4/1/5 Assignment 8 2-/3- NINAD JOG PHYS 402

$\boxed{1.}$ Particle of mass m in an infinite square well between $x=0$ and $x=L$ with a perturbation $\hat{H}' = a\delta(x - L/4)$

a) Find: $E_n^{(1)}$. The energy eigenvalues and eigenstates for the unperturbed system are: $E_n^{(0)} = \left(\frac{\pi^2\hbar^2}{2mL^2}\right)n^2$, $\phi_n^{(0)}(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

$$E_n^{(1)} = \langle n|H'|n\rangle = \frac{2a}{L}\int_0^L \sin^2\left(\frac{n\pi x}{L}\right)\delta(x - L/4)\,dx = \boxed{\frac{2a}{L}\sin^2\left(\frac{n\pi}{L}\right)}$$

i.e. $$E_n^{(1)} = \begin{cases} a/L & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is a multiple of } 4 \\ \frac{2a}{L} & \text{otherwise} \end{cases}$$

b) Second order shift in energy: $E_n^{(2)} = \sum_{k\neq n} \frac{|\langle k|H'|n\rangle|^2}{E_n^{(0)} - E_k^{(0)}}$

$$= \frac{\left(\frac{2a}{L}\right)^2 \sum_{k\neq n}\left|\int_0^L \sin\left(\frac{k\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)\delta(x - L/4)\,dx\right|^2}{\left(\frac{\pi^2\hbar^2}{2mL^2}\right)(k^2 - n^2)} = \boxed{\frac{8ma^2}{\pi^2\hbar^2}\sum_{k\neq n}\frac{\left(\sin\left(\frac{k\pi}{4}\right)\sin\left(\ldots\right)\right.}{k^2 - n^2}}$$

For the ground state, $n = 1$.

$$E_1^{(2)} = \frac{4ma^2}{\pi^2\hbar^2}\sum_{k\neq 1}\frac{\sin^2(k\pi/4)}{k^2 - 1} = \frac{4ma^2}{\pi^2\hbar^2}\left[\underbrace{\frac{1}{2^2-1}}_{k=2} + \underbrace{\frac{1}{2.(3^2-1)}}_{k=3} + \underbrace{\frac{1}{2(5^2-1)}}_{k=5} + \underbrace{\frac{1}{6^2-1}}_{k=6} + \ldots\right.$$

$$E_1^{(2)} = \frac{4ma^2}{\pi^2\hbar^2}\Big[\underbrace{\underset{k=2}{\frac{1}{3}} + \underset{k=3}{\frac{1}{16}} + \underset{k=5}{\frac{1}{48}} + \underset{k=6}{\frac{1}{35}} + \underset{k=7}{\frac{1}{96}} + \underset{k=9}{\frac{1}{160}} + \underset{k=10}{\frac{1}{99}} + \cdots}_{0.472}\Big]$$

$$\therefore \boxed{E_1^{(2)} = \frac{1.888\, ma^2}{\pi^2\hbar^2}}$$

c) What is the condition to be considered small, in terms of a, m, L and $\hbar$?

$$E_1 = E_1^{(0)} + E_1^{(1)} + E_1^{(2)} = \frac{\pi^2\hbar^2}{2mL^2} + \frac{a}{L} + \frac{1.89\, ma^2}{\pi^2\hbar^2}.$$

This is valid when $\frac{a}{L} \ll \frac{\pi^2\hbar^2}{2mL^2}$ i.e. when $\boxed{a \ll \frac{\pi^2\hbar^2}{2mL}}$

2.

a) $\hat{H} = \frac{A \hat{S}_1 \cdot \hat{S}_2}{\hbar^2}$

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$|1,1\rangle$
$|1,0\rangle$
$|1,-1\rangle$
$|0,0\rangle$

possible states

$$\hat{H}|1,1\rangle = \frac{A}{\hbar^2}\left(\frac{\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2}{2}\right)|1,1\rangle$$

$$= \frac{A}{2\hbar^2}\left(\hbar^2(1+1)(1) - 3/2\hbar^2\right)|1,1\rangle$$

$$= \frac{A}{4}|1,1\rangle$$

$$\hat{H}|1,0\rangle = \frac{A}{4}|1,0\rangle$$

$$\hat{H}|1,-1\rangle = \frac{A}{4}|1,0\rangle$$

$$\hat{H}|0,0\rangle = \frac{A}{\hbar^2}\left(\frac{\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2}{2}\right)|0,0\rangle$$

$$= \frac{A}{2\hbar^2}\left(0\hbar^2 - 3/2\hbar^2\right)|0,0\rangle$$

$$= -\frac{3A}{4}|0,0\rangle$$

unperturbed state vectors

$|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$ have energy $\frac{A}{4}$ — $|0,0\rangle$ has energy $\frac{-3A}{4}$

