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Atomic Wave Functions for the Configurations $s^n p^m$ studied by the Projection Operator Technique*

By

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Tables of angular momentum wave functions and energy matrices for the atomic configurations $s^n p^m$ are given in the cases of strong, weak and intermediate coupling. Also the transformation matrices between *LS*- and *jj*-coupling are calculated.

All these calculations are carried out as an application of the projection operator method for angular momenta, introduced by LÖWDIN.

On a calculé des fonctions propres du moment cinétique ainsi que les matrices correspondantes de l'énergie, pour les configurations atomiques $s^n p^m$. Les trois types de couplage, *LS*, *jj* et intermédiaire ont été étudiés, ainsi que les matrices de transformation entre ces couplages. Pour tous ces calculs on a utilisé la méthode des projecteurs pour le moment cinétique, introduite par LÖWDIN.

Eigenfunktionen des Drehimpulses und entsprechende Energiematrizen für die Atomkonfigurationen $s^n p^m$ sind für die drei Kopplungsfälle, *LS*, *jj* und intermediär tabelliert. Matrizen für Transformationen zwischen *LS*- und *jj*-Kopplung werden angegeben. Alle diese Rechnungen sind auf die von LÖWDIN eingeführte Projektionsoperatormethode gegründet.

Introduction

The projection operators for angular momentum, introduced by LÖWDIN [*4*] have up to now been applied in two cases: to the spin degeneracy problem [*6*] and for the construction of atomic state wave functions [*3, 7, 8*].

The present paper is an application of the methods developed by FIESCHI-LÖWDIN [*3, 7*] to configurations containing *s*- and/or *p*-electrons. We give tables of wave functions for the zero-order functions in the *LS*-scheme, the "coupled" functions in the *SLJM*- and *jjJM*-schemes, the electrostatic interaction matrices and the spin-orbit interaction matrices in the two schemes, the transformation matrix between *SLJM* and *jjJM*, and finally the energies in the intermediate coupling case.

The energy matrices and the transformation matrix are calculated in CONDON-SHORTLEY [*2*] for some of the configurations $s^n p^m$, and the zero order functions for

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the LS-scheme are given by COMPANION and ELLISON [1]. As far as we know, however, the other wave functions are not published anywhere. Since the signs of the matrix elements depend on the choice of phase of the wave function, we have made all the tables complete, so as to make them self-contained.

By this detailed application of projection operator techniques we wish to show the simplicity and directness they offer. We choose a simple anti-symmetric function, and keeping the antisymmetry, we select the components wanted. The procedure of applying projection operators in orbital angular momentum space, in spin space, and/or in total angular momentum space is quite elementary: it requires only the simple rules for the step operators and for the behaviour of determinants. The Clebsch-Gordan and fractional parentage coefficients enter only implicitly, so these two concepts are not even needed. The idempotency property of the projection operators together with the property of the special projection operators considered here of commutability with the Hamiltonian simplifies the calculation of matrix elements to a large extent.

Another point we want to stress, is that the projection operator method makes the whole procedure unified. One uses projection operators in orbital angular momentum space and/or in spin space to get the correct zero-order functions for LS-coupling ($SLM_L\, M_S$). Then one goes over to the $SLJM$-scheme by means of a projection operator in total angular momentum space. To get the connection between the one-electron functions ($nlm_l m_s$) and ($nljm$) one uses a projection operator in the total angular momentum space for one electron, and finally to go over from the one-electron functions ($nljm$) to the $jjJM$-scheme, one utilizes a projection operator in total angular momentum space. — In some cases the terms are degenerate (e.g. $(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}; \frac{3}{2}, \frac{3}{2})$ for sp^2), and it is advantageous to have the corresponding functions orthogonal. Since the functions are here expressed as projected functions, the orthogonalization procedure is most simply carried out by LÖWDIN's method [8]. — Then the fact that the functions are expressed as projected functions is used in every calculation of matrix elements.

We believe that these two principal advantages, simplification and unification, which the present method offers, might be valuable not only for teaching purposes but also for developing the theory for wave functions having higher accuracy.

Some Comments to the Tables

For both theory and notations, we refer to FIESCHI-LÖWDIN [3, 7], (see also the glossary at the end of the paper) but we make here some comments concerning details in the calculation.

For each configuration we give the table of possible functions, ($m_l(1)\; m_l(2) \ldots | \ldots m_l(N)$), which is then resolved so as to give the possible terms. Then we list the zero-order functions $^{2S+1}L\; (M_L,\, M_S)$. All functions (both zero-order and "coupled" functions) are normalized, and we also give the numerical factor by which they differ from the projected functions. After that there is a table of the functions in the $SLJM$-scheme: $^{2S+1}L_{JM}$, the electrostatic interaction matrix $\boldsymbol{H}'$ and the spin-orbit matrix $\boldsymbol{V}$ in the $SLJM$-scheme. For jj-coupling we give a table, with the possible functions ($m_1\, m_2 \ldots | \ldots m_N$), giving the possible terms, the functions ($j_1\, j_2 \ldots j_N;\, JM$) in the $jjJM$-scheme, the connection between functions ($m_1\, m_2 \ldots | \ldots m_N$) and ($m_l\,(1)\, m_l\,(2) \ldots | \ldots m_l\,(N)$) for that particular configuration, the transformation matrix $\boldsymbol{U}$ between the $SLJM$- and the $jjJM$-scheme and finally the two matrices $\boldsymbol{H}'$ and $\boldsymbol{V}$ in the $jjJM$-scheme. For intermediate coupling we give the energies explicitly in the case of second-order secular equations, but we only give the secular equation itself for higher orders.

In all the projections we need the coefficients $\varkappa^{\pm}_{lm_l} = \sqrt{(l \mp m_l)\,(l \pm m_l + 1)}$ and we have therefore condensed the tables pp 17 and 37 of Fieschi-Löwdin [3, 7] to Tab. 1.

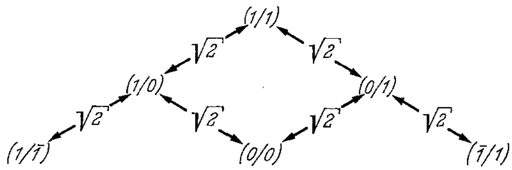
When making the $L^{\nu}_{-}\, L^{\nu}_{+}$ operations, the simplest way is probably to make L_{+}, L^2_{+}, L^3_{+}, ..., $L_{-}\,L_{+}$, $L_{-}\,L^2_{+}$, $L^2_{-}\,L^2_{+}$,... successively. It is however a little

Table 1. $\varkappa^{\pm}_{lm} = \sqrt{(l \mp m)\,(l \pm m + 1)}$

m \ l	$\frac{1}{2}$		1		$\frac{3}{2}$		2		$\frac{5}{2}$		3		$\frac{7}{2}$	
	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$	$\varkappa^+$	$\varkappa^-$
$\frac{7}{2}$													0	$\sqrt{7}$
3											0	$\sqrt{6}$		
$\frac{5}{2}$									0	$\sqrt{5}$			$\sqrt{7}$	$2\sqrt{3}$
2							0	2			$\sqrt{6}$	$\sqrt{10}$		
$\frac{3}{2}$					0	$\sqrt{3}$			$\sqrt{5}$	$2\sqrt{2}$			$2\sqrt{3}$	$\sqrt{15}$
1			0	$\sqrt{2}$			2	$\sqrt{6}$			$\sqrt{10}$	$\sqrt{12}$		
$\frac{1}{2}$	0	1			$\sqrt{3}$	2			$2\sqrt{2}$	3			$\sqrt{15}$	4
0			$\sqrt{2}$	$\sqrt{2}$			$\sqrt{6}$	$\sqrt{6}$			$\sqrt{12}$	$\sqrt{12}$		
$-\frac{1}{2}$	1	0			2	$\sqrt{3}$			3	$2\sqrt{2}$			4	$\sqrt{15}$
-1			$\sqrt{2}$	0			$\sqrt{6}$	2			$\sqrt{12}$	$\sqrt{10}$		
$-\frac{3}{2}$					$\sqrt{3}$	0			$2\sqrt{2}$	$\sqrt{5}$			$\sqrt{15}$	$2\sqrt{3}$
-2							2	0			$\sqrt{10}$	$\sqrt{6}$		
$-\frac{5}{2}$									$\sqrt{5}$	0			$2\sqrt{3}$	$\sqrt{7}$
-3											$\sqrt{6}$	0		
$-\frac{7}{2}$													$\sqrt{7}$	0

tedious to write up all these operations, and therefore we would propose the following algorithm, the idea of which has been given by Polo [9].

We write up the functions in rows corresponding to the M_L-values. The operation L_{+} can then be illustrated by an arrow to the next higher row and similarly for L_-. On the arrow we write the value of the corresponding $\varkappa^{\pm}_{lm_l}$. When all possible functions are written up, we have only to follow all possible paths, remembering the corresponding coefficients in each step. The algorithm is perhaps best illustrated by an example. We want the eigenfunction corresponding to ^1S of p^2. Any one of $(0 \mid 0)$, $(1 \mid \bar{1})$ or $(\bar{1} \mid 1)$ is possible as starting function for a projection. We choose $(0 \mid 0)$.



Polo - diagram

The projection operator $\mathcal{O}_{00}$ is, when $L_{\max} = 2$:

$$^L\mathcal{O}_{00} = 1 - \frac{L_- L_+}{2} + \frac{L_-^2 L_+^2}{12} \quad . \tag{1}$$

From $(0 \mid 0)$ L_+ takes us to $(1 \mid 0)$ or $(0 \mid 1)$. L_- will bring us back to $(0 \mid 0)$ or take us to $(1 \mid \bar{1})$ or $(\bar{1} \mid 1)$. Remembering the coefficients on the arrows we thus get

$$L_- L_+ (0 \mid 0) = 4\,(0 \mid 0) + 2\,(1 \mid \bar{1}) + 2\,(\bar{1} \mid 1) \quad . \tag{2}$$

In the same way we get

$$L_-^2 L_+^2 (0 \mid 0) = 16\,(0 \mid 0) + 8\,(1 \mid \bar{1}) + 8\,(\bar{1} \mid 1) \quad . \tag{3}$$

Here we must notice that it is possible to reach $(1 \mid 1)$ in two ways in the upward direction and also to reach $(0 \mid 0)$ in two ways on the way down. – Taking account of the numerical factors in $^L\mathcal{O}_{00}$, we then get

$$^L\mathcal{O}_{00}\,(0 \mid 0) = \frac{1}{3}\left\{(0|0) - (1|\bar{1}) - (\bar{1}|1)\right\} \quad . \tag{4}$$

Only in relatively few cases is it necessary to make any projection in spin space, since most of our starting functions represent already pure spin states. Even when this is not the case, the corresponding projection is much easier to handle than the orbital projection, since the coefficients $\varkappa^{\pm}_{lm_l}$ are in this case very simple. (1 and 0 as may be seen from Tab. 1.)

In this connection one must remember that a determinant changes sign, if two of its columns are interchanged.

E. g.

$$\begin{aligned} S_+ (1 \mid 0\bar{1}) &= S_+ (1\,\alpha,\, 0\beta,\, \bar{1}\beta) = (1\,\alpha,\, 0\,\alpha,\, \bar{1}\beta) + (1\,\alpha,\, 0\beta,\, \bar{1}\,\alpha) \\ &= (1\,\alpha,\, 0\,\alpha,\, \bar{1}\beta) - (1\,\alpha,\, \bar{1}\,\alpha,\, 0\beta) = (10 \mid \bar{1}) - (1\bar{1} \mid 0) \quad . \end{aligned} \tag{5}$$

We give functions only for the principal case ($M_L = L$, $M_S = S$ and later $M = J$), since the other cases are easily obtained by the step-down operators L_-, S_- or J_-. This makes also the checking very easy, depending on the relation

$$\left.\begin{matrix} S_+ \\ L_+ \end{matrix}\right\} \mathcal{O}_{LL}\, \mathcal{O}_{SS}\, \Psi \equiv 0 \quad . \tag{6}$$

We list results for $s^n\ p^m$, $n = 0$; $m = 2, 3, 4$; $n = 1$; $m = 1, 2, 3, 4, 5$. For p^4, sp^4, sp^5 we have used the "hole" theorem which says that the wave-functions of $s^n\ p^m$ can be correlated to those of $s^{2-n}\ p^{6-m}$ simply by the relation

$$(m_l\,(1)\,m_l\,(2)\,\ldots\,|\,\ldots\,m_l\,(N)) \qquad [m_l\,(1)\,m_l\,(2)\,\ldots\,|\,\ldots\,m_l\,(N)]\,, \tag{7}$$

where the square bracket has the same meaning as in FIESCHI-LÖWDIN [3, 7]. Obviously, it is very simple to get the functions for the almost closed shells, if one has those of the "complementary" shell, but we have anyhow given them here, since we thought that it might be useful to have them written down somewhere explicitly. — Here it should be pointed out that one has to be very careful with the phases by going over to the almost closed shells.

In going over from the $SLM_L\,M_S$-scheme to the $SLJM$-scheme, one gets first the ${}^{2S+1}L_{JM}$-functions as linear combinations of ${}^{2S+1}L\ (M_L,M_S)$-functions. Among them there are often cases with $M_L \neq L$ or $M_S \neq S$, so one has to use L_- or S_- to get the appropriate functions. By doing this, one has to be very careful with the numerical factors. E. g. S_- working on a ${}^3P$ as an entity gives a factor $\sqrt{2}$, but $S_- = \Sigma\, s_-\,(i)$ working upon the separate electron coordinates gives a factor 1 for each:

$$\begin{aligned} {}^3P\,(1{,}0) &= \frac{1}{\sqrt{2}} S_-\,{}^3P\,(1{,}1) = \frac{1}{\sqrt{2}} S_-\,(10| \\ &= \frac{1}{\sqrt{2}} \left\{ s_-\,(1) + s_-\,(2) \right\} (10| = \frac{1}{\sqrt{2}} \left\{ (1|0) - (0|1) \right\}\ . \end{aligned} \tag{8}$$

All the functions in the $SLJM$-scheme have been checked by the relation

$$J_+\ {}^{2S+1}L_{JJ} \equiv 0\ . \tag{9}$$

The same relation is used to check the functions in the $jjJM$-scheme, although J_+ in this case works as $\Sigma\, j_+\,(i)$.

