HW #6 solutions

(1) degenerate perturbation theory (1st-order)

(a) doubly-degenerate:

$$\begin{vmatrix} H_{11}^{(1)} - E^{(1)} & H_{12}^{(1)} \\ H_{12}^{(1)} & H_{22}^{(1)} - E^{(1)} \end{vmatrix} = 0$$

but $H_{11}^{(1)} = 4b$, $H_{12}^{(1)} = 2b$, $H_{22}^{(1)} = 6b$

$$\begin{vmatrix} 4b - E^{(1)} & 2b \\ 2b & 6b - E^{(1)} \end{vmatrix} = 0$$

expanding:

$$(4b - E^{(1)})(6b - E^{(1)}) - 4b^2 = 0$$

$$E^{(1)2} - 10b\,E^{(1)} + 20b^2 = 0$$

from quadratic eqn: $E^{(1)} = (5 \pm \sqrt{5})\,b$

(b) for the ground state $E^{(1)} = (5-\sqrt{5})b$

inserting into secular eqn:

$$\left[4b-(5-\sqrt{5})b\right]c_1 + 2b\,c_2 = 0$$

$$b(\sqrt{5}-1)c_1 + 2b\,c_2 = 0$$

$$c_1 = \frac{2}{1-\sqrt{5}}\,c_2$$

for the excited state $E^{(1)} = (5+\sqrt{5})b$

$$\left[4b-(5+\sqrt{5})b\right]c_1 + 2b\,c_2 = 0$$

$$c_1 = \frac{2}{1+\sqrt{5}}\,c_2$$

in each case, $c_1^2 + c_2^2 = 1$ since the basis is orthonormal

ground state: $\frac{4}{1.5279}c_2^2 + c_2^2 = 1$

so $c_2 = \cancel{0.2764}\ 0.526$ oops, forgot $\sqrt{\ }$

$\therefore\ c_1 = \cancel{-0.4472}\ -0.851$

$$\psi_1 = -0.\overset{851}{\cancel{4472}}\,\psi_1^{(0)} + 0.\overset{526}{\cancel{2764}}\,\psi_2^{(0)}$$

for the excited state:

$$\frac{4}{10.472} c_2^2 + c_2^2 = 1$$

$$c_2 = 0.851$$

$$c_1 = 0.526$$

$$\psi = 0.526\,\psi_1^{(0)} + 0.851\,\psi_2^{(0)}$$

(1) Consider:

$\alpha(1)\alpha(2)$

$\alpha(1)\beta(2)$

$\beta(1)\alpha(2)$

$\beta(1)\beta(2)$

(a)

$$S_z = s_z(1) + s_z(2)$$

$$S_z\alpha(1)\alpha(2) = \left(s_z(1) + s_z(2)\right)\alpha(1)\alpha(2)$$

$$= \tfrac{1}{2}\hbar\alpha(1)\alpha(2) + \tfrac{1}{2}\hbar\alpha(1)\alpha(2) = \hbar\alpha(1)\alpha(2)$$

$$S_z\alpha(1)\beta(2) = \tfrac{1}{2}\hbar\alpha(1)\beta(2) + \left(-\tfrac{1}{2}\hbar\right)\alpha(1)\beta(2) = 0$$

$$S_z\beta(1)\alpha(2) = -\tfrac{1}{2}\hbar\beta(1)\alpha(2) + \tfrac{1}{2}\hbar\beta(1)\alpha(2) = 0$$

$$S_z\beta(1)\beta(2) = -\tfrac{1}{2}\hbar\beta(1)\beta(2) - \tfrac{1}{2}\hbar\beta(1)\beta(2) = -\hbar\beta(1)\beta(2)$$

