VIRIAL THEOREM

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 3.31.

While examining the energy-time uncertainty relation, we derived the equation:

$$\frac{d}{dt}\langle Q\rangle=\frac{i}{\hbar}\langle[H,Q]\rangle+\left\langle\frac{\partial Q}{\partial t}\right\rangle \tag{1}$$

If we take $Q=xp$, we need the commutator $[\hat{H},xp]$. This is a straightforward calculation using derivatives, and remembering that $p=(\hbar/i)\partial/\partial x$. We also use

$$\hat{H} = \frac{p^2}{2m}+V \tag{2}$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x) \tag{3}$$

assuming that the potential is time-independent. To make using the derivatives easier (especially when using the product rule), it is best to apply the commutator to some arbitrary function f. The result is

$$\left[\hat{H},xp\right]f=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\left(x\frac{\hbar}{i}\frac{\partial}{\partial x}\right)f-\left(x\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)f \tag{4}$$

$$=-\frac{\hbar^3}{2im}\left(x\frac{\partial^3 f}{\partial x^3}+2\frac{\partial^2 f}{\partial x^2}\right)+\frac{\hbar}{i}xV\frac{\partial f}{\partial x}+\frac{\hbar^3}{2im}\left(x\frac{\partial^3 f}{\partial x^3}\right)-\frac{\hbar}{i}x\left(\frac{\partial V}{\partial x}f+V\frac{\partial f}{\partial x}\right) \tag{5}$$

$$=-\frac{\hbar^3}{im}\frac{\partial^2 f}{\partial x^2}-\frac{\hbar}{i}x\frac{\partial V}{\partial x}f \tag{6}$$

from which we get

$$\frac{i}{\hbar}[\hat{H},xp]=-\frac{\hbar^{2}}{m}\frac{\partial^{2}}{\partial x^{2}}-x\frac{\partial V}{\partial x} \tag{7}$$

The first term on the RHS is $2T$, so from 1, taking means of both sides gives the result:

$$\frac{d}{dt}\langle xp\rangle=2\langle T\rangle-\left\langle x\frac{dV}{dx}\right\rangle \tag{8}$$

In a stationary state, $\langle p\rangle=0$ and $d\langle x\rangle/dt=0$ (since the particle has no net motion) so the LHS is zero in this case and

$$2\langle T\rangle=\left\langle x\frac{dV}{dx}\right\rangle \tag{9}$$

This is known as the *virial theorem*. Actually, the theorem is more common in statistical mechanics, where its form is

$$2\langle T\rangle=-\sum_{k=1}^{N}\langle\mathbf{F}_{k}\cdot\mathbf{r}_{k}\rangle \tag{10}$$

where $\mathbf{F}_k$ is the force acting on particle k, located at position $\mathbf{r}_k$. For a conservative force, the force can be expressed as the negative gradient of a potential, which gives us the form we have derived here. The curious name 'virial' comes from the Latin word *vis*, which means 'energy' or 'force'.

For the harmonic oscillator, $V=m\omega^{2}\left\langle x^{2}\right\rangle/2$, so

$$\left\langle x\frac{dV}{dx}\right\rangle=m\omega^{2}\left\langle x^{2}\right\rangle \tag{11}$$

so $\langle T\rangle=m\omega^{2}\left\langle x^{2}\right\rangle/2=\langle V\rangle$. This agrees with the result we obtained by directly calculating the mean values earlier.

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