The matrix elements of the spin-orbit interaction are easily calculated in the $jjJM$-scheme, but the electrostatic interaction still involves rather cumbersome work, in spite of the simplifications introduced by the projection operator formalism. The electrostatic interaction is already calculated, however, in the $SLJM$-scheme, and since the $SLJM$-functions and the $jjJM$-functions are different orthonormal bases for describing the same subspace, we can find the unitary transformation, which connects them, from our knowledge of the functions, and then transform the matrices of electrostatic interaction, and spin-orbit interaction. This latter one could then be used for checking purposes since we know that it is diagonal in the $jjJM$-scheme, with the elements given by FIESCHI-LÖWDIN formulas (73), (74).

The transformation coefficients are overlap integrals between two functions which can both be expressed as JJ-projections. As usual we can then use the turn-over rule, which of course reduces considerably the number of terms in the integral.

The general integral is of the form

$$\begin{aligned} \int {}^{2S+1}L^*_{JJ} \cdot (j_1\,j_2\,\ldots\,j_N;\,JJ)\,(dx) &= \int [\text{const.}\ O_{JJ}\ {}^{2S+1}L\,(M_L,\,M_S)]^* \times \\ &\times [\text{const.}\ O_{JJ}\,(m_1\,m_2\,\ldots\,|\,\ldots\,m_N)]\,(dx)\ . \end{aligned} \tag{10}$$

Here we use the turn-over rule in that direction which is most advantageous; i. e. if ${}^{2S+1}L\ (M_L, M_S)$ contains fewer terms than $(m_1\, m_2 \ldots \mid \ldots m_N)$ we use it in "the ordinary way" and move the first O_{JJ} to the right, otherwise the second O_{JJ} to the left.

$$\begin{aligned} &\int {}^{2S+1}L\ (M_L, M_S)^*\ O_{JJ}\ (m_1\, m_2 \ldots \mid \ldots m_N)\ (dx) \\ &= \int [O_{JJ}\ {}^{2S+1}L\ (M_L, M_S)]^*\ (m_1\, m_2 \ldots \mid \ldots m_N)\ (dx)\ . \end{aligned} \tag{11}$$

The function ${}^{2S+1}L\ (M_L, M_S)$ is a sum of determinants built up of $(nl\, m_l\, m_s)$-functions, whereas $O_{JJ}\ (m_1\, m_2 \ldots \mid \ldots m_N)$ is a sum of $(m_1\, m_2 \ldots \mid \ldots m_N)$-determinants built up of $(nljm)$-functions. We must therefore transform the $(nljm)$-functions to (nlm_lm_s)-functions according to FIESCHI-LÖWDIN Chapt. IV. We need also the transformations between determinants of type $(\frac{3}{2}, \frac{1}{2} \mid$ and $(1 \mid 0)$. These are given for each configuration after the $jjJM$-functions. The integral

$$\int {}^{2S+1}L\ (M_L\, M_S)^* \cdot O_{JJ}\ (m_1\, m_2 \ldots \mid \ldots m_N)\ (dx)\ , \tag{12}$$

could then in principle be further simplified by remembering that ${}^{2S+1}L\ (M_L, M_S)$ is the result of an O_{LL} (and perhaps O_{SS}) projection on a single determinant.

$${}^{2S+1}L\ (M_L, M_S) = O_{LL} \cdot O_{SS} \cdot (m_l\,(1), m_l\,(2) \ldots \mid \ldots m_l\,(N))\ . \tag{13}$$

The turn-over rule could of course be used again

$$\int (m_l\,(1), m_l\,(2) \ldots \mid \ldots m_l\,(N))^* \cdot O_{LL} \cdot O_{SS} \cdot O_{JJ} \cdot (m_1 m_2 \ldots \mid \ldots m_N)\ (dx)\ , \tag{14}$$

and here we have the integral between a single determinant and a sum of similar determinants.

In practice, however, we have found it simpler not to make this last step. It would namely force us to make the operations $O_{LL} \cdot O_{SS} \cdot O_{JJ}\ (m_1\, m_2 \ldots \mid \ldots m_N)$ and this generally implies more work than to make the integration at the stage

$$\int {}^{2S+1}L\ (M_L, M_S)^* \cdot O_{JJ}\ (m_1\, m_2 \ldots \mid \ldots m_N)\ (dx)\ , \tag{15}$$

even if ${}^{2S+1}L\ (M_L, M_S)$ contains more than one term [5].

As an example we choose the matrix element between ${}^1S_{00}$ and $(\frac{3}{2}, \frac{3}{2}; 0,0)$:

$$\begin{aligned} (0, 0, 0, 0 \mid \boldsymbol{U} \mid \tfrac{3}{2}, \tfrac{3}{2}; 0, 0) &= \int {}^1S_{00}^*\ (\tfrac{3}{2}, \tfrac{3}{2}; 0, 0)\ (dx) \\ &= \int [\mathcal{O}_{00}\ {}^1S\ (0, 0)]^*\ \sqrt{2}\ \mathcal{O}_{00}\ (\tfrac{3}{2}, -\tfrac{3}{2} \mid (dx) \\ &= \sqrt{2} \int [\mathcal{O}_{00}\ {}^1S\ (0, 0)]^* \cdot (\tfrac{3}{2}, -\tfrac{3}{2} \mid (dx) \\ &= \sqrt{2} \int {}^1S\ (0, 0)^*\ (1 \mid \overline{1})\ (dx) \\ &= \sqrt{\frac{2}{3}} \int \{ (0 \mid 0) - (1 \mid \overline{1}) - (\overline{1} \mid 1) \}^* (1 \mid \overline{1})\ (dx) \\ &= -\sqrt{\frac{2}{3}}\ . \end{aligned}$$

For a discussion of the energy matrices for the almost closed shells, we refer to CONDON and SHORTLEY [2], XII:1 and XIII:1,2.

The intermediate coupling case is treated as in CONDON and SHORTLEY [2] XI.3.

Glossary

Notation	Definition	Eigenvalues
One particle operators and eigenvalues:		
$\vec{l}$	orbital angular momentum	l
l_z	z- component of $\vec{l}$	m_l
$\vec{s}$	spin angular momentum	$\frac{1}{2}$
s_z	z- component of $\vec{s}$	m_s
$\vec{j}$	$\vec{l}+\vec{s}$	j
j_z	$l_z + s_z$	$m = m_l + m_s$
Many particle operators and eigenvalues:		
$\vec{L}$	$\Sigma_i \vec{l}\,(i)$	L
L_z	$\Sigma_i\, l_z\,(i)$	M_L
$\vec{S}$	$\Sigma_i \vec{s}\,(i)$	S
S_z	$\Sigma_i\, s_z\,(i)$	M_S
$\vec{J}$	$\Sigma_i \vec{j}\,(i) = \vec{L}+\vec{S}$	J
J_z	$\Sigma_i\, j_z\,(i) = L_z + S_z$	M

One particle functions:

$(n\, l\, m_l\, m_s)$ eigenfunction of $\vec{l}^{\,2}$, $\vec{s}^{\,2}$, l_z and s_z .

$(n\, l\, j\, m)$ eigenfunction of $\vec{l}^{\,2}$, $\vec{s}^{\,2}$, $\vec{j}^{\,2}$ and j_z .

Many-particle functions:

LS-scheme: Slaterdeterminant $(m_l\,(1)\; m_l\,(2)\; \ldots \mid m_l\,(\nu)\; \ldots\; m_l\,(N))$ meaning $\det\left\{(n\, l\, m_l\,(1)\,\alpha)\; \ldots\; (n\, l\, m_l\,(\nu)\,\beta)\; \ldots\; (n\, l\, m_l\,(N)\,\beta)\right\}$ coupled to zero-order functions ${}^{2S+1}L\;(M_L,\, M_S)$ which are eigenfunctions of $\vec{L}^{\,2}$, $\vec{S}^{\,2}$, L_Z and S_Z.

jj-scheme: Slaterdeterminant $(m_1\, m_2\, \ldots \mid m_\nu\, m_{\nu+1}\, \ldots)$ meaning

$$\det\left\{(nl,\, l+\tfrac{1}{2},\, m_1)\,(n\, l,\, l+\tfrac{1}{2},\, m_2)\,\ldots\,(n\, l,\, l-\tfrac{1}{2},\, m_\nu)\,(n\, l,\, l-\tfrac{1}{2},\, m_{\nu+1})\,\ldots\right\}$$

Projection operator (total angular momentum).

$${}^{J}\mathcal{O}_{JM} = (2\,J+1)\,\frac{(J+M)!}{(J-M)!}\sum_{i=0}(-1)^i\,\frac{J_-^{J-M+i}\,J_+^{J-M+i}}{i!\,(2J+i+1)!}$$

$SLJM$-scheme: ${}^{2S+1}L_{JM}$ eigenfunctions of $\vec{L}^{\,2}$, $\vec{S}^{\,2}$, $\vec{J}^{\,2}$ and J_Z.

The electrostatic interaction is diagonal and spin-orbit interaction non-diagonal in this representation.

$jjJM$-scheme: $(j_1\, j_2\, \ldots\, j_N;\; J\, M)$ eigenfunctions of $\vec{j}_i^{\,2}$, $\vec{J}^{\,2}$ and J_z.

The electrostatic interaction is non-diagonal and spin-orbit interaction diagonal in this representation.

Table 2. p

$M_L \backslash M_S$	$\frac{1}{2}$	$-\frac{1}{2}$
1	$(1\mid$	$\mid 1)$
0	$(0\mid$	$\mid 0)$
−1	$(\bar{1}\mid$	$\mid \bar{1})$

$$\begin{array}{cc} 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{array} = {}^2P$$

$${}^2P\,(1, \tfrac{1}{2}) = (1\mid$$

SLJM

$${}^2P_{\frac{3}{2}\frac{3}{2}} = {}^2P\,(1,\tfrac{1}{2}) = \mathcal{O}_{\frac{3}{2}\frac{3}{2}}\,{}^2P\,(1,\tfrac{1}{2}) = (1\mid$$

$${}^2P_{\frac{1}{2}\frac{1}{2}} = \frac{1}{\sqrt{3}}\left\{{}^2P\left(0,\tfrac{1}{2}\right) - \sqrt{2}\,{}^2P\left(1,-\tfrac{1}{2}\right)\right\} = \sqrt{3}\,\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,{}^2P\left(0,\tfrac{1}{2}\right)$$

$$= \frac{1}{\sqrt{3}}\left(0\mid - \sqrt{\frac{2}{3}}\mid 1\right).$$

Note that this relation governs the phases of transformations between *SLJM*- and *jjJM*-schemes.

Table 3. p^2

$M_L \backslash M_S$	1	0	−1
2		$(1\mid 1)$	
1	$(10\mid$	$(1\mid 0)\ (0\mid 1)$	$\mid 10)$
0	$(1\bar{1}\mid$	$(1\mid\bar{1})\ (0\mid 0)\ (\bar{1}\mid 1)$	$\mid 1\bar{1})$
−1	$(\bar{1}0\mid$	$(\bar{1}\mid 0)\ (0\mid\bar{1})$	$\mid\bar{1}0)$
−2		$(\bar{1}\mid\bar{1})$	

$$\begin{array}{ccc} & 1 & \\ 1 & 2 & 1 \\ 1 & 3 & 1 \\ 1 & 2 & 1 \\ & 1 & \end{array} = \begin{array}{c} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{array} + \begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{array} + 1 = {}^1D + {}^3P + {}^1S$$

$${}^1D\,(2,0) = (1\mid 1)$$

$${}^3P\,(1,1) = (10\mid$$

$${}^1S\;(0,0) = \frac{1}{\sqrt{3}}\left\{(0\mid 0) - (1\mid\bar{1}) - (\bar{1}\mid 1)\right\} = \sqrt{3}\;\mathcal{O}_{00}\,(0\mid 0)\;.$$

SLJM

$${}^1D_{22} = {}^1D\,(2,0) = \mathcal{O}_{22}\,{}^1D\,(2,0) = (1\mid 1)$$

$${}^3P_{22} = {}^3P\,(1,1) = \mathcal{O}_{22}\,{}^3P\,(1,1) = (1\,0\mid$$

$${}^3P_{11} = \frac{1}{\sqrt{2}}\left\{{}^3P\,(1,0) - {}^3P\,(0,1)\right\} = \sqrt{2}\;\mathcal{O}_{11}\,{}^3P\,(1,0) = \frac{1}{\sqrt{2}}\left\{\frac{1}{\sqrt{2}}\left[(1\mid 0) - (0\mid 1)\right] - (1\,\bar{1}\mid\right\}$$

$${}^3P_{00} = \frac{1}{\sqrt{3}}\left\{{}^3P\,(0,0) - {}^3P(1,-1) - {}^3P\,(-1,1)\right\} = \sqrt{3}\;\mathcal{O}_{00}\,{}^3P\,(0,0)$$

$$= \frac{1}{\sqrt{3}}\left\{\frac{1}{\sqrt{2}}\left[(1\mid\bar{1}) - (\bar{1}\mid 1)\right] - \mid 10) - (0\bar{1}\mid\right\}$$

$${}^1S_{00} = {}^1S\,(0,0) = \mathcal{O}_{00}\,{}^1S\,(0,0) = \frac{1}{\sqrt{3}}\left\{(0\mid 0) - (1\mid\bar{1}) - (\bar{1}\mid 1)\right\}\;.$$

Electrostatic interaction in LS-coupling

$$E\,(^1S) = F_0 + 10\,F_2$$
$$E\,(^1D) = F_0 + F_2$$
$$E\,(^3P) = F_0 - 5\,F_2\ .$$

Spin-orbit interaction in LS-coupling

	$^1S_0$	$^3P_0$	$^3P_1$	$^3P_2$	$^1D_2$
$^1S_0$	0	$-2\sqrt{2}$			
$^3P_0$	$-2\sqrt{2}$	-2			
$^3P_1$			-1		
$^3P_2$				1	$\sqrt{2}$
$^1D_2$				$\sqrt{2}$	0

