The allowed terms for equivalent electrons, $n\mathbf{p}^2$

Application of the method described in the lecture for a pair of equivalent electrons.

For the electron configuration $n\mathrm{p}^2$ $l_1 = l_2 = 1$ and $s_1 = s_2 = 1/2$ for each electron, so $m_l = -1, 0, +1$ and $m_s = \pm 1/2$.

All possible combinations are listed in table 1. In the m_s column '+' refers to $m_s = +1/2$ and '$-$' refers to $m_s = -1/2$.

The states not allowed by the Pauli Exclusion Principle because $(m_{l_1}, m_{s_1}) = (m_{l_2}, m_{s_2})$ are eliminated and have an 'X' in the 'Pauli?' column.

The pairs of states that are the same when the electron labels are exchanged such as those labelled with ♣ and ♠ have one state of the pair eliminated to avoid double-counting and have an 'X' in the 'label?' column.

♣ : $\{(m_{l_1} = 1, m_{s_1} = +); (m_{l_2} = 1, m_{s_2} = -)\}$ and $\{(m_{l_1} = 1, m_{s_1} = -); (m_{l_2} = 1, m_{s_2} = +)\}$

♠ : $\{(m_{l_1} = 1, m_{s_1} = -); (m_{l_2} = 0, m_{s_2} = +)\}$ and $\{(m_{l_1} = 0, m_{s_1} = +); (m_{l_2} = 1, m_{s_2} = -)\}$

There are 15 states remaining which may be grouped according to their values of $M_L = m_{l_1} + m_{l_2}$ and $M_S = m_{s_1} + m_{s_2}$.

The largest value of M_L is $M_L = 2$, for which in this table $M_S = 0$. There must, therefore be a group of $M_L = +2, +1, 0, -1, -2$ (all possible values of M_L for $L = 2$) each with $M_S = 0$, so that $S = 0$.

Group these together and assign a term: $(2S + 1) = 1$, $L = 2 \Rightarrow D$.

The term is ^1D.

What's left? The largest M_L left is $M_L = 1$ (i.e. $L = 1$), so there must be a group of $M_L = +1, 0, -1$ all with the same M_S. Actually there are three - one with $M_S = +1$, one with $M_S = 0$ and one with $M_S = -1$. This means that not only is $L = 1$ but also $S = 1$.

Groups these together and assign a term: $(2S + 1) = 3$, $L = 1 \Rightarrow P$.

The term is ^3P

What's left? Only one state with $M_L = M_S = 0$, and so $L = S = 0$.

Assign a term to this: $(2S + 1) = 1$, $L = 0 \Rightarrow S$.

The term is ^1S

The allowed terms are therefore $^1S,^3P,^1D$.

The grouping of the allowed configurations is shown in table 2

m_{l_1}	m_{s_1}	m_{l_2}	m_{s_2}	Pauli?	label?
1	+	1	+	X	
1	+	1	−		♣
1	+	0	+		
1	+	0	−		
1	+	-1	+		
1	+	-1	−		
1	−	1	+		X ♣
1	−	1	−	X	
1	−	0	+		♠
1	−	0	−		
1	−	-1	+		
1	−	-1	−		
0	+	1	+		X
0	+	1	−		X ♠
0	+	0	+	X	
0	+	0	−		
0	+	-1	+		
0	+	-1	−		
0	−	1	+		X
0	−	1	−		X
0	−	0	+		X
0	−	0	−	X	
0	−	-1	+		
0	−	-1	−		
-1	+	1	+		X
-1	+	1	−		X
-1	+	0	+		X
-1	+	0	−		X
-1	+	-1	+	X	
-1	+	-1	−		
-1	−	1	+		X
-1	−	1	−		X
-1	−	0	+		X
-1	−	0	−		X
-1	−	-1	+		X
-1	−	-1	−	X	

Table 1: Table of the possible combinations of $m_{l_1}, m_{s_1}, m_{l_2}, m_{s_2}$

m_{l_1}	m_{s_1}	m_{l_2}	m_{s_2}	$M_L = m_{l_1} + m_{l_2}$	$M_S = m_{s_1} + m_{s_2}$
1	$+1/2$	1	$-1/2$	2	0
1	$-1/2$	0	$+1/2$	1	0
0	$+1/2$	0	$-1/2$	0	0
0	$-1/2$	-1	$+1/2$	-1	0
-1	$+1/2$	-1	$-1/2$	-2	0
1	$+1/2$	0	$+1/2$	1	1
1	$+1/2$	-1	$+1/2$	0	1
0	$+1/2$	-1	$+1/2$	-1	1
1	$+1/2$	0	$-1/2$	1	0
1	$-1/2$	-1	$+1/2$	0	0
0	$+1/2$	-1	$-1/2$	-1	0
1	$-1/2$	0	$-1/2$	1	-1
1	$-1/2$	-1	$-1/2$	0	-1
0	$-1/2$	-1	$-1/2$	-1	-1
1	$+1/2$	-1	$-1/2$	0	0

Table 2: Grouping of the allowed combinations of $m_{l_1}, m_{s_1}, m_{l_2}, m_{s_2}$