$\Rightarrow$ all eigenfunctions of S_z w/ eigenvalues $\hbar, 0, 0, -\hbar$

$$S^2(1,2) = s^2(1) + s^2(2) + s_-(1)s_+(2) + s_+(1)s_-(2) + 2s_z(1)s_z(2)$$

$$S^2\alpha(1)\alpha(2) = s^2(1)\alpha(1)\alpha(2) + s^2(2)\alpha(1)\alpha(2) + s_-(1)s_+(2)\alpha(1)\alpha(2)$$

$$+ s_+(1)s_-(2)\alpha(1)\alpha(2) + 2s_z(1)s_z(2)\alpha(1)\alpha(2)$$

$$= \tfrac{1}{2}\left(\tfrac{1}{2}+1\right)\hbar^2\alpha(1)\alpha(2) + \tfrac{3}{4}\hbar^2\alpha(1)\alpha(2) + 0$$

$$+ 0 + 2\left(\tfrac{1}{2}\hbar\right)\left(\tfrac{1}{2}\hbar\right)\alpha(1)\alpha(2)$$

$$= 2\hbar^2\alpha(1)\alpha(2)$$

$\therefore$ $\alpha(1)\alpha(2)$ is an eigenfunction w/ $S=1$

eigenvalue $= 2\hbar^2$

likewise,

$$S^2 \beta(1)\beta(2) = \frac{3}{4}\hbar^2 \beta(1)\beta(2) + \frac{3}{4}\hbar^2 \beta(1)\beta(2) + 0 + 0$$
$$+ 2\left(-\tfrac{1}{2}\hbar\right)\left(-\tfrac{1}{2}\hbar\right)\beta(1)\beta(2)$$
$$= 2\hbar^2 \beta(1)\beta(2)$$

✓ eigenfunction, $S = 1$
eigenvalue $= 2\hbar^2$

$$S^2 \alpha(1)\beta(2) = \frac{3}{4}\hbar^2 \alpha(1)\beta(2) + \frac{3}{4}\hbar^2 \alpha(1)\beta(2)$$
$$+ (\hbar)(\hbar)\beta(1)\alpha(2) + 0 + 2\left(\tfrac{1}{2}\hbar\right)\left(-\tfrac{1}{2}\hbar\right)\alpha(1)\beta(2)$$
$$= \hbar^2 \alpha(1)\beta(2) + \hbar^2 \beta(1)\alpha(2)$$

$\Rightarrow$ not an eigenfunction

$$S^2 \beta(1)\alpha(2) = \frac{3}{4}\hbar^2 \beta(1)\alpha(2) + \frac{3}{4}\hbar^2 \beta(1)\alpha(2) + 0$$
$$+ (\hbar)(\hbar)\alpha(1)\beta(2) + 2\left(-\tfrac{1}{2}\hbar\right)\left(\tfrac{1}{2}\hbar\right)\beta(1)\alpha(2)$$
$$= \hbar^2 \beta(1)\alpha(2) + \hbar^2 \alpha(1)\beta(2)$$

$\Rightarrow$ not an eigenfunction

(b) $$S^2\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] = \hbar^2\left[\alpha(1)\beta(2) + \beta(1)\alpha(2) + \beta(1)\alpha(2) + \alpha(1)\beta(2)\right]$$

(using results from part a)

$$= 2\hbar^2\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right]$$

$\Rightarrow$ eigenfunction w/ $S = 1$
eigenvalue $= 2\hbar^2$

$$S^2\left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right] = 0$$

Sz gives zero in both cases

$\Rightarrow$ eigenfunction w/ $S = 0$
eigenvalue $= 0\hbar^2$

(2)

obtain $\Theta_{1,0}$ from $\Theta_{1,-1}$

$\Theta_{1,0} = |1,0\rangle$ where $S=1, m_s=0$

$\Theta_{1,-1} = |1,-1\rangle$ $S=1, m_s=-1$

$$S_+|1,-1\rangle = \hbar\sqrt{1(1+1)-(-1)(-1+1)}\,|1,0\rangle = \sqrt{2}\,\hbar\,\Theta_{1,0}$$

$$|1,-1\rangle = \left|\tfrac{1}{2},-\tfrac{1}{2};\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = \left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle$$ where $s(1)=\frac{1}{2}$ $s(2)=\frac{1}{2}$ $m_s(1)=-\frac{1}{2}$ $m_s(2)=-\frac{1}{2}$