$\times\ \frac{1}{2}\zeta_{np}$

jj-coupling

$M \diagdown j_1 j_2$	$\frac{3}{2}, \frac{3}{2}$	$\frac{3}{2}, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}$
2	$(\frac{3}{2}, \frac{1}{2}\,\vert$	$(\frac{3}{2}\,\vert\,\frac{1}{2})$	
1	$(\frac{3}{2}, -\frac{1}{2}\,\vert$	$(\frac{3}{2}\,\vert -\frac{1}{2})\ (\frac{1}{2}\,\vert\,\frac{1}{2})$	
0	$(\frac{3}{2}, -\frac{3}{2}\,\vert\ (\frac{1}{2}, -\frac{1}{2}\,\vert$	$(\frac{1}{2}\,\vert -\frac{1}{2})\ (-\frac{1}{2}\,\vert\,\frac{1}{2})$	$\vert\,\frac{1}{2}, -\frac{1}{2})$
-1	$(-\frac{3}{2}, \frac{1}{2}\,\vert$	$(-\frac{3}{2}\,\vert\,\frac{1}{2})\ (-\frac{1}{2}\,\vert -\frac{1}{2})$	
-2	$(-\frac{3}{2}, -\frac{1}{2}\,\vert$	$(-\frac{3}{2}\,\vert -\frac{1}{2})$	

1 1
1 2
2 2 1 $= 2\ (J = 2) + 1\ (J = 1) + 2\ (J = 0)$
1 2
1 1

$$\left(\tfrac{3}{2}, \tfrac{3}{2}; 2, 2\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}\,\right| = \mathcal{O}_{22}\left(\tfrac{3}{2}, \tfrac{1}{2}\,\right|$$
$$\left(\tfrac{3}{2}, \tfrac{1}{2}; 2, 2\right) = \left(\tfrac{3}{2}\,\middle|\,\tfrac{1}{2}\right) = \mathcal{O}_{22}\left(\tfrac{3}{2}\,\middle|\,\tfrac{1}{2}\right)$$
$$\left(\tfrac{3}{2}, \tfrac{1}{2}; 1, 1\right) = \frac{1}{2}\left\{\sqrt{3}\left(\tfrac{3}{2}\,\middle|\,-\tfrac{1}{2}\right) - \left(\tfrac{1}{2}\,\middle|\,\tfrac{1}{2}\right)\right\} = \frac{2}{\sqrt{3}}\,\mathcal{O}_{11}\left(\tfrac{3}{2}\,\middle|\,-\tfrac{1}{2}\right)$$
$$\left(\tfrac{3}{2}, \tfrac{3}{2}; 0, 0\right) = \frac{1}{\sqrt{2}}\left\{\left(\tfrac{3}{2}, -\tfrac{3}{2}\,\right| - \left(\tfrac{1}{2}, -\tfrac{1}{2}\,\right|\right\} = \sqrt{2}\,\mathcal{O}_{00}\left(\tfrac{3}{2}, -\tfrac{3}{2}\,\right|$$
$$\left(\tfrac{1}{2}, \tfrac{1}{2}; 0, 0\right) = \left|\,\tfrac{1}{2}, -\tfrac{1}{2}\right) = \mathcal{O}_{00}\left|\,\tfrac{1}{2}, -\tfrac{1}{2}\right)\ .$$

Transformations

1. Uncoupled determinants

$$\left(\tfrac{3}{2}, \tfrac{1}{2}\,\right| = \sqrt{\frac{2}{3}}\,(10\,| + \frac{1}{\sqrt{3}}\,(1\,|\,1)\,;$$

$$\left|\,\tfrac{1}{2}, -\tfrac{1}{2}\right) = \frac{1}{3}\left\{\sqrt{2}\,(0\bar{1}\,| + \sqrt{2}\,|\,10) - (0\,|\,0) + 2\,(\bar{1}\,|\,1)\right\};$$

$$\left(\tfrac{3}{2}, -\tfrac{3}{2}\,\right| = (1\,|\,\bar{1})\,;$$

$$\left(\tfrac{1}{2}\,\middle|\,\tfrac{1}{2}\right) = -\,(0\,|\,1)\,;$$

$$(\tfrac{3}{2}\,|\,\tfrac{1}{2}) = \frac{1}{\sqrt{3}}(10\,| - \sqrt{\frac{2}{3}}(1\,|\,1); \qquad (\tfrac{1}{2}, -\tfrac{1}{2}\,| = \frac{1}{3}\{\sqrt{2}(0\bar{1}\,| + 2(0\,|\,0) - (\bar{1}\,|\,1) + \sqrt{2}\,|\,10)\};$$

$$(\tfrac{3}{2}| -\tfrac{1}{2}) = \sqrt{\frac{2}{3}}(1\bar{1}\,| - \frac{1}{\sqrt{3}}(1\,|\,0) .$$

2. Coupled JM-functions

	$(\frac{3}{2},\frac{3}{2};0,M)$	$(\frac{1}{2},\frac{1}{2};0\,M)$	
$^1S_{0M}$	$-\sqrt{2}$	-1	$\times \frac{1}{\sqrt{3}}$
$^3P_{0M}$	1	$-\sqrt{2}$	

	$(\frac{3}{2},\frac{3}{2};2,M)$	$(\frac{3}{2},\frac{1}{2};2\,M)$	
$^3P_{2M}$	$\sqrt{2}$	1	$\times \frac{1}{\sqrt{3}}$
$^1D_{2M}$	1	$-\sqrt{2}$	

$$^3P_{1M} = -(\tfrac{3}{2},\tfrac{1}{2};1,M)$$

Spin-Orbit Interaction in jj-Coupling

$$V(\tfrac{3}{2},\tfrac{3}{2}) = \zeta_{np}$$
$$V(\tfrac{3}{2},\tfrac{1}{2}) = -\frac{1}{2}\zeta_{np}$$
$$V(\tfrac{1}{2},\tfrac{1}{2}) = -2\zeta_{np}$$

Electrostatic interaction in jj-coupling

	$(\frac{3}{2},\frac{3}{2};0,M)$	$(\frac{1}{2},\frac{1}{2};0,M)$
$(\frac{3}{2},\frac{3}{2};0,M)$	F_0+5F_2	$5\sqrt{2}\,F_2$
$(\frac{1}{2},\frac{1}{2};0,M)$	$5\sqrt{2}\,F_2$	F_0

	$(\frac{3}{2},\frac{3}{2};2,M)$	$(\frac{3}{2},\frac{1}{2};2,M)$
$(\frac{3}{2},\frac{3}{2};2,M)$	F_0-3F_2	$-2\sqrt{2}\,F_2$
$(\frac{3}{2},\frac{1}{2};2,M)$	$-2\sqrt{2}\,F_2$	F_0-F_2

$$E(\tfrac{3}{2},\tfrac{1}{2};1,M) = F_0 - 5F_2$$

Intermediate coupling

$$\left.\begin{matrix}^1D_2'\\ ^1P_2'\end{matrix}\right\}: F_0 - 2F_2 + \frac{1}{4}\zeta \pm \sqrt{9F_2^2 - \frac{3}{2}F_2\zeta + \frac{9}{16}\zeta^2}$$

$$^3P_1: F_0 - 5F_2 - \frac{1}{2}\zeta$$

$$\left.\begin{matrix}^3P_0'\\ ^1S_0\end{matrix}\right\}: F_0 + \frac{5}{2}F_2 - \frac{1}{2}\zeta \pm \sqrt{\frac{225}{4}F_2^2 + \frac{15}{2}F_2\zeta + \frac{9}{4}\zeta^2}$$

Table 4. p^3

M_L \ M_S	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
2		$(10\,|\,1)$	$(1\,|\,01)$	
1		$(10\,|\,0)$ $(1\bar{1}\,|\,1)$	$(0\,|\,10)$ $(1\,|\,\bar{1}1)$	
0	$(10\bar{1}\,|$	$(10\,|\,\bar{1})$ $(1\bar{1}\,|\,0)$ $(0\bar{1}\,|\,1)$	$(1\,|\,0\bar{1})$ $(\bar{1}\,|\,01)$ $(0\,|\,1\bar{1})$	$|\,10\bar{1})$
−1		$(\bar{1}0\,|\,0)$ $(\bar{1}1\,|\,\bar{1})$	$(0\,|\,\bar{1}0)$ $(\bar{1}\,|\,1\bar{1})$	
−2		$(\bar{1}0\,|\,\bar{1})$	$(\bar{1}\,|\,0\bar{1})$	

$$
\begin{array}{cccc}
 & 1\ 1 & & 1\ 1 & & & & \\
 & 2\ 2 & & 1\ 1 & & 1\ 1 & & \\
1 & 3\ 3 & 1 = & 1\ 1 & + & 1\ 1 & + & 1\ 1\ 1\ 1 = {}^2D + {}^2P + {}^4S \\
 & 2\ 2 & & 1\ 1 & & 1\ 1 & & \\
 & 1\ 1 & & 1\ 1 & & & &
\end{array}
$$

$$
\begin{aligned}
{}^2D\left(2, \tfrac{1}{2}\right) &= (10\,|\,1) \\
{}^2P\left(1, \tfrac{1}{2}\right) &= \frac{1}{\sqrt{2}}\left\{(10\,|\,0) - (1\,\bar{1}\,|\,1)\right\} = \sqrt{2}\ {}^L\mathcal{O}_{11}\,{}^S\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,(10\,|\,0) \\
{}^4S\left(0, \tfrac{3}{2}\right) &= (1\,0\,\bar{1}\,|
\end{aligned}
$$

SLJM

$$
\begin{aligned}
{}^2D_{\frac{5}{2},\frac{5}{2}} &= {}^2D\left(2, \tfrac{1}{2}\right) = \mathcal{O}_{\frac{5}{2},\frac{5}{2}}\,{}^2D\left(2, \tfrac{1}{2}\right) = (1\,0\,|\,1) \\
{}^2D_{\frac{3}{2},\frac{3}{2}} &= \frac{1}{\sqrt{5}}\left\{2\,{}^2D\left(2, -\tfrac{1}{2}\right) - {}^2D\left(1, \tfrac{1}{2}\right)\right\} = \frac{\sqrt{5}}{2}\,\mathcal{O}_{\frac{3}{2},\frac{3}{2}}\,{}^2D\left(2, -\tfrac{1}{2}\right) \\
&= -\frac{1}{\sqrt{10}}\left\{2\sqrt{2}\,(1\,|\,1\,0) + (1\,\bar{1}\,|\,1) + (1\,0\,|\,0)\right\} \\
{}^2P_{\frac{3}{2},\frac{3}{2}} &= {}^2P\left(1, \tfrac{1}{2}\right) = \mathcal{O}_{\frac{3}{2},\frac{3}{2}}\,{}^2P\left(1, \tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\left\{(1\,0\,|\,0) - (1\,\bar{1}\,|\,1)\right\} \\
{}^2P_{\frac{1}{2},\frac{1}{2}} &= \frac{1}{\sqrt{3}}\left\{{}^2P\left(0, \tfrac{1}{2}\right) - \sqrt{2}\,{}^2P\left(1, -\tfrac{1}{2}\right)\right\} = \sqrt{3}\,\mathcal{O}_{\frac{1}{2},\frac{1}{2}}\,{}^2P\left(0, \tfrac{1}{2}\right) \\
&= \frac{1}{\sqrt{3}}\left\{\frac{1}{\sqrt{2}}\left[(1\,0\,|\,\bar{1}) - (0\,\bar{1}\,|\,1)\right] + (0\,|\,1\,0) - (1\,|\,1\bar{1})\right\} \\
{}^4S_{\frac{3}{2},\frac{3}{2}} &= {}^4S\left(0, \tfrac{3}{2}\right) = \mathcal{O}_{\frac{3}{2},\frac{3}{2}}\,{}^4S\left(0, \tfrac{3}{2}\right) = (1\,0\,\bar{1}\,|\ .
\end{aligned}
$$

Electrostatic interaction in LS-coupling

$$
\begin{aligned}
E\,({}^2P) &= 3\,F_0 \\
E\,({}^2D) &= 3\,F_0 - 6\,F_2 \\
E\,({}^4S) &= 3\,F_0 - 15\,F_2\ .
\end{aligned}
$$

Spin-orbit interaction in LS-coupling

	${}^2P_{\frac{1}{2}}$	${}^4S_{\frac{3}{2}}$	${}^2P_{\frac{3}{2}}$	${}^2D_{\frac{3}{2}}$	${}^2D_{\frac{5}{2}}$
${}^2P_{\frac{1}{2}}$	0				
${}^4S_{\frac{3}{2}}$		0	2	0	
${}^2P_{\frac{3}{2}}$		2	0	$-\sqrt{5}$	
${}^2D_{\frac{3}{2}}$		0	$-\sqrt{5}$	0	
${}^2D_{\frac{5}{2}}$					0

$\times\ \frac{1}{2}\,\zeta_{np}$

jj-coupling

M \ $j_1\, j_2\, j_3$	$\frac{3}{2}, \frac{3}{2}, \frac{3}{2}$	$\frac{3}{2}, \frac{3}{2}, \frac{1}{2}$	$\frac{3}{2}, \frac{1}{2}, \frac{1}{2}$
$\frac{5}{2}$		$\left(\frac{3}{2}, \frac{1}{2} \middle\vert \frac{1}{2}\right)$	
$\frac{3}{2}$	$\left(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}\right\vert$	$\left(\frac{3}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}\right)$ $\left(\frac{3}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}\right)$	$\left(\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}\right)$
$\frac{1}{2}$	$\left(\frac{3}{2}, \frac{1}{2}, -\frac{3}{2}\right\vert$	$\left(\frac{3}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}\right)$ $\left(\frac{1}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}\right)$ $\left(\frac{3}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}\right)$	$\left(\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}\right)$
$-\frac{1}{2}$	$\left(\frac{3}{2}, -\frac{1}{2}, -\frac{3}{2}\right\vert$	$\left(-\frac{3}{2}, \frac{3}{2} \middle\vert -\frac{1}{2}\right)$ $\left(-\frac{1}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}\right)$ $\left(-\frac{3}{2}, \frac{1}{2} \middle\vert \frac{1}{2}\right)$	$\left(-\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}\right)$
$-\frac{3}{2}$	$\left(\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}\right\vert$	$\left(-\frac{3}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}\right)$ $\left(-\frac{3}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}\right)$	$\left(-\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}\right)$
$-\frac{5}{2}$		$\left(-\frac{3}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}\right)$	

$$\begin{matrix} & 1 & \\ 1 & 2 & 1 \\ 1 & 3 & 1 \\ 1 & 3 & 1 \\ 1 & 2 & 1 \\ & 1 & \end{matrix} = \begin{matrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{matrix} + \begin{matrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{matrix} + \begin{matrix} 1 \\ 1 \end{matrix} = 1\left(J = \tfrac{5}{2}\right) + 3\left(J = \tfrac{3}{2}\right) + 1\left(J = \tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}; \tfrac{5}{2}, \tfrac{5}{2}\right) = \left(\tfrac{3}{2}, \tfrac{1}{2} \middle\vert \tfrac{1}{2}\right) = \mathcal{O}_{\frac{5}{2}, \frac{5}{2}} \left(\tfrac{3}{2}, \tfrac{1}{2} \middle\vert \tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}; \tfrac{3}{2}, \tfrac{3}{2}\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\right\vert = \mathcal{O}_{\frac{3}{2}, \frac{3}{2}} \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\right\vert$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}; \tfrac{3}{2}, \tfrac{3}{2}\right) = \frac{1}{\sqrt{5}}\left\{2\left(\tfrac{3}{2}, \tfrac{1}{2} \middle\vert -\tfrac{1}{2}\right) - \left(\tfrac{3}{2}, -\tfrac{1}{2} \middle\vert \tfrac{1}{2}\right)\right\} = \frac{\sqrt{5}}{2}\, \mathcal{O}_{\frac{3}{2}, \frac{3}{2}} \left(\tfrac{3}{2}, \tfrac{1}{2} \middle\vert -\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}; \tfrac{3}{2}, \tfrac{3}{2}\right) = \left(\tfrac{3}{2} \middle\vert \tfrac{1}{2}, -\tfrac{1}{2}\right) = \mathcal{O}_{\frac{3}{2}, \frac{3}{2}} \left(\tfrac{3}{2} \middle\vert \tfrac{1}{2}, -\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\left\{\left(\tfrac{3}{2}, -\tfrac{3}{2} \middle\vert \tfrac{1}{2}\right) - \left(\tfrac{1}{2}, -\tfrac{1}{2} \middle\vert \tfrac{1}{2}\right)\right\} = \sqrt{2}\, \mathcal{O}_{\frac{1}{2}, \frac{1}{2}} \left(\tfrac{3}{2}, -\tfrac{3}{2} \middle\vert \tfrac{1}{2}\right)$$

