Determination of allowed states of a multiparticle specified for given states of the subsystems

I. G. Kaplan and O. B. Rodimova

L. Ya. Karpov Physico-chemical Research Institute
Institute of Optics of the Atmosphere, Siberian Division, USSR Academy of Sciences

(Submitted October 25, 1973; resubmitted January 15, 1974)
Zh. Eksp. Teor. Fiz. **66**, 1560–1569 (May 1974)

A method is developed for finding the allowed states of a multiparticle system if the states of the subsystems (complex of impurity centers in the crystal, nucleon clusters in the nucleus, polyatomic molecules) are given. An advantage of the proposed procedure over those previously developed is its independence of the number of particles in the subsystems. Each subsystem is characterized by a spin value S_a and an irreducible representation $\Gamma^{(\alpha_a)}$ of a local point symmetry group. Depending on the value of S_a, the subsystems behave like bosons or fermions under permutation. Formulas are derived for the character of the reducible representation made up of the coordinate wave functions of the system, having a definite symmetry with respect to permutation of the subsystem; resolution of this representation into irreducible parts yields allowed representations $\Gamma^{(\alpha)}$ of the point symmetry group of the system. The allowed values of the spin S of the system are obtained from the tables of the reduction of the group of unitary transformations U_{2S_a+1} on the group of three-dimensional rotations. A connection is obtained between the developed method and the plethysm operation. It is shown that the permutation factors obtained in an earlier papers of the authors[9] can be expressed in terms of $3nj$ symbols, so that this procedure can likewise be made independent of the number of particles in the system, and a connection is indicated between the $3nj$ symbols and the plethysm coefficients. The case of allowance for the spin-orbit interaction within the subsystems is considered separately. Examples of the application of the developed method to various systems are given.

1. INTRODUCTION

In the investigation of composite systems (complexes of impurity ions in crystals, nucleon clusters in nuclei, polyatomic molecules, etc.) it is necessary to be able to find the allowed system states compatible with the specified states of the subsystems. A case that has been thoroughly investigated is the one in which the system is an aggregate of identical particles in a central field (nucleons in spherical nuclei, electrons in atoms). In this case, effective methods were developed for the classification of the allowed states[1-4]. The situation becomes much more complicated when the system consists of multiparticle subsystems and has an arbitrary spatial symmetry.

The first to solve the problem of classifying the states of such a composite system was Kotani[5], but his method called for cumbersome calculations of the spin factor. The breakdown of the total wave function into a coordinate function and a spin function, each symmetrized with respect to mutually-dual Young patterns, greatly facilitated the problem of classifying the states of a composite system[6,7]. In the general methods developed on the basis of this breakdown for the classification of states of multielectron systems[8,9], the permutations of the subsystems reduced to permutations of the particles among the subsystems. For systems with $N \gtrsim 12$ permuted particles, the use of the methods proposed in[8,9] is ineffective, since it calls for knowledge of the characters of the permutation groups π_N, the determination of which at large values of N is difficult.

In this paper we develop for the determination of allowed states of quantum-mechanical systems a method that does not depend on the number of particles in the subsystems. It is based on regarding a multiparticle system that has, in the general case, a complicated spatial structure as a unified particle–a fermion or a boson (in accordance with the value of the total spin S_a of the subsystem). The allowed values of the total spin of a system consisting of such "particles" is determined from the tables for the reduction of the group of unitary transformations U_{2S_a+1} on a group of three-dimensional rotations. We consider separately the case when the spin-orbital interaction inside the subsystems is taken into account. We discuss the connection between the developed method and methods that make use of the "plethysm" operation[4,10] (see Sec. 3 below).

2. DESCRIPTION OF METHOD

We consider a system with a point-group symmetry G, consisting of n subsystems containing n_a particles each. Without loss of generality we can assume the spin of each particle to be 1/2. Let the state of the subsystem be characterized by an irreducible representation $\Gamma^{(\alpha a)}$ of the local symmetry group G_a and a total spin S_a. We assume the subsystems to be identical if all the S_a coincide; the $\Gamma^{(\alpha a)}$ can be different in this case.

