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Autor(en): **Racah, Giulio**

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On the Calculation of Nuclear Levels

by **Giulio Racah**
The Hebrew University, Jerusalem, Israel.

We shall not discuss in this paper if the nuclear forces are charge-symmetrical, nor if the nuclear-shell model is correct; but, assuming that the forces are charge-symmetrical and that the nuclear-shell model has some significance, we consider the problem of calculating the nuclear levels in this approximation.

This problem does not involve fundamental difficulties, but only technical difficulties connected with the great number of terms which appear in a nuclear configuration. It suffices to remember that the configuration p^6 has 12 supermultiplets with 40 terms, d^5 has 77 supermultiplets with 244 terms, d^{10} has 472 supermultiplets with 2420 terms.

The calculation of the term energies and the tabulation of the results may be simplified very much by using the group-theoretical methods developed by the author for the calculation of the spectra of the atomic configurations f^n [1]).

The configurations p^n.

For spin-independent forces (WIGNER and MAJORANA interactions) the term-values of p^n were calculated by HUND[2]); he represented his results with two empirical formulas, which were later demonstrated by the author[3]):

$$V_W = \frac{n(n-1)}{2} F_0 + \left[6\,M - \frac{3}{2} L(L+1) - n(n-4)\right] F_2, \qquad (1)$$

$$V_M = M(F_0 + F_2) + \frac{3}{2}[n(n+1) - L(L+1)] F_2; \qquad (2)$$

here F_0 and F_2 are the well known parameters of SLATER[4]), and M is the eigenvalue of the Majorana operator, which depends only on the partition Σ characterizing the supermultiplet to which the term belongs.

For spin-dependent forces (BARTLETT and HEISENBERG interactions) some term values were calculated by FEENBERG and

Phillips[5]): using their equations (6), (7) and (8) we may obtain the general formula

$$V_B - V_H = \left[R(R+1) + S(S+1) + \frac{n(n-4)}{2}\right](F_0 - 5F_2), \tag{3}$$

and we may give to $V_B + V_H$ the more convenient form

$$V_B + V_H = [S(S+1) - R(R+1)]\left(F_0 + \frac{5}{2}F_2\right) + 6XF_2, \tag{4}$$

where X is a matrix which is diagonal with respect to R, S and L, but not with respect to Σ.

The whole problem is now reduced to the calculation of the matrix X, and the main result of the group-theoretical methods is that its elements are the product of two independent functions:

$$X = (\Sigma|X(R,S,L)|\Sigma') = (\Sigma|\Phi(R,S)|\Sigma')(\Sigma|\Psi(L)|\Sigma'). \tag{5}$$

The functions Φ and Ψ may be calculated separately, and their non-vanishing elements are given in Tables I—III.

Table I.

$\Phi(R, S)$ and $\Psi(L)$ for p^2 and p^4.

Conf.	Σ—Σ'	$\Phi(R,S)$ (11)	(31)	(13)	(33)	(51)	(15)	$\Psi(L)$ S	P	D	F
p^2	200—200		1	−1				−5/2		1/2	
p^4	211—310		$\sqrt{3}$	$\sqrt{3}$	2				$\sqrt{5/2}$		
	220—220	0			0	1	−1	−5/2		1/2	
	220—310				1					$-\sqrt{3}$	
	220—400	1						$2\sqrt{10}$		$-\sqrt{7}$	
	310—310		1	−1	0				3	−5/2	1/2

Table II.

$\Phi(R, S)$ and $\Psi(L)$ for p^3 and p^5.

Conf.	Σ—Σ'	$\Phi(R,S)$ (22)	(42)	(24)	44)	$\Psi(L)$ S	P	D	F
p^3	210—210	0	1/2	−1/2			−5/2	3/2	
	210—300	1					$\sqrt{10}$		
p^5	221—320	0	1	−1			$5\sqrt{3}/4$		
	221—410	1					$\sqrt{15}$		
	311—311	0	3/2	−3/2	0	5/2		−1/2	
	311—320	4	$\sqrt{5}$	$\sqrt{5}$				$3/2\sqrt{5}$	
	320—320	0	1/2	−1/2			−3	5/2	−1/2
	320—410	1					−3	$-\sqrt{14/5}$	2

Table III.

$\Phi\,(R,\,S)$ and $\Psi\,(L)$ for p^6.

