VIRIAL THEOREM

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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 $2T$ (T is the kinetic energy), 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', and is the same root as in the word 'virile'.

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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