

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:

$$H(\lambda + \Delta\lambda) = H(\lambda) + \frac{\partial H}{\partial \lambda} \Delta\lambda + \dots \quad (1)$$

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

$$E_{n1} = E_{n0} + \Delta E \quad (2)$$

$$= \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \Delta\lambda \right| \psi_n \rangle \quad (3)$$

$$\frac{E_{n0} + \Delta E}{\Delta\lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle \quad (4)$$

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

$$\frac{\partial E}{\partial \lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle \quad (5)$$

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:

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2 \quad (6)$$

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega \quad (7)$$

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

$$\frac{\partial E_n}{\partial \omega} = \langle \psi_n | \frac{\partial H}{\partial \omega} | \psi_n \rangle \quad (8)$$

$$= \langle \psi_n | m\omega x^2 | \psi_n \rangle \quad (9)$$

$$= \frac{2}{\omega} \langle V \rangle \quad (10)$$

From the energy expression, we have

$$\frac{\partial E_n}{\partial \omega} = \left(n + \frac{1}{2} \right) \hbar \quad (11)$$

Putting them together we get

$$\langle V \rangle = \frac{1}{2} \left(n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2} \quad (12)$$

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

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

$$\frac{\partial E_n}{\partial \hbar} = \langle \psi_n | \frac{\partial H}{\partial \hbar} | \psi_n \rangle \quad (13)$$

$$= - \langle \psi_n | \frac{\hbar}{m} \frac{d^2}{dx^2} | \psi_n \rangle \quad (14)$$

$$= \frac{2}{\hbar} \langle T \rangle \quad (15)$$

From the energy expression, we have

$$\frac{\partial E_n}{\partial \hbar} = \left(n + \frac{1}{2} \right) \omega \quad (16)$$

Putting them together we get

$$\langle T \rangle = \frac{1}{2} \left(n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2} \quad (17)$$

which again agrees with the virial theorem.

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

$$\frac{\partial E_n}{\partial \hbar} = \langle \psi_n | \left| \frac{\partial H}{\partial \hbar} \right| \psi_n \rangle \quad (18)$$

$$= \frac{\hbar^2}{2m^2} \langle \psi_n | \left| \frac{d^2}{dx^2} \right| \psi_n \rangle + \frac{\omega^2}{2} \langle \psi_n | x^2 | \psi_n \rangle \quad (19)$$

$$= -\frac{1}{m} \langle T \rangle + \frac{1}{m} \langle V \rangle \quad (20)$$

From the energy expression, we have

$$\frac{\partial E_n}{\partial m} = 0 \quad (21)$$

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

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