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 \( \lambda \). Then we can write a Taylor series:

\[
H(\lambda + \Delta \lambda) = H(\lambda) + \frac{\partial H}{\partial \lambda} \Delta \lambda + \ldots
\]  

(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

\[
E_{n1} = E_{n0} + \Delta E
\]

\[
= \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \Delta \lambda \right| \psi_n \rangle
\]  

(2)

\[
\frac{E_{n0} + \Delta E}{\Delta \lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle
\]

(3)

Taking the limit as \( \Delta \lambda \to 0 \) we get

\[
\frac{\partial E}{\partial \lambda} = \langle \psi_n \left| \frac{\partial H}{\partial \lambda} \right| \psi_n \rangle
\]  

(4)

The parameter \( \lambda \) 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:

\[
H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2
\]  

(5)

\[
E_n = \left( n + \frac{1}{2} \right) \hbar \omega
\]  

(6)

First, we take \( \lambda = \omega \):
FEYNMAN-HELLMANN THEOREM AND THE HARMONIC OSCILLATOR

\[
\frac{\partial E_n}{\partial \omega} = \langle \psi_n \big| \frac{\partial H}{\partial \omega} \big| \psi_n \rangle \\
= \langle \psi_n \big| m\omega^2 \big| \psi_n \rangle \\
= \frac{2}{\omega} \langle V \rangle
\]

From the energy expression, we have

\[
\frac{\partial E_n}{\partial \omega} = \left( n + \frac{1}{2} \right) \hbar
\]

Putting them together we get

\[
\langle V \rangle = \frac{1}{2} \left( n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2}
\]

This agrees with the virial theorem result \( \langle T \rangle = \langle V \rangle = \frac{E_n}{2} \).

Second, we’ll try \( \lambda = \hbar \):

\[
\frac{\partial E_n}{\partial \hbar} = \langle \psi_n \big| \frac{\partial H}{\partial \hbar} \big| \psi_n \rangle \\
= -\langle \psi_n \big| \frac{\hbar}{m} \frac{d^2}{dx^2} \big| \psi_n \rangle \\
= \frac{2}{\hbar} \langle T \rangle
\]

From the energy expression, we have

\[
\frac{\partial E_n}{\partial \hbar} = \left( n + \frac{1}{2} \right) \omega
\]

Putting them together we get

\[
\langle T \rangle = \frac{1}{2} \left( n + \frac{1}{2} \right) \hbar \omega = \frac{E_n}{2}
\]

which again agrees with the virial theorem.

Finally, we’ll try \( \lambda = m \):
\[ \frac{\partial E_n}{\partial \hbar} = \langle \psi_n \mid \frac{\partial H}{\partial \hbar} \mid \psi_n \rangle \]  
(18)

\[ = \frac{\hbar^2}{2m^2} \langle \psi_n \mid \frac{d^2}{dx^2} \mid \psi_n \rangle + \frac{\omega^2}{2} \langle \psi_n \mid x^2 \mid \psi_n \rangle \]  
(19)

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

From the energy expression, we have

\[ \frac{\partial E_n}{\partial m} = 0 \]  
(21)

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

Pingbacks

Pingback: Feynman-Hellmann theorem: hydrogen atom mean values
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