Σ—Σ'	$\Phi\,(R,\,S)$							$\Psi\,(L)$					
	(11)	(31)	(13)	(33)	(33)′	(51)	(15)	S	P	D	D'	F	G
222—420		1	1					$5\sqrt{3}/2$					
321—321		3/5	−3/5	−2/3	2/3	1	−1		5/2	−3/2			
321—A				1					$4\sqrt{5/3}$				
321—B					1				$4\sqrt{5/3}$				
321—420		1	1							$4\sqrt{21}/5$			
A—A	1			−1/3					−2			3	
B—B	−1				1/3				−2			3	
420—420		1	−1					−3		9/10	−3/2	3/2	−1/2

$\psi\,(\mathrm{A}) = [\psi\,(411) + \psi\,(330)]/\sqrt{2},\ \psi\,(\mathrm{B}) = [\psi\,(411) - \psi\,(330)]/\sqrt{2}.$

The configurations d^n.

The first problem which arises for the configurations d^n is a convenient classification of the different states with the same L which belong to the same partition. As the partition numbers classify the terms according to the representations of the five-dimensional linear group, and the quantum number L according to the representations of the three-dimensional rotation group, a couple of quantum numbers $W \equiv (w_1\,w_2)$ may be introduced, which classifies the terms according to the representations of the five-dimensional rotation group. The quantum numbers W do not solve completely our problem, but are sufficient for our purpose: no more than three terms with the same L may belong to the same representation W, when also 18 may belong to the same partition.

The term values for $n \leqslant 4$ were obtained by Jahn[6]) by very long calculations based on a previous method of the author[7]). With the new group-theoretical methods we obtained for d^n the following formulas, which correspond to Eqs. (1) to (4):

$$V_W = \frac{n(n-1)}{2}\,F_0 + \left[5M - \frac{n(n-11)}{2} - \frac{5}{4}\,\gamma(W)\right](F_2 + 9F_4) + [\,2X^{(1)} - \omega(L,W)]\,(F_2 - 5\,F_4) \tag{6}$$

$$V_M = MF_0 + \left[\frac{3}{2}\,M + \frac{5\,n(n+3)}{4} - \frac{5}{4}\,\gamma(W)\right](F_2 + 9\,F_4) + [2\,\omega(L,W) - X^{(1)}]\,(F_2 - 5\,F_4) \tag{7}$$

$$V_B - V_H = \left[R(R+1) + S(S+1) + \frac{n(n-4)}{2}\right]\left[F_0 - \frac{7}{2}(F_2 + 9F_4)\right] + X^{(2)}(F_2 - 5F_4) \tag{8}$$

$$V_B + V_H = [S(S+1) - R(R+1)]\left[F_0 + \frac{7}{3}(F_2 + 9F_4)\right] + X^{(3)}(F_2 - 5F_4) + X^{(4)}(F_2 + 9F_4) \tag{9}$$

with

$$\gamma(W) = w_1(w_1 + 3) + w_2(w_2 + 1)$$

and

$$\omega(L,W) = \frac{1}{2} L(L+1) - \frac{3}{4}\gamma(W);$$

and the problem is reduced to the calculation of the four matrices $X^{(r)}$. The elements of these matrices have now the general expression

$$(\Sigma W | X^{(r)}(R, S, L) | \Sigma' W') =$$

$$\sum_{1}^{a}{}_{\alpha} \sum_{1}^{b}{}_{\beta} (\Sigma W | A^{(r)}_{\alpha\beta} | \Sigma' W') (\Sigma | \Phi^{(r)}_{\alpha}(R,S) | \Sigma') (W | \Psi^{(r)}_{\beta}(L) | W') \tag{10}$$

with a, $b \leqslant 3$; and it may also be shown that

$$\Phi^{(1)}_1 = \delta(\Sigma, \Sigma'), \quad \Phi^{(1)}_2 = \Phi^{(1)}_3 = 0, \quad \Phi^{(3)}_{\alpha} = \Phi^{(4)}_{\alpha},$$

$$\Psi^{(4)}_1 = \delta(W, W'), \quad \Psi^{(4)}_2 = \Psi^{(4)}_3 = 0, \quad \Psi^{(1)}_{\beta} = \Psi^{(2)}_{\beta} = \Psi^{(3)}_{\beta} \tag{11}$$

Tables of these functions for the configurations d^n with $n \leqslant 5$ were calculated, and will be published elsewhere.

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