

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:

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

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,

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

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

$$\mathbf{r} \cdot \mathbf{p} = -i\hbar x \frac{\partial}{\partial x} - i\hbar y \frac{\partial}{\partial y} - i\hbar z \frac{\partial}{\partial z} \quad (3)$$

$$\hat{H} = T + V \quad (4)$$

$$= -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V \quad (5)$$

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.

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

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

For stationary states the time derivative is zero, so

$$2\langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle \quad (8)$$

For hydrogen,

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

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

$$\frac{\partial V}{\partial x} = \frac{e^2}{4\pi\epsilon_0} \frac{x}{r^3} \quad (10)$$

$$\frac{\partial V}{\partial y} = \frac{e^2}{4\pi\epsilon_0} \frac{y}{r^3} \quad (11)$$

$$\frac{\partial V}{\partial z} = \frac{e^2}{4\pi\epsilon_0} \frac{z}{r^3} \quad (12)$$

$$\mathbf{r} \cdot \nabla V = \frac{e^2}{4\pi\epsilon_0} \frac{x^2 + y^2 + z^2}{r^3} \quad (13)$$

$$= \frac{e^2}{4\pi\epsilon_0} \frac{1}{r} \quad (14)$$

$$= -V \quad (15)$$

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

$$V = \frac{1}{2} m \omega^2 r^2 \quad (16)$$

so

$$\nabla V = m\omega^2 \mathbf{r} \quad (17)$$

$$\mathbf{r} \cdot \nabla V = m\omega^2 r^2 \quad (18)$$

$$= 2V \quad (19)$$

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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