VIRIAL THEOREM IN 3-D

We’ve seen the virial theorem in one dimension, which states:

\[ 2\langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle \]  

where \( T \) is the kinetic energy.

We can derive the 3-d version of the virial theorem using a similar method. From the formula for the rate of change of an observable, we have,

\[ \frac{d}{dt} \langle r \cdot p \rangle = \frac{i}{\hbar} \langle [\hat{H}, r \cdot p] \rangle \]  

assuming that the potential is time-independent. (This is what Shankar refers to as Ehrenfest’s theorem.) In three dimensions, we have

\[ r \cdot p = -i\hbar x \frac{\partial}{\partial x} - i\hbar y \frac{\partial}{\partial y} - i\hbar z \frac{\partial}{\partial z} \]  

\[ \hat{H} = T + V \]  

\[ = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V \]  

Since each term in the commutator (except for the potential \( V \)) contains only one of the three spatial coordinates, any derivative term commutes with any other derivative term that contains a different variable. The remaining three non-zero commutators, one for each coordinate, can be calculated in the same way as in one dimension. We are therefore left with a simple generalization of the result for one dimension.
\[
\frac{i}{\hbar} [\hat{H}, \mathbf{r} \cdot \mathbf{p}] = -\frac{\hbar^2}{m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - x \frac{\partial V}{\partial x} - y \frac{\partial V}{\partial y} - z \frac{\partial V}{\partial z}
\]

\[
d\frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{p} \rangle = 2\langle T \rangle - \langle \mathbf{r} \cdot \nabla V \rangle
\]

For stationary states the time derivative is zero, so

\[
2\langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle
\]

For hydrogen,

\[
V = -\frac{e^2}{4\pi \epsilon_0} \frac{1}{r}
\]

so since \( r = \sqrt{x^2 + y^2 + z^2} \),

\[
\frac{\partial V}{\partial x} = \frac{e^2}{4\pi \epsilon_0} \frac{x}{r^3}
\]

\[
\frac{\partial V}{\partial y} = \frac{e^2}{4\pi \epsilon_0} \frac{y}{r^3}
\]

\[
\frac{\partial V}{\partial z} = \frac{e^2}{4\pi \epsilon_0} \frac{z}{r^3}
\]

\[
\mathbf{r} \cdot \nabla V = \frac{e^2}{4\pi \epsilon_0} \frac{x^2 + y^2 + z^2}{r^3}
\]

Thus we have

\[
2\langle T \rangle = -\langle V \rangle
\]

But we know that the total energy for the hydrogen atom in quantum state \( n \) is \( E_n = \langle T \rangle + \langle V \rangle = \langle T \rangle - 2\langle T \rangle = -\langle T \rangle \) so we get \( \langle T \rangle = -E_n \) and \( \langle V \rangle = 2E_n \).

For the 3-d harmonic oscillator

\[
V = \frac{1}{2} m \omega^2 r^2
\]

so
\[ \nabla V = m\omega^2 r \]  
\[ r \cdot \nabla V = m\omega^2 r^2 \]  
\[ = 2V \]

The total energy in state \( n \) is \( E_n = \langle T \rangle + \langle V \rangle = \frac{1}{2} (2 \langle V \rangle) + \langle V \rangle = 2 \langle V \rangle \) so \( \langle V \rangle = E_n/2 = \langle T \rangle \).

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