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:

$$H(\lambda+\Delta\lambda)=H(\lambda)+\frac{\partial H}{\partial\lambda}\Delta\lambda+\ldots \tag{1}$$

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

$$E_{n1}=E_{n0}+\Delta E \tag{2}$$

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

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

Taking the limit as $\Delta\lambda\to0$ we get

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

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:

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

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

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

$$\frac{\partial E_n}{\partial \omega} = \left\langle \psi_n \left| \frac{\partial H}{\partial \omega} \right| \psi_n \right\rangle \tag{8}$$

$$= \left\langle \psi_n \left| m\omega x^2 \right| \psi_n \right\rangle \tag{9}$$

$$= \frac{2}{\omega} \langle V \rangle \tag{10}$$

From the energy expression, we have

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

Putting them together we get

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

This agrees with the virial theorem result $\langle T \rangle = \langle V \rangle = E_n/2$.
Second, we'll try $\lambda = \hbar$:

$$\frac{\partial E_n}{\partial \hbar} = \left\langle \psi_n \left| \frac{\partial H}{\partial \hbar} \right| \psi_n \right\rangle \tag{13}$$

$$= -\left\langle \psi_n \left| \frac{\hbar}{m} \frac{d^2}{dx^2} \right| \psi_n \right\rangle \tag{14}$$

$$= \frac{2}{\hbar} \langle T \rangle \tag{15}$$

From the energy expression, we have

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

Putting them together we get

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

which again agrees with the virial theorem.
Finally, we'll try $\lambda = m$:

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

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

$$= -\frac{1}{m} \langle T \rangle + \frac{1}{m} \langle V \rangle \tag{20}$$

From the energy expression, we have

$$\frac{\partial E_n}{\partial m} = 0 \tag{21}$$

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

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