

## 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:

$$(0.1) \quad \frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} \langle [H, Q] \rangle + \left\langle \frac{\partial Q}{\partial t} \right\rangle$$

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

$$(0.2) \quad \hat{H} = \frac{p^2}{2m} + V$$

$$(0.3) \quad = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

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

$$(0.4)$$

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

$$(0.5)$$

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

$$(0.6)$$

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

from which we get

$$(0.7) \quad \frac{i}{\hbar} [\hat{H}, xp] = -\frac{\hbar^2}{m} \frac{\partial^2}{\partial x^2} - x \frac{\partial V}{\partial x}$$

The first term on the RHS is  $2T$ , so from 0.1, taking means of both sides gives the result:

$$(0.8) \quad \frac{d}{dt} \langle xp \rangle = 2\langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle$$

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

$$(0.9) \quad 2\langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle$$

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

$$(0.10) \quad 2\langle T \rangle = - \sum_{k=1}^N \langle \mathbf{F}_k \cdot \mathbf{r}_k \rangle$$

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

$$(0.11) \quad \left\langle x \frac{dV}{dx} \right\rangle = m\omega^2 \langle x^2 \rangle$$

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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