CB2070 Ex. 7

① a) $|\psi\rangle = \begin{pmatrix}\alpha_1\\ \beta_1\end{pmatrix}\otimes\begin{pmatrix}\alpha_2\\ \beta_2\end{pmatrix} = \begin{pmatrix}\alpha_1\alpha_2\\ \alpha_1\beta_2\\ \beta_1\alpha_2\\ \beta_1\beta_2\end{pmatrix}$

$$\hat{S}^2 = (\hat{S}_1 + \hat{S}_2)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{S}_1\cdot\hat{S}_2$$

$$\hat{S}_1^2 = \hat{S}_2^2 = \frac{3}{4}\hbar^2\begin{pmatrix}1&0\\0&1\end{pmatrix} = \frac{3}{4}\hbar^2\,\mathbb{1}^{2\times2}$$

To be fully precise: $\hat{S}^2 = (\hat{S}_1\otimes\mathbb{1}_2 + \hat{S}_2\otimes\mathbb{1}_1)^2$

$$= \hat{S}_1^2\otimes\mathbb{1}_2^2 + \mathbb{1}_1^2\otimes\hat{S}_2^2 + 2\,\hat{S}_1\otimes\hat{S}_2$$

$$\frac{3}{4}\hbar^2\,\mathbb{1}^{2\times2}\otimes\mathbb{1}^{2\times2} = \frac{3}{4}\hbar^2\,\mathbb{1}^{4\times4}$$

$$2(\hat{S}_{1,x}\otimes\hat{S}_{2,x} + \hat{S}_{1,y}\otimes\hat{S}_{2,y} + \hat{S}_{1,z}\otimes\hat{S}_{2,z})$$
$$= \hat{S}_{1,+}\otimes\hat{S}_{2,-} + \hat{S}_{1,-}\otimes\hat{S}_{2,+} + 2\hat{S}_{1,z}\otimes\hat{S}_{2,z}$$

$$\left.\begin{aligned}\hat{S}_+ &= \hat{S}_x + i\hat{S}_y\\ \hat{S}_- &= \hat{S}_x - i\hat{S}_y\end{aligned}\right\} \Rightarrow \begin{aligned}\hat{S}_x &= \tfrac{1}{2}(S_+ + S_-)\\ \hat{S}_y &= \tfrac{1}{2i}(S_+ - S_-)\end{aligned}$$

$$\Leftrightarrow \hat{S}_{1,x}\otimes\hat{S}_{2,x} = \frac{1}{4}(\hat{S}_{1,+}\otimes\hat{S}_{2,+} + \hat{S}_{1,+}\otimes\hat{S}_{2,-} + \hat{S}_{1,-}\otimes\hat{S}_{2,+} + \hat{S}_{1,-}\otimes\hat{S}_{2,-})$$
$$\hat{S}_{1,y}\otimes\hat{S}_{2,y} = -\frac{1}{4}(\quad '' \quad - \quad '' \quad - \quad '' \quad + \quad '' \quad)$$

$$\Leftrightarrow \hat{S}_{1,x}\otimes\hat{S}_{2,x} + \hat{S}_{1,y}\otimes\hat{S}_{2,y} = \frac{1}{2}(\hat{S}_{1,+}\otimes\hat{S}_{2,-} + \hat{S}_{1,-}\otimes\hat{S}_{2,+})$$

$$\Rightarrow \hat{S}^2 = 2\cdot\frac{3}{4}\hbar^2\,\mathbb{1}^{4\times4} + \hbar^2\left[\underbrace{\begin{pmatrix}0&1\\0&0\end{pmatrix}\otimes\begin{pmatrix}0&0\\1&0\end{pmatrix}}_{\begin{pmatrix}0 & \begin{smallmatrix}0&0\\1&0\end{smallmatrix}\\ 0 & 0\end{pmatrix}} + \underbrace{\begin{pmatrix}0&0\\1&0\end{pmatrix}\otimes\begin{pmatrix}0&1\\0&0\end{pmatrix}}_{\begin{pmatrix}0 & 0\\ \begin{smallmatrix}0&1\\0&0\end{smallmatrix} & 0\end{pmatrix}} + \frac{1}{2}\underbrace{\begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes\begin{pmatrix}1&0\\0&-1\end{pmatrix}}_{\begin{pmatrix}\begin{smallmatrix}1&0\\0&-1\end{smallmatrix} & 0\\ 0 & \begin{smallmatrix}-1&0\\0&1\end{smallmatrix}\end{pmatrix}}\right]$$

