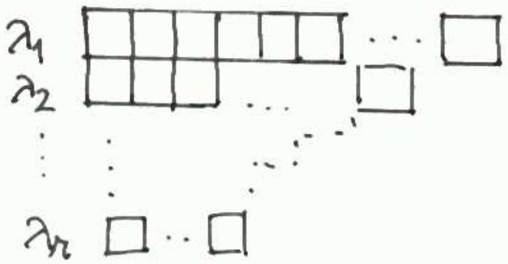
Molde ou diagrama de Young



$[\lambda] = (\lambda_1 \lambda_2 \dots \lambda_m)$

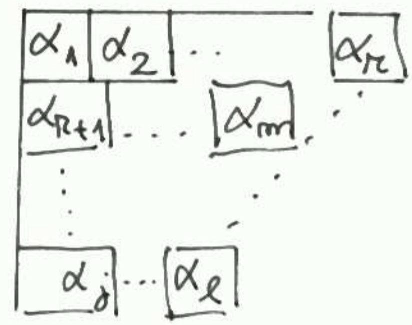
$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m$

$$\sum_i \lambda_i = n$$

$[\lambda]$ é chamada de partição de n

$\{[\lambda]\}$ são as rep. irredutíveis de S_n (permutações).

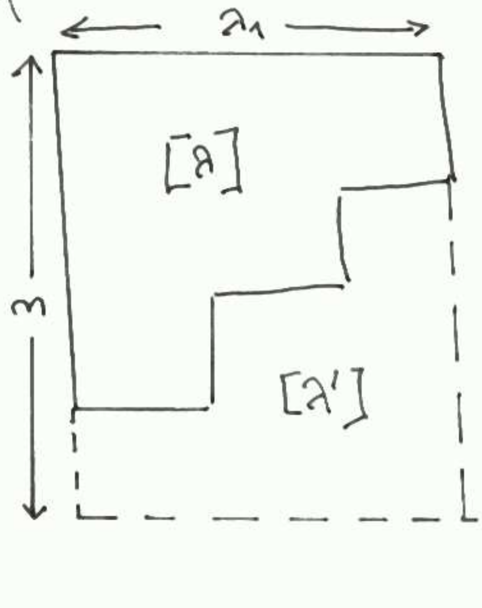
Tabela de Young



Uma tabela de Young pode representar:

- Componentes de tensores de uma dada simetria
- projetores de Young

Na redução de tensores para $SU(n)$, os moldes abaixo são equivalentes



$[\lambda] \equiv [\lambda']$

$[\lambda']$ é obtido de $[\lambda]$ completando um retângulo de lados $(\lambda_1 \times n)$.

TABLE 11–2

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = 1,\ SU(3)$

r	$[\lambda]$	J	$N([\lambda])$
0	[0]	$0 = S$	1
1	[1]	$1 = P$	3
2	[2]	$0, 2 = S\ D$	6
	$[11] \equiv [1]$	$1 = P$	3
3	[3]	$1, 3 = P\ F$	10
	[21]	$1, 2 = P\ D$	8
	$[111] \equiv [0]$	$0 = S$	1
4	[4]	$0, 2, 4 = S\ D\ G$	15
	[31]	$1, 2, 3 = P\ D\ F$	15
	$[22] \equiv [2]$	$0, 2 = S\ D$	6
	$[211] \equiv [1]$	$1 = P$	3
5	[41]	$1, 2, 3, 4 = P\ D\ F\ G$	24
	$[32] \equiv [31]$	$1, 2, 3 = P\ D\ F$	15
	$[311] \equiv [2]$	$0, 2 = S\ D$	6
	$[221] \equiv [1]$	$1 = P$	3
6	[42]	$0, (2)^2, 3, 4 = S\ D^2\ F\ G$	27
	$[411] \equiv [3]$	$1, 3 = P\ F$	10
	$[33] \equiv [3]$	$1, 3 = P\ F$	10
	$[321] \equiv [21]$	$1, 2 = P\ D$	8
	$[222] \equiv [0]$	$0 = S$	1

TABLE 11–3

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = \frac{3}{2},\ SU(4)$

r	$[\lambda]$	J	$N([\lambda])$
0	[0]	0	1
1	[1]	$\frac{3}{2}$	4
2	[2]	1, 3	10
	[11]	0, 2	6
3	[21]	$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$	20
4	[22]	$0, (2)^2, 4$	20
	[211]	1, 2, 3	15

