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

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

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?

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 $\left(\psi_n, \dfrac{\hat{\vec{p}}^2}{2m}\psi_n\right) = \dfrac{1}{2}\big(\psi_n, \vec{r}\cdot\vec{\nabla}V(\vec{r})\psi_n\big)$; also written as $\big\langle\hat{T}\big\rangle_n = \dfrac{1}{2}\big\langle\vec{r}\cdot\vec{\nabla}V(\vec{r})\big\rangle_n$ with $\hat{T} = \dfrac{\hat{\vec{p}}^2}{2m}$ the kinetic energy operator.

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

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

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