Transformations

1. Uncoupled determinants

	$(10\bar{1}\vert$	$(10\vert 0)$	$(1\bar{1}\vert 1)$	$(1\vert 10)$
$\left(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}\right\vert$	$\sqrt{2}$	2	-1	$\sqrt{2}$
$\left(\frac{3}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}\right)$	2	$-\sqrt{2}$	$-\sqrt{2}$	-1
$\left(\frac{3}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}\right)$	-1	$-\sqrt{2}$	$-\sqrt{2}$	2
$\left(\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}\right)$	$\sqrt{2}$	-1	2	$\sqrt{2}$

$\times \frac{1}{3}$;

$$\left(\tfrac{3}{2}, \tfrac{1}{2} \middle\vert \tfrac{1}{2}\right) = -(10 \vert 1)$$

$$\left(\tfrac{3}{2}, -\tfrac{3}{2} \middle\vert \tfrac{1}{2}\right) = -\frac{1}{\sqrt{3}}(10 \vert \bar{1}) - \sqrt{\frac{2}{3}}(1 \vert \bar{1}\, 1)$$

$$\left(\tfrac{1}{2}, -\tfrac{1}{2} \middle\vert \tfrac{1}{2}\right) = \sqrt{\frac{2}{3}}(0 \vert 10) - \frac{1}{\sqrt{3}}(0\, \bar{1} \vert 1)$$

2. Coupled JM-functions

$${}^2D_{\frac{5}{2}, M} = -\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}; \tfrac{5}{2}, M\right) \qquad {}^2P_{\frac{1}{2}, M} = -\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}; \tfrac{1}{2}, M\right)$$

	$\left(\frac{3}{2}, \frac{3}{2}, \frac{3}{2}; \frac{3}{2}, M\right)$	$\left(\frac{3}{2}, \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, M\right)$	$\left(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}; \frac{3}{2}, M\right)$
${}^4S_{\frac{3}{2}, M}$	2	$\sqrt{10}$	2
${}^2P_{\frac{3}{2}, M}$	3	0	-3
${}^2D_{\frac{3}{2}, M}$	$-\sqrt{5}$	$2\sqrt{2}$	$-\sqrt{5}$

$\times \frac{1}{3\sqrt{2}}$

Spin-orbit interaction in jj-coupling

$$V\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2}\right) = \frac{3}{2}\,\zeta_{np}$$
$$V\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2}\right) = 0$$
$$V\left(\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2}\right) = -\frac{3}{2}\,\zeta_{np}$$

Electrostatic interaction in jj-coupling

$$E\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};\tfrac{5}{2},M\right) = 3\,F_0 - 6\,F_2 \qquad E\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};\tfrac{1}{2},M\right) = 3\,F_0$$

	$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};\tfrac{3}{2},M\right)$	$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};\tfrac{3}{2},M\right)$	$\left(\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2};\tfrac{3}{2},M\right)$
$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};\tfrac{3}{2},M\right)$	$3\,F_0 - 5\,F_2$	$-\sqrt{10}\,F_2$	$-5\,F_2$
$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};\tfrac{3}{2},M\right)$	$-\sqrt{10}\,F_2$	$3\,F_0 - 11\,F_2$	$-\sqrt{10}\,F_2$
$\left(\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2};\tfrac{3}{2},M\right)$	$-5\,F_2$	$-\sqrt{10}\,F_2$	$3\,F_0 - 5\,F_2$

Intermediate coupling

$$^2D_{\frac{5}{2}} \;:\; 3\,F_0 - 6\,F_2$$
$$^2P_{\frac{1}{2}} \;:\; 3\,F_0$$

$$\left.\begin{matrix} ^4S'_{\frac{3}{2}} \\ ^2P'_{\frac{3}{2}} \\ ^2D'_{\frac{3}{2}} \end{matrix}\right\} : 3\,F_0 + \text{roots of equation } \lambda^3 + 21 F_2 \lambda^2 + (90 F_2^2 - \tfrac{9}{4}\zeta^2)\,\lambda - \frac{99}{4}\,F_2\zeta^2 = 0.$$

Table 5. p^4

The correspondence between configurations p^4 and p^2 is used throughout this table. Only information not directly available in Tab. 3 is given.

$$^1D\,(2,0) = (1\,0 \mid 1\,0)$$
$$^3P\,(1,1) = (1\,0\,\bar{1} \mid 1)$$
$$^1S\;(0,0) = \frac{1}{\sqrt{3}}\left\{(1\,\bar{1} \mid 1\,\bar{1}) - (0\,\bar{1} \mid 1\,0) - (1\,0 \mid 0\,\bar{1})\right\} = \sqrt{3}\;\mathcal{O}_{00}\,(1\,\bar{1} \mid 1\,\bar{1})$$

SLJM

$$^1D_{22} = (1\,0 \mid 1\,0)$$
$$^3P_{22} = (1\,0\,\bar{1} \mid 1)$$
$$^3P_{11} = \frac{1}{2}\,(1\,\bar{1} \mid 1\,0) - \frac{1}{2}\,(1\,0 \mid 1\,\bar{1}) - \frac{1}{\sqrt{2}}\,(1\,0\,\bar{1} \mid 0)$$
$$^3P_{00} = \frac{1}{\sqrt{6}}\,(0\,\bar{1} \mid 1\,0) - \frac{1}{\sqrt{6}}\,(1\,0 \mid 0\,\bar{1}) - \frac{1}{\sqrt{3}}\,(1 \mid 1\,0\,\bar{1}) - \frac{1}{\sqrt{3}}\,(1\,0\,\bar{1} \mid \bar{1})$$
$$^1S_{00} = \frac{1}{\sqrt{3}}\,\left\{(1\,\bar{1} \mid 1\,1) - (0\,\bar{1} \mid 1\,0) - (1\,0 \mid 0\,1)\right\}$$

jj-coupling

$$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2};2,2\right)=\left(\tfrac{3}{2},\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};2,2\right)=\left(\tfrac{3}{2},\tfrac{3}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};1,1\right)=\frac{1}{2}\left\{\sqrt{3}\left(\tfrac{3}{2},\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2}\right)-\left(\tfrac{3}{2},\tfrac{1}{2},-\tfrac{3}{2}\,\middle|\,\tfrac{1}{2}\right)\right\}$$

$$=\frac{2}{\sqrt{3}}\,\mathcal{O}_{11}\left(\tfrac{3}{2},\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,-\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2};0,0\right)=\frac{1}{\sqrt{2}}\left\{\left(\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right)-\left(\tfrac{3}{2},-\tfrac{3}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right)\right\}$$

$$=\sqrt{2}\,\mathcal{O}_{00}\left(\tfrac{1}{2},-\tfrac{1}{2}\,\middle|\,\tfrac{1}{2},-\tfrac{1}{2}\right)$$

$$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};0,0\right)\ \left(\tfrac{3}{2},\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{3}{2}\right|$$

Correspondences

P^4	P^2
$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2};J,M\right)$	$\left(\tfrac{1}{2},\tfrac{1}{2};J,M\right)$
$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2};J,M\right)$	$-\left(\tfrac{3}{2},\tfrac{1}{2};J,M\right)$
$\left(\tfrac{3}{2},\tfrac{3}{2},\tfrac{1}{2},\tfrac{1}{2};J,M\right)$	$\left(\tfrac{3}{2},\tfrac{3}{2};J,M\right)$

Interactions:

Substitute $6F_0-10F_2$ for F_0 and $-\zeta$ for ζ in Tab. 3.

Table 6. *sp*

$M_L \diagdown M_S$	1	0	−1
1	$(1\,s\,\vert$	$(1\,\vert\,s)\ (s\,\vert\,1)$	$\vert\,1\,s)$
0	$(0\,s\,\vert$	$(0\,\vert\,s)\ (s\,\vert\,0)$	$\vert\,0\,s)$
−1	$(\bar{1}\,s\,\vert$	$(\bar{1}\,\vert\,s)\ (s\,\vert\,\bar{1})$	$\vert\,\bar{1}\,s)$

$$\begin{matrix}1&2&1\\1&2&1\\1&2&1\end{matrix}=\begin{matrix}1&1&1\\1&1&1\\1&1&1\end{matrix}+\begin{matrix}1\\1\\1\end{matrix}={}^3P+{}^1P$$

$${}^3P\,(1,1)=(1\,s\,|$$

$${}^1P\,(1,0)=\frac{1}{\sqrt{2}}\left\{(1\,|\,s)+(s\,|\,1)\right\}=\sqrt{2}\,\mathcal{O}_{00}\,(1\,|\,s)$$

SLJM

$${}^3P_{22}={}^3P(1,1)=\mathcal{O}_{22}\,{}^3P\,(1,1)=(1\,s\,|$$

$${}^3P_{11}=\frac{1}{\sqrt{2}}\left\{{}^3P\,(1,0)-{}^3P\,(0,1)\right\}=\sqrt{2}\,\mathcal{O}_{11}\,{}^3P\,(1,0)=\frac{1}{2}\,(1\,|\,s)-\frac{1}{2}\,(s\,|\,1)-\frac{1}{\sqrt{2}}\,(0\,s|$$

$${}^1P_{11}={}^1P\,(1,0)=\mathcal{O}_{11}\,{}^1P\,(1,0)=\frac{1}{\sqrt{2}}\left\{(1\,|\,s)+(s\,|\,1)\right\}$$

$${}^3P_{00}=\frac{1}{\sqrt{3}}\left\{{}^3P\,(0,0)-{}^3P\,(1,-1)-{}^3P\,(-1,1)\right\}=\sqrt{3}\,\mathcal{O}_{00}\,{}^3P\,(0,0)$$

$$=\frac{1}{\sqrt{6}}\,(0\,|\,s)-\frac{1}{\sqrt{6}}\,(s\,|\,0)-\frac{1}{\sqrt{3}}\,|1\,s)-\frac{1}{\sqrt{3}}\,(\bar{1}\,s\,|$$

Electrostatic interaction in LS-coupling

$$E\,(^1P) = F_0 + G_1$$
$$E\,(^3P) = F_0 - G_1$$

Spin-orbit interaction in LS-coupling

	$^3P_2$	$^3P_1$	$^1P_1$	$^3P_0$
$^3P_2$	1			
$^3P_1$		-1	$\sqrt{2}$	
$^1P_1$		$\sqrt{2}$	0	
$^3P_0$				-2

$\times \frac{1}{2}\zeta_{np}$

jj-coupling (the s-electron is underlined)

$M \setminus j_1 j_2$	$\tfrac{3}{2}, \underline{\tfrac{1}{2}}$	$\tfrac{1}{2}, \underline{\tfrac{1}{2}}$
2	$(\tfrac{3}{2}\,\vert\,\underline{\tfrac{1}{2}})$	
1	$(\tfrac{3}{2}\,\vert -\underline{\tfrac{1}{2}})\ (\tfrac{1}{2}\,\vert\,\underline{\tfrac{1}{2}})$	$\vert\,\tfrac{1}{2}, \underline{\tfrac{1}{2}})$
0	$(\tfrac{1}{2}\,\vert -\underline{\tfrac{1}{2}})\ (-\tfrac{1}{2}\,\vert\,\underline{\tfrac{1}{2}})$	$\vert\,\tfrac{1}{2}, -\underline{\tfrac{1}{2}})\ \vert -\tfrac{1}{2}, \underline{\tfrac{1}{2}})$
-1	$(-\tfrac{3}{2}\,\vert\,\underline{\tfrac{1}{2}})\ (-\tfrac{1}{2}\,\vert -\underline{\tfrac{1}{2}})$	$\vert -\tfrac{1}{2}, -\underline{\tfrac{1}{2}})$
-2	$(-\tfrac{3}{2}\,\vert -\underline{\tfrac{1}{2}})$	

1
2 1
2 2 $= 1\ (J = 2) + 2\ (J = 1) + 1\ (J = 0)$
2 1
1

$$(\tfrac{3}{2}, \underline{\tfrac{1}{2}}; 2, 2) = (\tfrac{3}{2}\,|\,\underline{\tfrac{1}{2}}) = \mathcal{O}_{22}\,(\tfrac{3}{2}\,|\,\underline{\tfrac{1}{2}})$$
$$(\tfrac{3}{2}, \underline{\tfrac{1}{2}}; 1, 1) = \frac{1}{2}\left\{(\tfrac{1}{2}\,|\,\underline{\tfrac{1}{2}}) - \sqrt{3}\,(\tfrac{3}{2}\,| -\underline{\tfrac{1}{2}})\right\} = 2\,\mathcal{O}_{11}\,(\tfrac{1}{2}\,|\,\underline{\tfrac{1}{2}})$$
$$(\tfrac{1}{2}, \underline{\tfrac{1}{2}}; 1, 1) = |\,\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = \mathcal{O}_{11}\,|\,\tfrac{1}{2}, \underline{\tfrac{1}{2}})$$
$$(\tfrac{1}{2}, \underline{\tfrac{1}{2}}; 0, 0) = \frac{1}{\sqrt{2}}\left\{|\tfrac{1}{2}, -\underline{\tfrac{1}{2}}) - |-\tfrac{1}{2}, \underline{\tfrac{1}{2}})\right\} = \sqrt{2}\,\mathcal{O}_{00}\,|\,\tfrac{1}{2}, -\underline{\tfrac{1}{2}})$$