TABLE 11-4

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = 2,\ SU(5)$

r	[λ]	S	P	D	F	G	H	I	K	L	M	N	O	Q	$N([\lambda])$
		$J = 0$	1	2	3	4	5	6	7	8	9	10	11	12	
0	[0]	1													1
1	[1]	·	·	1											5
2	[2]	1	·	1	·	1									15
	[11]	·	1	·	1										10
3	[3]	1	·	1	1	1	·	1							35
	[21]		1	2	1	1	1								40
4	[4]	1	·	2	·	2	1	1	·	1					70
	[31]	·	2	2	3	2	2	1	1						105
	[22]	2	·	2	1	2	·	1							50
	[211]	·	2	1	2	1	1								45
5	[41]	1	2	3	4	4	3	3	2	1	1				224
	[32]	1	2	4	3	4	3	2	1	1					175
	[311]	·	3	2	4	2	3	1	1						126
	[221]	1	1	3	2	2	1	1							75
	[2111]	·	1	1	1	1									24
6	[42]	3	2	7	5	8	5	6	3	3	1	1			420
	[411]	·	4	3	6	4	5	3	3	1	1				280
	[33]	·	3	1	5	2	3	2	2	·	1				175
	[321]	1	4	6	6	6	5	3	2	1					280
	[3111]	1	1	2	2	2	1	1							70
7	[43]	1	4	7	7	8	8	6	5	4	2	1	1		560
	[421]	3	6	10	11	12	10	9	6	4	2	1			700
	[331]	·	5	4	7	5	6	3	3	1	1				315
	[4111]	·	2	3	3	3	3	2	1	1					160
	[322]	2	2	5	4	5	3	3	1	1					210
	[3211]	1	3	4	5	4	3	2	1						175
8	[44]	4	1	6	4	8	4	7	3	4	2	2	·	1	490
	[431]	2	9	12	16	15	15	12	10	6	4	2	1		1050
	[422]	4	3	10	7	11	7	8	4	4	1	1			560
	[4211]	1	6	6	9	8	8	5	4	2	1				450
9	[441]	4	5	11	11	14	11	12	8	7	4	3	1	1	980
	[432]	3	9	14	16	17	16	13	10	7	4	2	1		1120
	[4311]	2	7	10	12	12	11	9	6	4	2	1			720
	[4221]	2	5	8	9	9	8	6	4	2	1				480
10	[442]	6	5	15	12	18	13	15	9	9	4	4	1	1	1176
	[4411]	·	7	7	11	9	11	7	7	4	3	1	1		700
	[4321]	4	10	14	18	18	15	13	9	5	3	1			1024
	[4222]	2	1	5	3	5	3	3	1	1					200

TABLE 11–5

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = \frac{5}{2}$, $SU(6)$

r	[λ]	J	$N([\lambda])$
0	[0]	0	1
1	[1]	$\frac{5}{2}$	6
2	[2]	1, 3, 5	21
	[11]	0, 2, 4	15
3	[21]	$\frac{1}{2}, \frac{3}{2}, (\frac{5}{2})^2, (\frac{7}{2})^2, \frac{9}{2}, \frac{11}{2}, \frac{13}{2}$	70
	[111]	$\frac{3}{2}, \frac{5}{2}, \frac{9}{2}$	20
4	[22]	$(0)^2, (2)^3, 3, (4)^3, 5, (6)^2, 8$	105
	[211]	$(1)^2, (2)^2, (3)^3, (4)^2, (5)^2, 6, 7$	105
5	[221]	$(\frac{1}{2})^2, (\frac{3}{2})^3, (\frac{5}{2})^4, (\frac{7}{2})^4, (\frac{9}{2})^4, (\frac{11}{2})^3, (\frac{13}{2})^2, \frac{15}{2}, \frac{17}{2}$	210
	[2111]	$\frac{1}{2}, (\frac{3}{2})^2, (\frac{5}{2})^2, (\frac{7}{2})^2, (\frac{9}{2})^2, \frac{11}{2}, \frac{13}{2}$	84
6	[222]	$(1)^3, 2, (3)^5, (4)^2, (5)^3, (6)^2, (7)^2, 9$	175
	[2211]	$(0)^2, 1, (2)^5, (3)^3, (4)^5, (5)^2, (6)^3, 7, 8$	189
	[21111]	1, 2, 3, 4, 5	35

