27/10/2025 Lecture 24. Hellman-Feynman Theorem

E.g. of application of V.T.

$$2\langle\hat{T}\rangle = n\langle\hat{V}\rangle \quad — (1)$$

for V being a homogeneous function of n^{th} degree.

$$\because \quad E = \langle\hat{H}\rangle = \langle\hat{T}\rangle + \langle\hat{V}\rangle \quad — (2)$$

We have that

$$\langle\hat{T}\rangle = \frac{n}{2}\left(E - \langle\hat{T}\rangle\right)$$

$$\Rightarrow \quad \boxed{\langle\hat{T}\rangle = \frac{n}{n+2} E} \quad — (3)$$

Similarly,

$$\boxed{\langle\hat{V}\rangle = \frac{2}{n+2} E} \quad — (4)$$

$n \to$ degree of homogeneity.

Q. Calculate the expectation value of $\hat{x}^2$ for a Q.H.O. in the v^{th} excited state.

For a Q.H.O. $V(x) = \frac{1}{2}kx^2$ — (5)

$\Rightarrow V$ is homogeneous with degree 2.

Now, $E_v = (v+\frac{1}{2})\hbar\omega$ — (6)

$\therefore$ From (4) we have.

$$\langle \hat{V} \rangle_v = \frac{1}{2} k \langle \hat{x}^2 \rangle = \frac{2}{2+2}\left(v+\frac{1}{2}\right)\hbar\omega \quad \text{— (7)}$$

$$\Rightarrow \langle x^2 \rangle_v = \frac{1}{m\omega^2} \cdot \left(v+\frac{1}{2}\right)\hbar\omega \qquad (k = m\omega^2)$$

$$= \frac{\hbar}{(m\omega)}\left(v+\frac{1}{2}\right) \quad \text{— (8)}$$

$|||^{ly}$ $\langle \hat{p}^2 \rangle_v = 2m \langle \hat{T} \rangle_v = 2m \cdot \left(\frac{2}{2+2}\right)\left(v+\frac{1}{2}\right)\hbar\omega$

$$\Rightarrow \langle \hat{p}^2 \rangle_v = \left(v+\frac{1}{2}\right) m\hbar\omega \quad -(9)$$

Note that since $\langle \hat{x} \rangle = \langle \hat{p} \rangle = 0$ in all states we have.

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle}$$

$$\Delta x = \sqrt{\langle x^2 \rangle}$$

$\therefore$ in the v^{th} excited state.

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{m\omega}}\left(\sqrt{v+\frac{1}{2}}\right) \cdot \sqrt{\left(v+\frac{1}{2}\right)} \sqrt{m\hbar\omega}$$

$$= \left(v+\frac{1}{2}\right)\hbar \geq \frac{\hbar}{2} \quad -(10)$$

$\Rightarrow$ H.U.P. satisfied. since $v = 0, 1, 2, \ldots$

Does the V.T. really work? Let's calculate $\langle \hat{x}^2 \rangle$ explicitly

Now, $$\hat{a}_{\mp} = \frac{1}{\sqrt{2}}\left(\hat{\xi} \pm i\hat{\pi}\right) \quad -⑪$$

$$\Rightarrow \quad \hat{\xi} = \frac{1}{\sqrt{2}}\left(\hat{a}_- + \hat{a}_+\right) \quad -⑫$$

& $$\hat{x} = \sqrt{\frac{\hbar}{m\omega}}\,\hat{\xi}$$

$$\therefore \quad \hat{x}^2 = \frac{\hbar}{2m\omega}\left((\hat{a}_- + \hat{a}_+)(\hat{a}_- + \hat{a}_+)\right)$$

$$= \frac{\hbar}{2m\omega}\left[\hat{a}_-^2 + \hat{a}_+^2 + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+\right]$$

$$= \frac{\hbar}{2m\omega}\left[\hat{a}_-^2 + \hat{a}_+^2 + 2\hat{a}_-\hat{a}_+ - 1\right] \quad -⑬$$

(using $[\hat{a}_-, \hat{a}_+] = 1$)

$$\langle v | \hat{x}^2 | v \rangle = \frac{\hbar}{2m\omega}\Big\{\cancel{\langle v | \hat{a}_-^2 | v \rangle}^{\,0} + \underbrace{\cancel{\langle v | \hat{a}_+^2 | v \rangle}}_{0} + 2\langle v | \hat{a}_-\hat{a}_+ | v \rangle - 1\Big\}$$

$$= \frac{\hbar}{m\omega}\left\{ \langle v|v\rangle \left(\sqrt{v+1}\right)^2 - \frac{1}{2}\right\}$$

$$\left(\begin{array}{l} \text{using } \hat{a}_+|v\rangle = \sqrt{v+1}\,|v+1\rangle \\ \quad \& \quad \hat{a}_-|v\rangle = \sqrt{v}\,|v-1\rangle \end{array}\right.$$

$$= \left(v + \tfrac{1}{2}\right)\frac{\hbar}{m\omega} \quad \text{— (14)}$$

which agrees with (8).