With respect to space rotation, the multiparticle subsystem can be regarded as a single particle with spin S_a, inasmuch as the transformation properties of the spin wave function for an aggregate of $2S_a$ particles with spin 1/2 and of one particle with spin S_a are identical (see[11], Sec. 97). Depending on whether S_a is integer or half-integer (or, equivalently, whether the number of particles in the subsystem is even or odd), the wave function of the system should be subject, with respect to permutations of the subsystems, to either Bose or Fermi statistics. It can be represented in the form (see[12]):

$$\Psi = (f_\lambda)^{-1/2} \sum_r \Phi_r^{[\lambda]} \Omega_{\bar{r}}^{[\tilde{\lambda}]}, \tag{1}$$

where $\Phi_r^{[\lambda]}$ is the coordinate wave function of the system, symmetrized with respect to the r column of the representation $\Gamma^{[\lambda]}$ of the permutation group of the subsystems π_n, $\Gamma_{\bar{r}}^{[\tilde{\lambda}]}$ is the spin function symmetrized over the column $\bar{r}$ of the representation $\Gamma^{[\tilde{\lambda}]}$, and f_λ

is the dimensionality of the representation $\Gamma^{[\lambda]}$. The Young patterns $[\lambda]$ and $[\bar{\lambda}]$ are related as follows:

$$[\bar{\lambda}] = \begin{cases} [\lambda] - \text{for boson subsystems} \\ [\tilde{\lambda}] - \text{for fermion subsystems,} \end{cases} \quad (2)$$

where $[\tilde{\lambda}]$ is the Young pattern dual to the pattern $[\lambda]$.

Each subsystem is characterized by a coordinate wave function $\varphi_i^{(\alpha a)}$ belonging to the basis of the representation $\Gamma^{(\alpha a)}$ with dimensionality f_{α_a}.[1)] In the zeroth approximation in the interaction, the coordinate wave function of the system can be constructed from products of the coordinate functions of the subsystems

$$\Phi_0 = \varphi_{i_1}^{(\alpha_1)} \varphi_{i_2}^{(\alpha_2)} \dots \varphi_{i_n}^{(\alpha_n)} \quad (3)$$

with the aid of the Young operators $\omega_{rt}^{[\lambda]}$ [12]:

$$\Phi_{rt}^{[\lambda]} = \omega_{rt}^{[\lambda]} \Phi_0. \quad (4)$$

Altogether, it is possible to make up $f_{\alpha_1}, f_{\alpha_2}, \dots f_{\alpha_n}$ products (3). For each of them we can construct f_λ^2 functions (4). (The subscripts r and t run through f_λ values each). The functions $\Phi_{rt}^{[\lambda]}$ with fixed subscript t are transformed into one another upon permutation of the subsystems and consequently form a basis of the representation $\Gamma^{[\lambda]}$, and in the construction of the total wave function they enter in a single bilinear combination (1) and correspond to one physical state. The total number of independent states having the permutation symmetry of the Young pattern $[\lambda]$ is $f_\lambda f_{\alpha_1} f_{\alpha_2} \dots f_{\alpha_n}$ The coordinate functions (4) that describe these states form the basis of a certain representation $U_{\alpha_1 \dots \alpha_n}^{[\lambda]}$ in the general case reducible, of the point symmetry group G.

The operation of the point group $\mathscr{R}$ on the wave function (4) is equivalent to a certain permutation P of the wave functions of the individual subsystems and to a point transformation R of these functions. The character of the representation induced on the coordinate functions (4) can be represented in the form of two factors, one of which depends on the permutation symmetry of the coordinate function (the permutation factor), while the other depends on the symmetry with respect to the point transformations (orbital factor):

$$X^{[\lambda]}(\mathscr{R}) = X^{[\lambda]}(P) X^{(\alpha_1 \dots \alpha_n)}(\mathscr{R}). \quad (5)$$

It is easy to show (cf.[9]) that for the permutation P with cyclic structure $\{1^{n_1} 2^{n_2} \dots k^{n_k}\}$ [2)] the factors that enter in (5) are equal to

$$X^{[\lambda]}(P) = \chi^{[\lambda]}(P), \quad (6)$$

$$X^{(\alpha_1 \dots \alpha_n)}(\mathscr{R}) = [\chi^{(\alpha_1)}(R)]^{n_1} [\chi^{(\alpha_2)}(R^2)]^{n_2} \dots [\chi^{(\alpha_k)}(R^k)]^{n_k} \tau(\mathscr{R}), \quad (7)$$

where $\chi^{[\lambda]}(P)$ is the character of the representation $\Gamma^{[\lambda]}$ of the permutation group of the subsystems π_N, and $\chi^{(\alpha i)}(\mathscr{R})$ is the character of the representation $\Gamma^{(\alpha i)}$ of the local symmetry group of the subsystems contained in the cycle $\{i\}$. The representations $\Gamma^{(\alpha i)}$ of all the subsystems that enter in the cycle $\{i\}$ should coincide, since otherwise the character vanishes; $\tau(\mathscr{R})$ is the number of different system conformations that remain invariant under the operation $\mathscr{R}$. If the $\Gamma^{(\alpha i)}$ coincide for all the subsystems, then $\tau(\mathscr{R}) = 1$.