$E_1^{(0)} = E_{1,1}^{(0)} = E_{1,-1}^{(0)} = E_{1,0}^{(0)}$ $\qquad$ $E_0^{(0)}$

b) $E_0^{(1)} = \langle 0,0| \frac{B}{\hbar} \hat{S}_{1z} |0,0\rangle$

$$|0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$E_0^{(1)} = \frac{1}{2}(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|)\frac{B}{\hbar}\hat{S}_{1z}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

$$= \frac{B}{2\hbar}(\langle\uparrow\downarrow|\hat{S}_{1z}|\uparrow\downarrow\rangle + \langle\downarrow\uparrow|\hat{S}_{1z}|\downarrow\uparrow\rangle)$$

$$= \frac{B}{2\hbar}\left(\frac{\hbar}{2} - \frac{\hbar}{2}\right) = 0$$

$$\begin{pmatrix} ①\ \langle 1,1|\hat{H}'|1,1\rangle & \langle 1,0|\hat{H}'|1,1\rangle & \langle 1,-1|\hat{H}'|1,1\rangle \\ \langle 1,1|\hat{H}'|1,0\rangle & ②\ \langle 1,0|\hat{H}'|1,0\rangle & \langle 1,-1|\hat{H}'|1,0\rangle \\ \langle 1,1|\hat{H}'|1,-1\rangle & \langle 1,0|\hat{H}'|1,-1\rangle & ③\ \langle 1,-1|\hat{H}|1,-1\rangle \end{pmatrix}$$

$$|1,1\rangle \longleftrightarrow |\uparrow\uparrow\rangle$$
$$|1,-1\rangle \longleftrightarrow |\downarrow\downarrow\rangle$$
$$|1,0\rangle \longleftrightarrow \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

due to orthogonality, only the diagonal matrix elements are nonzero

① $\frac{B}{\hbar}\langle\uparrow\uparrow|\hat{S}_{1z}|\uparrow\uparrow\rangle = \frac{B}{2}$

② $\frac{B}{2\hbar}(\langle\uparrow\downarrow| + \langle\downarrow\uparrow|)\hat{S}_{1z}(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) =$

$\frac{B}{2\hbar}(\langle\uparrow\downarrow|\hat{S}_{1z}|\downarrow\uparrow\rangle + \langle\downarrow\uparrow|\hat{S}_{1z}|\uparrow\downarrow\rangle) = 0$

③ $\frac{B}{\hbar} \langle \downarrow\downarrow | \hat{S}_{1z} | \downarrow\downarrow \rangle = \frac{-B}{2}$

$$\begin{pmatrix} B/2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -B/2 \end{pmatrix}$$

$$E_{1,1}^{(1)} = \frac{B}{2}$$
$$E_{1,0}^{(1)} = 0$$
$$E_{1,-1}^{(1)} = \frac{-B}{2}$$

in sum:

$$E_{1,1} = \frac{A}{4} + \frac{B}{2} + O(B^2)$$

$$E_{1,0} = \frac{A}{4} + O(B^2)$$

$$E_{1,-1} = \frac{A}{4} - \frac{B}{2} + O(B^2)$$

$$E_0 = -\frac{3A}{4} + O(B^2)$$

c)

$$E_0^{(2)} = \sum_{(n,j)\neq(0,0)} \frac{|\langle n,j | \hat{H}' | 0,0 \rangle|^2}{E_0 - E_{n,j}} = \frac{|\langle 1,0 | \hat{H}' | 0,0 \rangle|^2}{E_0 - E_{1,0}}$$

only non vanishing term

$$E_0^{(2)} = \frac{\left| \frac{B}{2\hbar}\left(\langle \uparrow\downarrow | + \langle \downarrow\uparrow | \right) \hat{S}_{1z} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \right|^2}{\left(-\frac{3A}{4} - \frac{A}{4} \right)}$$

$$= \frac{-\left(\frac{B}{2}\right)^2}{A} = \frac{-B^2}{4A}$$

$$E_{1,1}^{(2)} = \sum_{(n,j)\neq(1,1)} \frac{|\langle n,j|\hat{H}'|1,1\rangle|^2}{E_{1,1} - E_{nj}} = 0$$

likewise

$$E_{1,-1}^{(2)} = 0$$

$$E_{1,0}^{(2)} = \sum_{(n,j)\neq(1,0)} \frac{|\langle n,j|\hat{H}'|1,0\rangle|^2}{E_{1,0} - E_{nj}} = \frac{|\langle 0,0|\hat{H}'|1,0\rangle|^2}{E_{10} - E_0}$$

$$= \frac{\left(\frac{B}{2}\right)^2}{\left(\frac{A}{4} + \frac{3A}{4}\right)}$$

$$= \frac{B^2}{4A}$$

$$\boxed{\begin{aligned} E_0 &= -\frac{3A}{4} - \frac{B^2}{4A} + O(B^3) \\ E_{1,1} &= \frac{A}{4} + \frac{B}{2} + O(B^3) \\ E_{1,0} &= \frac{A}{4} + \frac{B^2}{4A} + O(B^3) \\ E_{1,-1} &= \frac{A}{4} - \frac{B}{2} + O(B^3) \end{aligned}}$$

