1)

175(11): Expectation Value of $[r^2, \hat{p}^2]\phi$ for Particle in a Sphere

First consider:

$$[r^2, \hat{p}^2] = [r^2, \hat{\underline{p}}]\cdot\hat{\underline{p}} + \hat{\underline{p}}\cdot[r^2, \hat{\underline{p}}] \quad -(1)$$

where:

$$\begin{aligned}[r^2, \hat{\underline{p}}]\phi &= r^2\hat{\underline{p}}\phi - \hat{\underline{p}}(r^2\phi) \\ &= -i\hbar\left(r^2\underline{\nabla}\phi - \underline{\nabla}(r^2\phi)\right) \\ &= -i\hbar\left(r^2\underline{\nabla}\phi - r^2\underline{\nabla}\phi - \phi\underline{\nabla}r^2\right) \\ &= i\hbar(\underline{\nabla}r^2)\phi \quad -(2)\end{aligned}$$

where:

$$\underline{\nabla}r^2 = \frac{\partial}{\partial x}r^2\underline{i} + \frac{\partial}{\partial y}r^2\underline{j} + \frac{\partial}{\partial z}r^2\underline{k} \quad -(3)$$

and

$$r^2 = x^2 + y^2 + z^2 \quad -(4)$$

So

$$\underline{\nabla}r^2 = 2\underline{r} \quad -(5)$$

and

$$[r^2, \hat{\underline{p}}]\phi = 2i\hbar\underline{r}\phi. \quad -(6)$$

Therefore:

$$[r^2, \hat{p}^2]\phi = 2i\hbar(\underline{r}\cdot\hat{\underline{p}} + \hat{\underline{p}}\cdot\underline{r})\phi$$

where the anti-commutator is:

$$\{\underline{r}, \hat{\underline{p}}\}\phi = (\underline{r}\cdot\hat{\underline{p}} + \hat{\underline{p}}\cdot\underline{r})\phi \quad -(7)$$

and the commutator is:

$$[\underline{r}, \hat{\underline{p}}]\phi = (\underline{r}\cdot\hat{\underline{p}} - \hat{\underline{p}}\cdot\underline{r})\phi \quad -(8)$$

Therefore:

$$\boxed{[r^2, \hat{p}^2]\phi = 2i\hbar\{\underline{r}, \underline{\hat{p}}\}\phi} \quad -(9)$$

Here:

$$(\underline{r}\cdot\underline{\hat{p}} + \underline{\hat{p}}\cdot\underline{r})\phi = \underline{r}\cdot\underline{\hat{p}}\phi + \underline{\hat{p}}\cdot(\underline{r}\phi)$$

$$= -i\hbar\left(\underline{r}\cdot\underline{\nabla}\phi + \underline{\nabla}\cdot(\underline{r}\phi)\right)$$

$$= -i\hbar\left(\underline{r}\cdot\underline{\nabla}\phi + (\underline{\nabla}\cdot\underline{r})\phi + \underline{r}\cdot\underline{\nabla}\phi\right)$$

$$= -i\hbar\left(2\underline{r}\cdot\underline{\nabla}\phi + 3\phi\right). \quad -(10)$$

Here:

$$\underline{r}\cdot\underline{\nabla}\phi = X\frac{\partial\phi}{\partial X} + Y\frac{\partial\phi}{\partial Y} + Z\frac{\partial\phi}{\partial Z} \quad -(11)$$

so:

$$\{\underline{r}, \underline{\hat{p}}\}\phi = -i\hbar\left(2\left(X\frac{\partial\phi}{\partial X} + Y\frac{\partial\phi}{\partial Y} + Z\frac{\partial\phi}{\partial Z}\right) + 3\phi\right) \quad -(12)$$

and

$$\boxed{[r^2, \hat{p}^2]\phi = 2\hbar^2\left(2\left(X\frac{\partial\phi}{\partial X} + Y\frac{\partial\phi}{\partial Y} + Z\frac{\partial\phi}{\partial Z}\right) + 3\phi\right)} \quad -(13)$$

Example

Consider:

$$[Z^2, p_Z^2]\phi = 2\hbar^2\left(Z\frac{\partial\phi}{\partial Z} + \phi\right) \quad -(14)$$

for two wave functions.

3) Use:

$$\frac{\partial \varphi}{\partial z} = -\frac{\sin\theta}{r}\frac{\partial \varphi}{\partial \theta} \quad -(15)$$

and

$$z = r\cos\theta \quad -(16)$$

$$y = r\sin\theta\sin\phi \quad -(17)$$

$$x = r\sin\theta\cos\phi . \quad -(18)$$

1) For $l = 0,\ m_l = 0$:

$$\frac{\partial \varphi}{\partial z} = 0, \quad \varphi = \frac{1}{(4\pi)^{1/2}} \quad -(19)$$

so

$$[z^2, p_z^2]\varphi = 2\hbar^2\varphi = 2\hbar^2 \quad -(20)$$

and

$$\langle [z^2, p_z^2] \rangle = 2\hbar^2, \quad l = 0,\ m = 0 \quad -(21)$$

The wave functions are normalized as:

$$\int_0^{2\pi}\int_0^{\pi} Y_{lm}^{*}\, Y_{l'm'} \sin\theta\, d\theta\, d\phi = \delta_{ll'}\delta_{mm'} \quad -(22)$$

so for φ of eq (19):

$$\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi} \sin\theta\, d\theta\, d\phi = 1 \quad -(23)$$

2) For $l = 1,\ m_l = 0$:

$$\varphi = \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2}\cos\theta \quad -(24)$$

so:

+)

$$\frac{\partial \phi}{\partial z} = -\frac{\sin\theta}{r} \cdot \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2} \frac{\partial}{\partial\theta} \cos\theta$$

$$= \frac{1}{2r}\left(\frac{3}{\pi}\right)^{1/2} \sin^2\theta \quad -(25)$$

So

$$z\frac{\partial\phi}{\partial z} = \frac{1}{2}\sin^2\theta\cos\theta\left(\frac{3}{\pi}\right)^{1/2} \quad -(26)$$

and

$$\boxed{[z^2, p_z^2]\phi = 2\hbar^2\left(1 + \frac{1}{2}\left(\frac{3}{\pi}\right)^{1/2}\sin^2\theta\cos\theta\right)\phi}$$

$$-(27)$$

The normalization in this case is:

$$\frac{3}{4\pi}\int_0^{2\pi}\int_0^{\pi} \cos^2\theta\sin\theta \, d\theta \, d\phi = 1 \quad -(28)$$

because:

$$\int_0^{\pi} \cos^2\theta\sin\theta \, d\theta = -\frac{1}{3}\cos^3\theta \Big|_0^{\pi} = \frac{2}{3}$$

$$-(29)$$

So:

$$\langle [z^2, p_z^2] \rangle = 2\hbar^2 \, (l = 1, m = 0) \quad -(30)$$

ecause:

$$\langle \sin^2\theta\cos\theta \rangle = \frac{3}{4\pi}\int_0^{2\pi}\int_0^{\pi} \sin^2\theta\cos^3\theta \, d\theta \, d\phi \quad -(31)$$

$$= 0$$

ing:

$$\int_0^{\pi} \sin^2\theta\cos^3\theta \, d\theta = \frac{1}{30}\sin^3\theta\left(3\cos(2\theta) + 7\right)\Big|_0^{\pi} = 0.$$

$$-(32)$$