The expansion of the representation (5) into irreducible representations $\Gamma^{(\alpha)}$ of the point symmetry group of the system G yields irreducible representations $\Gamma^{(\alpha)}$ that are compatible with the permutation symmetry of the coordinate Young pattern $[\lambda]$. The corresponding values of the electron spin of the system should be obtained as a result of expanding the representation of the group G induced on the spin functions $\Omega_r^{[\bar{\lambda}]}$.

The spin functions of a system of identical particles, each having a spin S_a, transforms in accordance with the irreducible representation $U_{2S_a+1}^{[\bar{\lambda}]}$ of the group of unitary transformations in $(2S_a + 1)$-dimensional vector space (see[12]). The group of three-dimensional rotations R_3 is a subgroup of the group of unitary transformations U_{2S_a+1}, so that when the unitary operations are limited to rotations in three-dimensional space, the irreducible representations $U_{2S_a+1}^{[\bar{\lambda}]}$ become in the general case reducible and break up into irreducible representations $D^{(S)}$ of the group R_3 (reduction on a subgroup):

$$U_{2S_a+1}^{[\bar{\lambda}]} = \sum_S a(U_{2S_a+1}^{[\bar{\lambda}]} \to D^{(S)}) D^{(S)}, \quad (8)$$

where the coefficient a is equal to the multiplicity with which the representation $D^{(S)}$ enters in the expansion (8). According to the tables of the reduction $U_{2S_a+1} \to R_3$ (see[12], Appendix 3, and also[1,2]), it is easy to determine the values of S corresponding to the Young pattern $[\bar{\lambda}]$. These are indeed the allowed values of the multiplicities for the terms obtained by expanding the representation (5).

Thus, the procedure for finding the allowed terms of the system can be represented schematically in the form

$$\begin{array}{c} U_{\alpha_1 \dots \alpha_n}^{[\lambda]} \to U_{2S_a+1}^{[\bar{\lambda}]} \\ \downarrow \\ \Gamma^{(\alpha)} \to D^{(S)} \end{array} \quad (9)$$

With the exception of $S_a = 1/2$, each Young pattern $[\bar{\lambda}]$ usually corresponds to several values of the spin S. The procedure (9) is carried out in succession for each allowed Young pattern of n cells, after which identical terms are summed.

We can also write out expressions for the character of the irreducible representation containing all the terms of a given multiplicity. To this end it is necessary to sum the character (5) over all $[\lambda]$, multiplying it each time by the multiplicity of the representation $D^{(S)}$ in the expansion (8):

$$X^{(S)}(\mathscr{R}) = \sum_\lambda X^{[\lambda]}(\mathscr{R}) a(U_{2S_a+1}^{[\bar{\lambda}]} \to D^{(S)}). \quad (10)$$

Since the orbital factor in (5) does not depend on $[\lambda]$, it can be taken outside the summation sign in (10). As a result, the character of (10), like (5), can be represented in the form of the product of the orbital factor $X^{(\alpha_1 \dots \alpha_n)}(\mathscr{R})$ by the permutation factor $X^{(S)}(P)$:

$$X^{(S)}(\mathscr{R}) = X^{(S)}(P) X^{(\alpha_1 \dots \alpha_n)}(\mathscr{R}), \quad (11)$$

where $X^{(\alpha_1 \dots \alpha_n)}(\mathscr{R})$ is given by formula (7), and

$$X^{(S)}(P) = \sum_\lambda \chi^{[\lambda]}(P) a(U_{2S_a+1}^{[\bar{\lambda}]} \to D^{(S)}). \quad (12)$$

In the case of a system consisting of several groups of identical subsystems, one first uses the procedure (9) to determine the allowed states for each group. Direct products of the allowed coordinate representations of each group are then set up, and their expansion into irreducible parts yields the allowed coordinate representations of the system. The corresponding values of the total electron spin are obtained by vector addition of the spins of the individual groups.

We also write a formula for the character of the

representation containing all the terms of a given multiplicity. To do this, we recognize that this representation is a direct product of those representations (10) whose spins S_i yield the spin S by vector addition. For two groups of identical subsystems, the formula for the character of the representation is

$$X^{(S)}(\mathfrak{R}) = \sum_{S_1}\sum_{S_2} X^{(S_1)}(\mathfrak{R}) X^{(S_2)}(\mathfrak{R}) \alpha(S_1 \times S_2 \to S) \tau(\mathfrak{R}), \qquad (13)$$

where $\tau(\mathfrak{R})$ is the number of system conformations that remain invariant upon permutation of the different groups of identical subsystems, and the expressions for $X^{(S_i)}(\mathfrak{R})$ are given by formulas (11) and (12). Inasmuch as in the expansion of the direct product

$$D^{(S_1)} \times D^{(S_2)} = \sum \alpha(S_1 \times S_2 \to S) D^{(S)} \qquad (14)$$

the multiplicity of the representations $D^{(S)}$ does not exceed unity, the coefficient $\alpha(S_1 \times S_2 \to S)$ in (13) is equal to 1 or to 0. The generalization to the case of several groups of identical subsystems is obvious.

