QM II
Phys 652

Solution of HW #8

Problem #1

Consider Lecture #20, p.3:

$$(H_0 - E_n^{(0)})|n^{(2)}\rangle = (E_n^{(1)} - V)|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle$$

multiply by $\langle k^{(0)}|$ $\Rightarrow$ $(k \neq n)$

$$\langle k^{(0)}|H_0 - E_n^{(0)}|n^{(2)}\rangle = E_n^{(1)}\langle k^{(0)}|n^{(1)}\rangle -$$

$$- \langle k^{(0)}|V|n^{(1)}\rangle + E_n^{(2)}\underbrace{\langle k^{(0)}|n^{(0)}\rangle}_{=0 \text{ (since } k\neq n)}$$

$\Downarrow$

$$(E_k^{(0)} - E_n^{(0)})\langle k^{(0)}|n^{(2)}\rangle = E_n^{(1)}\underbrace{\langle k^{(0)}|n^{(1)}\rangle}_{= \text{Eq. (23.3)}\ \frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}} -$$

$$- \langle k^{(0)}|V\underbrace{|n^{(1)}\rangle}_{= \leftarrow \text{Lect \#20 p.6}\ \sum_{k'\neq n} \frac{\langle k'^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)} - E_{k'}^{(0)}}|k'^{(0)}\rangle};$$

So,

$$\langle k^{(0)}|n^{(2)}\rangle = \frac{\overbrace{E_n^{(1)}}^{=V_{nn}}}{E_k^{(0)}-E_n^{(0)}}\;\frac{\langle k^{(0)}|V|n^{(0)}\rangle}{E_n^{(0)}-E_k^{(0)}} -$$

$$-\frac{1}{E_k^{(0)}-E_n^{(0)}}\sum_{k'\neq n}\frac{\overbrace{\langle k'^{(0)}|V|n^{(0)}\rangle}^{=V_{k'n}}}{E_n^{(0)}-E_{k'}^{(0)}}\;\underbrace{\langle k^{(0)}|V|k'^{(0)}\rangle}_{=V_{kk'}} =$$

$$= \frac{V_{nn}V_{kn}}{-(E_n^{(0)}-E_k^{(0)})^2} + \frac{1}{E_n^{(0)}-E_k^{(0)}}\sum_{k'\neq n}\frac{V_{k'n}V_{kk'}}{E_n^{(0)}-E_{k'}^{(0)}}$$

$$|n^{(2)}\rangle = \underbrace{\sum_k |k^{(0)}\rangle\langle k^{(0)}|}_{I}n^{(2)}\rangle =$$

$$= \sum_{\substack{k,k'\\ \neq n}}\frac{V_{k'n}V_{kk'}\,|k^{(0)}\rangle}{(E_n^{(0)}-E_{k'}^{(0)})(E_n^{(0)}-E_k^{(0)})} - \sum_{k\neq n}\frac{V_{nn}V_{kn}\,|k^{(0)}\rangle}{(E_n^{(0)}-E_k^{(0)})^2} -$$

if you use $\langle n^{(0)}|n\rangle = 0$ convention

$$-\frac{1}{2}|n^{(0)}\rangle\underbrace{\langle n^{(1)}|n^{(1)}\rangle}_{=\sum_{k\neq n}\frac{|V_{kn}|^2}{(E_n^{(0)}-E_k^{(0)})^2}|n^{(0)}\rangle}$$

if you use $\langle n^{(0)}|n^{(2)}\rangle = -\frac{1}{2}\langle n^{(1)}|n^{(1)}\rangle$ from convention $\langle n|n\rangle = 1$, there is this extra term!

