Virial theorem in QM

Preliminary material

Heisenberg EOM:

for $\hat{x}$: $$\hat{p} = \frac{im}{\hbar}\left[\hat{H}, \hat{x}\right] \qquad (1)$$

for $\hat{x}\hat{p}$: $$\frac{i}{\hbar}\left[H, \hat{x}\hat{p}\right] = \frac{d}{dt}\left(\hat{x}\hat{p}\right) \qquad (2)$$

$[V, p]$ commutator:

$$[\hat{V}, \hat{p}]\,\varphi(x) = \hat{V}\hat{p}\,\varphi(x) - \hat{p}\hat{V}\varphi(x)$$

$$= \frac{\hbar}{i}\hat{V}\frac{d}{dx}\varphi - \frac{\hbar}{i}\frac{d}{dx}(V\varphi)$$

$$= \cancel{\frac{\hbar}{i}\hat{V}\varphi'} - \frac{\hbar}{i}V'\varphi - \cancel{\frac{\hbar}{i}V\varphi'}$$

$$= -\frac{\hbar}{i}\hat{V}'\varphi(x)$$

$$\boxed{[\hat{V}, \hat{p}] = -\frac{\hbar}{i}\frac{d\hat{V}}{dx}\varphi(x)} \qquad (3)$$

$$[\hat{H}, \hat{x}\hat{p}] = \underbrace{\underbrace{\hat{H}\hat{x}}_{\underbrace{[H,x]}_{(1)\Rightarrow \frac{\hbar}{im}\hat{p}} + \hat{x}\hat{H}}}\hat{p} - \hat{x}\hat{p}\hat{H}$$

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

$$= 2\frac{\hbar}{i}\hat{T} + \hat{x}\underbrace{[\hat{H}, \hat{p}]}_{\underbrace{[\hat{V}, \hat{p}]}_{(3)\Rightarrow -\frac{\hbar}{i}\hat{\nabla}\hat{V}}}$$

$$\underbrace{\frac{i}{\hbar}[\hat{H}, \hat{x}\hat{p}]}_{(2)\Rightarrow \frac{d}{dt}(\hat{x}\hat{p})} = 2\hat{T} - \hat{x}\hat{\nabla}V$$

$$\underbrace{\frac{d}{dt}\langle\Psi|\hat{x}\hat{p}|\Psi\rangle}_{\substack{\emptyset \text{ in stationary} \\ \text{states} \\ \Psi = e^{-i\omega t}\phi(x)}} = 2\hat{T} - \langle\Psi|x\hat{\nabla}V|\Psi\rangle$$

$$2\langle \hat{T} \rangle = \langle \hat{x}\, \hat{\nabla} \hat{V} \rangle$$

– a general fo.

Cb: $V = -\frac{1}{r}$

$$\hat{\nabla} = \frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial \vartheta} + \frac{1}{r \sin\vartheta}\frac{\partial}{\partial \varphi}$$

$$\hat{\nabla} V = \frac{1}{r^2}$$

$$\langle \hat{\underline{x}}\, \hat{\underline{\nabla}} \hat{V} \rangle = \langle \psi | \frac{r}{r^2} | \psi \rangle = \langle \frac{1}{r} \rangle = -\langle V \rangle$$

$$\boxed{2\langle T \rangle = -\langle V \rangle}$$