In the case when the spin-orbit interaction is large, representation of the wave functions of the subsystem in the form (1) is incorrect. The wave function of the system can be either symmetrical or antisymmetrical, depending on whether the number of particles in the subsystem is even or odd. The scheme (9) for finding the allowed states is replaced by

$$U^{[n],[1^n]}_{\alpha_1 \ldots \alpha_n} \to \Gamma^{(\alpha)}. \qquad (9a)$$

The characters of the reducible representations are obtained in this case from formulas (6) and (7), where $[\lambda]$ can assume only two values, $[n]$ and $[1^n]$.

3. DISCUSSION OF VARIOUS METHODS OF CALCULATING THE PERMUTATION FACTOR

In the preceding section, expression (11) for the character of the representation whose expansion yields all the allowed terms of a given multiplicity was represented in the form of a product of two factors, orbital and permutation. The calculation of the orbital factor is trivial, since it calls only for knowledge of the characters of the irreducible representations of the local point symmetry group of the subsystem. To find the permutation factor it is necessary to know the coefficients of the expansion of the unitary group $U^{[\lambda]}_{2S_a+1}$ on the group of three-dimensional rotations. Tables of these expansions for $S_a = 1/2(1/2)3$ are given in[1,2,12].

In the present section we discuss alternative methods of calculating the permutation factor. Methods of calculating the permutation factor in terms of the characters of the permutation groups of the system particles were given in[8,9]. In contrast to the expressions for the permutation factor of[8], which contains directly the characters of the permutation groups of all the system particles, the permutation factor in our paper[9] is expressed in terms of the transformation matrices of the permutation group, thus opening the possibility of a different approach to its calculation.

For a permutation with a cyclic structure $\{1^{n_1}2^{n_2}\ldots k^{n_k}\}$, the permutation factor in formula (34) of[9] can be expressed in the form[3)]

$$X^{[\lambda]}(P) = \sum_{\lambda^{(1)}\ldots\lambda^{(k)}} \alpha(\lambda^{(1)} \times \ldots \times \lambda^{(k)} \to \lambda) w_1(\lambda_a, \lambda^{(1)})^{n_1} \ldots w_k(\lambda_a, \lambda^{(k)})^{n_k} \qquad (15)$$

For each cycle of length m, the Young pattern $\lambda^{(m)}$ consists of $n_a m$ cells, and the summation in (34) of[9] over λ_{interm} is replaced in (15) by a coefficient α that indicates the multiplicity of a given $\Gamma^{[\lambda]}$ in the expansion of the external product $\Gamma^{[\lambda^{(1)}]} \times \ldots \times \Gamma^{[\lambda^{(k)}]}$, and

$$w_m(\lambda_a, \lambda^{(m)}) = \sum_{\lambda_{interm}} \langle (\underbrace{\lambda_a \ldots \lambda_a}_{m}) \lambda_{interm} \| P \| (\lambda_a \ldots \lambda_a) \lambda_{interm} \rangle^{[\lambda^{(m)}]}. \qquad (16)$$

The permutation P belongs to the class $\{m^{n_a}\}$, and λ_{interm} is the set of (m–2) intermediate Young patterns that arise when m patterns $[\lambda_a]$ are combined into a common pattern $[\lambda^{(m)}]$. The values of w_m for $mn_a \le 8$ permuted electrons are tabulated in[9]. For larger values of mn_a, the values of w_m can be obtained easily if the corresponding characters of the representations are known. It is the latter circumstance which imposes limitations on the applicability of this method.

The limitations connected with the number of particles in the system can be eliminated by using the connection between the transformation matrices of the permutation groups and the 3nj symbols of the group of three-dimensional rotations. The identity of the invariants of the permutation group and of the invariants of the unitary-transformation group was established by Kramer[13] (see also[14]). For particles with spin 1/2, the invariants of the unitary group are equivalent to 3nj-symbols, since each irreducible representation $U^{[\lambda]}$ corresponds to a definite irreducible representation $D^{(j)}$ of the group R_3. The matrices $\langle \| P \| \rangle$ actually effect the transition from one scheme of connecting the spin angular momenta to another, and for a cycle of length m they are expressed in terms of 3(m–1)j symbols. When writing down w_m concretely in terms of the 3(m–1)j symbols, it must be recognized that the Young patterns contained in w_m pertain to the coordinate wave functions, whereas the spin angular momenta are connected with the permutation-group representation that is conjugate to the coordinate representation, i.e., the permutation matrices are connected in these representations by the factor $(-1)^p$, where p is the parity of the permutation. Thus

