量化 Quiz 6 ；2015.5.20

1、He excited state $1s^1 2p^1$

請寫出 singlet & triplet 近似波函數 (先用 P_z)

50%

ANS：空間 (orbital) 部分

$$\phi_1 = \frac{1}{\sqrt{2}}[1s(1)2p_z(2) + 1s(2)2p_z(1)] \longrightarrow \text{symmetric}$$

$$\phi_2 = \frac{1}{\sqrt{2}}[1s(1)2p_z(2) - 1s(2)2p_z(1)] \longrightarrow \text{antisymmetric}$$

spin 部分

$$\left.\begin{aligned} \phi_{s1} &= \alpha(1)\alpha(2) \\ \phi_{s2} &= \beta(1)\beta(2) \\ \phi_{s3} &= \alpha(1)\beta(2)+\alpha(2)\beta(1) \end{aligned}\right\} \text{symmetric}$$

$$\phi_{s4} = \alpha(1)\beta(2)-\alpha(2)\beta(1) \longrightarrow \text{antisymmetric}$$

total wave function 須滿足 anti-symmetric (Pauli Principle)

$$\left.\begin{aligned} \psi_1 &= \frac{1}{\sqrt{2}}\{1s(1)2p_z(2)-1s(2)2p_z(1)][\alpha(1)\alpha(2)] \\ \psi_2 &= \frac{1}{\sqrt{2}}\{1s(1)2p_z(2)-1s(2)2p_z(1)][\beta(1)\beta(2)] \\ \psi_3 &= \frac{1}{\sqrt{2}}\{1s(1)2p_z(2)-1s(2)2p_z(1)][\alpha(1)\beta(2)+\alpha(2)\beta(1)] \end{aligned}\right\} \text{triplet}$$

$$\psi_4 = \frac{1}{\sqrt{2}}\{1s(1)2p_z(2)+1s(2)2p_z(1)][\alpha(1)\beta(2)-\alpha(2)\beta(1)] \longrightarrow \text{singlet}$$

P_x, P_y 与 P_z 相似

2、A=1～10

中性原子，基態term symbol　　1) ^{2S+1}L 40%　　2) $^{2S+1}L_J$ 10%

ANS：

$$\begin{array}{cccc} s & p & d & \\ \uparrow & \uparrow & \uparrow & \\ \end{array}$$

$L = 0, 1, 2, 3 \cdots$

$|L-S| \le J \le |L+S|$

	S	L	J	^{2S+1}L	$^{2S+1}L_J$	
H: $\frac{\uparrow}{1s}$	$\frac{1}{2}$	0	$\frac{1}{2}$	^2S ,	$^2S_{\frac{1}{2}}$	
He: $\frac{\uparrow\downarrow}{1s}$	0	0	0	^1S ,	$^1S_0$	
Li: $\frac{\uparrow}{2s}$	$\frac{1}{2}$	0	$\frac{1}{2}$	^2S ,	$^2S_{\frac{1}{2}}$	
Be: $\frac{\uparrow\downarrow}{2s}$	0	0	0	^1S ,	$^1S_0$	
B: 2p $\frac{\uparrow}{1}\,\frac{\ }{0}\,\frac{\ }{-1}$	$\frac{1}{2}$	1	$\frac{1}{2},\frac{3}{2}$	^2P ,	$^2P_{\frac{1}{2}}$	[軌域电子未超过半填滿取J值小的]
C: 2p $\frac{\uparrow}{1}\,\frac{\uparrow}{0}\,\frac{\ }{-1}$	1	1	0,1,2	^3P ,	$^3P_0$	
N: 2p $\frac{\uparrow}{1}\,\frac{\uparrow}{0}\,\frac{\uparrow}{-1}$	$\frac{3}{2}$	0	$\frac{3}{2}$	^4S ,	$^4S_{\frac{3}{2}}$	
O: 2p $\frac{\uparrow\downarrow}{1}\,\frac{\uparrow}{0}\,\frac{\uparrow}{-1}$	1	1	0,1,2	^3P ,	$^3P_2$	[軌域电子超过半填滿取J值最大的]
F: 2p $\frac{\uparrow\downarrow}{1}\,\frac{\uparrow\downarrow}{0}\,\frac{\uparrow}{-1}$	$\frac{1}{2}$	1	$\frac{1}{2},\frac{3}{2}$	^2P ,	$^2P_{\frac{3}{2}}$	
Ne: 2p $\frac{\uparrow\downarrow}{1}\,\frac{\uparrow\downarrow}{0}\,\frac{\uparrow\downarrow}{-1}$	0	0	0	^1S ,	$^1S_0$	