$$= \hbar^2\begin{pmatrix}2&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&2\end{pmatrix}$$

b) 2 el op., since op. has off-diagonals

c) Edges are already decoupled and inner 2×2 is diagonalized by equal lin. combs, so eigpairs are $2\hbar^2 : (\uparrow\uparrow)$, $2\hbar^2 : (\uparrow\downarrow + \downarrow\uparrow)$

$0 : \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$, $2\hbar^2 : (\downarrow\downarrow)$

c)+d) States 1, 2 and 4 are triplets ($S = 1$) with $M_S = 1, 0, -1$, respectively and state 3 is a singlet with $S = 0$ and $M_S = 0$, uniquely characterizing the eigenfunctions

(2) a) $\chi_1 = \phi_s \alpha \qquad \chi_2 = \phi_{11} \alpha$

$$\Rightarrow |\Psi\rangle = |\chi_1 \chi_2\rangle = \phi_s^1 \alpha^1 \phi_{11}^2 \alpha^2 - \phi_{11}^1 \alpha^1 \phi_s^2 \alpha^2$$

$$= \alpha_1 \alpha_2 (\phi_s^1 \phi_{11}^2 - \phi_{11}^1 \phi_s^2)$$

b) $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 = \hat{J}_z^2 + \hbar \hat{J}_z + \hat{J}_- \hat{J}_+$

$$\Leftrightarrow \hat{J}_x^2 + \hat{J}_y^2 = \hbar \hat{J}_z + \hat{J}_- \hat{J}_+ = \hbar \hat{J}_z + \hat{J}_x^2 + \hat{J}_y^2 \underbrace{+ i \hat{J}_x \hat{J}_y - i \hat{J}_y \hat{J}_x}_{= i \underbrace{[\hat{J}_x, \hat{J}_y]}_{= i\hbar \hat{J}_z} = -\hbar \hat{J}_z}$$

c) $\hat{J}_z |\Psi\rangle = (\hat{L}_z + \hat{S}_z)|\Psi\rangle = 2\hbar |\Psi\rangle$

$\longrightarrow \hat{S}_z |\alpha_1 \alpha_2\rangle = \hbar$

$\longrightarrow \hat{L}_z |\phi_s^1 \phi_{11}^2\rangle = (\hat{L}_{z_1} + \hat{L}_{z_2}) |\phi_s^1 \phi_{11}^2\rangle = \underbrace{\hat{L}_{z_1} |\phi_s^1\rangle}_{=0} + \underbrace{\hat{L}_{z_2} |\phi_{11}^2\rangle}_{=\hbar}$ - perm.

d) $\hat{J}^2 |\Psi\rangle = \left[\hat{J}_z^2 + \hbar \hat{J}_z + \hat{J}_- \hat{J}_+\right] |\Psi\rangle$

$\Rightarrow \hbar \hat{J}_z |\Psi\rangle = 2\hbar^2 |\Psi\rangle$

$\Rightarrow \hat{J}_z^2 |\Psi\rangle = 4\hbar^2 |\Psi\rangle$

$\Rightarrow \hat{J}_- \hat{J}_+ |\Psi\rangle = 0$, because $\hat{J}_+ |\Psi\rangle = 0$, because 1 and 1 can't be linearly combinated to something higher than 2, which is the eigenvalue of $|\Psi\rangle$

e) $^{2S+1}L_J \longrightarrow {}^3P_2$