TABLE 11–6

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = 3$, $SU(7)$, for $r \leq 4$

r	[λ]	$J =$ 0	1	2	3	4	5	6	7	8	9	10	11	12	$N([\lambda])$
0	[0]	1													1
1	[1]	·	·	·	1										7
2	[2]	1	·	1	·	1	·	1							28
	[11]	·	1	·	1	·	1								21
3	[3]	·	1	·	2	1	1	1	1	·	1				84
	[21]	·	1	2	2	2	2	1	1	1					112
	[111]	1	·	1	1	1	·	1							35
4	[4]	2	·	2	1	3	1	3	1	2	1	1	·	1	210
	[31]	·	3	3	5	4	5	4	4	2	2	1	1		378
	[22]	2	·	4	1	4	2	3	1	2	·	1			196
	[211]	·	3	2	4	3	4	2	2	1	1				210

TABLE 11–7

ANGULAR-MOMENTUM ANALYSIS OF THE $(j)^r$-CONFIGURATION

$j = \frac{7}{2}$, $SU(8)$, for $r \leq 4$

r	$[\lambda]$	J	$N([\lambda])$
0	[0]	0	1
1	[1]	$\frac{7}{2}$	8
2	[2]	$1, 3, 5, 7$	36
	[11]	$0, 2, 4, 6$	28
3	[21]	$\frac{1}{2}, \frac{3}{2}, (\frac{5}{2})^2, (\frac{7}{2})^3, (\frac{9}{2})^2, (\frac{11}{2})^2, (\frac{13}{2})^2, \frac{15}{2}, \frac{17}{2}, \frac{19}{2}$	168
	[111]	$\frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}, \frac{15}{2}$	56
4	[22]	$0^3, 2^4, 3^2, 4^5, 5^2, 6^5, 7^2, 8^3, 9, 10^2, 12$	336
	[211]	$1^3, 2^3, 3^5, 4^4, 5^5, 6^4, 7^4, 8^2, 9^2, 10, 11$	378
	[1111]	$0, 2^2, 4^2, 5, 6, 8$	70

wave functions form the basis for an irreducible representation $D^{(j)}$ of $O^+(3)$, with j half-integral]. For systems of identical particles having *integral* spin, the total wave function must be *symmetric* under any interchange.

For many-electron atoms, we start from the single-particle orbits in some averaged central field. The state of a single electron is characterized by quantum numbers n, l, m_l, m_s. The first quantum number gives the energy, l and m_l label the basis functions of the representation $D^{(l)}$ of the rotation group which is provided by the orbital (external) motion, and m_s labels the basis functions of the representation $D^{(1/2)}$ of the rotation group which is provided by the internal motion (spin). The perturbation consists of the Coulomb interaction between the electrons and of terms involving the electron spins.

For light atoms, the terms containing the electron spins make a contribution to the energy which is small compared to that from the Coulomb repulsion. The approximation procedure which starts from this assumption is called Russell-Saunders coupling (L-S coupling). In L-S coupling, we treat the orbital wave functions and the spin functions of the electrons separately. If there are r electrons in single-particle orbits with angular momentum l, the product of the orbital wave functions will be an rth-rank tensor with respect to $SU(2l+1)$. Since the Coulomb repulsion is symmetric in the coordinates of all the electrons, the Coulomb energy will depend strongly on the symmetry of the coordinate wave function. Thus the appropriate linear combinations are the irreducible rth-rank tensors.

TABLE 11-8

TERMS FOR ELECTRON CONFIGURATION $(p)^r$

	Orbital	Spin	Multiplet
$r = 1$	[1] $L = 1$	[1] $S = \frac{1}{2}$	^2P
$r = 2$	[2] $L = 2, 0$	[1^2] $S = 0$	^1S, ^1D
	[1^2] $L = 1$	[2] $S = 1$	^3P
$r = 3$	[21] $L = 2, 1$	[21] $S = \frac{1}{2}$	^2P, ^2D
	[1^3] $L = 0$	[3] $S = \frac{3}{2}$	^4S