Hence, V.T. is verified in this case.

Other examples in assignment.

Hellman-Feynman Theorem

Consider a system with a Hamiltonian depending on a parameter λ.

$$\hat{H} \equiv \hat{H}(\lambda)$$ eg. $\lambda \to e, m, \hbar, c, k, \omega,$ etc

(Family of problems)

$\Rightarrow$ The eigenvalues & eigenstates also depend on the parameter.

i.e. $$\hat{H}(\lambda)\,|\Psi_\lambda\rangle = E(\lambda)\,|\Psi_\lambda\rangle \quad -(15)$$

If $$E(\lambda) = \langle \Psi_\lambda | \hat{H}(\lambda) | \Psi_\lambda \rangle$$ where $\langle \Psi_\lambda | \Psi_\lambda \rangle = 1$ $-(16)$

then

$$\frac{dE}{d\lambda} = \left\langle \frac{\partial \Psi_\lambda}{\partial \lambda} \right| \hat{H}(\lambda) \left| \Psi_\lambda \right\rangle + \left\langle \Psi_\lambda \right| \hat{H}(\lambda) \left| \frac{\partial \Psi_\lambda}{\partial \lambda} \right\rangle + \left\langle \Psi_\lambda \right| \frac{\partial \hat{H}(\lambda)}{\partial \lambda} \left| \Psi_\lambda \right\rangle$$

$$= \left(\left\langle \frac{\partial \Psi_\lambda}{\partial \lambda} \middle| \Psi_\lambda \right\rangle + \left\langle \Psi_\lambda \middle| \frac{\partial \Psi_\lambda}{\partial \lambda} \right\rangle \right) E(\lambda)$$

$$+ \left\langle \Psi_\lambda \middle| \frac{\partial \hat{H}}{\partial \lambda} \middle| \Psi_\lambda \right\rangle \quad (\text{using } 15)$$

$$= E(\lambda) \frac{\partial}{\partial \lambda} \langle \Psi_\lambda | \Psi_\lambda \rangle$$

$$+ \left\langle \Psi_\lambda \middle| \frac{\partial \hat{H}(\lambda)}{\partial \lambda} \middle| \Psi_\lambda \right\rangle$$

$$= \left\langle \Psi_\lambda \middle| \frac{\partial \hat{H}(\lambda)}{\partial \lambda} \middle| \Psi_\lambda \right\rangle \quad (\because |\Psi_\lambda\rangle \text{ is normalized}) \quad — (17)$$

$$\therefore \boxed{\frac{dE(\lambda)}{d\lambda} = \left\langle \Psi_\lambda \middle| \frac{\partial \hat{H}(\lambda)}{\partial \lambda} \middle| \Psi_\lambda \right\rangle} \quad — (18)$$

This is called the Hellmann-Feynman Theorem

Variational Principle & Variation Theorem

Let $|\Psi\rangle$ be an arbitrary normalized state in the Hilbert space of the system described by the hamiltonian $\hat{H}$.
Then, the energy estimated by $|\Psi\rangle$ provides an upper bound to the exact ground state energy of $\hat{H}$.

i.e. $$\boxed{\langle \Psi | \hat{H} | \Psi \rangle \geq E_0} \quad -(1)$$

Proof:

Let $$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle \quad -(2)$$

Then, $$|\Psi\rangle = \sum_n |\phi_n\rangle c_n \quad -(3)$$

$c_n \in \mathbb{C}$.

$\because$ $\hat{H}$ is Hermitian $$\langle \phi_m | \phi_n \rangle = \delta_{mn} \quad -(4)$$

Then $\langle \Psi | \hat{\mathcal{H}} | \Psi \rangle - E_0$

$$= \langle \Psi | \hat{\mathcal{H}} - E_0 \hat{\mathbb{1}} | \Psi \rangle$$

$$= \sum_m \sum_n c_m^* \langle \phi_m | (\hat{H} - E_0 \hat{\mathbb{1}}) | \phi_n \rangle c_n$$

$$= \sum_m \sum_n |c_n|^2 (E_n - E_0) \delta_{mn}$$

$$= \sum_n |c_n|^2 (E_n - E_0) \quad - (5)$$

Each term in the sum is greater than or equal to 0.

$$\therefore \langle \Psi | \hat{H} | \Psi \rangle - E_0 \geq 0$$

$$\text{or } \langle \Psi | \hat{H} | \Psi \rangle \geq E_0 \quad - (6)$$

Hence proved.