\frac{1}{2}}P_l^m(x)=P_{l+1}^{m+1}(x)-P_{l-1}^{m+1}(x)$

$$
\begin{aligned}
&\hat{L}_-Y_{lm}(\theta,\phi)\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{e^{i(m-1)\phi}}{(2l+1)\sin\theta}[(l-m+1)(l+m)P_{l-1}^m(\cos\theta)-(l+m)(l-m+1)P_{l+1}^m(\cos\theta)]\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\frac{e^{i(m-1)\phi}}{(2l+1)\sin\theta}[(l-m+1)(l+m)(2l+1)(1-\cos^2\theta)^{\frac{1}{2}}P_l^{m-1}(\cos\theta)]\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}[(l-m+1)(l+m)P_l^{m-1}(\cos\theta)]e^{i(m-1)\phi}\\
=&\hbar(-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m+1)!}{(l+m-1)!}}\sqrt{(l-m+1)(l+m)}P_l^{m-1}(\cos\theta)e^{i(m-1)\phi}\\
=&\hbar\sqrt{l(l+1)-m(m-1)}Y_{l,m\pm1}(\theta,\phi)
\end{aligned}\tag{39}
$$

(c)

$$\begin{aligned}
&\left[\frac{(l+m)(l-m)}{(2l-1)(2l+1)}\right]^{\frac{1}{2}} Y_{l-1,m} + \left[\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}} Y_{l+1,m} \\
=&\left[\frac{(l+m)(l-m)}{(2l-1)(2l+1)}\right]^{\frac{1}{2}} (-1)^m\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m-1)!}{(l+m-1)!}}P_{l-1}^m(\cos\theta)e^{im\phi} \\
&+\left[\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}} (-1)^m\sqrt{\frac{(2l+3)}{4\pi}\frac{(l-m+1)!}{(l+m+1)!}}P_{l+1}^m(\cos\theta)e^{im\phi} \\
=&(-1)^m e^{im\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}[(l+m)P_{l-1}^m(\cos\theta)+(l-m+1)P_{l+1}^m(\cos\theta)] \\
&\text{(using the recursion formula } (l+1-m)P_{l+1}^m(x)-(2l+1)xP_l^m(x)+(l+m)P_{l-1}^m(x)=0) \\
=&(-1)^m e^{im\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}(2l+1)\cos\theta P_l^m(\cos\theta) \\
=&(-1)^m e^{im\phi}\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\cos\theta P_l^m(\cos\theta) \\
=&\cos\theta Y_{lm}
\end{aligned} \tag{40}$$

$$\begin{aligned}
&\pm\left[\frac{(l\mp m)(l\mp m-1)}{(2l-1)(2l+1)}\right]^{1/2} Y_{l-1,m\pm1} \mp \left[\frac{(l\pm m+2)(l\pm m+1)}{(2l+1)(2l+3)}\right]^{1/2} Y_{l+1,m\pm1} \\
=&\pm\left[\frac{(l\mp m)(l\mp m-1)}{(2l-1)(2l+1)}\right]^{1/2} (-1)^{m\pm1}\sqrt{\frac{(2l-1)}{4\pi}\frac{(l-1-m\mp1)!}{(l-1+m\pm1)!}}P_{l-1}^{m\pm1}(\cos\theta)e^{i(m\pm1)\phi} \\
&\mp\left[\frac{(l\pm m+2)(l\pm m+1)}{(2l+1)(2l+3)}\right]^{1/2} (-1)^{m\pm1}\sqrt{\frac{(2l+3)}{4\pi}\frac{(l+1-m\mp1)!}{(l+1+m\pm1)!}}P_{l+1}^{m\pm1}(\cos\theta)e^{i(m\pm1)\phi} \\
=&(-1)^{m\pm1}\frac{e^{i(m\pm1)\phi}}{\sqrt{4\pi(2l+1)}}\pm\left[\sqrt{(l\mp m)(l\mp m-1)\frac{(l-1-m\mp1)!}{(l-1+m\pm1)!}}P_{l-1}^{m\pm1}(\cos\theta)\right. \\
&\left.-\sqrt{(l\pm m+2)(l\pm m+1)\frac{(l+1-m\mp1)!}{(l+1+m\pm1)!}}P_{l+1}^{m\pm1}(\cos\theta)\right]
\end{aligned} \tag{41}$$