Solutions of HW #1 (ctd)

QM II Phys 652

Problem #1

2D harmonic oscillator $\Rightarrow$

$$\underbrace{H_0}_{= H_{0x} + H_{0y}} = \frac{P_x^2 + P_y^2}{2m} + \frac{K(x^2+y^2)}{2} \quad ; \quad V = \alpha x y$$

$$\Psi^{(0)} = \Psi_x(x)\Psi_y(y)$$

$\Psi^{(0)}$: unperturbed

$$E^{(0)}_{n_x, n_y} = \hbar\omega_0 (n_x + n_y + 1), \quad \omega_0 = \sqrt{\frac{K}{m}}$$

recall Phys 651

The lowest energy level $\Rightarrow$ $n_x = n_y = 0 \Rightarrow E_{0,0} = \hbar\omega_0$;

non-degenerate

Higher levels: $\left.\begin{array}{l} n_x = 1, n_y = 0 \\ n_x = 0, n_y = 1 \end{array}\right] \Rightarrow E_{0,1} = E_{1,0} = 2\hbar\omega_0$

double-degenerate

$\left.\begin{array}{l} n_x = 1, n_y = 1 \\ n_x = 2, n_y = 0 \\ n_x = 0, n_y = 2 \end{array}\right] \Rightarrow E_{1,1} = E_{2,0} = E_{0,2} = 3\hbar\omega_0$

triple-degenerate

⋮

so on

Take the lowest degenerate level $\Rightarrow E_{1,0} = E_{0,1}$

$\Downarrow$

need to compose a 2×2 matrix $\hat{V}$;

choose the basis $\{|n_x, n_y\rangle\} = \overset{①}{|\underset{n_x}{1}, \underset{n_y}{0}\rangle}, \overset{②}{|0,1\rangle}$

$\hat{V}_{11} = \langle 1,0|V|1,0\rangle$

$\hat{V}_{12} = \langle 1,0|V|0,1\rangle$

$\hat{V}_{21} = \langle 0,1|V|1,0\rangle$

$\hat{V}_{22} = \langle 0,1|V|0,1\rangle$

$V = \alpha x y$

$x = \sqrt{\frac{\hbar}{m\omega_0}} \frac{\sqrt{2}}{2} (a + a^+)$

$y = \sqrt{\frac{\hbar}{m\omega_0}} \frac{\sqrt{2}}{2} (b + b^+)$

x acting on $\mathcal{E}_x$, $y \Rightarrow$ on $\mathcal{E}_y$

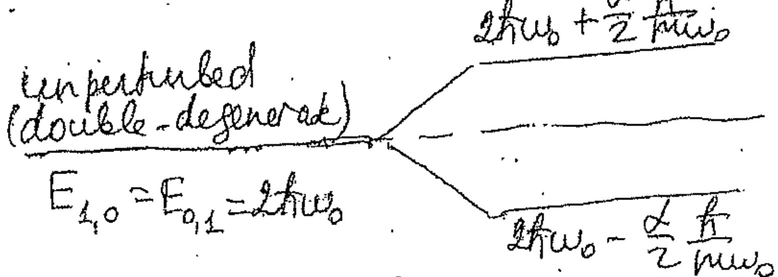
$$V_{11} = \langle \overset{n_x}{1}, \overset{n_y}{0} | \alpha x y | \overset{n_x}{1}, \overset{n_y}{0} \rangle \overset{\alpha}{=} \alpha \langle 1|x|1\rangle \cdot \langle 0|y|0\rangle = \alpha \frac{\hbar}{m\omega_0} \frac{1}{2} \langle 1|a + a^+|1\rangle \cdot \langle 0|b + b^+|0\rangle = 0 = V_{22}$$

$$V_{12} = \alpha \frac{\hbar}{m\omega_0} \frac{1}{2} \langle 1|\underbrace{a}_{0} + \underbrace{a^+|0\rangle}_{|1\rangle} \langle 0|\underbrace{b}_{|0\rangle} + \underbrace{b^+|1\rangle}_{0} =$$

$$= \frac{\alpha}{2} \frac{\hbar}{m\omega_0} = V_{21}$$

So, $\hat{V}^{(n=n_x+n_y=1)} = \begin{pmatrix} 0 & \frac{\alpha}{2}\frac{\hbar}{m\omega_0} \\ \frac{\alpha}{2}\frac{\hbar}{m\omega_0} & 0 \end{pmatrix}$

$$\det\begin{pmatrix} -E^{(1)}_{n=1} & \frac{\alpha}{2}\frac{\hbar}{m\omega_0} \\ \frac{\alpha}{2}\frac{\hbar}{m\omega_0} & -E^{(1)}_{n=1} \end{pmatrix} = 0 \Rightarrow E^{(1)}_{n=1} = \pm\frac{\alpha}{2}\frac{\hbar}{m\omega_0}$$



