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CLEBSCH-GORDAN COEFFICIENTS FOR THE COREPRESENTATIONS OF SHUBNIKOV POINT GROUPS

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Recently, generalized crystallographic groups, two-coloured(Shubnikov) [1-3] and (multi)-coloured [4-5], are widely used in group-theoretical analysis of different physical properties of crystals with magnetic symmetry. A generalized group is called antiunitary, if the "colour load" of the group elements contains the antiunitary operator of time-inversion Θ [6]. The antiunitary groups A consist of unitary $g_i=u_i$ and antiunitary $g_j=a_j$ operators. The wave functions and the operators of physical quantities transform in the common way under the action of the operators $g\in A$,

$$g\psi^{\alpha}_{a} = \sum_{a'} \psi^{\alpha}_{a'} D^{\alpha}(g)_{a'a} , \tag{1}$$

but the mapping $g\rightarrow D^{\alpha}(g)$ is not a homomorphism, i.e. the set of matrices $D^{\alpha} = \{ D^{\alpha}(g), \ g\in A\}$ does not form a representation of the group A. Wigner [6] called this set of matrices a corepresentation (corep for short [2]). He had proved that for quantum mechanical systems with an antiunitary symmetry, the irreducible coreps (not the ordinary representations) defined the transformation properties of the wave functions, the degeneracy of the levels, selection rules, the correlation between the matrix elements, etc. The need of a further development of the corepresentation theory, and in particular, the creation of a generalized theory of the irreducible tensorial sets, is obvious. One of the basic elements of such a theory is the set of Clebsch-Gordan Coefficients (CGC) for coreps.

The CGC for the coreps of antiunitary groups are introduced for the first time in [7] (see also [8]), where equations for the calculation of the CGC and examples for their applications are given. Orthogonality relations for the matrix elements of the coreps, projection operators and two generalizations of Wigner-Eckart theorem are also given in [7]. The CGC for the coreps are also discussed in the papers [9-12], whose results are in a good agreement with those of [7]. In recent papers [13] it is reported about the calculation of the CGC for the Shubnikov point groups, but only in the case of even under space-inversion, basic functions (the tables of the coefficients are not contained in [13]).
Another method for the calculation of the CGC for the coreps, completely different from the methods given in [7-13], was proposed in [14]

(see also [15]). The method is based on the generalized Racah lemma [14] which can be written in the following matrix form:

$$\left(\bigoplus_{\beta_1\beta_2} U^{\beta_1\beta_2}\right) X^{\alpha_1\alpha_2} = \left(S^{\alpha_1} \otimes S^{\alpha_2}\right)^{-1} U^{\alpha_1\alpha_2} \left(\oplus S^{\alpha}\right) \tag{2}$$

The matrices $U^{\alpha_1\alpha_2}$ and $U^{\beta_1\beta_2}$ reduce $D^{\alpha_1} \otimes D^{\alpha_2}$ and $D^{\beta_1} \otimes D^{\beta_2}$ (D^{α} are the coreps of the group A and D^{β} of the group B, where $B \subset A$). The matrices S^{α_i} reduce the subduction ($D^{\alpha_i} \downarrow B$). The so-called "isoscalar factors" form the matrix $X^{\alpha_1\alpha_2}$, which can be unitary for the ordinary representations, but it should be orthogonal (i.e. all isoscalar factors - real) in the case of coreps.

The calculation of the CGC for coreps using (2) has the following advantages in comparison with the methods, previously used: a) The phases of the CGC for some different groups are well-correlated with those of their common supergroup; b) In many cases the CGC for the subgroups coincide with the coefficients of the supergroup; c) Some of the "intermediate" results in the process of calculation of the CGC (such as isoscalar factors, etc.) have a self-dependent significance and they are not less useful than the "main" result.

The CGC for the single-valued and double-valued corepresentations of all 90 antiunitary Shubnikov point groups (58 black-and-white and 32 grey) were calculated and tabulated by this method. The complete tables are published in [15-19].

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