

P.31.3

The Schrödinger equation for the linear harmonic oscillator is

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \underbrace{\frac{1}{2} m \omega^2 q^2}_{V_0} \right) \psi_n(q) = E_n \psi_n(q) \quad \text{--- (1)}$$

With a constant force added, the perturbation potential is

$$V = \alpha q \quad (\alpha = \text{constant})$$

We can write the total potential energy as

$$\begin{aligned} V_0 + V &= \frac{1}{2} m \omega^2 q^2 + \alpha q = \frac{1}{2} m \omega^2 \left(q^2 + \underbrace{\left(\frac{2\alpha}{m\omega^2} \right)}_{\beta} q \right) \\ &= \frac{1}{2} m \omega^2 \left(q^2 + \beta q + \frac{\beta^2}{4} - \frac{\beta^2}{4} \right) \quad (\text{completing squares}) \\ &= \frac{1}{2} m \omega^2 \left\{ \left(q + \frac{\beta}{2} \right)^2 - \frac{\beta^2}{4} \right\} \\ &= \frac{1}{2} m \omega^2 \left(q + \frac{\beta}{2} \right)^2 - \frac{1}{2} m \omega^2 \cdot \frac{1}{4} \cdot \frac{4\alpha^2}{(m\omega^2)^2} \\ &= \frac{1}{2} m \omega^2 \underbrace{\left(q + \frac{\beta}{2} \right)^2}_{q'^2} - \frac{\alpha^2}{2m\omega^2} \\ &= \frac{1}{2} m \omega^2 q'^2 - \frac{\alpha^2}{2m\omega^2}, \quad \text{where } q' \equiv q + \frac{\beta}{2} \end{aligned}$$

Then Schrödinger equation becomes

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2} m \omega^2 q'^2 - \frac{\alpha^2}{2m\omega^2} \right) \psi_n(q) = E_n' \psi_n(q) \quad \text{--- (2)}$$

new energy eigenvalues

i.e.

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dq^2} + \frac{1}{2} m \omega^2 q'^2 \right) \psi_n(q) = \left(E_n' + \frac{\alpha^2}{2m\omega^2} \right) \psi_n(q) \quad \text{--- (2)}$$

In (2), make the coordinate transformation

$$q \rightarrow q + \frac{\beta}{2} = q', \quad \psi_n(q) \rightarrow \psi_n'(q')$$

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P31.3 Then (2) \Rightarrow

cont'd $\left(-\frac{\hbar^2}{2m} \frac{d^2}{dq'^2} + \frac{1}{2} m \omega^2 q'^2 \right) \psi'_n(q') = \left(E'_n + \frac{\alpha^2}{2m\omega^2} \right) \psi'_n(q') \quad (3)$

But (3) is the same equation as (1), with

$$E'_n + \frac{\alpha^2}{2m\omega^2} = \left(n + \frac{1}{2} \right) \hbar \omega$$

$$\therefore \boxed{E'_n = \left(n + \frac{1}{2} \right) \hbar \omega - \frac{\alpha^2}{2m\omega^2}} \quad (4)$$

These are the exact new energy eigenvalues

Now let's do perturbation (this turns out to be the harder way!) From (31.13) and (31.37) in text, we have, up to second-order:

$$\boxed{E_n = E_n^{(0)} + \overbrace{\langle n | V | n \rangle}^{\propto q} + \sum_{m \neq n} \frac{|\langle m | V | n \rangle|^2}{E_n^{(0)} - E_m^{(0)}} + \dots} \quad (5)$$

where $|n\rangle$ and $E_n^{(0)}$ are the unperturbed eigenstates and energy eigenvalues of the unperturbed Hamiltonian H_0 , i.e.

$$H_0 |n\rangle = \hbar \omega \left(n + \frac{1}{2} \right) |n\rangle, \quad E_n^{(0)} = \hbar \omega \left(n + \frac{1}{2} \right)$$

$$\psi_n^{(0)}(q) = \langle q | n \rangle = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-Q^2/2} H_n(Q) \quad \left[\begin{array}{l} \text{see eq. (14.37)} \\ \text{and (14.57) in text} \end{array} \right]$$

\uparrow $Q \equiv \sqrt{\frac{m\omega}{\hbar}} q$, $H_n(Q)$ is the n -th Hermite polynomial
 dimensionless coordinate $H_n(Q) = (-1)^n e^{Q^2} \frac{d^n}{dQ^n} e^{-Q^2}; n = 0, 1, 2, 3, \dots \quad \left[\begin{array}{l} \text{see eq. (14.54) in} \\ \text{text} \end{array} \right]$

Now the unperturbed Hamiltonian ~~has~~ is symmetric under reflection:

$$H_0(q) = H_0(-q)$$

$\therefore \psi_n^{(0)}(q)$ has definite parity (either even or odd under reflection)

$$\therefore \langle n | V | n \rangle = \alpha \int_{-\infty}^{\infty} dq \, q \, \psi_n^{(0)*}(q) \psi_n^{(0)}(q) = 0$$

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\therefore There is no first-order correction to $E_n^{(0)}$.

so we have to calculate the 2nd order term in (5).

