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Abstract

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ON THE DECOMPOSITION OF DIRECT PRODUCTS OF IRREDUCIBLE REPRESENTATIONS OF SPACE GROUPS

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In recent years, in solid-state physics, in interpreting experimental material, selection rules that take into account the full symmetry of the crystal, i.e., its space group, have been used more and more widely. Comparison of these selection rules with experimental data on absorption coefficients makes it possible to draw definite conclusions about the structure of the electronic, excitonic, and phonon spectra of a crystal. In addition to the study of direct and indirect optical transitions, these selection rules can be used in the analysis of processes of scattering of current carriers by thermal vibrations, spin waves, combination scattering of light, the Jahn–Teller effect in crystals, etc. The determination of these selection rules reduces to the decomposition of direct products of irreducible representations of the space group of the crystal into irreducible components. Numerous works have been devoted to the consideration of this question and to the physical applications of selection rules.

Lax and Hopfield ⁽¹⁾ considered irreducible representations of the space group O_h^7 for each branch of phonon vibrations of crystals with the diamond structure. Selection rules for transitions in crystals with the zinc-blende structure (T_d^2) were found by Birman ⁽²⁾. G. F. Koster ^(3, 4) obtained selection rules for transitions between different irreducible sets of states and for intervalley transitions in crystals with the zinc-blende structure, taking into account spin-orbit interaction and the time-reversal operation. Birman ⁽⁵⁾ compared two methods of obtaining selection rules: the method using the symmetry elements of the entire space group (the full-group method), and the method using the symmetry elements that constitute a subgroup of the space group (the subgroup method).

However, in all previous works only selection rules were found, while the actual decomposition of the direct product of representations into irreducible representations, i.e., the construction from the basis functions of the direct product of such combinations that belong to definite irreducible representations, was not carried out. Meanwhile, for example, in describing exciton states in dielec-

tric crystals it is necessary to be able to construct, from the wave functions of the particle and the hole, such combinations as correspond to the irreducible representation of the space group characterizing the exciton state. Thus, it is necessary to be able to calculate Clebsch–Gordan (C.G.) coefficients for space groups. In the work of Overhauser ⁽⁶⁾, devoted to the theory of excitons in alkali-halide crystals, the simplest case of these coefficients was considered for the product of two representations with quasi-momenta k and k' equal to zero, when the indicated C.G. coefficients coincide with the corresponding quantities for the point group O_h . In general form, the problem of calculating C.G. coefficients for space groups has not been considered. Therefore, in the present work we shall briefly describe one possible method for calculating them.

A space group includes the operations of the translation subgroup, the operations of the point group, products of point-group operations by translations, and operations containing translations that do not belong to the translation subgroup. We shall consider symmorphic groups, which have no nontrivial screw axes or glide planes. However, the results obtained are not difficult to generalize to the case of nonsymmorphic groups, using, for example, the apparatus of loaded representations ⁽⁷⁾.

We shall denote the basis functions of the irreducible representation D^{kA} of the full space group (k is the vector defining the star of the representation, A is the symbol of the irreducible representation of the point group G_k of the vector k) by the symbol

$$|k_i A \alpha\rangle; \quad (1)$$

here the index i runs over all rays of the star k ; α enumerates the rows of the representation A .

It is important to note that all basis functions corresponding to different rays of the star k_i are obtained from the function of one ray k by means of a fixed set of operations σ_i :

$$G(\sigma_i)|k A \alpha\rangle = |k_i A \alpha\rangle. \quad (2)$$

In the decomposition of the direct product of two representations D^{kA} and $D^{k'B}$ into irreducible components

$$D^{kA} \times D^{k'B} = \sum_{k''C} N_{k''C} D^{k''C} \quad (3)$$

the integers $N_{k''C}$ are given by the formula

$$N_{k''C} = \frac{v_3}{n_{k''}} \sum_{g \in G_{k_{i0}} G_{k'_{j0}} G_{k''}} \chi_C^*(g) \chi_A(\sigma_{i0}^{-1} g \sigma_{i0}) \chi_B(\sigma_{j0}^{-1} g \sigma_{j0}), \quad (4)$$

where σ_{j_0} is the operation which carries the vector k' into k'_{j_0} in accordance with condition (3) ($\sigma_{j_0}k' = k'_{j_0} + B_s$; B_s is a reciprocal-lattice vector satisfying the relation $k_{i_0} + k'_{j_0} = k'' + B_q$); v_3 is the number of stars k'' in the product of the stars k and k' , i.e., the number of combinations of rays k_i and k'_j that give, in the sum, the vector k'' , $k_i + k'_j = k'' + B_r$; $n_{k''}$ is the order of the group $G_{k''}$. The summation of products of ordinary characters of the point groups χ must be carried out over the intersection of all three little groups $G_{k_{i_0}}$, $G_{k'_{j_0}}$, and $G_{k''}$.