Transformations

1. Uncoupled determinants

$$(\tfrac{3}{2}\,|\,\underline{\tfrac{1}{2}}) = (1\,s|\ ; \qquad |\,\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = \frac{1}{\sqrt{3}}\,(0\,s| + \sqrt{\frac{2}{3}}\,(s\,|\,1)$$
$$(\tfrac{1}{2}\,|\,\underline{\tfrac{1}{2}}) = \sqrt{\frac{2}{3}}\,(0\,s| - \sqrt{\frac{1}{3}}\,(s\,|\,1)\ |\,\tfrac{1}{2}, -\underline{\tfrac{1}{2}}) = \frac{1}{\sqrt{3}}\,(0\,|\,s) - \sqrt{\frac{2}{3}}\,|\,1\,s)$$

2. Coupled JM-functions

$$^3P_{2M} = (\tfrac{3}{2}, \underline{\tfrac{1}{2}}; 2, M) \qquad ^3P_{0M} = (\tfrac{1}{2}, \underline{\tfrac{1}{2}}; 0, M)$$

$$\begin{array}{c|cc|}
 & \left(\tfrac{3}{2},\tfrac{1}{2};1,M\right) & \left(\tfrac{1}{2},\tfrac{1}{2};1,M\right) \\
\hline
{}^3P_{1M} & -1 & -\sqrt{2} \\
{}^1P_{1M} & -\sqrt{2} & 1 \\
\hline
\end{array} \times \frac{1}{\sqrt{3}}$$

Spin-orbit interaction in jj-coupling

$$V\left(\tfrac{3}{2},\tfrac{1}{2}\right) = \frac{1}{2}\zeta_{np}$$

$$V\left(\tfrac{1}{2},\tfrac{1}{2}\right) = -\zeta_{np}.$$

Electrostatic interaction in jj-coupling

$$E\left(\tfrac{3}{2},\tfrac{1}{2};2,M\right) = F_0 - G_1 \qquad E\left(\tfrac{1}{2},\tfrac{1}{2};0,M\right) = F_0 - G_1$$

$$\begin{array}{c|cc|}
 & \left(\tfrac{3}{2},\tfrac{1}{2};1,M\right) & \left(\tfrac{1}{2},\tfrac{1}{2};1,M\right) \\
\hline
\left(\tfrac{3}{2},\tfrac{1}{2};1,M\right) & F_0 + \frac{1}{3}G_1 & -\frac{2\sqrt{2}}{3}G_1 \\
\left(\tfrac{1}{2},\tfrac{1}{2};1,M\right) & -\frac{2\sqrt{2}}{3}G_1 & F_0 - \frac{1}{3}G_1 \\
\hline
\end{array}$$

Intermediate coupling

$${}^3P_{22} \;:\; F_0 - G_1 + \frac{1}{2}\zeta$$

$$\left.\begin{array}{l}{}^3P_{11}\\ {}^1P_{11}\end{array}\right\} : \; F_0 - \frac{1}{4}\zeta \pm \sqrt{G_1^2 + \frac{1}{2}\zeta G_1 + \frac{9}{16}\zeta^2}$$

$${}^3P_{00} \;:\; F_0 - G_1 - \zeta\;.$$

Table 7. sp^2

$M_L \setminus M_S$	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
2		$(1\,s \vert 1)$	$(1 \vert 1\,s)$	
1	$(10\,s \vert$	$(10 \vert s)$ $(0\,s \vert 1)$ $(1\,s \vert 0)$	$(1 \vert s\,0)$ $(0 \vert s\,1)$ $(s \vert 10)$	$\vert 10\,s)$
0	$(1\bar{1}\,s \vert$	$(1\bar{1} \vert s)$ $(1\,s \vert \bar{1})$ $(\bar{1}\,s \vert 1)$ $(0\,s \vert 0)$	$(1 \vert \bar{1}\,s)$ $(\bar{1} \vert 1\,s)$ $(s \vert 1\bar{1})$ $(0 \vert 0\,s)$	$\vert 1\bar{1}\,s)$
−1	$(0\bar{1}\,s \vert$	$(\bar{1}0 \vert s)$ $(0\,s \vert \bar{1})$ $(\bar{1}\,s \vert 0)$	$(\bar{1} \vert s\,0)$ $(0 \vert s\,\bar{1})$ $(s \vert \bar{1}0)$	$\vert 0\bar{1}\,s)$
−2		$(\bar{1}\,s \vert \bar{1})$	$(\bar{1} \vert \bar{1}\,s)$	

$$\begin{array}{cccc}
 & 1 & 1 & \\
1 & 3 & 3 & 1 \\
1 & 4 & 4 & 1 \\
1 & 3 & 3 & 1 \\
 & 1 & 1 &
\end{array}
=
\begin{array}{cc}
1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1
\end{array}
+
\begin{array}{cccc}
 & & & \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ & & &
\end{array}
+
\begin{array}{cc}
 & \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \\ &
\end{array}
+
\begin{array}{cc}
 & \\ & \\ 1 & 1 \\ & \\ &
\end{array}
= {}^2D + {}^4P + {}^2P + {}^2S$$

$$^2D\ (2, \tfrac{1}{2}) = (1\,s\,|\,1)$$
$$^4P\ (1, \tfrac{3}{2}) = (1 0\,s\,|$$
$$^2P\ (1, \tfrac{1}{2}) = \frac{1}{\sqrt{6}}\left\{2\,(1 0\,|\,s) - (0\,s\,|\,1) + (1\,s\,|\,0)\right\} = \sqrt{\frac{3}{2}}\,{}^S\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,(1 0\,|\,s)$$
$$^2S\ (0, \tfrac{1}{2}) = \frac{1}{\sqrt{3}}\left\{(0\,s\,|\,0) - (1\,s\,|\,\overline{1}) - (\overline{1}\,s\,|\,1)\right\} = \sqrt{3}\,{}^L\mathcal{O}_{00}\,(0\,s\,|\,0)\ .$$

SLJM

$$^2D_{\frac{5}{2},\frac{5}{2}} = {}^2D\left(2, \tfrac{1}{2}\right) = \mathcal{O}_{\frac{5}{2},\frac{5}{2}}\,{}^2D\left(2, \tfrac{1}{2}\right) = (1\,s\,|\,1)$$
$$^4P_{\frac{5}{2},\frac{5}{2}} = {}^4P\left(1, \tfrac{3}{2}\right) = \mathcal{O}_{\frac{5}{2},\frac{5}{2}}\,{}^4P\left(1, \tfrac{3}{2}\right) = (1\,0\,s\,|$$

$$^2D_{\frac{3}{2}\frac{3}{2}} = \frac{1}{\sqrt{5}}\left\{{}^2D\left(1, \tfrac{1}{2}\right) - 2\,{}^2D\left(2, -\tfrac{1}{2}\right)\right\} = \sqrt{5}\,\mathcal{O}_{\frac{3}{2}\frac{3}{2}}\,{}^2D\left(1, \tfrac{1}{2}\right)$$
$$= \frac{1}{\sqrt{10}}\left\{(1\,s\,|\,0) + (0\,s\,|\,1)\right\} - \frac{2}{\sqrt{5}}\,(1\,|\,s\,1)$$

$$^4P_{\frac{3}{2}\frac{3}{2}} = \frac{1}{\sqrt{5}}\left\{\sqrt{2}\,{}^4P\left(1, \tfrac{1}{2}\right) - \sqrt{3}\,{}^4P\left(0, \tfrac{3}{2}\right)\right\} = \sqrt{\frac{5}{2}}\,\mathcal{O}_{\frac{3}{2}\frac{3}{2}}\,{}^4P\left(1, \tfrac{1}{2}\right)$$
$$= \sqrt{\frac{2}{15}}\left\{(1\,0\,|\,s) - (1\,s\,|\,0) + (0\,s\,|\,1)\right\} - \sqrt{\frac{3}{5}}\,(1\,\overline{1}\,s\,|$$

$$^2P_{\frac{3}{2}\frac{3}{2}} = {}^2P\left(1, \tfrac{1}{2}\right) = \mathcal{O}_{\frac{3}{2}\frac{3}{2}}\,{}^2P\left(1, \tfrac{1}{2}\right) = \frac{1}{\sqrt{6}}\left\{2\,(1\,0\,|\,s) - (0\,s\,|\,1) + (1\,s\,|\,0)\right\}$$

$$^4P_{\frac{1}{2}\frac{1}{2}} = \frac{1}{\sqrt{6}}\left\{\sqrt{2}\,{}^4P\left(0, \tfrac{1}{2}\right) - {}^4P\left(1, -\tfrac{1}{2}\right) - \sqrt{3}\,{}^4P\left(-1, \tfrac{3}{2}\right)\right\} = \sqrt{3}\,\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,{}^4P\left(0, \tfrac{1}{2}\right)$$
$$= \frac{1}{3}\left\{(1\,\overline{1}\,|\,s) - (1\,s\,|\,\overline{1}) - (s\,\overline{1}\,|\,1)\right\} -$$
$$- \frac{1}{3\sqrt{2}}\left\{(0\,|\,s\,1) - (1\,|\,s\,0) - (s\,|\,0\,1)\right\} - \frac{1}{\sqrt{2}}\,(0\,\overline{1}\,s\,|$$

$$^2P_{\frac{1}{2}\frac{1}{2}} = \frac{1}{\sqrt{3}}\left\{{}^2P\left(0, \tfrac{1}{2}\right) - \sqrt{2}\,{}^2P\left(1, -\tfrac{1}{2}\right)\right\} = \sqrt{3}\,\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,{}^2P\left(0, \tfrac{1}{2}\right)$$
$$= \frac{1}{3\sqrt{2}}\left\{2(1\,\overline{1}\,|\,s) - (\overline{1}\,s\,|\,1) + (1\,s\,|\,\overline{1})\right\} - \frac{1}{3}\left\{(1\,|\,0\,s) - (0\,|\,1\,s) + 2\,(s\,|\,0\,1)\right\}$$

$$^2S_{\frac{1}{2}\frac{1}{2}} = {}^2S\left(0, \tfrac{1}{2}\right) = \mathcal{O}_{\frac{1}{2}\frac{1}{2}}\,{}^2S\left(0, \tfrac{1}{2}\right) = \frac{1}{\sqrt{3}}\left\{(0\,s\,|\,0) - (1\,s\,|\,\overline{1}) - (\overline{1}\,s\,|\,1)\right\}$$

Electrostatic interaction in LS-coupling

$$E\ (^2D) = F_0 + F_2 - G_1$$
$$E\ (^4P) = F_0 - 5\,F_2 - 2\,G_1$$
$$E\ (^2P) = F_0 - 5\,F_2 + G_1$$
$$E\ (^2S) = F_0 + 10\,F_2 - G_1$$

$$\left\{F_0 = F_0\,(np, np) + 2\,F_0\,(ns, np),\ G_1 = G_1\,(ns, np)\right\}$$

Spin-orbit interaction in LS-coupling

	$^2D_{\frac{5}{2}}$	$^4P_{\frac{5}{2}}$
$^2D_{\frac{5}{2}}$	0	$-\sqrt{2}$
$^4P_{\frac{5}{2}}$	$-\sqrt{2}$	1

$\times\ \frac{1}{2}\,\zeta_{np}$

$$
\begin{array}{c|ccc|}
 & {}^2D_{\frac32} & {}^4P_{\frac32} & {}^2P_{\frac32} \\
\hline
{}^2D_{\frac32} & 0 & \sqrt{3} & \sqrt{15} \\
{}^4P_{\frac32} & \sqrt{3} & -2 & \sqrt{5} \\
{}^2P_{\frac32} & \sqrt{15} & \sqrt{5} & 2 \\
\hline
\end{array} \times \frac{1}{6}\zeta_{np}
\qquad
\begin{array}{c|ccc|}
 & {}^4P_{\frac12} & {}^2P_{\frac12} & {}^2S_{\frac12} \\
\hline
{}^4P_{\frac12} & -5 & \sqrt{2} & 4\sqrt{3} \\
{}^2P_{\frac12} & \sqrt{2} & -4 & -2\sqrt{6} \\
{}^2S_{\frac12} & 4\sqrt{3} & -2\sqrt{6} & 0 \\
\hline
\end{array} \times \frac{1}{6}\zeta_{np}
$$

jj-coupling (the *s*-electron is underlined)