$$\left(s_+(1)+s_+(2)\right)\left|-\tfrac{1}{2},-\tfrac{1}{2}\right\rangle = \hbar\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)-\left(-\tfrac{1}{2}\right)\left(-\tfrac{1}{2}+1\right)}\,\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle$$
$$+\hbar\sqrt{\tfrac{1}{2}\left(\tfrac{1}{2}+1\right)-\left(-\tfrac{1}{2}\right)\left(-\tfrac{1}{2}+1\right)}\,\left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle$$
$$=\hbar\left(\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle + \left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle\right)$$

$$\Rightarrow \quad \Theta_{10} = \frac{1}{\sqrt{2}}\left(\left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle + \left|-\tfrac{1}{2},\tfrac{1}{2}\right\rangle\right)$$
$$= \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)+\beta(1)\alpha(2)\right]$$

(b) $\Theta_{11} = \cancel{\alpha\beta} \; \alpha(1)\alpha(2)$

$\cancel{\beta}\, \Theta_{1,-1} = \beta(1)\beta(2)$

$\Theta_{10} = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right]$

let $\Theta_{00} = c_1\alpha(1)\alpha(2) + c_2\beta(1)\beta(2) + c_3\alpha(1)\beta(2) + c_4\beta(1)\alpha(2)$

using Schmidt orthogonalization:

$$\Theta_{00} = c_1\alpha(1)\alpha(2) + c_2\beta(1)\beta(2) + c_3\alpha(1)\beta(2) + c_4\beta(1)\alpha(2)$$
$$- \alpha(1)\alpha(2)\langle\alpha(1)\alpha(2)\,|\,c_1\alpha(1)\alpha(2) + c_2\beta(1)\beta(2) + \cdots\rangle$$
$$- \beta(1)\beta(2)\langle\beta(1)\beta(2)\,|\,c_1\alpha(1)\alpha(2) + c_2\beta(1)\beta(2) + \cdots\rangle$$
$$- \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right]\left\langle \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right] \,\middle|\, c_1\alpha(1)\alpha(2)\right.$$
$$\left. + c_2\beta(1)\beta(2) + c_3\alpha(1)\beta(2) + c_4\beta(1)\alpha(2)\right\rangle$$

remember: $\langle\alpha|\beta\rangle = 0$

$$\Theta_{00} = c_1\alpha(1)\alpha(2) + c_2\beta(1)\beta(2) + c_3\alpha(1)\beta(2) + c_4\beta(1)\alpha(2)$$
$$- \alpha(1)\alpha(2)\cdot c_1 \quad - \beta(1)\beta(2)\cdot c_2$$
$$- \frac{1}{2}\left[\alpha(1)\beta(2) + \beta(1)\alpha(2)\right](c_3 + c_4)$$

$$= c_3\alpha(1)\beta(2) + c_4\beta(1)\alpha(2) - \frac{1}{2}c_3\alpha(1)\beta(2) - \frac{1}{2}c_3\beta(1)\alpha(2)$$
$$- \frac{1}{2}c_4\alpha(1)\beta(2) - \frac{1}{2}c_4\beta(1)\alpha(2)$$

$$= \frac{1}{2}c_3\alpha(1)\beta(2) + \frac{1}{2}c_4\beta(1)\alpha(2) - \frac{1}{2}c_3\beta(1)\alpha(2) - \frac{1}{2}c_4\alpha(1)\beta(2)$$

$$\Theta_{00} = \frac{1}{2}\left[(c_3 - c_4)\alpha(1)\beta(2) - (c_3 - c_4)\beta(1)\alpha(2)\right]$$

$$= \frac{1}{2}C\left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right]$$

to normalize, $\left(\frac{1}{2}C\right)^2 = \frac{1}{2}$

$$\therefore \quad C = \sqrt{2}$$

$$\Theta_{00} = \frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right]$$