PHYS 5002: Homework #4

1 Square Root of an Operator

a.) We begin by describing how you define the square root of an operator. If you have ever computed the square root of a matrix, then this will be familiar.

Consider a nonnegative operator $\hat{O}$ (nonnegative means that all eigenvalues satisfy $\lambda \geq 0$). In its eigenbasis, it is represented as a diagonal matrix, with eigenvalues on the diagonal.

$$\left\langle m \middle| \hat{O} \middle| n \right\rangle = \begin{pmatrix} o_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & o_n \end{pmatrix}$$

To make the square root, we use the same eigenvectors but take the square root of each eigenvalue

$$\left\langle m \middle| \sqrt{\hat{O}} \middle| n \right\rangle = \begin{pmatrix} \pm\sqrt{o_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \pm\sqrt{o_n} \end{pmatrix}$$

Obviously, any pattern of + or − signs gives a valid square root operator, such that $\left(\sqrt{\hat{O}}\right)^2 = \hat{O}$, but, of course, we would like to define it uniquely if we can. Show that there is only one choice of $\sqrt{\hat{O}}$ that is also positive semidefinite (nonnegative).

Explain further why any operator that commutes with $\hat{O}$ must also commute with $\sqrt{\hat{O}}$.

b.) Using the definition $\hat{r}^2 = \hat{r}_x^2 + \hat{r}_y^2 + \hat{r}_z^2$ and $[\hat{r}_\alpha, \hat{p}_\beta] = i\hbar\delta_{\alpha\beta}$ find $[\hat{p}_\alpha, \hat{r}^2]$.

c.) Use the Leibniz rule to show

$$[\hat{p}_\alpha, \hat{r}] = -i\hbar\frac{\hat{r}_\alpha}{\hat{r}}$$

Note: you may assume $[\hat{p}_\alpha, \hat{r}]$ commutes with $\hat{r}$.

d.) Use the Jacobi identity to evaluate $[\hat{r}^2, [\hat{r}, \hat{p}_\alpha]]$, but you cannot assume that $[\hat{r}, [\hat{r}, \hat{p}_\alpha]] = 0$ anymore. Instead use the result from part (c) before you made that assumption. You should be able to prove that $[\hat{r}^2, [\hat{r}, \hat{p}_\alpha]] = 0$.

But then, part (a) implies $[\hat{r}, [\hat{r}, \hat{p}_\alpha]] = 0$, so your calculation in part (c) is justified.

e.) Use Leibniz rule on $[\hat{p}_\alpha, \frac{\hat{r}}{\hat{r}}]$ to find $[\hat{p}_\alpha, \frac{1}{\hat{r}}]$.

2 Projected Momentum Operators in Spherical Coordinates

In spherical coordinates we have

$$\begin{aligned} \mathbf{e}_r &= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\ \mathbf{e}_\theta &= (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \\ \mathbf{e}_\phi &= (-\sin\phi, \cos\phi, 0) \end{aligned}$$

Using the quantum analog $\hat{\mathbf{e}}_r = \frac{\hat{\mathbf{r}}}{\hat{r}}$, we determined a Hermitian radial momentum $\hat{p}_r = \frac{1}{2}(\hat{\mathbf{e}}_r \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \hat{\mathbf{e}}_r)$ in the lecture, and put it into canonical form with all coordinate operators on the left. In doing so, we found a quantum correction.

a.) Carry out the same calculation for the θ component of momentum to find

$$\hat{p}_\theta = \frac{1}{2}(\hat{\mathbf{e}}_\theta \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \hat{\mathbf{e}}_\theta)$$

and move all coordinate operators to the left. Express your final answer in terms of $\cos\hat{\theta}, \sin\hat{\theta}, \cos\hat{\phi}, \sin\hat{\phi}, \hat{r}$ and $\hat{p}_x, \hat{p}_y, \hat{p}_z$. This case also has a quantum correction. Note that $\cos\hat{\theta} = \frac{\hat{r}_z}{\hat{r}}, \sin\hat{\theta}\cos\hat{\phi} = \frac{\hat{r}_x}{\hat{r}}$, and $\sin\hat{\theta}\sin\hat{\phi} = \frac{\hat{r}_y}{\hat{r}}$

b.) Repeat for the ϕ component

$$\hat{p}_\phi = \frac{1}{2}(\hat{\mathbf{e}}_\phi \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \hat{\mathbf{e}_\phi}).$$

Note that this notation for $\hat{p}_\theta$ and $\hat{p}_\phi$ is not the same as what many authors use (because they discuss the canonical momentum, not the projection along the spherical unit vectors). For us, it is the component of angular momentum along the corresponding unit vector direction.

3 The Laguerre Polynomial

a.) The Laguerre polynomial is defined by

$$L_k^{2l+1}(x) = \sum_{j=0}^{k} \binom{2l+k+1}{k-j} \frac{(-x)^j}{j!}$$

where $\binom{m}{n} = \frac{m!}{n!(m-n)!}$ is the binomial coefficient.