M \ $j_1 j_2 j_3$	$\frac32, \frac32, \underline{\frac12}$	$\frac32, \frac12, \underline{\frac12}$	$\frac12, \frac12, \underline{\frac12}$
$\frac52$	$(\frac32, \frac12 \mid \underline{\frac12})$	$(\frac32 \mid \frac12, \underline{\frac12})$	
$\frac32$	$(\frac32, -\frac12 \mid \underline{\frac12})$ $(\frac32, \frac12 \mid -\underline{\frac12})$	$(\frac32 \mid -\frac12, \underline{\frac12})$ $(\frac32 \mid \frac12, -\underline{\frac12})$ $(\frac12 \mid \frac12, \underline{\frac12})$	
$\frac12$	$(\frac32, -\frac32 \mid \underline{\frac12})$ $(\frac32, -\frac12 \mid -\underline{\frac12})$ $(\frac12, -\frac12 \mid \underline{\frac12})$	$(\frac32 \mid -\frac12, -\underline{\frac12})$ $(\frac12 \mid \frac12, -\underline{\frac12})$ $(\frac12 \mid -\frac12, \underline{\frac12})$ $(-\frac12 \mid \frac12, \underline{\frac12})$	$\mid \frac12, -\frac12, \underline{\frac12})$
$-\frac12$	$(\frac32, -\frac32 \mid -\underline{\frac12})$ $(\frac12, -\frac32 \mid \underline{\frac12})$ $(\frac12, -\frac12 \mid -\underline{\frac12})$	$(-\frac32 \mid \frac12, \underline{\frac12})$ $(-\frac12 \mid -\frac12, \underline{\frac12})$ $(-\frac12 \mid \frac12, -\underline{\frac12})$ $(\frac12 \mid -\frac12, -\underline{\frac12})$	$\mid \frac12, -\frac12, -\underline{\frac12})$
$-\frac32$	$(\frac12, -\frac32 \mid -\underline{\frac12})$ $(-\frac12, -\frac32 \mid \underline{\frac12})$	$(-\frac32 \mid \frac12, -\underline{\frac12})$ $(-\frac32 \mid -\frac12, \underline{\frac12})$ $(-\frac12 \mid -\frac12, -\underline{\frac12})$	
$-\frac52$	$(-\frac12, -\frac32 \mid -\underline{\frac12})$	$(-\frac32 \mid -\frac12, -\underline{\frac12})$	

$$
\begin{array}{ccc}
1 & 1 & \\
2 & 3 & \\
3 & 4 & 1 \\
3 & 4 & 1 \\
2 & 3 & \\
1 & 1 &
\end{array}
=
\begin{array}{cc}
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1 \\
1 & 1
\end{array}
+
\begin{array}{cc}
 & \\
1 & 2 \\
1 & 2 \\
1 & 2 \\
1 & 2 \\
 &
\end{array}
+
\begin{array}{ccc}
1 & 1 & 1 \\
1 & 1 & 1
\end{array}
= 2\left(J = \tfrac52\right) + 3\left(J = \tfrac32\right) + 3\left(J = \tfrac12\right)
$$

$$\left(\tfrac32, \tfrac32, \underline{\tfrac12}; \tfrac52, \tfrac52\right) = \left(\tfrac32, \tfrac12 \mid \underline{\tfrac12}\right) = \mathcal{O}_{\frac52 \frac52}\left(\tfrac32, \tfrac12 \mid \underline{\tfrac12}\right)$$

$$\left(\tfrac32, \tfrac12, \underline{\tfrac12}; \tfrac52, \tfrac52\right) = \left(\tfrac32 \mid \tfrac12, \underline{\tfrac12}\right) = \mathcal{O}_{\frac52 \frac52}\left(\tfrac32 \mid \tfrac12\ \underline{\tfrac12}\right)$$

$$\left(\tfrac32, \tfrac32, \underline{\tfrac12}; \tfrac32, \tfrac32\right) = \frac{1}{\sqrt{5}}\left\{\left(\tfrac32, -\tfrac12 \mid \underline{\tfrac12}\right) - 2\left(\tfrac32, \tfrac12 \mid -\underline{\tfrac12}\right)\right\} = \sqrt{5}\,\mathcal{O}_{\frac32 \frac32}\left(\tfrac32, -\tfrac12 \mid \underline{\tfrac12}\right)$$

$$\left(\tfrac32, \tfrac12, \underline{\tfrac12}; \tfrac32, \tfrac32\right)' = \frac{1}{2\sqrt{5}}\left\{4\left(\tfrac32 \mid -\tfrac12, \underline{\tfrac12}\right) - \sqrt{3}\left(\tfrac12 \mid \tfrac12, \underline{\tfrac12}\right) - \left(\tfrac32 \mid \tfrac12, -\underline{\tfrac12}\right)\right\}$$

$$= \frac{\sqrt{5}}{2}\,\mathcal{O}_{\frac32 \frac32}\left(\tfrac32 \mid -\tfrac12, \underline{\tfrac12}\right)$$

$$\left(\tfrac32, \tfrac12, \underline{\tfrac12}; \tfrac32, \tfrac32\right)'' = \frac{1}{\sqrt{10}}\left\{2\left(\tfrac12 \mid \tfrac12, \underline{\tfrac12}\right) - \sqrt{3}\left(\tfrac32 \mid -\tfrac12, \underline{\tfrac12}\right) - \sqrt{3}\left(\tfrac32 \mid \tfrac12, -\underline{\tfrac12}\right)\right\}$$

$$= \sqrt{\frac{5}{2}}\,\mathcal{O}_{\frac32 \frac32}\left(\tfrac12 \mid \tfrac12, \underline{\tfrac12}\right)$$

Orthogonalization of the two latter functions yields:

$$\left(\tfrac32, \tfrac12, \underline{\tfrac12}; \tfrac32, \tfrac32\right)_{\mathrm{I}} = \left(\tfrac32, \tfrac12, \underline{\tfrac12}; \tfrac32, \tfrac32\right)'$$

$$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right)_{\mathrm{II}} = \frac{1}{2}\left\{ \sqrt{3}\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right)' + 4\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right)'' \right\}$$

$$= \frac{1}{2}\left\{ \left(\tfrac{1}{2} \middle| \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2} \middle| \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) \right\}$$

$$= \frac{1}{2}\, \mathcal{O}_{\frac{3}{2}\frac{3}{2}} \left\{ \sqrt{3}\left(\tfrac{3}{2} \middle| -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) + 4\left(\tfrac{1}{2} \middle| \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) \right\}$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\left\{ \left(\tfrac{1}{2}, -\tfrac{1}{2} \middle| \underline{\tfrac{1}{2}}\right) - \left(\tfrac{3}{2}, -\tfrac{3}{2} \middle| \underline{\tfrac{1}{2}}\right) \right\} = \sqrt{2}\, \mathcal{O}_{\frac{1}{2}\frac{1}{2}} \left(\tfrac{1}{2}, -\tfrac{1}{2} \middle| \underline{\tfrac{1}{2}}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \frac{1}{\sqrt{6}}\left\{ \left(\tfrac{1}{2} \middle| \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) + \left(\tfrac{1}{2} \middle| -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \left(-\tfrac{1}{2} \middle| \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2} \middle| -\tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) \right\}$$

$$= \sqrt{6}\, \mathcal{O}_{\frac{1}{2}\frac{1}{2}} \left(\tfrac{1}{2} \middle| \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)$$

$$\left(\tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \left| \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = \mathcal{O}_{\frac{1}{2}\frac{1}{2}} \left| \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right)$$

Transformations

1. Uncoupled determinants

$$\left(\tfrac{3}{2}, \tfrac{1}{2} \middle| \underline{\tfrac{1}{2}}\right) = \sqrt{\frac{2}{3}}\,(1\,0\,s| - \frac{1}{\sqrt{3}}\,(1\,s\,|\,1); \quad \left(\tfrac{3}{2}, -\tfrac{1}{2} \middle| \underline{\tfrac{1}{2}}\right) = \frac{1}{\sqrt{3}}\,(1\,\bar{1}\,s| - \sqrt{\frac{2}{3}}\,(1\,s\,|\,0)$$

$$\left(\tfrac{3}{2} \middle| \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = \frac{1}{\sqrt{3}}\,(1\,0\,s| + \sqrt{\frac{2}{3}}\,(1\,s\,|\,1); \quad \left(\tfrac{3}{2} \middle| -\tfrac{1}{2},\right) = \sqrt{\frac{2}{3}}\,(1\,\bar{1}\,s) - \sqrt{\frac{1}{3}}\,(1\,s\,|\,0)$$

$$\left(\tfrac{1}{2} \middle| \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) = (0\,|\,s\,1); \qquad \left(\tfrac{1}{2} \middle| \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = (0\,s\,|\,1)$$

$$\left(\tfrac{1}{2}, -\tfrac{1}{2} \middle| \underline{\tfrac{1}{2}}\right) = \frac{1}{3}\left\{ \sqrt{2}\,(0\,\bar{1}\,s| - 2\,(0\,s\,|\,0) - (s\,\bar{1}\,|\,1) - \sqrt{2}\,(s\,|\,0\,1) \right\}$$

$$\left| \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = \frac{1}{3}\left\{ \sqrt{2}\,(0\,\bar{1}\,s| + (0\,s\,|\,0) + 2\,(s\,\bar{1}\,|\,1) - \sqrt{2}\,(s\,|\,0\,1) \right\}$$

2. Coupled JM-functions

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$
${}^2D_{\frac{5}{2}, M}$	-1	$\sqrt{2}$
${}^4P_{\frac{5}{2}, M}$	$\sqrt{2}$	1

$\times \frac{1}{\sqrt{3}}$

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{I}}$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{II}}$
${}^2D_{\frac{3}{2}, M}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{2\sqrt{6}}$	$\frac{\sqrt{10}}{4}$
${}^4P_{\frac{3}{2}, M}$	$-\frac{1}{3}$	$-\frac{2\sqrt{2}}{3}$	0
${}^2P_{\frac{3}{2}, M}$	$-\frac{\sqrt{5}}{3}$	$\frac{\sqrt{10}}{12}$	$-\frac{\sqrt{6}}{4}$

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$\left(\tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$
${}^4P_{\frac{1}{2}, M}$	$-\frac{\sqrt{2}}{3}$	$-\frac{1}{\sqrt{3}}$	$-\frac{2}{3}$
${}^2P_{\frac{1}{2}, M}$	$\frac{1}{3}$	$-\sqrt{\frac{2}{3}}$	$\frac{\sqrt{2}}{3}$
${}^2S_{\frac{1}{2}, M}$	$-\sqrt{\frac{2}{3}}$	0	$\frac{1}{\sqrt{3}}$

Spin-orbit interaction in jj-coupling

$$V\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}\right) = \zeta_{np}$$

$$V\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = -\frac{1}{2}\zeta_{np}$$

$$V\left(\tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) = -2\zeta_{np}$$

Electrostatic interaction in jj-coupling

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$
$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$	$F_0 - 3F_2 - \frac{5}{3}G_1$	$-2F_2 - \frac{1}{3}G_1$
$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{5}{2}, M\right)$	$-2F_2 - \frac{1}{3}G_1$	$F_0 - F_2 - \frac{4}{3}G_1$

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{I}}$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{II}}$
$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)$	$F_0 - 3F_2$	$-\frac{1}{\sqrt{2}}(F_2 + G_1)$	$\sqrt{\frac{15}{2}}\left(-F_2 + \frac{1}{3}G_1\right)$
$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{I}}$	$-\frac{1}{\sqrt{2}}(F_2 + G_1)$	$F_0 - \frac{19}{4}F_2 - \frac{7}{4}G_1$	$\frac{\sqrt{15}}{4}\left(F_2 - \frac{1}{3}G_1\right)$
$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, M\right)_{\mathrm{II}}$	$\sqrt{\frac{15}{2}}\left(-F_2 + \frac{1}{3}G_1\right)$	$\frac{\sqrt{15}}{4}\left(F_2 - \frac{1}{3}G_1\right)$	$F_0 - \frac{5}{4}F_2 - \frac{1}{4}G_1$

	$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$\left(\tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$
$\left(\tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$F_0 + 5F_2 - G_1$	$-\sqrt{\frac{2}{3}}G_1$	$-5\sqrt{2}F_2$
$\left(\tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$-\sqrt{\frac{2}{3}}G_1$	$F_0 - 5F_2$	$-\frac{2}{\sqrt{3}}G_1$
$\left(\tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, M\right)$	$-5\sqrt{2}F_2$	$-\frac{2}{\sqrt{3}}G_1$	$F_0 - G_1$

Intermediate coupling

$$\left.\begin{array}{l} {}^2D'_{\frac{5}{2}} \\ {}^4P_{\frac{5}{2}} \end{array}\right\} : F_0 - 2F_2 - \frac{3}{2}G_1 - \frac{\zeta}{4} \pm \frac{1}{2}\sqrt{(4F_2 + 3G_1)^2 + 4\zeta(6F_2 + G_1) + \frac{9}{4}\zeta^2}$$

For $J = 3/2$ and $1/2$ we refer to the corresponding third order secular determinantal equations.

Table 8. sp^3

$M_L \backslash M_S$	2	1	0	−1	−2
2		$(s\,10 \mid 1)$	$(s\,1 \mid 0\,1)\ (1\,0 \mid s\,1)$	$(1 \mid s\,1\,0)$	
1		$(s\,1\,0 \mid 0)\ (s\,1\,\bar{1} \mid 1)$	$(s\,1 \mid 1\,\bar{1})\ (s\,0 \mid 1\,0)\ (1\,0 \mid s\,0)\ (1\,\bar{1} \mid s\,1)$	$(1 \mid s\,1\,\bar{1})\ (0 \mid s\,1\,0)$	
0	$(s\,1\,0\,\bar{1} \mid$	$(s\,1\,0 \mid \bar{1})\ (s\,1\,\bar{1} \mid 0)$ $(s\,0\,\bar{1} \mid 1)\ (1\,0\,\bar{1} \mid s)$	$(s\,1 \mid 0\,\bar{1})\ (s\,0 \mid 1\,\bar{1})\ (s\,\bar{1} \mid 1\,0)$ $(1\,0 \mid s\,\bar{1})\ (1\,\bar{1} \mid s\,0)\ (0\,\bar{1} \mid s\,1)$	$(s \mid 1\,0\,\bar{1})\ (1 \mid s\,0\,\bar{1})$ $(0 \mid s\,1\,\bar{1})\ (\bar{1} \mid s\,1\,0)$	$\mid s\,1\,0\,\bar{1})$
−1		$(s\,0\,\bar{1} \mid 0)\ (s\,1\,\bar{1} \mid \bar{1})$	$(s\,\bar{1} \mid 1\,\bar{1})\ (s\,0 \mid 0\,\bar{1})\ (0\,\bar{1} \mid s\,0)\ (1\,\bar{1} \mid s\,\bar{1})$	$(\bar{1} \mid s\,1\,\bar{1})\ (0 \mid s\,0\,\bar{1})$	
−2		$(s\,0\,\bar{1} \mid \bar{1})$	$(s\,\bar{1} \mid 0\,\bar{1})\ (0\,\bar{1} \mid s\,\bar{1})$	$(\bar{1} \mid s\,0\,\bar{1})$	

$$\begin{matrix} & 1\ 2\ 1 & & 1\ 1\ 1 & & 1 \\ & 2\ 4\ 2 & & 1\ 1\ 1 & & 1 & & 1\ 1\ 1 & & 1 \\ 1\ 4\ 6\ 4\ 1 & & = & 1\ 1\ 1 & + & 1 & + & 1\ 1\ 1 & + & 1 & + & 11111 & + & 111 & = {}^3D + {}^1D + {}^3P + {}^1P + {}^5S + {}^3S \\ & 2\ 4\ 2 & & 1\ 1\ 1 & & 1 & & 1\ 1\ 1 & & 1 \\ & 1\ 2\ 1 & & 1\ 1\ 1 & & 1 \end{matrix}$$

$${}^2D\ (2{,}1) = (s\ 01 \mid 1)$$

$${}^1D\ (2{,}0) = \frac{1}{\sqrt{2}}\left\{(s\ 1 \mid 01) - (10 \mid s\ 1)\right\} = \sqrt{2}\ {}^S\mathcal{O}_{00}\ (s\ 1 \mid 01)$$

$${}^3P\ (1{,}1) = \frac{1}{\sqrt{2}}\left\{(s\ 01 \mid 0) - (s\ \bar{1}1 \mid 0)\right\} = \sqrt{2}\ {}^L\mathcal{O}_{11}\ (s\ 01 \mid 0)$$

$${}^1P\ (1{,}0) = \frac{1}{2}\left\{(s\ 0 \mid 01) + (01 \mid s\ 0) - (s\ 1 \mid \bar{1}1) - (\bar{1}1 \mid s\ 1)\right\} = 2\ {}^L\mathcal{O}_{11}\ {}^S\mathcal{O}_{00}\ (s\ 0 \mid 01)$$

$${}^5S\ (0{,}2) = (s\ \bar{1}01 \mid$$

$${}^3S\ (0{,}1) = \frac{1}{\sqrt{12}}\left\{(s\,\bar{1}1 \mid 0) + (s\,0\bar{1} \mid 1) + (s\,10 \mid \bar{1}) + 3\,(10\bar{1} \mid s)\right\} = \sqrt{12}\ {}^L\mathcal{O}_{00}\ {}^S\mathcal{O}_{11}\ (s\ \bar{1}1 \mid 0)$$