TABLE 11-9

TERMS FOR ELECTRON CONFIGURATION $(d)^r$

	Orbital	Spin	Multiplet
$r = 1$	[1] $L = 2$	[1] $S = \frac{1}{2}$	^2D
$r = 2$	[2] $L = 4, 2, 0$	[1^2] $S = 0$	^1S, ^1D, ^1G
	[1^2] $L = 3, 1$	[2] $S = 1$	^3P, ^3F
$r = 3$	[21] $L = 5, 4, 3, (2)^2, 1$	[21] $S = \frac{1}{2}$	^2P, $(^2D)^2$, ^2F, ^2G, ^2H
	[1^3] $L = 3, 1$	[3] $S = \frac{3}{2}$	^4P, ^4F
$r = 4$	[1^4] $L = 2$	[4] $S = 2$	^5D
	[21^2] $L = 5, 4, (3)^2, 2, (1)^2$	[31] $S = 1$	
	[2^2] $L = 6, (4)^2, 3, (2)^2, (0)^2$	[2^2] $S = 0$	
$r = 5$	[1^5] $L = 0$	[5] $S = \frac{5}{2}$	^6S
	[21^3] $L = 4, 3, 2, 1$	[41] $S = \frac{3}{2}$	
	[2^21] $L = 6, 5, (4)^2, (3)^2, (2)^3, 1, 0$	[32] $S = \frac{1}{2}$	

Problems. (1) Use Table 11-6 to construct the table of terms arising from the configuration $(f)^r$ $(l = 3)$.

(2) The arguments used here can also be applied to the classification of rotational states of homonuclear diatomic molecules. Apply them to the classification of the states of ortho- and para-hydrogen and ortho- and para-deuterium. Write the partition function for these molecules in their ground-electronic and vibrational state.

The next step in the perturbation procedure would be to include the spin-dependent terms in the Hamiltonian. The product of the representations D^J and D^S then splits into representations D^J. The spin-dependent terms cause a splitting of the multiplets.

11-4 Seniority in atomic spectra. For the configuration $(p)^r$, the symmetry pattern [λ] and the angular momentum L completely characterized the state: a multiplet occurred only once for a given symmetry.

TABLE 11–14

TOTAL ANGULAR MOMENTA IN THE CONFIGURATION $(j)^r$

		J
$j = \frac{3}{2}$	$r = 1$	$\frac{3}{2}$
	2	2, 0
$j = \frac{5}{2}$	$r = 1$	$\frac{5}{2}$
	2	4, 2, 0
	3	$\frac{9}{2}, \frac{5}{2}, \frac{3}{2}$
$j = \frac{7}{2}$	$r = 1$	$\frac{7}{2}$
	2	6, 4, 2, 0
	3	$\frac{15}{2}, \frac{11}{2}, \frac{9}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$
	4	$8, 6, 5, (4)^2, (2)^2, 0$
$j = \frac{9}{2}$	$r = 1$	$\frac{9}{2}$
	2	8, 6, 4, 2, 0
	3	$\frac{21}{2}, \frac{17}{2}, \frac{15}{2}, \frac{13}{2}, \frac{11}{2}, (\frac{9}{2})^2, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$
	4	$12, 10, 9, (8)^2, 7, (6)^3, 5, (4)^3, 3, (2)^2, (0)^2$
	5	$\frac{25}{2}, \frac{21}{2}, \frac{19}{2}, (\frac{17}{2})^2, (\frac{15}{2})^2, (\frac{13}{2})^2, (\frac{11}{2})^2, (\frac{9}{2})^3, (\frac{7}{2})^2, (\frac{5}{2})^2, \frac{3}{2}, \frac{1}{2}$

$\frac{3}{2}$, and hence $J = \frac{3}{2}$ is contained in the representation. Striking out $\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$, we exhaust the table, so the configuration $(\frac{5}{2})^3$ contains $J = \frac{9}{2}, \frac{5}{2}, \frac{3}{2}$.

There is a simple check on the angular-momentum analysis. The tensor of symmetry $[1^r]$ with respect to $SU(2j+1)$ has $\binom{2j+1}{r}$ independent components. (This is the number of ways of selecting the r indices $i_1 > i_2 > \cdots > i_r$ from the $2j+1$ values $j, j-1, \ldots, -j$.) Since a representation $D^{(J)}$ of the rotation group has dimension $2J+1$, we must have

$$\sum_{J \text{ in } [1^r]} (2J+1) = \binom{2j+1}{r}. \tag{11–14}$$

In the last example,

$$\binom{2j+1}{r} = \binom{6}{3} = 20 = \left(2 \cdot \frac{9}{2} + 1\right) + \left(2 \cdot \frac{5}{2} + 1\right) + \left(2 \cdot \frac{3}{2} + 1\right).$$

We tabulate the results through $j = \frac{9}{2}$ (Table 11–14).