

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:

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

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

$$\hat{H} = \frac{p^2}{2m} + V \quad (2)$$

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

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

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

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

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

from which we get

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

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

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

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

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

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

$$2 \langle T \rangle = - \sum_{k=1}^N \langle \mathbf{F}_k \cdot \mathbf{r}_k \rangle \quad (10)$$

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, $V = m\omega^2 \langle x^2 \rangle / 2$, so

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

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

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