SLJM

$${}^3D_{33} = {}^3D\ (2{,}1) = \mathcal{O}_{33}\ {}^3D\ (2{,}1) = (s\ 0\ 1 \mid 1)$$

$${}^3D_{22} = \sqrt{\frac{2}{3}}\ {}^3D\ (2{,}0) - \sqrt{\frac{1}{3}}\ {}^3D\ (1{,}1) = \sqrt{\frac{3}{2}}\ \mathcal{O}_{22}\ {}^2D\ (2{,}0)$$

$${}^1D_{22} = {}^1D\ (2{,}0) = \mathcal{O}_{22}\ {}^1D\ (2{,}0) = \frac{1}{\sqrt{2}}\left\{(s\ 1 \mid 0\ 1) - (1\ 0 \mid s\ 1)\right\}$$

$${}^3P_{22} = {}^3P\ (1{,}1) = \mathcal{O}_{22}\ {}^3P\ (1{,}1) = \frac{1}{\sqrt{2}}\left\{(s\ 0\ 1 \mid 0) - (s\ \bar{1}\ 1 \mid 0)\right\}$$

$${}^5S_{22} = {}^5S\ (0{,}2) = \mathcal{O}_{22}\ {}^5S\ (0{,}2) = (s\ \bar{1}\ 0\ 1 \mid$$

$${}^3D_{11} = \sqrt{\frac{3}{10}}\ {}^3D\ (1{,}0) - \frac{1}{\sqrt{10}}\ {}^3D\ (0{,}1) - \sqrt{\frac{3}{5}}\ {}^3D\ (2, -1) = \sqrt{\frac{10}{3}}\ \mathcal{O}_{11}\ {}^3D\ (1{,}0)$$

$$= \sqrt{\frac{3}{40}}\left\{(s\ 0 \mid 1\ 0) - (s\ 1 \mid \bar{1}\ 1) + (\bar{1}\ 1 \mid s\ 1) + (01 \mid s\ 0)\right\} -$$

$$- \sqrt{\frac{1}{60}}\left\{(s\ \bar{1}\ 0 \mid 1) + 2\,(s\ \bar{1}\ 1 \mid 0) + (s\ 0\ 1 \mid \bar{1})\right\} - \sqrt{\frac{3}{5}}\,(1 \mid s\ 0\ 1)$$

$$
\begin{aligned}
{}^3P_{11} &= \frac{1}{\sqrt{2}}\left\{{}^3P\,(1{,}0) - {}^3P\,(0{,}1)\right\} = \sqrt{2}\;\mathcal{O}_{11}\,{}^3P\,(1{,}0)\\
&= \frac{\sqrt{2}}{4}\left\{(s\,0\mid 1\,0) + (0\,1\mid s\,0) + (s\,1\mid \bar{1}\,1) + (1\,\bar{1}\mid s\,1)\right\} - \frac{1}{2}\left\{(s\,0\,1\mid \bar{1}) - (s\,\bar{1}\,0\mid 1)\right\}
\end{aligned}
$$

$$
{}^1P_{11} = {}^1P\,(1{,}0) = \mathcal{O}_{11}\,{}^1P\,(1{,}0) = \frac{1}{2}\left\{(s\,0\mid 0\,1) + (0\,1\mid s\,0) - (s\,1\mid \bar{1}\,1) - (\bar{1}\,1\mid s\,1)\right\}
$$

$$
{}^3S_{11} = {}^3S\,(0{,}1) = \mathcal{O}_{11}\,{}^3S\,(0{,}1) = \frac{1}{\sqrt{12}}\left\{(s\,\bar{1}\,1\mid 0) + (s\,0\,\bar{1}\mid 1) + (s\,1\,0\mid \bar{1}) + 3\,(1\,0\,\bar{1}\mid s)\right\}
$$

$$
\begin{aligned}
{}^3P_{00} &= \frac{1}{\sqrt{3}}\left\{{}^3P\,(0{,}0) - {}^3P\,(1,-1) - {}^3P\,(-1,1)\right\} = \sqrt{3}\;\mathcal{O}_{00}\,{}^3P\,(0{,}0)\\
&= \frac{1}{2\sqrt{3}}\left\{(s\,1\mid \bar{1}\,0) + (s\,\bar{1}\mid 1\,0) + (0\,1\mid s\,\bar{1}) + (0\,\bar{1}\mid s\,1)\right\} -\\
&\quad - \frac{1}{\sqrt{6}}\left\{(s\,\bar{1}\,1\mid \bar{1}) - (s\,\bar{1}\,0\mid 0)\right\} - \frac{1}{\sqrt{6}}\left\{(0\mid s\,0\,1) - (1\mid s\,\bar{1}\,1)\right\}
\end{aligned}
$$

Electrostatic interaction in LS-coupling

$$
\begin{array}{lll}
E\,({}^3D) = F_0 - 6\,F_2 - 2\,G_1 & E\,({}^1D) = F_0 - 6\,F_2 & \left\{F_0 = 3\,F_0\,(ns, np) + \right.\\
E\,({}^3P) = F_0 \qquad\qquad - 2\,G_1 & E\,({}^1P) = F_0 & \qquad \left. + 3\,F_0\,(np, np)\right\}\\
E\,({}^5S) = F_0 - 15\,F_2 - 3\,G_1 & E\,({}^3S) = F_0 - 15\,F_2 + G_1 &
\end{array}
$$

Spin-orbit interaction in LS-coupling

$$
\begin{array}{c|cccc|}
 & {}^3D_2 & {}^1D_2 & {}^3P_2 & {}^5S_2\\
\hline
{}^3D_2 & 0 & 0 & -\sqrt{3} & 0\\
{}^1D_2 & 0 & 0 & \sqrt{2} & 0\\
{}^3P_2 & -\sqrt{3} & \sqrt{2} & 0 & 2\\
{}^5S_2 & 0 & 0 & 2 & 0\\
\hline
\end{array}
\times \frac{1}{2}\,\zeta_{np}
\qquad\qquad
\begin{array}{c|cccc|}
 & {}^3D_1 & {}^3P_1 & {}^1P_1 & {}^3S_1\\
\hline
{}^3D_1 & 0 & \sqrt{5} & \sqrt{10} & 0\\
{}^3P_1 & \sqrt{5} & 0 & 0 & 2\\
{}^1P_1 & \sqrt{10} & 0 & 0 & 2\sqrt{2}\\
{}^3S_1 & 0 & 2 & 2\sqrt{2} & 0\\
\hline
\end{array}
\times \frac{1}{2\sqrt{3}}\,\zeta_{np}
$$

$$
V\left({}^3D_3\right) = 0 \qquad\qquad V\left({}^3P_0\right) = 0
$$

jj-coupling (the s-electron is underlined)

$M \setminus j_1 j_2 j_3 j_4$	$\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \underline{\frac{1}{2}}$	$\frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \underline{\frac{1}{2}}$	$\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \underline{\frac{1}{2}}$
3		$\left(\frac{3}{2}, \frac{1}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right)$	
2	$\left(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2} \middle\vert \underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{3}{2}, \frac{1}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, \underline{\frac{1}{2}}\right)$
1	$\left(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2} \middle\vert -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, \frac{1}{2}, -\frac{3}{2} \middle\vert \underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2}, \frac{1}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, \underline{\frac{1}{2}}\right)$
0	$\left(\frac{3}{2}, \frac{1}{2}, -\frac{3}{2} \middle\vert -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{1}{2}, -\frac{3}{2} \middle\vert \underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{3}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{1}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right)$	$\left(\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(-\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, \underline{\frac{1}{2}}\right)$
−1	$\left(\frac{3}{2}, -\frac{1}{2}, -\frac{3}{2} \middle\vert -\underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \middle\vert \underline{\frac{1}{2}}\right)$	$\left(\frac{3}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{1}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(\frac{1}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right) \left(-\frac{1}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, \underline{\frac{1}{2}}\right)$	$\left(-\frac{1}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(-\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, \underline{\frac{1}{2}}\right)$
−2	$\left(\frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \middle\vert -\underline{\frac{1}{2}}\right)$	$\left(\frac{1}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(-\frac{1}{2}, -\frac{3}{2} \middle\vert \frac{1}{2}, -\underline{\frac{1}{2}}\right) \left(-\frac{1}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, \underline{\frac{1}{2}}\right)$	$\left(-\frac{3}{2} \middle\vert \frac{1}{2}, -\frac{1}{2}, -\underline{\frac{1}{2}}\right)$
−3		$\left(-\frac{1}{2}, -\frac{3}{2} \middle\vert -\frac{1}{2}, -\underline{\frac{1}{2}}\right)$	

$$\begin{matrix} & 1 & \\ 1 & 3 & 1 \\ 2 & 5 & 2 \\ 2 & 6 & 2 \\ 2 & 5 & 2 \\ 1 & 3 & 1 \\ & 1 & \end{matrix} = 1\,(J = 3) + 4\,(J = 2) + 4\,(J = 1) + 1\,(J = 0)$$

$$\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};3,3\right) = \left(\tfrac32,\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right)$$

$$\left(\tfrac32,\tfrac32,\tfrac32,\underline{\tfrac12};2,2\right) = \left(\tfrac32,\tfrac12,-\tfrac12\,\middle|\,\underline{\tfrac12}\right)$$

$$\left.\begin{aligned}
\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};2,2\right)_{\mathrm{I}} &= \frac{1}{\sqrt{30}}\left\{5\left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,\underline{\tfrac12}\right) - 2\left(\tfrac32,-\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right) - \left(\tfrac32,\tfrac12\,\middle|\,\tfrac12,-\underline{\tfrac12}\right)\right\} = \sqrt{\frac65}\,\mathcal{O}_{22}\left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,\underline{\tfrac12}\right)\\
\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};2,2\right)_{\mathrm{II}} &= \frac{1}{\sqrt5}\left\{\left(\tfrac32,-\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right) - 2\left(\tfrac32,\tfrac12\,\middle|\,\tfrac12,-\underline{\tfrac12}\right)\right\} = \frac{1}{\sqrt5}\,\mathcal{O}_{22}\left\{2\left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,\underline{\tfrac12}\right) + 5\left(\tfrac32,-\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right)\right\}
\end{aligned}\right\}\ \text{orthogonalized}$$

$$\left(\tfrac32,\tfrac12,\tfrac12,\underline{\tfrac12};2,2\right) = \left(\tfrac32\,\middle|\,\tfrac12,-\tfrac12,\underline{\tfrac12}\right)$$

$$\left(\tfrac32,\tfrac32,\tfrac32,\underline{\tfrac12};1,1\right) = \frac12\left\{\sqrt3\left(\tfrac32,\tfrac12,-\tfrac12\,\middle|\,-\underline{\tfrac12}\right) - \left(\tfrac32,\tfrac12,-\tfrac32\,\middle|\,\underline{\tfrac12}\right)\right\} = \frac{2}{\sqrt3}\,\mathcal{O}_{11}\left(\tfrac32,\tfrac12,-\tfrac12\,\middle|\,-\underline{\tfrac12}\right)$$

$$\left.\begin{aligned}
\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};1,1\right)_{\mathrm{I}} &= \frac{1}{\sqrt{20}}\left\{2\sqrt3\left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,-\underline{\tfrac12}\right) - \sqrt3\left(\tfrac32,-\tfrac12\,\middle|\,\tfrac12,-\underline{\tfrac12}\right) - \sqrt3\left(\tfrac32,-\tfrac12\,\middle|\,-\tfrac12,\underline{\tfrac12}\right) + \left(\tfrac32,-\tfrac32\,\middle|\,\tfrac12,\underline{\tfrac12}\right) +\right.\\
&\quad \left. + \left(\tfrac12,-\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right)\right\} = \sqrt{\frac53}\,\mathcal{O}_{11}\left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,-\underline{\tfrac12}\right)\\
\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};1,1\right)_{\mathrm{II}} &= \frac{1}{\sqrt2}\left\{\left(\tfrac32,-\tfrac32\,\middle|\,\tfrac12,\underline{\tfrac12}\right) - \left(\tfrac12,-\tfrac12\,\middle|\,\tfrac12,\underline{\tfrac12}\right)\right\} = \frac{1}{\sqrt6}\,\mathcal{O}_{11}\left\{2\sqrt3\left(\tfrac32,-\tfrac32\,\middle|\,\tfrac12,\underline{\tfrac12}\right) - \left(\tfrac32,\tfrac12\,\middle|\,-\tfrac12,-\underline{\tfrac12}\right)\right\}
\end{aligned}\right\}\ \text{orthogonalized}$$

$$\left(\tfrac32,\tfrac12,\tfrac12,\underline{\tfrac12};1,1\right) = \frac12\left\{\left(\tfrac12\,\middle|\,\tfrac12,-\tfrac12,\underline{\tfrac12}\right) - \sqrt3\left(\tfrac32\,\middle|\,\tfrac12,-\tfrac12,-\underline{\tfrac12}\right)\right\} = 2\,\mathcal{O}_{11}\left(\tfrac12\,\middle|\,\tfrac12,-\tfrac12,\underline{\tfrac12}\right)$$

$$\left(\tfrac32,\tfrac32,\tfrac12,\underline{\tfrac12};0,0\right) = \frac12\left\{\left(\tfrac32,-\tfrac32\,\middle|\,-\tfrac12,\underline{\tfrac12}\right) - \left(\tfrac32,-\tfrac32\,\middle|\,\tfrac12,-\underline{\tfrac12}\right) - \left(\tfrac12,-\tfrac12\,\middle|\,-\tfrac12,\underline{\tfrac12}\right) + \left(\tfrac12,-\tfrac12\,\middle|\,\tfrac12,-\underline{\tfrac12}\right)\right\} = 2\,\mathcal{O}_{00}\left(\tfrac32,-\tfrac32\,\middle|\,-\tfrac12,\underline{\tfrac12}\right)$$