$$\begin{aligned} w_2 &= \langle \lambda_{1a}\lambda_{1b} \| P_{ab} \| \lambda_{1a}\lambda_{1b} \rangle^{[\lambda]} = (-1)^{n_a} \langle S_{1a}S_{1b} | P_{ab} | S_{1a}S_{1b} \rangle^S \\ &= (-1)^{n_a} \langle S_{1a}S_{1b} | S_{1b}S_{1a} \rangle^S = (-1)^{n_a}(-1)^{2S_1 - S} = (-1)^S, \end{aligned} \qquad (17)$$

$$\begin{aligned} w_3 &= \sum_{\bar\lambda} \langle (\lambda_{1a}\lambda_{1b})\bar\lambda\lambda_{1c} \| P_{abc} \| (\lambda_{1a}\lambda_{1b})\bar\lambda\lambda_{1c} \rangle^{[\lambda]} \\ &= \sum_{\bar S} \langle (S_{1a}S_{1b})\bar S S_{1c} | P_{abc} | (S_{1a}S_{1b})\bar S S_{1c} \rangle^S = \sum_{\bar S} \langle (S_{1a}S_{1b})\bar S S_{1c} | (S_{1b}S_{1c})\bar S S_{1a} \rangle^S \\ &= \sum_{\bar S} (-1)^{S_1 + \bar S - S} (2\bar S + 1) W(S_1 S_1 S S_1;\ \bar S \bar S) \equiv \sum_{\bar S} (-1)^{\bar S} (2\bar S + 1) \begin{Bmatrix} S_1 & S_1 & \bar S \\ S_1 & S & \bar S \end{Bmatrix}. \end{aligned}$$

Since extensive tables of 6j and 9j symbols are available[15,16], the calculation of w_m by formulas (17) entails no difficulty. For systems having more than four subsystems, the procedure for calculating w_m becomes more complicated, since they are expressed in terms of 12j symbols or symbols of higher order.

The permutation factors can also be expressed in terms of the "plethysm" coefficients. The plethysm operation was introduced by Littlewood[17,18] and used in[4,19,20] to classify states in atoms, and in[10] to classify terms of impurity complexes. For the group of unitary transformations U_k, the plethysm operation can be formulated in the following manner. We expand into irreducible parts the representation obtained by multiplying directly the representations $U_k^{[\lambda_a]}$ ($[\lambda_a]$ is a Young pattern of n cells) by itself m times. The obtained representations $(U_k^{[\lambda_a]})^{[\lambda]}$ ($[\lambda]$ is a Young pattern of m cells) are irreducible with respect to the operations of the group U_l, where l is the dimension-

ality of the representation $U_k^{[\lambda_a]}$, but are reducible with respect to the group U_k. The plethysm coefficients are defined as the coefficients for the expansion of the representation $(U_k^{[\lambda_a]})^{[\lambda]}$ on the irreducible representations $U_k^{[\lambda']}$ ($[\lambda']$ is a Young pattern of $n_a m$ cells):

$$(U_k^{[\lambda_a]})^{[\lambda]} = \sum_{\lambda'} \alpha(\lambda_a \otimes \lambda \to \lambda') U_k^{[\lambda']}, \qquad (18)$$

where the symbol $\otimes$ denotes the plethysm operation.

For subsystems consisting of particles with spin 1/2, states with a total spin S_a are described by a spin function that belongs to the representation $U_2^{[\tilde{\lambda}_a]}$ of the group U_2, where the Young pattern $[\tilde{\lambda}_a]$ consists of two rows of lengths $\tilde{\lambda}_a^{(1)}$ and $\tilde{\lambda}_a^{(2)}$ ($\tilde{\lambda}_a^{(1)} - \tilde{\lambda}_a^{(2)} = 2S_a$). The construction of the basis of the representation $U_{2S_a+1}^{[\lambda]}$ out of the wave functions of m subsystems (each subsystem being in a state with spin S_a) is equivalent to constructing the basis of the representation $U_2^{[\lambda_a]})^{(\lambda)}$. Since each Young pattern $[\lambda']$ of $n_a m$ cells corresponds uniquely to a total spin S, the determination of the expansion

$$(U_2^{[\tilde{\lambda}_a]})^{[\tilde{\lambda}]} = \sum_{\tilde{\lambda}'} \alpha(\tilde{\lambda}_a \otimes \tilde{\lambda} \to \tilde{\lambda}') U_2^{[\tilde{\lambda}']} \qquad (19)$$

is fully equivalent to a determination of the expansion (8). Therefore the coefficients of the expansion (8) are equal to the plethysm coefficients

$$\alpha(U_{2S_a+1}^{[\tilde{\lambda}]} \to D^{(s)}) \equiv \alpha(\tilde{\lambda}_a \otimes \tilde{\lambda} \to \tilde{\lambda}'). \qquad (20)$$

