

FEYNMAN-HELLMANN THEOREM AND THE HARMONIC OSCILLATOR

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 6.32.

A useful theorem known as the Feynman-Hellmann theorem can be derived as follows. Suppose that the hamiltonian of a quantum system is a function of some parameter λ . Then we can write a Taylor series:

$$(0.1) \quad H(\lambda + \Delta\lambda) = H(\lambda) + \frac{\partial H}{\partial \lambda} \Delta\lambda + \dots$$

If the second term is small, we can treat it as a perturbation on $H(\lambda)$ so if the wave function is non-degenerate, or a 'good' linear combination of degenerate states, we have

$$(0.2) \quad E_{n1} = E_{n0} + \Delta E$$

$$(0.3) \quad = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \Delta\lambda \right| \psi_n \rangle$$

$$(0.4) \quad \frac{E_{n0} + \Delta E}{\Delta\lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle$$

Taking the limit as $\Delta\lambda \rightarrow 0$ we get

$$(0.5) \quad \frac{\partial E}{\partial \lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle$$

The parameter λ can be any quantity that appears in the hamiltonian, even physical constants such as \hbar . As an example, we can look again at the 1-d harmonic oscillator:

$$(0.6) \quad H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2$$

$$(0.7) \quad E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

First, we take $\lambda = \omega$:

$$(0.8) \quad \frac{\partial E_n}{\partial \omega} = \langle \psi_n | \frac{\partial H}{\partial \omega} | \psi_n \rangle$$

$$(0.9) \quad = \langle \psi_n | m\omega x^2 | \psi_n \rangle$$

$$(0.10) \quad = \frac{2}{\omega} \langle V \rangle$$

From the energy expression, we have

$$(0.11) \quad \frac{\partial E_n}{\partial \omega} = \left(n + \frac{1}{2} \right) \hbar$$

Putting them together we get

$$(0.12) \quad \langle V \rangle = \frac{1}{2} \left(n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2}$$

This agrees with the virial theorem result $\langle T \rangle = \langle V \rangle = E_n/2$.

Second, we'll try $\lambda = \hbar$:

$$(0.13) \quad \frac{\partial E_n}{\partial \hbar} = \langle \psi_n | \frac{\partial H}{\partial \hbar} | \psi_n \rangle$$

$$(0.14) \quad = - \langle \psi_n | \frac{\hbar}{m} \frac{d^2}{dx^2} | \psi_n \rangle$$

$$(0.15) \quad = \frac{2}{\hbar} \langle T \rangle$$

From the energy expression, we have

$$(0.16) \quad \frac{\partial E_n}{\partial \hbar} = \left(n + \frac{1}{2} \right) \omega$$

Putting them together we get

$$(0.17) \quad \langle T \rangle = \frac{1}{2} \left(n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2}$$

which again agrees with the virial theorem.

Finally, we'll try $\lambda = m$:

$$(0.18) \quad \frac{\partial E_n}{\partial \hbar} = \langle \psi_n | \frac{\partial H}{\partial \hbar} | \psi_n \rangle$$

$$(0.19) \quad = \frac{\hbar^2}{2m^2} \langle \psi_n | \frac{d^2}{dx^2} | \psi_n \rangle + \frac{\omega^2}{2} \langle \psi_n | x^2 | \psi_n \rangle$$

$$(0.20) \quad = -\frac{1}{m} \langle T \rangle + \frac{1}{m} \langle V \rangle$$

From the energy expression, we have

$$(0.21) \quad \frac{\partial E_n}{\partial m} = 0$$

which leads to $\langle T \rangle = \langle V \rangle$, again in agreement with the virial theorem.

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