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Pset-6 P4
Shlok Vaibhav Singh
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Given that $\widehat{H} = \dfrac{1}{2m}\widehat{p}^2 + V(\widehat{x})$ and $H|a\rangle = E_{a'}|a\rangle$

a) $[[\widehat{x},\ \widehat{H}], \widehat{x}]] = 2\widehat{x}\widehat{H}\widehat{x} - \widehat{H}\widehat{x}^2 - \widehat{x}^2\widehat{H}$

$\widehat{H}$ contains $V(\widehat{x})$ which will commute with $\widehat{x}$

$\Rightarrow [[\widehat{x},\ \widehat{H}], \widehat{x}]] = 2\widehat{x}\dfrac{\widehat{p}^2}{2m}\widehat{x} - \dfrac{\widehat{p}^2}{2m}\widehat{x}^2 - \widehat{x}^2\dfrac{\widehat{p}^2}{2m}$

$\Rightarrow [[\widehat{x},\ \widehat{H}], \widehat{x}]] = \left[\ \widehat{x},\ \widehat{p}^2\right]\dfrac{\widehat{x}}{2m} - \dfrac{\widehat{x}}{2m}\left[\ \widehat{x},\ \widehat{p}^2\right]$

$\Rightarrow [[\widehat{x},\ \widehat{H}], \widehat{x}]] = \dfrac{i\hbar}{m}[\widehat{p},\ \widehat{x}] = \dfrac{\hbar^2}{m}$

$$\langle a|2\widehat{x}\widehat{H}\widehat{x} - \widehat{H}\widehat{x}^2 - \widehat{x}^2\widehat{H}|a\rangle = \frac{\hbar^2}{m}|a\rangle \qquad \Big(Assuming\ |a\rangle\ is\ normalized\Big) \qquad (1)$$

Since by completenss of eigenkets, $\sum_{a'}|a'\rangle\langle a'| = \mathbb{1}$, the first term is $\langle a|2\widehat{x}\widehat{H}\widehat{x}|a\rangle$ and is recasted into $\sum_{a'}2\langle a|\widehat{x}|a'\rangle\langle a'|\widehat{H}\widehat{x}|a\rangle$, now since :

$$\boxed{\langle a'|H = E_a\langle a'|}$$

the term further simplifies to : $\sum_{a'}2\langle a|\widehat{x}|a'\rangle\langle a'|\widehat{x}|a\rangle E_{a'}$

since $\widehat{x}$ is Hermitian , $\langle a|\widehat{x}|a'\rangle = \langle a'|\widehat{x}|a\rangle^*$, so that the first term is $\sum_{a'}2|\langle a|\widehat{x}|a'\rangle|^2E_{a'}$

the second term is $-\langle a|\widehat{H}\widehat{x}^2|a\rangle = -E_a\langle a|\widehat{x}^2|a\rangle$, by noting that $\sum_{a'}|a'\rangle\langle a'| = \mathbb{1}$:

this simplifies to : $-E_a\sum_{a'}\langle a|\widehat{x}|a'\rangle\langle a'|\widehat{x}|a\rangle = -E_a\sum_{a'}|\langle a|\widehat{x}|a'\rangle|^2$

the third term is similar to second term, putting these three simplifications together in (2) :

$$\sum_{a'}|\langle a|\widehat{x}|a'\rangle|^2(E_{a'} - E_a) = \frac{\hbar^2}{2m}$$

This is the Thomas-Reiche-Kuhn Sum rule

b) To show: $\langle a|\hat{p}|a'\rangle = \frac{im}{\hbar}(E_a - E_{a'})\langle a|\hat{x}|a'\rangle$ and

$$\langle a|\hat{p}^2|a\rangle = \frac{m^2}{\hbar^2}\sum_{a'}(E_a - E_{a'})^2|\langle a|\hat{x}|a'\rangle|^2$$

$$[\hat{H},\ \hat{x}] = \frac{\hat{p}^2}{2m}\hat{x} - \hat{x}\frac{\hat{p}^2}{2m} = -\frac{i\hbar\hat{p}}{m}$$