As a result, when calculating the permutation factor by means of formula (12) we can use the plethysm coefficients in place of the coefficients for the reduction of the group of unitary transformations on the group of three-dimensional rotations. The published plethysm tables cover the values $n_a m \leq 18$[21].

We note that the determination of the plethysm of the spin states in[10] in the case of identical ion spins is fully equivalent to the reduction $U_{2S_a+1} \to R_3$, although the meaning of the designations of the Young patterns in the spin plethysm in[10] is not standard and calls for additional explanations. The procedure called in[10] "plethysm of the set $(\Gamma_{i_1} \ldots \Gamma_{i_m})$ with $[\lambda]$" actually reduces to calculation of the character of the representation by formulas (5)–(7) of the present paper. In the case of a complex consisting of several groups of identical subsystems, the procedure of the present paper differs essentially from that of[10].

In view of the different methods of calculating the permutation factor, a mutual relation exists between the quantities in formulas (12) and (15). To establish this relation, we consider the operation $\mathscr{R}$, which is equivalent to permutation with cyclic structure $\{n\}$. Formula (15) reduces in this case to one factor $w_n(\lambda_a, \lambda')$. Using (20), we obtain an expression for w_n in terms of the plethysm coefficients:

$$w_n(\lambda_a, \lambda') = \sum_{\lambda} \chi^{[\lambda]}(\{n\}) \alpha(\tilde{\lambda}_a \otimes \tilde{\lambda} \to \tilde{\lambda}'). \qquad (21)$$

Since w_n is expressed in terms of 3nj symbols, see (17), a mutual relation exists between the plethysm coefficients and the 3nj symbols of the group R_3.

4. EXAMPLES

1. Complex of three subsystems: let $G = D_3$, $G_a = C_3$, $\Gamma^{(\alpha_a)} = E$, $S_a = 3/2$. To find the characters of the coordinate representation we use formulas (6) and (7), which yield in our case the following expressions for the characters corresponding to the operations of the group D_3:

$$X(E) = \chi^{[\lambda]}(\{1^3\})[\chi^{(E)}(E)]^3, \quad X(C_3) = \chi^{[\lambda]}(\{3\})\chi^{(E)}(C_3^3),$$
$$X(U_2) = \chi^{[\lambda]}(\{21\})\chi^{(E)}(U_2^2)\chi^{(E)}(U_2).$$

The corresponding values of the multiplicities are obtained from the tables of the reduction $U_4^{[\lambda]} \to D^{(S)}$. The results of the analysis are given in Table I. Thus, the following multiplets are allowed (the number in the parentheses indicates the multiplicity of the given multiplet):

$$\overset{2,\ 4,\ 6,\ 8,\ 10}{(2)\ (6)\ (5)\ (2)\ (3)} A_1, \ \overset{2,\ 4,\ 6,\ 8,\ 10}{(2)\ (6)\ (3)\ (2)} A_2, \ \overset{2,\ 4,\ 6,\ 8,\ 10}{(2)\ (10)\ (8)\ (6)\ (2)} E.$$

2. Three-dimensional ion cluster FeCrFe[22]: $G = G_{2v}$, $\Gamma^{(\alpha_a)} = D^{(0)}$, $S_{Fe} = 5/2$, $S_{Cr} = 3/2$. We have two groups of identical atoms with $N' = 2$ and $N'' = 1$. Owing to the absence of orbital degeneracy, the formula for the characters is given by expression (6):

$$X(\mathfrak{R}) = \chi^{[\lambda']}(P).$$

The spins S' corresponding to the obtained coordinate states are obtained from the tables of the reduction $U_6^{[\lambda']} \to D^{(S')}$. The allowed values of the total spin are the resultants of the vector addition of the spins S' and $S_{Cr} = 3/2$. Using Table II, we obtain the following multiplets:

$$\overset{2,\ 4,\ 6,\ 8,\ 10,\ 12}{(2)\ (2)\ (2)} A_1, \ \overset{2,\ 4,\ 6,\ 8,\ 10,\ 12,\ 14}{(2)\ (2)\ (2)\ (2)} B_2.$$

