

Virial theorem in quantum mechanics

- ① If the potential energy $U(\vec{r})$ satisfies
- $$\vec{r} \cdot \frac{\partial U}{\partial \vec{r}} = nU(\vec{r})$$

and

- ② the system is in one of the bound states (discrete spectra, finite motion)

$$2\bar{K} = n\bar{U} \quad \text{--- mean potential energy}$$

mean kinetic energy

Proof

$$\dot{p} = -\frac{\partial U}{\partial x} \quad \leftarrow \text{force}$$

$$x\dot{p} = -x \frac{\partial U}{\partial x} = -nU$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{\partial K}{\partial p} = \frac{\partial \frac{p^2}{2m}}{\partial p} = \frac{p}{m}$$

$$p\dot{x} = 2K$$

$$x\dot{p} + p\dot{x} = \left(-x \frac{\partial H}{\partial x} + p \frac{\partial H}{\partial p} \right) = -n\bar{U} + 2\bar{K}$$

$$\frac{d}{dt}(xp) = -n\bar{U} + 2\bar{K}$$

so far classical

• Averaging over a quantum-mechanical state $|n\rangle$: $H|n\rangle = E_n|n\rangle$.

• $\frac{d}{dt} \hat{A} = \frac{i}{\hbar} [H, \hat{A}]$ quantum equation of motion

$$-n \langle n | U | n \rangle + 2 \langle n | K | n \rangle =$$

$$= \frac{i}{\hbar} \langle n | H x p - x p H | n \rangle =$$

$$= \frac{i}{\hbar} E_n \cdot \langle x p \rangle - \langle x p \rangle = 0$$

$$\boxed{2\bar{K} = n\bar{U}}$$

Hermiticity?

$$\begin{aligned} \langle x p \rangle &= \\ &= \langle (x p)^\dagger \rangle^* \\ &= \langle p x \rangle^* \end{aligned}$$

Examples:

① Harmonic oscillator $U_2 = \frac{kx^2}{2}$

$$n=2$$

$$\boxed{\bar{K} = \bar{U}}$$

② Anharmonic oscillator $U_4 = \frac{g x^4}{2}$

pure

$$n=4$$

$$\boxed{\bar{K} = 2\bar{U}}$$

③ Coulomb potential $U_c = -\frac{e^2}{r}$

$$r \cdot \frac{\partial U_c}{\partial r} = + \frac{e^2}{r^2} \cdot r = -U_c$$

$$n=-1$$

$$\boxed{\bar{K} = -\frac{1}{2}\bar{U}}$$

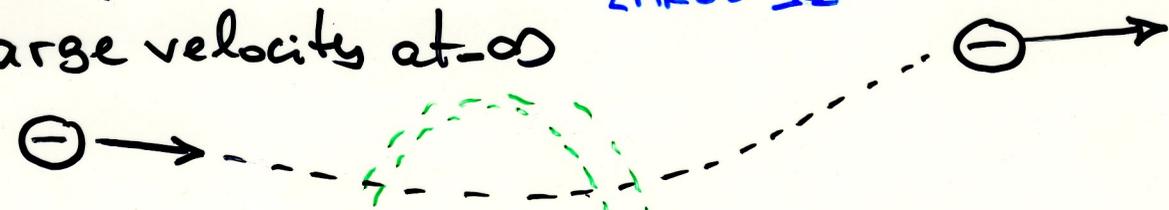
Does it work in any energy eigenstate $|n\rangle$?

Physics tells us NO:

VERY large velocity at $-\infty$

LARGE \bar{K}

and at $+\infty$



Coulomb field

$$U_c = -\frac{e^2}{r}$$

very small potential energy \bar{U}_c

Evidently

$$\bar{K} \gg |\bar{U}_c|$$

in scattering eigenstates (infinite motion)

$|n\rangle$

Formalism tells us YES:

$$\bar{K} = -\frac{1}{2}\bar{U}_c$$

$$\langle n | H \times p - x p H | n \rangle = 0$$

The problem lies in $\langle xp \rangle = \infty$
 for scattering states

Infinite motion $\langle x \rangle = \infty$

A more careful QM derivation
 of the virial theorem

(p and x don't commute)

$$\frac{d}{dt} \langle xp \rangle = \frac{dx}{dt} \cdot p + x \cdot \frac{dp}{dt} = \frac{i}{\hbar} \left\{ [H, x] \cdot p + x \cdot [H, p] \right\}$$

$$[H, x] = \left[\frac{p^2}{2m}, x \right] = \frac{1}{2m} \left(p [p, x] + [p, x] p \right)$$

$$\boxed{[H, x] = -i\hbar \cdot \frac{p}{m}} \quad \boxed{[H, p] = i\hbar \frac{\partial U}{\partial x}}$$

$$[H, p] = [U, p] = \left[U, -i\hbar \frac{\partial}{\partial x} \right] = i\hbar \frac{\partial U}{\partial x}$$

$$\frac{d}{dt} \langle xp \rangle = \frac{i}{\hbar} \cdot (-i\hbar) \left\{ \frac{p^2}{m} - x \frac{\partial U}{\partial x} \right\}$$

\downarrow \downarrow
 $2K$ nU

We obtain the operator identity

$$\frac{i}{\hbar} [H, xp] = \frac{d}{dt}(xp) = 2K - nU$$

$$x \frac{\partial U}{\partial x} = nU$$

a property of the potential

Now average over a quantum-mechanical eigenstate

$$\frac{i}{\hbar} \langle m | \underbrace{Hxp - Hxp}_0 | m \rangle = \langle m | 2K - nU | m \rangle$$

$$\langle m | xp | m \rangle < \infty$$

← for bound (normalizable) states

$$H|m\rangle = E_m|m\rangle$$

$$2\bar{K} = n\bar{U}$$

in any bound state of H