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Academician S. V. VONSOVSKII, V. I. CHEREPANOV,
A. N. MEN' , A. E. NIKIFOROV

GROUP-THEORETICAL CLASSIFICATION OF THE STATES OF A PAIR OF EXCHANGE-COUPLED IONS IN A CRYSTAL

In connection with the creation of optical quantum generators on the lines of pairs of exchange-coupled impurity ions in crystals ([1]), a group-theoretical classification of the states of the pair is of interest.

The problem of determining the possible states of a pair of interacting impurity ions in a crystal is, in principle, analogous to the problem of determining the state of a diatomic molecule ([2]); however, it is necessary to take into account the influence of the symmetry of the crystalline field. The symmetry group of the pair of ions A and B in the crystal G_k is defined as the intersection of the point group G_C, corresponding to the midpoint C of the segment AB^*, with the group $D_{\infty h}$ (or $C_{\infty v}$, for unlike impurity ions), whose axial axis coincides with AB, i.e. $G_k = G_C \cap D_{\infty h}(C_{\infty v})$. Since $D_{\infty h} = C_{\infty v} + I_C C_{\infty v}$ (where I_C is inversion at the point C), one may write:

$$G_k = G_k^J \quad \text{(for unlike ions A and B);} \tag{1a}$$

$$G_k = G_k^J + I_0 G_k^J \quad \text{(for like ions A and B),} \tag{1b}$$

where $G_k^J = G_C \cap C_{\infty v}$, and I_0 is any one of the elements of the intersection $C_C \cap I_C C_{\infty v}$. Equality (1) is the decomposition of the group G_k into cosets with respect to the invariant subgroup G_k^J. The group G_k^J contains symmetry elements that do not interchange the ions A and B, while $I_0 G_k^J$, on the contrary, contains elements that interchange the ions A and B. On the other hand, it is easy to show that the subgroup G_k^J coincides with the intersection of the groups $G_A \times G_B \cap C_{\infty v}$, containing only such pairs of elements g_A (from the group G_A) and $\tilde{g}_B$ (from the group G_B) that transform all points of space in the same way.**

As for a molecule, the classification of states may be carried out in various ways. We shall consider the simplest one, in which one starts from the states of a pair of noninteracting ions in the crystalline field.

In contrast to a diatomic molecule, it is necessary to consider not two, but three different cases: 1) different ions, 2) identical ions in nonequivalent positions (identical nonequivalent ions), 3) identical ions in equivalent positions (identical equivalent ions).

Let us first consider the first two cases, which admit a common treatment, since in both cases $G_k = G_k^J$. Let the states of the individual ions be determined by the quantum numbers $\chi_1\Gamma_1\mu_1$ and $\chi_2\Gamma_2\mu_2$, where $\Gamma_1\mu_1$ and $\Gamma_2\mu_2$ are the index and row of irreducible representations*** of the groups G_A and G_B, respectively, and χ_1 and χ_2 are additional quantum numbers.

Writing the wave functions of the pair of noninteracting ions in the form of antisymmetrized (with respect to permutations of electrons between the ions) products of the wave functions of the individual ions and considering them as a basis of a representation of the group G_k, it is easy to obtain the formula for the characters of this representation

$$X(g_A\tilde{g}_B) = X^{(\Gamma_1)}(g)X^{(\Gamma_2)}(\tilde{g}). \tag{2}$$

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* The point group G_C of an ideal crystal without the impurity is meant. Analogously, G_k is determined by Kaplyanskii and Przhevuskii (private communication).

** Such elements can only be rotations about the common symmetry axis AB or reflections in symmetry planes containing this axis.

*** We note that Γ_i is a double-valued representation of the double group if N_i (the number of electrons of the i-th ion) is an odd number.

Using these characters, one can decompose the given representation into irreducible representations of the group G_k, which determines the possible terms arising in the interaction of the ions of the pair.