Writing the Laguerre polynomial as

$$L_k^{2l+1}(x) = \sum_{j=0}^{k} a_j^{2l+1;k} x^j$$

compute the ratio $\frac{a_{j+1}^{2l+1;k}}{a_j^{2l+1;k}}$ and express your result in simplest terms as the ratio of one integer in the numerator divided by the product of two integers in the denominator.

b.) Under the assumption that the state $|n, l = n-1\rangle$ is normalized, show that the eigenstate of hydrogen can be written as

$$|n,l\rangle = (-i)^{n-l-1}\left(\frac{na_0}{2\hat{r}}\right)^{n-l-1}\sqrt{\frac{(2n-1)!(n-l-1)!}{(n+1)!}}\,L_{n-l-1}^{2l+1}\left(\frac{2\hat{r}}{na_0}\right)|n,l=n-1\rangle$$

To do this, we must first verify that

$$\hat{B}_r^\dagger(l)\hat{B}_r^\dagger(l+1)\cdots\hat{B}_r^\dagger(n-2)\,|n,l=n-1\rangle = \left(\frac{-i\hbar}{\sqrt{2\mu}na_0}\right)^{n-l-1}\left(\frac{na_0}{2\hat{r}}\right)^{n-l-1}\frac{(2n-1)!}{(n+l)!}\frac{(n-l-1)!\,l!}{(n-1)!} \times L_{n-l-1}^{2l+1}\left(\frac{2\hat{r}}{na_0}\right)|n,l=n-1\rangle$$

We do this by computing the coefficient of the $\hat{r}^0$ term. Verify from the string of radial raising operators that this coefficient is

$$\left(\frac{i\hbar}{\sqrt{2m}na_0}\right)^{n-l-1}\frac{(2n-1)!\,l!}{(n+l)!(n-1)!}\,|n,l=n-1\rangle$$

Show you get the same result from the Laguerre polynomial.

4 Factorizing the Hydrogen Atom

We solve for the eigenstates of hydrogen using the full Schrödinger methodology. This has us start with the ground state for a given l and compute the excited states with $n > l+1$ using the procedure of interchanging $\hat{A}^\dagger$ and $\hat{A}$ and refactorizing.

We work in the angular momentum l subspace, so our first Hamiltonian is

$$\begin{aligned}\hat{H}_0^{(l)} = \hat{H}_l &= \hat{B}_r^\dagger(l)\hat{B}_r(l) + \tilde{E}_l \\ &= \hat{A}_0^\dagger(l)\hat{A}_0(l) + E_0\end{aligned}$$

The ground state of $\hat{H}_l$ satisfies $\hat{B}(l)\,|n{=}l+1, l\rangle = 0$ and $E_0 = \tilde{E}_l$. Denote $|\phi_0\rangle = |n{=}l+1, l\rangle$

The first auxiliary Hamiltonian is

$$\hat{H}_1^{(l)} = \hat{A}_0^{(l)}\hat{A}_0^{\dagger(l)} + E_0$$

Show that

$$\begin{aligned}\hat{H}_1^{(l)} = \hat{H}_{l+1} &= \hat{B}_r^\dagger(l+1)\hat{B}_r(l+1) + \tilde{E}_{l+1} \\ &= \hat{A}_1^\dagger\hat{A}_1 + E_1.\end{aligned}$$

We form $|\phi_1\rangle$ via

$$\hat{A}_1\,|\phi_1\rangle = 0 \implies \hat{B}_r(l+1)\,|\phi_1\rangle = 0$$

and $|\psi_1\rangle$ via

$$\hat{A}_0^\dagger\,|\phi_1\rangle = \hat{B}_r^\dagger(l)\,|\phi_1\rangle = \hat{B}_r^\dagger(l)\,|n = l+2, l+1\rangle$$

Explain how this $|\psi_2\rangle$ is correctly the state $|n{=}l+2, l\rangle$ and how $E_1 = \tilde{E}_{l+1}$. Complete the calculation to find all eigenstates and energies. Note this is essentially a "bookkeeping" exercise as all the hard work has already been done.

5 Decomposing Kinetic Energy into Radial and Angular Momentum

We derive $\hat{\mathbf{p}}^2 = \hat{p}_r^2 + \frac{\hat{\mathbf{L}}^2}{\hat{r}^2}$ in a different way.

a.) Assume that $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ are both vector operators. They need not commute. Then,

$$\begin{aligned}(\hat{\mathbf{A}} \times \hat{\mathbf{B}})^2 &= \sum_{ijklm} \varepsilon_{ijk}\varepsilon_{lmk}\hat{A}_i\hat{B}_j\hat{A}_l\hat{B}_m \\ &= \sum_{ijlm}(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})\hat{A}_i\hat{B}_j\hat{A}_l\hat{B}_m \\ &= \hat{\mathbf{A}}^2\hat{\mathbf{B}}^2 + \sum_{ij}\hat{A}_i[\hat{B}_j, \hat{A}_i]\hat{B}_j \\ &\quad - (\hat{\mathbf{A}} \cdot \hat{\mathbf{B}})^2 - \sum_{ij}\Big(\hat{A}_i\hat{B}_j[\hat{A}_j, \hat{B}_i] - \hat{A}_i\hat{B}_i[\hat{A}_j, \hat{B}_j]\Big)\end{aligned}$$

assuming $[\hat{A}_i, \hat{A}_j] = [\hat{B}_i, \hat{B}_j] = 0$.

b.) Pick $\hat{\mathbf{A}} = \hat{\mathbf{r}}$ and $\hat{\mathbf{B}} = \hat{\mathbf{p}}$ to show

$$(\hat{\mathbf{r}} \times \hat{\mathbf{p}})^2 = \hat{\mathbf{r}}^2\hat{\mathbf{p}}^2 - (\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 + i\hbar\,\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}$$

Use this to then verify that

$$\hat{\mathbf{p}}^2 = \hat{p}_r^2 + \frac{\hat{\mathbf{L}}^2}{\hat{r}^2}.$$

Hint: You need

$$\frac{1}{\hat{r}^2}(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})^2 = \frac{1}{\hat{r}}(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}})\frac{1}{\hat{r}}(\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}) + \text{quantum correction}.$$