VIRIAL THEOREM IN 3-D

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.40.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 13, Exercise 13.1.5.

[If some equations are too small to read easily, use your browser's magnifying option (Ctrl + on Chrome, probably something similar on other browsers).]

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

$$2\langle T\rangle=\left\langle x\frac{dV}{dx}\right\rangle \tag{1}$$

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,

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{p}\rangle=\frac{i}{\hbar}\langle[\hat{H},\mathbf{r}\cdot\mathbf{p}]\rangle \tag{2}$$

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

$$\begin{aligned}
\mathbf{r}\cdot\mathbf{p} &= -i\hbar x\frac{\partial}{\partial x}-i\hbar y\frac{\partial}{\partial y}-i\hbar z\frac{\partial}{\partial z} && (3)\\
\hat{H} &= T+V && (4)\\
&= -\frac{\hbar^{2}}{2m}\left(\frac{\partial^{2}}{\partial x^{2}}+\frac{\partial^{2}}{\partial y^{2}}+\frac{\partial^{2}}{\partial z^{2}}\right)+V && (5)
\end{aligned}$$

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.

$$\frac{i}{\hbar}[\hat{H}, \mathbf{r}\cdot\mathbf{p}] = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) - x\frac{\partial V}{\partial x} - y\frac{\partial V}{\partial y} - z\frac{\partial V}{\partial z} \tag{6}$$

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{p}\rangle = 2\langle T\rangle - \langle\mathbf{r}\cdot\nabla V\rangle \tag{7}$$

For stationary states the time derivative is zero, so

$$2\langle T\rangle = \langle\mathbf{r}\cdot\nabla V\rangle \tag{8}$$

For hydrogen,

$$V = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{9}$$

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

$$\begin{aligned}
\frac{\partial V}{\partial x} &= \frac{e^2}{4\pi\epsilon_0}\frac{x}{r^3} && (10)\\
\frac{\partial V}{\partial y} &= \frac{e^2}{4\pi\epsilon_0}\frac{y}{r^3} && (11)\\
\frac{\partial V}{\partial z} &= \frac{e^2}{4\pi\epsilon_0}\frac{z}{r^3} && (12)\\
\mathbf{r}\cdot\nabla V &= \frac{e^2}{4\pi\epsilon_0}\frac{x^2+y^2+z^2}{r^3} && (13)\\
&= \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} && (14)\\
&= -V && (15)
\end{aligned}$$

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

$$V = \frac{1}{2}m\omega^2 r^2 \tag{16}$$

so

$$\nabla V = m\omega^2 \mathbf{r} \tag{17}$$
$$\mathbf{r}\cdot\nabla V = m\omega^2 r^2 \tag{18}$$
$$= 2V \tag{19}$$

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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