Transformations

1. Uncoupled determinants

	$(s\,1\,0\,\bar{1}\,|$	$(s\,1\,\bar{1}\,|\,1)$	$(s\,1\,0\,|\,0)$	$(s\,1\,|\,1\,0)$	
$(\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}\,|\,\underline{\frac{1}{2}})$	$-\sqrt{2}$	1	-2	$-\sqrt{2}$	
$(\frac{3}{2}, \frac{1}{2}\,|\,-\frac{1}{2}, \underline{\frac{1}{2}})$	-2	$\sqrt{2}$	$\sqrt{2}$	1	$\times\,\frac{1}{3}$
$(\frac{3}{2}, -\frac{1}{2}\,|\,\frac{1}{2}, \underline{\frac{1}{2}})$	1	$\sqrt{2}$	$\sqrt{2}$	-2	
$(\frac{3}{2}\,|\,\frac{1}{2}, -\frac{1}{2}, \underline{\frac{1}{2}})$	$-\sqrt{2}$	-2	1	$-\sqrt{2}$	

$$(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}\,|\,-\underline{\tfrac{1}{2}}) = \frac{1}{3}\left\{\sqrt{2}\,(1\,0\,\bar{1}\,|\,s) - (1\,\bar{1}\,|\,1\,s) + 2\,(1\,0\,|\,0\,s) + \sqrt{2}\,(1\,|\,1\,0\,s)\right\}$$

$$(\tfrac{3}{2}, \tfrac{1}{2}\,|\,-\tfrac{1}{2}, -\underline{\tfrac{1}{2}}) = \frac{1}{3}\left\{2\,(10\,\bar{1}\,|\,s) - \sqrt{2}\,(1\,\bar{1}\,|\,1\,s) - \sqrt{2}\,(10\,|\,0\,s) - (1\,|\,10\,s)\right\}$$

$$(\tfrac{3}{2}, -\tfrac{3}{2}\,|\,\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = \frac{1}{\sqrt{3}}\left\{(s\,10\,|\,\bar{1}) - \sqrt{2}\,(s\,1\,|\,1\,\bar{1})\right\}$$

$$(\tfrac{1}{2}\,|\,\tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = -\frac{1}{\sqrt{3}}\left\{\sqrt{2}\,(s\,0\,\bar{1}\,|\,1) + (s\,0\,|\,10)\right\}$$

$$(\tfrac{3}{2}, -\tfrac{3}{2}\,|\,-\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = \frac{1}{\sqrt{3}}\left\{\sqrt{2}\,(s\,1\,\bar{1}\,|\,\bar{1}) - (s\,1\,|\,0\,\bar{1})\right\}; \quad (\tfrac{3}{2}, \tfrac{1}{2}\,|\,\tfrac{1}{2}, \underline{\tfrac{1}{2}}) = (s\,10\,|\,1)$$

2. Coupled JM-functions

$$^3D_{3M} = (\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 3, M)$$

	$(\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \underline{\frac{1}{2}}; 2, M)$	$(\frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 2, M)_{\mathrm{I}}$	$(\frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 2, M)_{\mathrm{II}}$	$(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 2, M)$
$^5S_{2M}$	$\frac{\sqrt{2}}{3}$	$\frac{2\sqrt{30}}{15}$	$-\frac{\sqrt{5}}{15}$	$\frac{\sqrt{2}}{3}$
$^3P_{2M}$	$\frac{\sqrt{2}}{2}$	0	0	$-\frac{\sqrt{2}}{2}$
$^1D_{2M}$	$\frac{1}{3}$	$-\frac{\sqrt{15}}{15}$	$\frac{4\sqrt{10}}{15}$	$\frac{1}{3}$
$^3D_{2M}$	$-\frac{\sqrt{6}}{6}$	$\frac{\sqrt{10}}{5}$	$\frac{2\sqrt{15}}{15}$	$-\frac{\sqrt{6}}{6}$

	$(\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \underline{\frac{1}{2}}; 1, M)$	$(\frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 1, M)_{\mathrm{I}}$	$(\frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 1, M)_{\mathrm{II}}$	$(\frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \underline{\frac{1}{2}}; 1, M)$
$^3S_{1M}$	$\frac{\sqrt{2}}{3}$	$\frac{\sqrt{5}}{3}$	0	$-\frac{\sqrt{2}}{3}$
$^1P_{1M}$	$\frac{\sqrt{3}}{3}$	0	$-\frac{\sqrt{3}}{3}$	$\frac{\sqrt{3}}{3}$
$^3P_{1M}$	$\frac{\sqrt{6}}{6}$	0	$\frac{\sqrt{6}}{3}$	$\frac{\sqrt{6}}{6}$
$^3D_{1M}$	$\frac{\sqrt{10}}{6}$	$-\frac{2}{3}$	0	$-\frac{\sqrt{10}}{6}$

$$^3P_{0M} = (\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 0, M)$$

Spin-orbit interaction in jj-coupling

$$V\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{\underline{2}}\right) = \tfrac{3}{2}\zeta_{np} \qquad V\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{\underline{2}}\right) = 0 \qquad V\left(\tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{\underline{2}}\right) = -\tfrac{3}{2}\zeta_{np}$$

The electrostatic interaction matrices in *jj*-coupling are omitted but they can be found from the *LS*-scheme with proper transformations.

For the case of intermediate coupling we refer to the corresponding secular determinantal equations.

Table 9. sp^4

The correspondence between configurations sp^4 and sp^2 is used throughout this table. Only information not directly available in Tab. 7 is given.

$$^2D\left(2, \tfrac{1}{2}\right) = (10\,s \mid 10)$$

$$^4P\left(1, \tfrac{3}{2}\right) = (10\bar{1}\,s \mid 1)$$

$$^2P\left(1, \tfrac{1}{2}\right) = \frac{1}{\sqrt{6}}\left\{2\,(10\bar{1} \mid 1\,s) + (10\,s \mid 1\bar{1}) - (1\bar{1}\,s \mid 10)\right\} = \sqrt{\frac{3}{2}}\;{}^S\mathcal{O}_{\frac{1}{2}\frac{1}{2}}\;{}^L\mathcal{O}_{11}\,(10\bar{1} \mid 1\,s)$$

$$^2S\left(0, \tfrac{1}{2}\right) = \frac{1}{\sqrt{3}}\left\{(1\bar{1}\,s \mid 1\bar{1}) - (0\bar{1}\,s \mid 10) - (10\,s \mid 0\bar{1})\right\} = \sqrt{3}\;{}^L\mathcal{O}_{00}\,(1\bar{1}\,s \mid 1\bar{1})$$

SLJM

$$^2D_{\frac{5}{2}\frac{5}{2}} = (10\,s \mid 10)$$

$$^4P_{\frac{5}{2}\frac{5}{2}} = (10\bar{1}\,s \mid 1)$$

$$^2D_{\frac{3}{2}\frac{3}{2}} = \frac{1}{\sqrt{5}}\left\{\frac{1}{\sqrt{2}}\left[(1\bar{1}\,s \mid 10) + (10\,s \mid 1\bar{1})\right] - 2\,(10 \mid 10\,s)\right\}$$

$$^4P_{\frac{3}{2}\frac{3}{2}} = \frac{1}{\sqrt{5}}\left\{\sqrt{\frac{2}{3}}\left[-(10\bar{1} \mid 1\,s) - (1\bar{1}\,s \mid 10) + (10\,s \mid 1\bar{1})\right] - \sqrt{3}\,(10\bar{1}\,s \mid 0)\right\}$$

$$^2P_{\frac{3}{2}\frac{3}{2}} = \frac{1}{\sqrt{6}}\left\{2\,(10\bar{1} \mid 1\,s) + (10\,s \mid 1\bar{1}) - (1\bar{1}\,s \mid 10)\right\}$$

$$^4P_{\frac{1}{2}\frac{1}{2}} = \frac{1}{3\sqrt{2}}\Big\{\sqrt{2}\left[-(10\bar{1} \mid 0\,s) - (0\bar{1}\,s \mid 10) + (10\,s \mid 0\bar{1})\right] -$$
$$- \left[(10 \mid 1\bar{1}\,s) - (1\bar{1} \mid 10\,s) + (1\,s \mid 10\bar{1})\right] - 3\,(10\bar{1}\,s \mid \bar{1})\Big\}$$

$$^2P_{\frac{1}{2}\frac{1}{2}} = \frac{1}{3\sqrt{2}}\left\{2\,(10\bar{1} \mid 0\,s) + (10\,s \mid 0\bar{1}) - (0\bar{1}\,s \mid 10)\right\} -$$
$$- \frac{1}{3}\left\{(1\bar{1} \mid 10\,s) - (10 \mid 1\bar{1}\,s) + 2\,(1\,s \mid 10\bar{1})\right\}$$

$$^2S_{\frac{1}{2}\frac{1}{2}} = \frac{1}{\sqrt{3}}\left\{(1\bar{1}\,s \mid 1\bar{1}) - (0\bar{1}\,s \mid 10) - (10\,s \mid 0\bar{1})\right\}$$

jj-coupling (the *s*-electron is underlined)

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{\underline{2}}; \tfrac{5}{2}, \tfrac{5}{2}\right) = \left(\tfrac{3}{2}\,\tfrac{1}{2} \mid \tfrac{1}{2}, -\tfrac{1}{2}, \tfrac{1}{\underline{2}}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{\underline{2}}; \tfrac{5}{2}, \tfrac{5}{2}\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \mid \tfrac{1}{2}, \tfrac{1}{\underline{2}}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right) = \frac{1}{\sqrt{5}}\left\{\left(\tfrac{3}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - 2\left(\tfrac{3}{2}, \tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)\right\}$$

$$\begin{aligned}\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right)_{\mathrm{I}} = {} & \frac{1}{2\sqrt{5}}\left\{4\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \right. \\ & \left. - \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)\right\}\end{aligned}$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{3}{2}, \tfrac{3}{2}\right)_{\mathrm{II}} = \frac{1}{2}\left\{\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)\right\}$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \frac{1}{\sqrt{2}}\left\{\left(\tfrac{3}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \left(\tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right)\right\}$$

$$\begin{aligned}\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = {} & \frac{1}{\sqrt{6}}\left\{\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) + \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \right. \\ & \left. - \left(\tfrac{3}{2}, -\tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, -\tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)\right\}\end{aligned}$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \underline{\tfrac{1}{2}}; \tfrac{1}{2}, \tfrac{1}{2}\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \underline{\tfrac{1}{2}}\right)$$

Interactions:

Substitute $6\,F_0(np, np) + 4\,F_0(ns, np) - 10\,F_2(np, np) - G_1(ns, np)$ for F_0 and $-\zeta$ for ζ in Tab. 7.

Table 10. sp^5

The correspondence between configurations sp^5 and sp is used throughout this table. Only information not directly available in Tab. 6 is given.

$${}^3P\,(1, 1) = (10\,\bar{1}\,s \mid 10)$$

$${}^1P\,(1, 0) = \frac{1}{\sqrt{2}}\left\{(10\,\bar{1} \mid 10\,s) + (10\,s \mid 10\,\bar{1})\right\} = \sqrt{2}\ {}^S\mathcal{O}_{00}\,(10\,\bar{1} \mid 10\,s)$$

SLJM

$${}^3P_{22} = (10\,\bar{1}\,s \mid 10)$$

$${}^3P_{11} = \frac{1}{2}\left\{(10\,\bar{1} \mid 10\,s) - (10\,s \mid 10\,\bar{1})\right\} - \frac{1}{\sqrt{2}}(10\,\bar{1}\,s \mid 1\,\bar{1})$$

$${}^1P_{11} = \frac{1}{\sqrt{2}}\left\{(10\,\bar{1} \mid 10\,s) - (10\,s \mid 10\,\bar{1})\right\}$$

$${}^3P_{00} = \frac{1}{\sqrt{6}}\left\{(10\,\bar{1} \mid 1\,\bar{1}\,s) - (1\,\bar{1}\,s \mid 10\,\bar{1})\right\} - \frac{1}{\sqrt{3}}(10\,\bar{1}\,s \mid 0\,\bar{1}) - \frac{1}{\sqrt{3}}(10 \mid 10\,\bar{1}\,s)$$

jj-coupling (the s-electron is underlined)

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 2, 2\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right)$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 1, 1\right) = \frac{1}{2}\left\{\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right) - \sqrt{3}\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2} \,\middle|\, \tfrac{1}{2}, -\tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right)\right\}$$

$$\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 1, 1\right) = \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, \underline{\tfrac{1}{2}}\right)$$

$$\begin{aligned}\left(\tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{3}{2}, \tfrac{1}{2}, \underline{\tfrac{1}{2}}; 0, 0\right) = {} & \frac{1}{\sqrt{2}}\left\{\left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, \tfrac{1}{2}, -\underline{\tfrac{1}{2}}\right) - \right. \\ & \left. - \left(\tfrac{3}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{3}{2} \,\middle|\, -\tfrac{1}{2}, \underline{\tfrac{1}{2}}\right)\right\}\end{aligned}$$

Interactions

Substitute $10\,F_0(np, np) + 5\,F_0(ns, np) - 24\,F_2(np, np) - 2\,G_1(ns, np)$ for F_0 and $-\zeta$ for ζ in Tab. 6.

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