VIRIAL THEOREM IN 3-D

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

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:

$$2\langle T\rangle=\left\langle x\frac{dV}{dx}\right\rangle \tag{0.1}$$

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,

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{p}\rangle=\frac{i}{\hbar}\langle[\hat{H},\mathbf{r}\cdot\mathbf{p}]\rangle \tag{0.2}$$

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

$$\begin{aligned}
\mathbf{r}\cdot\mathbf{p} &= -i\hbar x\frac{\partial}{\partial x}-i\hbar y\frac{\partial}{\partial y}-i\hbar z\frac{\partial}{\partial z} && (0.3)\\
\hat{H} &= T+V && (0.4)\\
&= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V && (0.5)
\end{aligned}$$

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.

$$\frac{i}{\hbar}[\hat{H},\mathbf{r}\cdot\mathbf{p}] = -\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-x\frac{\partial V}{\partial x}-y\frac{\partial V}{\partial y}-z\frac{\partial V}{\partial z} \tag{0.6}$$

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{p}\rangle = 2\langle T\rangle-\langle\mathbf{r}\cdot\nabla V\rangle \tag{0.7}$$

For stationary states the time derivative is zero, so

$$2\langle T\rangle=\langle\mathbf{r}\cdot\nabla V\rangle \tag{0.8}$$

For hydrogen,

$$V=-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} \tag{0.9}$$

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

$$\frac{\partial V}{\partial x} = \frac{e^2}{4\pi\varepsilon_0}\frac{x}{r^3} \tag{0.10}$$

$$\frac{\partial V}{\partial y} = \frac{e^2}{4\pi\varepsilon_0}\frac{y}{r^3} \tag{0.11}$$

$$\frac{\partial V}{\partial z} = \frac{e^2}{4\pi\varepsilon_0}\frac{z}{r^3} \tag{0.12}$$

$$\mathbf{r}\cdot\nabla V = \frac{e^2}{4\pi\varepsilon_0}\frac{x^2+y^2+z^2}{r^3} \tag{0.13}$$

$$= \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} \tag{0.14}$$

$$= -V \tag{0.15}$$

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

$$V=\frac{1}{2}m\omega^2r^2 \tag{0.16}$$

so

$$\nabla V = m\omega^2 \mathbf{r} \tag{0.17}$$

$$\mathbf{r}\cdot\nabla V = m\omega^2 r^2 \tag{0.18}$$

$$= 2V \tag{0.19}$$

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 $\langle V\rangle = E_n/2 = \langle T\rangle$.

PINGBACKS

Pingback: Momentum space in 3-d
Pingback: Fine structure of hydrogen: relativistic correction
Pingback: runge lenz vector and closed orbits