$$\Rightarrow \langle a|[\hat{H},\ \hat{x}]|a'\rangle = -\langle a|\frac{i\hbar\hat{p}}{m}|a'\rangle$$

$$\Rightarrow (E_a - E_{a'})\langle a|\hat{x}|a'\rangle = -\langle a|\frac{i\hbar\hat{p}}{m}|a'\rangle$$

$$\Rightarrow \langle a|\hat{p}|a'\rangle = \frac{im}{\hbar}(E_a - E_{a'})\langle a|\hat{x}|a'\rangle$$

or $\langle a'|\hat{p}|a\rangle = \frac{-im}{\hbar}(E_a - E_{a'})\langle a'|\hat{x}|a\rangle$ ($\hat{x}$ and $\hat{p}$ are Hermitian)

Multiplying both equations:

$$\Rightarrow \langle a|\hat{p}|a'\rangle\langle a'|\hat{p}|a\rangle = \frac{m^2}{\hbar^2}(E_a - E_{a'})^2\langle a|\hat{x}|a'\rangle\langle a'|\hat{x}|a\rangle$$

Summing over all a':

$$\Rightarrow \sum_{a'}\langle a|\hat{p}|a'\rangle\langle a'|\hat{p}|a\rangle = \frac{m^2}{\hbar^2}\sum_{a'}(E_a - E_{a'})^2\langle a|\hat{x}|a'\rangle\langle a'|\hat{x}|a\rangle$$

By completeness of eigenkets, $\sum_{a'}|a'\rangle\langle a'| = \mathbb{1}$, thus

$$\langle a|\hat{p}^2|a\rangle = \frac{m^2}{\hbar^2}\sum_{a'}(E_a - E_{a'})^2|\langle a|\hat{x}|a'\rangle|^2$$

c) Virial's theoram:

$$[\widehat{xp},\ \hat{H}] = \widehat{xp}\hat{H} - \hat{H}\widehat{xp}$$

$$\langle a|[\widehat{xp},\ \hat{H}]|a\rangle = E\langle a|\widehat{xp} - \widehat{xp}]|a\rangle = 0$$

$$\widehat{xp}\hat{H} - \hat{H}\widehat{xp} = \hat{x}\frac{\hat{p}^3}{2m} + \widehat{xp}V(\hat{x}) - V(\hat{x})\widehat{xp} - \frac{\hat{p}^2}{2m}\widehat{xp}$$

$$\Rightarrow \frac{i\hbar}{m}\hat{p}^2 + \hat{x}\,[\hat{p},\ V(\hat{x})]$$

since $[\hat{p},\ V(\hat{x})] = -i\hbar\frac{\partial V(\hat{x})}{\partial x}$

$$\Rightarrow \widehat{xp}\hat{H} - \hat{H}\widehat{xp} = \frac{i\hbar}{m}\hat{p}^2 - i\hbar\hat{x}\frac{\partial V(\hat{x})}{\partial x}$$

$$\Rightarrow \langle a|\hat{p}^2|a\rangle - \langle a|\hat{x}\frac{\partial V(\hat{x})}{\partial x}|a\rangle = 0$$

$$\Rightarrow \langle a|\frac{\hat{p}^2}{2m}|a\rangle = \frac{1}{2}\langle a|\hat{x}\frac{\partial V(\hat{x})}{\partial x}|a\rangle$$

Since this relation holds for each eigenket, it will hold for any superposition of eigenkets, so this holds for any wavefunction:

$$\Rightarrow \langle \Psi|\frac{\hat{p}^2}{2m}|\Psi\rangle = \frac{1}{2}\langle \Psi|\hat{x}\frac{\partial V(\hat{x})}{\partial x}|\Psi\rangle$$

$$\Rightarrow \boxed{2\langle T\rangle = \langle x\frac{dV(x)}{dx}\rangle}$$

For $V = \alpha x^n$, $2\langle T\rangle = \alpha\langle V\rangle$