3. Particle in a 2-D box: $V = \begin{cases} 0 & \text{for } 0<x<L \text{ and } 0<y<L \\ \infty & \text{otherwise} \end{cases}$

a) The eigenenergies are $\boxed{E_{nk}^{(0)} = \dfrac{\pi^2\hbar^2}{2mL^2}(n^2+k^2)}$, since the x & y directions are independent.

and the eigenvalues are: $\psi_{nk}^{(0)}(x,y) = \dfrac{2}{L}\sin\left(\dfrac{n\pi x}{L}\right)\sin\left(\dfrac{k\pi y}{L}\right)$, $n = 1,2,3,\ldots$, $k = 1,2,3\ldots$

The first excited state is doubly degenerate since it can be formed with $n=1$ and $k=2$ OR $n=2$ and $k=1$.

b) Perturbation: $\hat{H}' = a\cos\left(\dfrac{\pi x}{L}\right)\cos\left(\dfrac{\pi y}{L}\right)$

Let $|\alpha\rangle = |n=1, k=2\rangle = \dfrac{2}{L}\sin\left(\dfrac{\pi x}{L}\right)\sin\left(\dfrac{2\pi y}{L}\right)$

$|\beta\rangle = |n=2, k=1\rangle = \dfrac{2}{L}\sin\left(\dfrac{2\pi x}{L}\right)\sin\left(\dfrac{\pi y}{L}\right)$

Find: $H' = \begin{pmatrix} \langle\alpha|H'|\alpha\rangle & \langle\alpha|H'|\beta\rangle \\ \langle\beta|H'|\alpha\rangle & \langle\beta|H'|\beta\rangle \end{pmatrix}$

$$\langle\alpha|H'|\alpha\rangle = \frac{4a}{L^2}\int_0^L\int_0^L \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{2\pi y}{L}\right)\cos\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi y}{L}\right)dy\,dx$$

Let $\dfrac{\pi x}{L} = u$, $\dfrac{\pi y}{L} = v$ $\Rightarrow \langle\alpha|H'|\alpha\rangle = \dfrac{4a}{\pi^2}\displaystyle\int_0^\pi \sin^2 u\cos u\,du \int_0^\pi \sin^2 2v\cos v\,dv$

$\displaystyle\int_0^\pi \sin^2 u\cos u\,du = \int_0^0 t^2\,dt = 0$ ($\sin u = t$) $\Rightarrow \boxed{\langle\alpha|H'|\alpha\rangle = 0}$,

Similarly, $\boxed{\langle\beta|H'|\beta\rangle = 0}$

$$\langle\alpha|H'|\beta\rangle = \frac{4a}{\pi^2}\int_0^\pi du\,\sin u\sin 2u\cos u\int_0^\pi \sin v\sin 2v\cos v\,dv = \frac{4a}{\pi^2}\left[\frac{1}{2}\int_0^\pi \sin^2 2u\,du\right]^2$$

$$= \frac{a}{4\pi^2}\left(\int_0^{2\pi}\sin^2 t\,dt\right)^2 = \frac{a}{4\pi^2}\cdot\pi^2 = \frac{a}{4} \Rightarrow \boxed{H' = \frac{a}{4}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} = \begin{pmatrix} W_{\alpha\alpha} & W_{\alpha\beta} \\ W_{\beta\alpha} & W_{\beta\beta} \end{pmatrix}$$

This is the pauli sigma matrix, so its eigenstates and eigenvalues are:

$|\psi_+\rangle = \dfrac{1}{\sqrt{2}}(|\alpha\rangle + |\beta\rangle)$ and $|\psi_-\rangle = \dfrac{1}{\sqrt{2}}(|\alpha\rangle - |\beta\rangle)$, $E_\pm = \pm\dfrac{a}{4}$

The first order correction is:

$$E_\pm^{(1)} = \frac{1}{2}\left[W_{\alpha\alpha} + W_{\beta\beta} \pm \sqrt{(W_{\alpha\alpha} - W_{\beta\beta})^2 + 4|W_{\alpha\beta}|^2}\right]$$

$$E_\pm^{(1)} = \pm\frac{a}{8}\cdot 2\cdot 1 = \boxed{\pm\frac{a}{4}}$$