$\frac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle)$

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

eigenvectors

$\Rightarrow$ $V = \alpha xy$ removes degeneracy

Problem

$$S_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad S_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix};$$

$$S_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

(a) $H = AS_z^2 + B(S_x^2 - S_y^2) \Rightarrow$

$$S_z^2 = \hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad S_x^2 - S_y^2 = \hbar^2\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ \cdot & \cdot & \cdot \end{pmatrix}$$

$$H = \hbar^2 \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ B & 0 & A \end{pmatrix}$$

<u>Eigenvalues:</u> $\det \begin{bmatrix} \hbar^2 A - \lambda & 0 & \hbar^2 B \\ 0 & -\lambda & 0 \\ \hbar^2 B & 0 & \hbar^2 A - \lambda \end{bmatrix} \doteq 0$

$\Downarrow$

1) $\lambda_1 = 0$

2) $\lambda_{2,3} = A\hbar^2 \pm B\hbar^2$

<u>Eigenvectors:</u>

1) $\lambda_1 = 0$: $|\lambda_1 = 0\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

2) $\lambda_2 = A\hbar^2 + B\hbar^2 \Rightarrow$

$$|\lambda_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

3) $\lambda_3 = A\hbar^2 - B\hbar^2 \Rightarrow$

$$|\lambda_3\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

$\Downarrow$

Energy diagram

$\leftarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{2}} \left(|\underset{S}{1}, \underset{m_s}{1}\rangle + |1, -1\rangle \right)$

$B\hbar^2$ } - - - - - $A\hbar^2$

$B\hbar^2$ }

$\leftarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{2}} \left(|1, 1\rangle - |1, -1\rangle \right)$

$E = 0 \Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \Rightarrow |1, 0\rangle$

(b) $H = \underbrace{H_0}_{= AS_z^2} + \underbrace{V}_{= B(S_x^2 - S_y^2)}$

(i)

$$H_0 |s, m_s\rangle = A S_z^2 |s, m_s\rangle = \underbrace{A\hbar^2 m_s^2}_{= E^{(0)}} |s, m_s\rangle$$

$E^{(0)}$ ← unperturbed

Since it's a spin-1 particle

⇓

$m_s = 0, \pm 1$ ⇒ have a non-degenerate level $E^{(0)}_{m_s=0} = 0$ and a double-degenerate level $E^{(0)}_{m_s=\pm 1} = A\hbar^2$

(ii) $E^{(1)}_{m_s=0} = \langle \underset{s}{1}, \underset{m_s}{0} | V | 1, 0\rangle =$

$= B \langle 1, 0 | S_x^2 - S_y^2 | 1, 0 \rangle = B(\langle S_x^2\rangle - \langle S_y^2\rangle)$

$= 0$ (recall Worksheet #3)

(iii) Double-degenerate level $E^{(0)}_{m_s=\pm 1} = A\hbar^2$

⇓

compose 2x2 matrix ⇩

Choose the basis: $\overset{①}{|\underset{s}{1}, \underset{m_s}{1}\rangle}$; $\overset{②}{|\underset{s}{1}, \underset{m_s}{-1}\rangle}$

Then, $V_{11} = \langle 1,1 | B(S_x^2 - S_y^2) | 1,1 \rangle \underset{\text{see (ii)}}{=} 0 = V_{22}$

$V_{12} = \langle 1,1 | B(S_x^2 - S_y^2) | 1,-1 \rangle = \frac{B}{2} \langle 1,1 | S_+^2 | 1,-1 \rangle$

$$S_x^2 - S_y^2 = \left(\frac{S_+ + S_-}{2}\right)^2 - \left(\frac{S_+ - S_-}{2i}\right)^2 = \frac{S_+^2 + S_-^2}{2}$$