3. The molecule CD_4 in the absence of an external field: $G = T_d$, $G_a = O_3$, $\Gamma(C) = D^{(1)}$, $\Gamma(D) = D^{(0)}$, $S_C = S_D = 1$. The formula for the character in which account is taken of the presence of two groups of identical atoms ($N' = 4$, $N'' = 1$) takes in this case the simple form:

$$X(\mathfrak{R}) = \chi^{[\lambda']}(P)\chi^{(C)}(R).$$

The C atom is assumed to be in the ground state $1s^2 2s^2 2p^3 (^3P)$ and the characters $\chi^{(1)}(R)$ corresponding to the operations of the group T_d are equal to

$$\chi^{(1)}(E) = 3, \quad \chi^{(1)}(C_3) = 0, \quad \chi^{(1)}(C_2) = \chi^{(1)}(S_4) = -1, \quad \chi^{(1)}(\sigma_d) = 1.$$

We have the following set of allowed multiplets (see Table III):

$$\overset{1,\ 3,\ 5,\ 7,\ 9}{(2)\ (3)\ (2)} A_1, \ \overset{1,\ 3,\ 5}{(2)\ (3)\ (4)} A_2, \ \overset{1,\ 3,\ 5,\ 7,\ 9}{(2)\ (2)\ (2)} E,$$
$$\overset{1,\ 3,\ 5,\ 7,\ 9}{(2)\ (5)\ (5)\ (3)} F_1, \ \overset{1,\ 3,\ 5,\ 7,\ 9,\ 11}{(2)\ (7)\ (6)\ (5)\ (2)} F_2.$$

TABLE I

S	$\tilde{\lambda}$	λ	E	$2C_3$	$3U_2$	$\Gamma^{(\alpha)}$
$^3/_2$, $^5/_2$, $^9/_2$	[3]	[1³]	8	2	2	$3A_1, A_2, 2E$
$^1/_2$, $^3/_2$, $^5/_2$, $^7/_2$	[21]	[21]	16	−2	0	$2A_1, 2A_2, 6E$
$^3/_2$	[1³]	[3]	8	2	−2	$A_1, 3A_2, 2E$

TABLE II

S	S'	$\tilde{\lambda}'$	λ'	E	C_2	σ_1	σ_2	$\Gamma^{(\alpha)}$
$^1/_2$, $(^3/_2)^2$, $(^5/_2)^2$, $(^7/_2)^2$, $(^9/_2)^2$, $^{11}/_2$, $^{13}/_2$	1, 3, 5	[2]	[1²]	1	−1	−1	1	B_2
$^1/_2$, $(^3/_2)^2$, $(^5/_2)^2$, $(^7/_2)^2$, $^9/_2$, $^{11}/_2$	0, 2, 4	[1²]	[2]	1	1	1	1	A_1

TABLE III

S	S'	$\tilde{\lambda}'$	λ'	E {1⁴}	$8C_3$ {31}	$3C_2$ {2²}	$6\sigma_d$ {21²}	$6S_4$ {4}	$\Gamma^{(\alpha)}$
$1^2, 2, 3^2, 4, 5$	0, 2, 4	[4]	[4]	3	0	−1	1	−1	F_2
$0, 1^2, 2^2, 3^2, 4$	1, 2, 3	[31]	[31]	9	0	1	1	1	A, E, F_1, F_2
$1^2, 2, 3$	0, 2	[2²]	[2²]	6	0	−2	0	0	F_1, F_2
$0, 1, 2$	1	[21²]	[21²]	9	0	1	−1	−1	A_2, E, F_1, F_2

4. Pair of atoms in even states with strong spin-orbit interaction. The total angular momentum of each atom is $J_a = 1$. Let

$$G=\mathbf{D}_{\infty h}, \quad G_a=\mathbf{O}_3, \quad \Gamma^{(\alpha_a)}=D^{(1)}.$$

The classification of the states is in accordance with the scheme (9a), and the expressions obtained from formulas (6) and (7) for the characters of the representations are

$$X(E)=\chi^{[\lambda]}(\{1^2\})[\chi^{(1)}(E)]^2, \quad X(C_\varphi)=\chi^{[\lambda]}(\{1^2\})[\chi^{(1)}(\varphi)]^2,$$
$$X(U_2)=\chi^{[\lambda]}(\{1^2\})[\chi^{(1)}(U_2)]^2, \quad X(I)=\chi^{[\lambda]}(\{2\})\chi^{(1)}(E),$$
$$X(IC_\varphi)=\chi^{[\lambda]}(\{2\})\chi^{(1)}(2\varphi), \; X(IU_2)=\chi^{[\lambda]}(\{2\})\chi^{(1)}(E).$$