Then

$$\begin{aligned}
&\left[\frac{(l-m)(l-m-1)}{(2l-1)(2l+1)}\right]^{1/2}Y_{l-1,m+1}-\left[\frac{(l+m+2)(l+m+1)}{(2l+1)(2l+3)}\right]^{1/2}Y_{l+1,m+1}\\
=&(-1)^{m+1}\frac{e^{i(m+1)\phi}}{\sqrt{4\pi(2l+1)}}\left[\sqrt{(l-m)(l-m-1)\frac{(l-1-m-1)!}{(l-1+m+1)!}}P_{l-1}^{m+1}(\cos\theta)\right.\\
&\left.-\sqrt{(l+m+2)(l+m+1)\frac{(l+1-m-1)!}{(l+1+m+1)!}}P_{l+1}^{m+1}(\cos\theta)\right]\\
=&(-1)^{m+1}e^{i(m+1)\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}\left[P_{l-1}^{m+1}(\cos\theta)-P_{l+1}^{m+1}(\cos\theta)\right]\\
&\text{(using the recursion formula }(2l+1)(1-x^2)^{\frac{1}{2}}P_l^m(x)=P_{l+1}^{m+1}(x)-P_{l-1}^{m+1}(x))\\
=&(-1)^{m+1}e^{i(m+1)\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}\left[(2l+1)(1-\cos^2\theta)^{\frac{1}{2}}P_{l+1}^{m}(\cos\theta)\right]\\
=&(-1)^{m+1}e^{i(m+1)\phi}\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\sin\theta P_{l+1}^{m}(\cos\theta)\\
=&\sin\theta e^{i\phi}Y_{lm}
\end{aligned}\tag{42}$$

and

$$\begin{aligned}
&-\left[\frac{(l+m)(l+m-1)}{(2l-1)(2l+1)}\right]^{1/2}Y_{l-1,m-1}+\left[\frac{(l-m+2)(l-m+1)}{(2l+1)(2l+3)}\right]^{1/2}Y_{l+1,m-1}\\
=&(-1)^{m-1}\frac{e^{i(m-1)\phi}}{\sqrt{4\pi(2l+1)}}-\left[\sqrt{(l+m)(l+m-1)\frac{(l-1-m+1)!}{(l-1+m-1)!}}P_{l-1}^{m-1}(\cos\theta)\right.\\
&\left.-\sqrt{(l-m+2)(l-m+1)\frac{(l+1-m+1)!}{(l+1+m-1)!}}P_{l+1}^{m-1}(\cos\theta)\right]\\
=&(-1)^{m}e^{i(m-1)\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}[(l+m)(l+m-1)P_{l-1}^{m-1}(\cos\theta)\\
&-(l-m+2)(l-m+1)P_{l+1}^{m-1}(\cos\theta)]\\
&\text{(using the recursion formula }(2l+1)(1-x^2)^{\frac{1}{2}}P_l^m(x)=(l+m)(l+m-1)P_{l-1}^{m-1}(x)\\
&\qquad-(l-m+2)(l-m+1)P_{l+1}^{m-1}(x))\\
=&(-1)^{m}e^{i(m-1)\phi}\sqrt{\frac{1}{4\pi(2l+1)}\frac{(l-m)!}{(l+m)!}}[(2l+1)(1-\cos^2\theta)^{\frac{1}{2}}P_{l}^{m}(\cos\theta)]\\
=&(-1)^{m}e^{i(m-1)\phi}\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\sin\theta P_{l}^{m}(\cos\theta)\\
=&\sin\theta e^{-i\phi}Y_{lm}
\end{aligned}$$

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Therefore,

$$\sin\theta e^{\pm i\phi}Y_{lm}=\pm\left[\frac{(l\mp m)(l\mp m-1)}{(2l-1)(2l+1)}\right]^{1/2}Y_{l-1,m\pm1}\mp\left[\frac{(l\pm m+2)(l\pm m+1)}{(2l+1)(2l+3)}\right]^{1/2}Y_{l+1,m\pm1}\tag{43}$$

$\square$