In the third case it is necessary to distinguish two possibilities: a) the ions of the pair are in different states ($\chi_1\Gamma_1 \neq \chi_2\Gamma_2$), b) the ions of the pair are in the same state ($\chi_1\Gamma_1 = \chi_2\Gamma_2 = \chi\Gamma$). In case a), in constructing the wave functions of the pair it is necessary to take into account degeneracy with respect to the exchange of states

Table 1

States	Pair of order I (D_3)	Pair of order II (C_i)	Pair of order III (C_2)	Pair of order IV (C_1)	Pair of order V (S_6)	Approximate classification (C_3) (for all pairs)
$\overline{2A} \times \overline{2A}$	A_1+3A_2	A_g+3A_u	$A+3B$	$4A$	A_g+3A_u	$4A$

States	Pair of order I (D_3)	Pair of order II (C_i)	Pair of order III (C_2)	Pair of order IV (C_1)	Pair of order V (S_6)	Approximate classification (C_3) (for all pairs)
$\overline{E} \times \overline{E}$	$2A_2 + E$	$A_g + 3A_u$	$A + 3B$	$4A$	$A_g + A_u + E_g$	$2A + E$
$(\overline{2A} \times \overline{E}) + (\overline{E} \times \overline{2A})$	$4E$	$4A_g + 4A_u$	$4A + 4B$	$8A$	$2E_u + 2E_g$	$4E$
$(\overline{2A} \times \overline{2A}^*) + (\overline{2A}^* \times \overline{2A})$	$4A_1 + 4A_2$	$4A_g + 4A_u$	$4A + 4B$	$8A$	$4A_u + 4A_g$	$8A$
$(\overline{E} \times \overline{E}^*) + (\overline{E}^* \times \overline{E})$	$2A_1 + 2A_2 + 2E$	$4A_g + 4A_u$	$4A + 4B$	$8A$	$2A_u + 2A_g + E_u + E_g$	$4A + 2E$
$(\overline{2A} \times \overline{E}^*) + (\overline{E}^* \times \overline{2A})$	$4E$	$4A_g + 4A_u$	$4A + 4B$	$8A$	$2E_u + 2E_g$	$4E$
$(\overline{E} \times \overline{2A}^*) + (\overline{2A}^* \times \overline{E})$	$4E$	$4A_g + 4A_u$	$4A + 4B$	$8A$	$2E_u + 2E_g$	$4E$

$$X(g_A\tilde{g}_B) = X^{(\Gamma_1)}(g)X^{(\Gamma_2)}(\tilde{g}) + X^{(\Gamma_2)}(g)X^{(\Gamma_1)}(\tilde{g}), \qquad X(I_0 g_A\tilde{g}_B) = 0; \tag{3a}$$

$$X(g_A\tilde{g}_B) = X^{(\Gamma)}(g)X^{(\Gamma)}(\tilde{g}), \qquad X(I_0 g_A\tilde{g}_B) = (-1)^N X^{(\Gamma)}(g\tilde{g}), \tag{3b}$$

where N is the number of electrons in each of the ions. In the particular case when G_A, G_B, and G_C are rotation groups, the results of Wigner' s work [2] are obtained.

As an example, let us determine the terms of pairs of identical equivalent Cr^{3+} ions in ruby ($G_A = G_B = C_3$), when each ion of the pair is in one of the two states ${}^4T_2$ ($\overline{2A}$ or $\overline{E}$) of the ground doublet, or when one of the ions of the pair is excited into one of the two states ${}^2T_3$ ($\overline{E}^*$ or $\overline{2A}^*$) of the lowest excited doublet.*

The decomposition (1b) for pairs of orders from the first to the fifth** has the form
I. $D_3 = C_3 + U_2 C_3$. II. $C_i = C_1 + I_{CC} 1$. III. $C_2 = C_1 + C_2 C_1$. IV. $C_1 = C_1$. V. $S_6 + I_{CC} 3$. Table 1 gives the terms of these pairs, determined using formulas (3a) and (3b). The last column of the table gives the approximate classification of the terms.

Institute of Metal Physics
Academy of Sciences of the USSR

Ural State University
named after A. M. Gorky

Institute of Metallurgy, Sverdlovsk

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* By an asterisk we distinguish excited states from ground states, since we do not write out the additional quantum numbers.

** The arrangement of pairs is meant in order of increasing distance between the ions of the pair.

Note: Figure translations are in progress. See original paper for figures.