Pert. Theory examples

Useful rules & tricks

... continued example

$H_0 \rightarrow$ Particle in a box

i.e. $\frac{p^2}{2m}$ with $0 \leq x \leq L$

Notation $H = H_0 + \lambda V$

.... λ can be set to 1 after deriving the formulae for $E_n^{(1)}, E_n^{(2)} \ldots$

Here we are given

pert. $V(x) = \alpha \, \delta(x - L/2)$

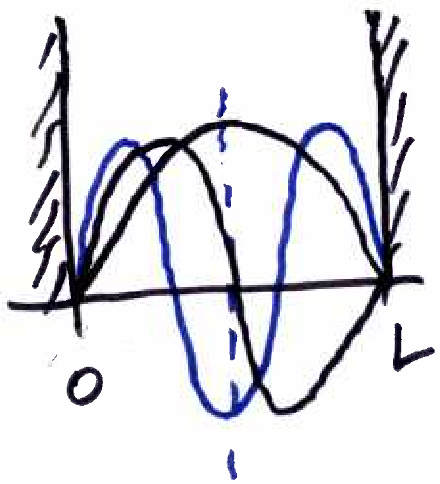
dim. of α : Energy - Length

$$E_n^{(1)} = \begin{cases} \frac{2}{L}\alpha & n = 1, 3 \ldots \\ 0 & n = 2, 4 \ldots \end{cases}$$

$E_1^{(2)}$:

$$V_{1k} = \frac{2}{L}\alpha \int \sin\frac{\pi}{L}x \, \sin\frac{k\pi}{L}x \, dx \, \delta(x - L/2)$$

$$= \frac{2}{L}\alpha \, (-1)^{\left(\frac{k-1}{2}\right)} \quad k = 3, 5, \ldots$$



Check : $k = 3 \quad (-1)^1$
$k = 5 \quad (-1)^2$

Thus $|V_{1k}|^2 = \left(\frac{2}{L}\alpha\right)^2 \quad k = 3, 5, \ldots$ & zero for k even

$$E_1^{(2)} = \sum_{k \neq 1} \frac{|V_{k1}|^2}{E_1 - E_k} = \left(\frac{2}{L}\alpha\right)^2$$

$$E_1 - E_k = \frac{\pi^2 \hbar^2}{2mL^2}(1 - k^2) \qquad k \text{ odd}$$

$$\therefore E_1^{(2)} = \sum_{r=1}^{\infty} \left(\frac{2}{L}\alpha\right)^2 \times \frac{2mL^2}{\pi^2 \hbar^2} \times \frac{1}{1-(2r+1)^2}$$

$$\frac{1}{1-(3)^2} + \frac{1}{1-(5)^2} + \cdots = \frac{1}{2}\left(\frac{1}{1+3} + \frac{1}{1-3} + \frac{1}{1+5} + \frac{1}{1-5}\right)$$

$$\frac{1}{1-k^2} = \frac{1}{2}\left(\frac{1}{1+k} + \frac{1}{1-k}\right)$$

$$\frac{1}{1-(2k+1)^2} = \frac{1}{2}\left(\frac{1}{1+k+1} + \frac{1}{1-k-1}\right)$$

$$\frac{1}{1-(2r+1)^2} \qquad \frac{1}{1-(2r+3)^2}$$

$$\frac{1}{2}\left(\frac{1}{1-(2r+1)} + \frac{1}{1+(2r+1)}\right)$$

$$\frac{1}{2}\left(\frac{1}{1-(2r+3)} + \frac{1}{1+(2r+3)}\right)$$

.... Finally only $\frac{1}{2}\left(\frac{1}{1-3}\right) = -\frac{1}{4}$ survives

$$\therefore E_1^{(2)} = \frac{8m\alpha^2}{\pi^2\hbar^2}\left(-\frac{1}{4}\right) = -\frac{2m\alpha^2}{\pi^2\hbar^2}$$

Check validity of pert scheme:

Need $\frac{V_{ij}}{E_i^{(0)} - E_j^{(0)}} < 1 \sim \frac{\alpha \times L}{\frac{\pi^2\hbar^2}{2mL^2}} \sim \frac{\alpha L m}{\pi^2\hbar^2}$

Thus (αL) is a suitable expansion param.

CDEEP
IIT Bombay

PH 422 L 12 / Slide 5

Note about H.O. related problems:

Use $x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^{\dagger})$

$p = \frac{1}{i}\sqrt{\frac{m\hbar\omega}{2}}\,(a - a^{\dagger})$

with $[a, a^{\dagger}] = 1$ $\quad \because [x, p] = i\hbar$

$N = a^{\dagger}a$ $\quad N|n\rangle = n|n\rangle$ ... eigenstates & eigenvalues of N

$E_n = (n + \frac{1}{2})\hbar\omega$

$a^{\dagger}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$a|n\rangle = \sqrt{n}\,|n-1\rangle$

Examples (contd.)

Stark effect

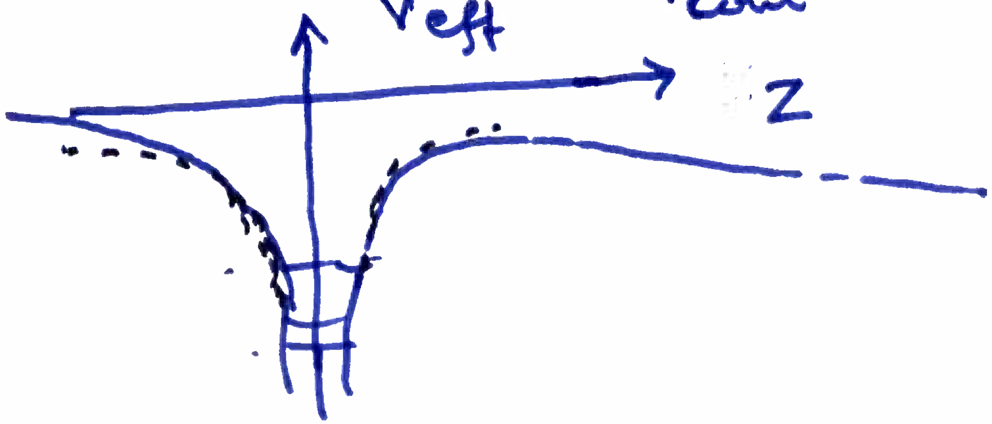
H atom in an ext $\vec{E}$ field

$$H = H_0 + \lambda V$$

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \quad ; \quad \lambda V = (-e)|\vec{E}|z$$

for $\vec{E} = |\vec{E}|\,\hat{k}$

Note $V_{eff} = V_{coul} + \lambda V_{pert}$



$$E_n^{(1)} = \langle \psi_n^{(0)} | z | \psi_n^{(0)} \rangle$$
$$= 0$$

Lecture 13

Note that atomic states $|\psi_n^{(0)}\rangle$ are eigenstates of parity.

This is because $\mathcal{P}\vec{x}\mathcal{P}^\dagger = -\vec{x}$ & $\mathcal{P}\vec{p}\mathcal{P}^\dagger = -\vec{p}$

but H_0 involves only $|\vec{p}|^2$ & $1/|\vec{x}| \equiv 1/r$

Thus $[H_0, \mathcal{P}] = 0$ or $\mathcal{P} H_0 \mathcal{P}^\dagger = H_0$

Thus $|\psi_n^{(0)}\rangle$ are also eigenstates of $\mathcal{P}$.