$- \frac{B}{2} \overbrace{\langle 1,1 | S_-^2 | 1,-1 \rangle}^{0} = \frac{B}{2} \langle 1,1 | S_+ S_+ | 1,-1 \rangle =$

$= \frac{B}{2} \cdot \hbar \sqrt{1 \cdot 2 + 1 \cdot 0} \langle 1,1 | S_+ | 1,0 \rangle = B\hbar^2 = V_{21}$

$S_+ |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s+1)} \, |s, m_s + 1\rangle$

So, $\hat{V} = \begin{pmatrix} 0 & B\hbar^2 \\ B\hbar^2 & 0 \end{pmatrix}$

Find $E^{(1)}_{m_s = \pm 1} \Rightarrow \det \begin{bmatrix} -E^{(1)} & B\hbar^2 \\ B\hbar^2 & -E^{(1)} \end{bmatrix} = 0 \Rightarrow$

$$E^{(1)}_{m_s = \pm 1} = \pm B\hbar^2$$

Eigenstates: $E^{(1)}_{m_s=1} = B\hbar^2 \Rightarrow \begin{bmatrix} -B\hbar^2 & B\hbar^2 \\ B\hbar^2 & -B\hbar^2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0$

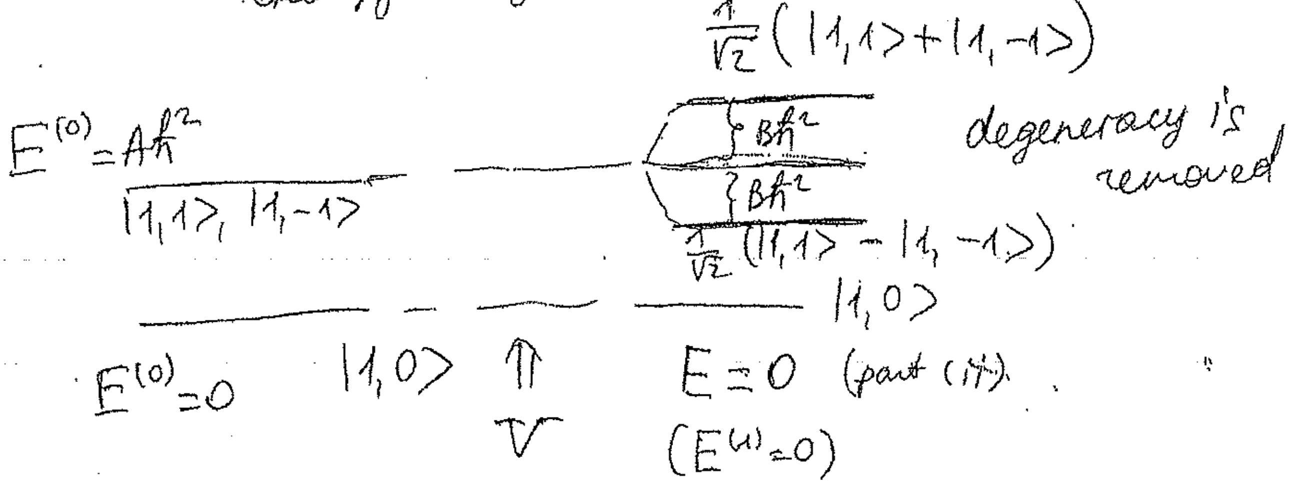
$$\Downarrow$$

$$\underline{\frac{1}{\sqrt{2}}\left(|1,1\rangle + |1,-1\rangle\right)}$$

$E^{(1)}_{m_s=-1} = -B\hbar^2 \Rightarrow \underline{\frac{1}{\sqrt{2}}\left(|1,1\rangle - |1,-1\rangle\right)}$

$\Downarrow$

energy diagram



(iv) Perturbation theory yielded exactly the same result as in the case of the exact solution