We present below the values of the characters and the allowed multiplets for the case when the atom contains an even number of electrons ($[\lambda] = [2]$):

$[\lambda]$	$\frac{E}{\{1^2\}}$	$\frac{2C_\varphi}{\{1^2\}}$	$\frac{U_2}{\{1^2\}}$	$\frac{I}{\{2\}}$	$\frac{2IC_\varphi}{\{2\}}$	$\frac{IU_2}{\{2\}}$	$\Gamma^{(\alpha)}$
[2]	9	$[\chi^{(1)}(\varphi)]^2$	1	3	$\chi^{(1)}(2\varphi)$	3	$2\Sigma_g^+, \Sigma_u^-, \Pi_g, \Pi_u, \Delta_g$

[1)]The coordinate wave function of the subsystem is also an "internal" symmetry $[\lambda_a]$ relative to permutations of the subsystem particles. In the formulas derived below, however, this circumstance is not utilized directly.

[2)]We recall that $n_1 + 2n_2 + \ldots + kn_k = n$.

[3)]In [9] the term permutation factor is used for the factors $w_m(\lambda_a, \lambda^{(m)})$ that enter in (15).

[4)]A detailed exposition of the application of the developed procedure to impurity ions in a crystal will be published in Fiz. Tverd. Tela. [Sov. Physics–Solid State].

[1]H. A. Jahn. Proc. Roy. Soc., **A201**, 516 (1950).
[2]B. H. Flowers. Proc. Roy. Soc., **A212**, 248 (1952); **A215**, 398 (1952). A. R. Edmonds, B. H. Flowers, Proc. Roy Soc., **A214**, 515 (1952).
[3]V. G. Neudachin and Yu. F. Smirnov, Nuklonnye assotsiatsii v legkikh yadrakh (Nucleon Clusters in Light Nuclei), Nauka, 1969.
[4]B. G. Wybourne, Symmetry Principles and Atomic Spectroscopy, N. Y., 1970.
[5]M. Kotani, Proc. Phys.-Math. Soc., Japan, **19**, 460 (1937).
[6]I. G. Kaplan, Zh. Eksp. Teor. Fiz. **37**, 1050 (1959) [Sov. Phys.-JETP **10**, 747 (1960)].
[7]I. G. Kaplan, ibid. **51**, 169 (1966) [**24**, 114 (1967)].
[8]V. I. Cherepanov and A. A. Shchetkov, ibid. **55**, 1805 (1968) [**28**, 953 (1969)].
[9]I. G. Kaplan and O. B. Rodimova, ibid. **55**, 1881 (1968) [**28**, 995 (1969)].
[10]B. A. Men', A. N. Men', and V. I. Cherepanov, Dokl. Akad. Nauk SSSR **209**, 333 (1973) [Sov. Phys.-Doklady **18**, 187 (1973)].
[11]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, 1963.
[12]I. G. Kaplan, Simmetriya mnogoelektronnykh sistem (Symmetry of Many-Electron Systems), Nauka 1969.
[13]P. Kramer, Zs. f. Phys., **205**, 181 (1967); **216**, 68 (1968).
[14]V. I. Kuklin, Yu. F. Smirnov and L. Majling, Nucl. Phys., A **103**, 681 (1967).
[15]A. F. Nikiforov, B. V. Uvarov, and Yu. L. Levitan, Tablitsy koeffitsienov Raka (Tables of Racah Coefficients), VTsAN SSSR, 1962.
[16]Ya. I. Vizbaraĭte, I. I. Gelmbotskiĭ, R. I. Karaziya, G. D. Strotskite, and V. I. Uldukite, Tablitsy ^{9}j-koeffitsientov dlya tselykh znachenii parametrov s odnim parametrom, ravnym edinitse (Tables of 9j coefficients for integer values of the parameters with one parameter equal to unity), VTsAN SSSR (1968).
[17]D. E. Littlewood, J. Lond. Math. Soc., **11**, 49 (1936).
[18]D. E. Littlewood, Theory of Group Characters and Matrix Representations of Groups, N. Y., 1958, 2nd ed.
[19]P. R. Smith and B. G. Wybourne, J. Math. Phys., 8, 2434 (1967); **9**, 1040 (1968).
[20]B. G. Wybourne, J. Math. Phys., **10**, 467 (1969).
[21]V. Vanagas, Algebraicheskie metody v teorii yadra Algebraic Methods in the Theory of the Nucleus) Vil'nyus, 1971.
[22]R. L. Martin, in: Fizicheskie metody issledovaniya i svoĭstva neorganicheskikh soedinenii (Physical Methods of Investigation and Properties of Inorganic Compounds) [Russian translation], Mir, 1970.

Translated by J. G. Adashko
160