The matrix elements in this correction term are given by

$$\langle m | V | n \rangle = \alpha C_m C_n \int_{-\infty}^{\infty} dq \, q e^{-Q^2} H_m(Q) H_n(Q)$$

$$\text{where } C_n = \left(\frac{m\omega}{\pi \hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}}, \quad Q \equiv \sqrt{\frac{m\omega}{\hbar}} q$$

$$\therefore \langle m | V | n \rangle = \alpha C_m C_n \left(\frac{\hbar}{m\omega} \right) \int_{-\infty}^{\infty} dQ \cdot Q H_m(Q) H_n(Q) e^{-Q^2}$$

(Note all the normalization constants and wave functions are real)

From Eq. (14.71) of text, we have the recursion relation

$$Q H_m(Q) = \frac{H_{m+1}(Q)}{2} + m H_{m-1}(Q)$$

$$\therefore \langle m | V | n \rangle = \alpha C_m C_n \left(\frac{\hbar}{m\omega} \right) \int_{-\infty}^{\infty} dQ e^{-Q^2} H_n(Q) \left(\frac{H_{m+1}(Q)}{2} + m H_{m-1}(Q) \right)$$

note that this is mass of the oscillator, do not confuse with the numerical index m .

$$\langle m | V | n \rangle = \alpha C_m C_n \left(\frac{\hbar}{m\omega} \right) \left[\frac{1}{2} \int_{-\infty}^{\infty} dQ e^{-Q^2} H_n H_{m+1} + m \int_{-\infty}^{\infty} dQ e^{-Q^2} H_n H_{m-1} \right] \quad (6)$$

From the orthonormality condition of the $\psi_n^{(0)}$'s, we have

$$\delta_{ij} = \int_{-\infty}^{\infty} dq \, \psi_i^{(0)}(q) \psi_j^{(0)}(q) = C_i C_j \int_{-\infty}^{\infty} dq e^{-Q^2} H_i(Q) H_j(Q) \quad \left(q = \sqrt{\frac{\hbar}{m\omega}} Q \right)$$

$$= C_i C_j \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} dQ e^{-Q^2} H_i(Q) H_j(Q)$$

$$\therefore \int_{-\infty}^{\infty} dQ e^{-Q^2} H_i(Q) H_j(Q) = \sqrt{\frac{m\omega}{\hbar}} \frac{\delta_{ij}}{C_i C_j}$$

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∴ Eq. (6) becomes

$$\begin{aligned}
 \langle m | V | n \rangle &= \alpha C_m C_n \left(\frac{\hbar}{m\omega} \right) \left[\frac{1}{2} \sqrt{\frac{m\omega}{\hbar}} \frac{\delta_{n,m+1}}{C_n C_{m+1}} + m \sqrt{\frac{m\omega}{\hbar}} \frac{\delta_{n,m-1}}{C_n C_{m-1}} \right] \\
 &= \frac{\alpha}{2} \sqrt{\frac{\hbar}{m\omega}} \left(\frac{C_m}{C_{m+1}} \right) \delta_{n,m+1} + \alpha m \sqrt{\frac{\hbar}{m\omega}} \left(\frac{C_m}{C_{m-1}} \right) \delta_{n,m-1} \\
 &= \alpha \sqrt{\frac{\hbar}{m\omega}} \left\{ \frac{1}{2} \left(\frac{C_m}{C_{m+1}} \right) \delta_{n,m+1} + m \left(\frac{C_m}{C_{m-1}} \right) \delta_{n,m-1} \right\} \\
 \therefore |\langle m | V | n \rangle|^2 &= \alpha^2 \frac{\hbar}{m\omega} \left\{ \frac{1}{4} \left(\frac{C_m}{C_{m+1}} \right)^2 \delta_{n,m+1} + m^2 \left(\frac{C_m}{C_{m-1}} \right)^2 \delta_{n,m-1} \right\}
 \end{aligned}$$

The cross terms in the square vanishes since

$$\delta_{n,m-1} \cdot \delta_{n,m+1} = 0 \text{ for any pair } (n, m)$$

and $\delta_{n,m}^2 = \delta_{n,m}$.

Thus

$$\sum_{m \neq n} \frac{|\langle m | V | n \rangle|^2}{E_n^{(0)} - E_m^{(0)}} = \frac{\alpha^2 \hbar}{m\omega} \left[\frac{\frac{1}{4} \left(\frac{C_{n-1}}{C_n} \right)^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{(n+1)^2 \left(\frac{C_{n+1}}{C_n} \right)^2}{E_n^{(0)} - E_{n+1}^{(0)}} \right]$$

$$E_n^{(0)} - E_{n-1}^{(0)} = \hbar\omega ; \quad E_n^{(0)} - E_{n+1}^{(0)} = -\hbar\omega$$

and from by using $C_n = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}}$, we have

$$\frac{C_{n-1}}{C_n} = \frac{2^{n/2} \sqrt{n!}}{2^{(n-1)/2} \sqrt{(n-1)!}} = \sqrt{2n} ; \quad \frac{C_{n+1}}{C_n} = \frac{2^{n/2} \sqrt{n!}}{2^{(n+1)/2} \sqrt{(n+1)!}} = \frac{1}{\sqrt{2(n+1)}}$$

$$\begin{aligned}
 \therefore \sum_{m \neq n} \frac{|\langle m | V | n \rangle|^2}{E_n^{(0)} - E_m^{(0)}} &= \frac{\alpha^2 \hbar}{m\omega} \left[\frac{2n}{4\hbar\omega} - \frac{(n+1)^2}{\hbar\omega} \cdot \frac{1}{2(n+1)} \right] \\
 &= \frac{\alpha^2 \hbar}{2 \cdot m\omega \cdot \hbar\omega} [n - (n+1)] = -\frac{\alpha^2}{2m\omega^2}
 \end{aligned}$$

$$\therefore E_n^{(2)} = \left(n + \frac{1}{2} \right) \hbar\omega - \frac{\alpha^2}{2m\omega^2}$$

in agreement with our exact result earlier.