The Clebsch-Gordan coefficients of the space group can be determined with the aid of the projection operator $P_{\gamma'\gamma}^C$ for the point group $G_{k''}$, which carries the function $|k_i A \alpha'\rangle |k'_j B \beta'\rangle$ into the function $|k''_s C \gamma'\rangle$

$$\langle k_i A \alpha', k'_j B \beta' | k''_s C \gamma' \rangle = \frac{\langle k_i A \alpha', k'_j B \beta' | \sigma_s P_{\gamma'\gamma}^C | k_{i_0} A \alpha, k'_{j_0} B \beta \rangle}{\langle k_{i_0} A \alpha, k'_{j_0} B \beta | P_{\gamma'\gamma}^C | k_{i_0} A \alpha, k'_{j_0} B \beta \rangle^{1/2}}. \quad (5)$$

Here σ_s carries the vector k'' into k''_s ($\sigma_s k'' = k''_s + B_q$) in accordance with condition (3),

$$P_{\gamma'\gamma}^C = \frac{n_C}{n_{k''}} \sum_h D_{\gamma'\gamma}^C(h) \hat{G}(h),$$

n_C is the dimension of the representation C ; the quantities α, β, k_{i_0} , and k'_{j_0} in the numerator and denominator of (5) are fixed arbitrarily, but under the condition that

$$k_{i_0} + k'_{j_0} = k'' + B_r.$$

The numerator of (5) is computed by the formula

$$\frac{n_C}{n_{k''}} \sum_h \langle k_i A \alpha' | \sigma_s h | k_{i_0} A \alpha \rangle \langle k'_j B \beta' | \sigma_s h | k'_{j_0} B \beta \rangle \langle k''_s C \gamma' | \sigma_s h | k'' C \gamma \rangle = \frac{n_C}{n_{k''}} \sum_h D_{\alpha'\alpha}^A(\sigma_i^{-1} \sigma_s h \sigma_{i_0}) D_{\beta'\beta}^B(\sigma_j^{-1} \sigma_s h \sigma_{j_0})$$

* k_{i_0}, k'_{j_0} are one such combination.

where $D_{\alpha'\alpha}^A(h')$ are elements of the matrices of irreducible representations of point groups, given, for example, in (8). The operations σ_i and σ_j are chosen from condition (3).

Although formally in (6) the summation is over all operations h of the small group $G_{k''}$, nevertheless, in fact, only those operations which simultaneously satisfy the three conditions make a nonzero contribution:

$$\sigma_s h k_{i_0} = k_i + B_v,$$

$$\sigma_s h k'_{j0} = k'_j + B_w,$$

$$\sigma_s h k'' = k''_s + B_q.$$

Table 1

Clebsch-Gordan coefficients of the group O_h^1
 $\langle k_i A \alpha, k'_j B \beta | k''_s C \gamma \rangle$ in the case $k A \alpha = M_1$,
 $k' B \beta = M_2$, $k'' = \Gamma$ (a —edge of the cube)

$M_1 k_i$	$M_2 k'_j$	Γ_2	$\Gamma_{12} u$	$\Gamma_{12} v$
$\frac{\pi}{a} \frac{\pi}{a} 0$	$\frac{\pi}{a} \frac{\pi}{a} 0$	$\frac{1}{\sqrt{3}}$	$\sqrt{\frac{2}{3}}$	0
$\frac{\pi}{a} 0 \frac{\pi}{a}$	$\frac{\pi}{a} 0 \frac{\pi}{a}$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{2}}$
$0 \frac{\pi}{a} \frac{\pi}{a}$	$0 \frac{\pi}{a} \frac{\pi}{a}$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{2}}$

For example, if at least one of the vectors k_i , k'_j , or k''_s corresponds to a general point of the Brillouin zone, then in (6) only the identity operation h should be taken into account.

The denominator in (5) is calculated in an analogous way. If $N_{h''C} > 1$, then the calculation by formula (5) should be carried out with several different choices of the quantities k_{i0} , k'_{j0} , α , β , and the required number of independent sets of C.G.C. obtained in this way should be orthonormalized so that they possess the necessary orthonormality properties

$$\sum_{k''_s C \gamma'} \langle k_i A \alpha, k'_j B \beta | k''_s C \gamma' \rangle \langle k_{i0} A' \alpha', k'_{j0} B' \beta' | k''_s C \gamma' \rangle = \delta_{k_i A \alpha k'_j B \beta}^{k_{i0} A' \alpha' k'_{j0} B' \beta'},$$

$$\sum_{\substack{k_i A \alpha \\ k'_j B \beta}} \langle k_i A \alpha, k'_j B \beta | k''_{s0} C \gamma \rangle \langle k_i A \alpha, k'_j B \beta | k''_{s0} C' \gamma' \rangle = \delta_{k''_{s0} C \gamma}^{k''_{s0} C' \gamma'}. \quad (7)$$

Using formula (5), we have calculated the C.G.C. for the cubic groups O_h^1 and O_h^5 . As an example, Table 1 gives the C.G.C. for the symmetry group of the simple cubic lattice O_h^1 for the case $A = M_1$, $B = M_2$, and $C = \Gamma$ (in the notation of (9)).

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

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