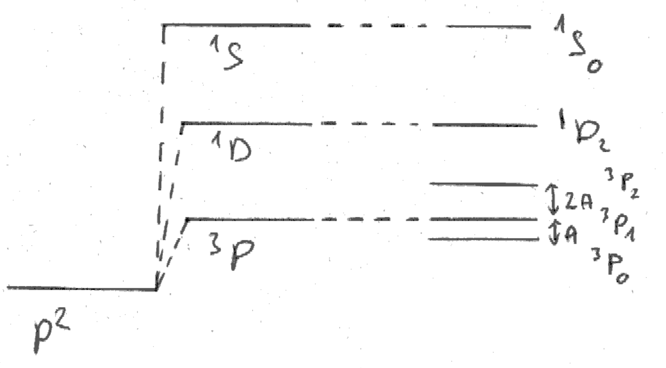

Atomic terms of p^2 configuration

$\ell = 2,\ s = 1$

$\Rightarrow (2\ell+1)\times(2s+1)$ possible spin-orbitals for two e^-

$\Rightarrow$ There are $\binom{6}{2} = 15$ states belonging to p^2 conf.

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^1D atomic term ($L=2,\ S=0,\ J=L=2$) has 5 states:

$M_L = -2, -1, 0, 1, 2$

As $p_1(1)\,p_1(2)$ is the only product with $M_L = 2$,

$$\psi^{M_L=2}_{^1D_2} = p_1(1)\,p_1(2)\,{}^1\eta\ ,\ \text{where}\ {}^1\eta = \frac{1}{\sqrt{2}}\left(\alpha(1)\beta(2) - \alpha(2)\beta(1)\right)$$

Similarly, $\psi^{M_L=-2}_{^1D_2} = p_{-1}(1)\,p_{-1}(2)\,{}^1\eta$

$$\left(\hat{L}^-_1 + \hat{L}^-_2\right)\psi^{M_L=2}_{^1D_2} \sim \psi^{M_L=1}_{^1D_2}$$

$\hat{L}^- = \hat{L}_x - i\hat{L}_y$

$\hat{L}^- \phi_{L,M_L} = \sqrt{(L+M_L)(L-M_L+1)}\cdot \phi_{L,M_L-1}$ (*)

$\hat{L}^- = \hat{L}^-_1 + \hat{L}^-_2$

$$\Longrightarrow \psi^{M_L=1}_{^1D_2} = \left\{p_1(1)\,p_0(2) + p_0(1)\,p_1(2)\right\}{}^1\eta$$

$$\xrightarrow{\text{up-down sym.}} \psi^{M_L=-1}_{^1D_2} = \left\{p_{-1}(1)\,p_0(2) + p_0(1)\,p_{-1}(2)\right\}{}^1\eta$$

Note that $p_1(1)\,p_0(2) + p_0(1)\,p_1(2)$ is the only sym. comb. with $M_L = 1$.

The symmetric combination with $M_L = 0$ is

$$a\cdot p_0(1)\,p_0(2) + b\left(p_1(1)\,p_{-1}(2) + p_{-1}(1)\,p_1(2)\right)$$

(From (*) $a = b = \sqrt{2}$)

$$\Downarrow$$

$$\psi^{M_L=0}_{^1D_2} = \left\{a\,p_0(1)\,p_0(2) + b\left(p_1(1)\,p_{-1}(2) + p_{-1}(1)\,p_1(2)\right)\right\}{}^1\eta$$

What about the ^3D states? $p_1(1)\,p_1(2)\,\frac{1}{\sqrt{2}}\left(\alpha(1)\beta(2) + \alpha(2)\beta(1)\right) =$

$p_1(1)\,p_1(2)\,{}^3\eta_0$ is a sym. function $\Longrightarrow$ there are no ^3D states!

$\Psi_{^1S_0}^{M_L=0}$ is the lin. comb. of products with $M_L=0$:

$P_0(1)\,P_0(2)$, $P_{-1}(1)\,P_1(2)$, and $P_1(1)\,P_{-1}(2)$

$\Psi_{^1S_0}^{M_L=0}$ must be orthogonal to $\Psi_{^1D_2}^{M_L=0}$ $\Longrightarrow$

$$\Psi_{^1S_0}^{M_L=0} = \left\{ b\,P_0(1)P_0(2) - \frac{a}{2}\left(P_1(1)P_{-1}(2) + P_1(1)P_{-1}(2)\right)\right\}{}^1\eta$$

—o—

$\Psi_{^3S_1}^{M_L=0}$ should contain the $P_0(1)\,P_0(2)$ spatial part, but $P_0(1)\,P_0(2)\,{}^3\eta$ is not anti-sym. $\Longrightarrow$ no such a state!

—o—

There are 3 triplet spin conf. and 3 anti-sym. spatial conf.:

${}^3\eta_1 = \alpha(1)\,\alpha(2)$	$P_1(1)\,P_0(2) - P_0(1)\,P_1(2)$	$M_L=1$
${}^3\eta_0 = \frac{1}{\sqrt{2}}\left(\alpha(1)\,\beta(2) + \alpha(1)\,\beta(2)\right)$	$P_1(1)\,P_{-1}(2) - P_{-1}(1)\,P_1(2)$	$M_L=0$
${}^3\eta_{-1} = \beta(1)\,\beta(2)$	$P_0(1)\,P_{-1}(2) - P_{-1}(1)\,P_0(2)$	$M_L=-1$

Coupling these functions provides the $3\times3=9$ ${}^3P$ states. For example, $\Psi_{^1P_2}^{M_J=2} = \left(P_1(1)\,P_0(2) - P_0(1)\,P_1(2)\right){}^3\eta_1$