

Virial Theorem

$V(x, y, z)$ is homogeneous of degree n in x, y, z if

$$V(\alpha x, \alpha y, \alpha z) = \alpha^n V(x, y, z).$$

It follows that

$$\left. \frac{d}{d\alpha} V(\alpha x, \alpha y, \alpha z) \right|_{\alpha=1} = x \frac{\partial V}{\partial x} + y \frac{\partial V}{\partial y} + z \frac{\partial V}{\partial z} = nV$$

that is

$$\vec{r} \cdot \vec{\nabla} V = nV,$$

Now

$$\begin{aligned} [H, r, p] &= \left[\frac{\vec{p}^2}{2m} + V(\vec{r}), r, p \right] \\ &= \sum_{i=1}^3 \left[\frac{\vec{p}^2}{2m}, r_i \right] p_i + \sum_{i=1}^3 r_i [V(\vec{r}), p_i] \end{aligned}$$

$$= \sum_{i=1}^3 \left(-\frac{i\hbar}{2m} \frac{\partial p^2}{\partial p_i} p_i + i\hbar r_i \frac{\partial V(\vec{r})}{\partial r_i} \right)$$

$$= -\frac{i\hbar}{m} \vec{p}^2 + i\hbar \vec{r} \cdot \vec{\nabla} V(\vec{r}),$$

Now take the mean value of $[H, r, p]$

in an e -state of H

$$H|E\rangle = E|E\rangle.$$

We find

$$\begin{aligned} \langle E|[H, \vec{r} \cdot \vec{p}]|E\rangle &= \langle E|H\vec{r} \cdot \vec{p} - \vec{r} \cdot \vec{p}H|E\rangle \\ &= \langle E|E\vec{r} \cdot \vec{p} - \vec{r} \cdot \vec{p}E|E\rangle = 0 \end{aligned}$$

Thus

$$\langle E|\frac{\vec{p}^2}{m}|E\rangle = \langle E|\vec{r} \cdot \vec{\nabla} V|\vec{r}\rangle|E\rangle.$$

So $\vec{r} \cdot \vec{\nabla} V(\vec{r})$ is homogeneous of degree n , then

$$\langle E|\frac{\vec{p}^2}{2m}|E\rangle = \frac{n}{2} \langle E|V|E\rangle$$

or the mean value \bar{K} of the kinetic energy is $\frac{n}{2}$ times the mean value \bar{V} of the potential energy in any stationary state

$$\bar{K} = \frac{n}{2} \bar{V}.$$

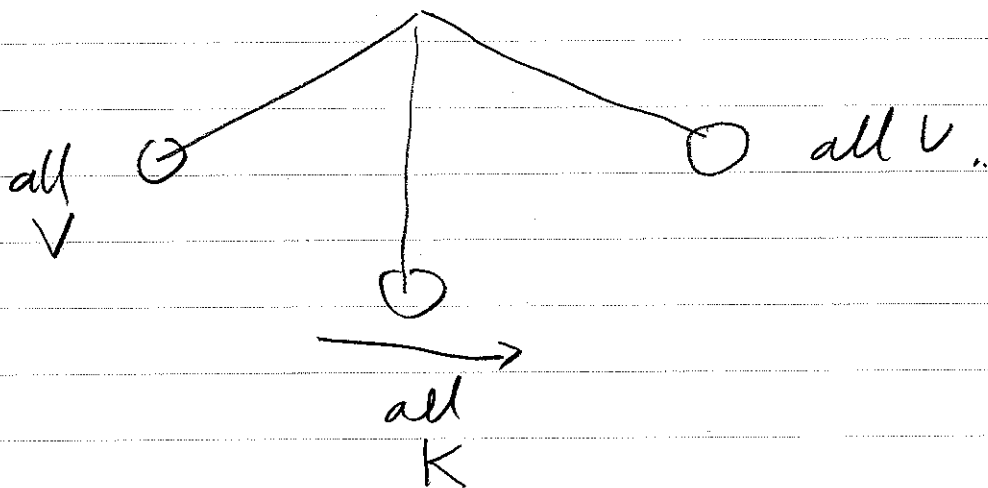
For the harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \text{ and } V(\alpha x) = \alpha^2 V(x)$$

so $n = 2$ and

$$\bar{K} = \bar{V}$$

which makes sense since



For the hydrogen atom

$$V = -\frac{e^2}{r} = -\frac{e^2}{\sqrt{x^2 + y^2 + z^2}} \quad \text{so}$$

$$V(\alpha x, \alpha y, \alpha z) = \alpha^{-1} V(x, y, z) \quad \text{and } n = -1.$$

So for the H-atom

$$\bar{K} = -\frac{1}{2} \bar{V}$$

in any e-state of H.