Heisenberg Eqn of Motion

The Hydrogen atom is so well-studied that there are many many tricks for evaluating things! I will give one example...

$$\frac{d\hat{Q}}{dt} = \frac{i}{\hbar}[\hat{H},\hat{Q}]$$

$$\Longrightarrow \quad \frac{d}{dt}\langle\hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle$$

Consider $\hat{Q} = \hat{x}\hat{p}$

$$[\hat{H},\hat{Q}] = [\hat{H},\hat{x}\hat{p}]$$

$$= [\hat{p}^2/2m + V(x), \hat{x}\hat{p}]$$

$$[\hat{A},\hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A}$$

$$= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A}$$

Similarly $[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$

$$= [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$$

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

$$= \hat{x}\left(V(x)\frac{\hbar}{i}\frac{\partial}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}V(x)\right)$$

$$= -\hat{x}\frac{\hbar}{i}\frac{\partial V}{\partial x}$$

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

$\hat{T}$

$$\frac{d}{dt}\langle \hat{x}\hat{p}\rangle = \frac{i}{\hbar}\left\{ -\frac{\hbar}{i}\langle \hat{x}\frac{dV}{dx}\rangle + 2\frac{\hbar}{i}\langle \hat{T}\rangle \right.$$

$$= 2\langle \hat{T}\rangle - \langle \hat{x}\frac{dV}{dx}\rangle$$

For a stationary state

$$\psi(x t) = \phi(x)\, e^{-iEt/\hbar}$$

$$\frac{d}{dt}\langle \hat{x}\hat{p}\rangle = \frac{d}{dt}\int dx\; e^{iEt/\hbar}\phi^*(x)\,\hat{x}\hat{p}\,e^{-iEt/\hbar}\phi(x)$$

$$= \phi$$

Hence $\quad 2\langle \hat{T}\rangle = \langle \hat{x}\frac{dV}{dx}\rangle$ (see page V-3)
For 1D oscillator

Can show similarly in 3D that

$$2\langle \hat{T}\rangle = \langle \vec{r}\cdot\vec{\nabla}V\rangle$$

Hydrogen atom $\quad V = -e^2/r$

$$\vec{\nabla}V = \hat{x}\frac{d}{dx}\left(-\frac{e^2}{r}\right) + \cdots$$

$$(x^2+y^2+z^2)^{-1/2}$$

$$= \hat{x}\left(\frac{e^2}{2r^3}\,2x\right) + \cdots$$

$$= \frac{e^2}{r^3}\,\vec{r}$$

$$\vec{r}\cdot\vec{\nabla}V = e^2/r$$

We learn $2\langle\hat{T}\rangle = -\langle\hat{V}\rangle$

$$\langle\hat{T}\rangle + \langle V\rangle = E_n$$

$$\left.\begin{aligned}\langle\hat{T}\rangle &= -E_n \\ \langle V\rangle &= 2E_n\end{aligned}\right\}\text{ recall } E_n < 0!$$

Same as for classical circular orbit

$$mv^2/r = GMm/r^2$$

$$\frac{1}{2}mv^2 = \frac{1}{2}GMm/r$$

$$\uparrow \qquad\qquad \uparrow$$

$$T = -\frac{1}{2}V$$

For 1D oscillator $V = \frac{1}{2}m\omega^2x^2$

$$\frac{dV}{dx} = m\omega^2 x$$

$$x\frac{dV}{dx} = m\omega^2x^2 = 2V$$

$$2\langle\hat{T}\rangle = 2\langle V\rangle \longrightarrow \langle T\rangle = \langle V\rangle$$

True also classically $x(t) = A\cos\omega t$

$$\langle V\rangle = \langle\tfrac{1}{2}m\omega^2x^2\rangle = \tfrac{1}{2}m\omega^2A^2\,\tfrac{1}{2}$$

$$v = -\omega A\sin\omega t$$

$$\langle T\rangle = \tfrac{1}{2}m\,\langle\omega^2A^2\sin^2\omega t\rangle = \tfrac{1}{2}m\omega^2A^2\tfrac{1}{2}$$

$$\langle V \rangle = 2 E_n$$

$$\left\langle \frac{-e^2}{r} \right\rangle = 2 \frac{-e^2}{2a_0} \frac{1}{n^2}$$

$$\langle 1/r \rangle = 1/a_0 \; 1/n^2$$