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TENSOR FIELDS IN CRYSTALS AND COLOUR GROUPS

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The theory of permutational colour groups is used to construct tables of the $k = 0$ irreducible representations whose basis functions are linear combinations of the components of tensor fields defined on the atoms of a crystal. As examples of their use, these tables are shown to be applicable in determining the $k = 0$ vibrational modes of a crystal and in applying the Tensor Field Criterion in the Landau theory of continuous phase transitions.

1. Tensor fields

It is often necessary in solid state physics problems to find the irreducible representations of the space group G of a crystal whose basis functions are linear combinations of components of tensors defined on the atoms of the crystal. Consider a q-component tensor field $T(r_i)_\alpha$, $(\alpha = 1, 2, \ldots, q)$, defined on the atoms at positions r_i, $(i = 1, 2, 3, \ldots)$, of a simple crystal[1]) generated by G from $r = r_1$. The components of this tensor field constitute a set of basis functions for a representation D_G^{TF}, called the tensor field representation, of the space group G. The structure of this representation is that of a direct product:

$$D_G^{\mathrm{TF}} = D_G^{\mathrm{PERM}} \times D_G^{\mathrm{T}}, \tag{1}$$

D_G^{T} is the tensor representation whose basis functions are the q components of the tensor T. D_G^{PERM} is the permutation representation, the representation which characterizes how the atoms of the crystal permute under elements of the space group of the crystal. The tensor field representation is in general reducible.

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Using the theory of permutational colour groups, Kotzev, Litvin and Birman[2]) have derived and tabulated all $k=0$ irreducible representations contained in the permutation representation D_G^{PERM} for all possible crystals of all possible space group symmetries. For a single simple crystal generated by G from r, they have shown that the $k=0$ irreducible representations contained in D_G^{PERM} are identical with the irreducible representations contained in the permutation representation D_R^{S} associated with the permutational colour point group $R(S)$, where R is the point group of the space group G and S is the site symmetry group of the atom at position r. Consequently, the $k=0$ irreducible representations contained in the tensor field representation D_G^{TF} of a crystal generated by G from r are those irreducible representations contained in the direct product

$$D_R^{\mathrm{S}} \times D_R^{\mathrm{T}}, \tag{2}$$

where D_R^{T} is the tensor representation of the point group R of the space group G.

2. $k=0$ vibrational modes

In lattice vibrational problems, one needs to determine the irreducible representations of the space group G of the crystal whose basis functions are combinations of components of a three-component tensor, the displacements, of each of the atoms[3]). These irreducible representations are contained in the tensor field representation, see eq. (1), $D_G^{\mathrm{TF}} = D_G^{\mathrm{PERM}} \times D_G^{\mathrm{V}}$, where D_G^{V} is the polar vector representation. For a single simple crystal, the $k=0$ irreducible representations contained in this representation are, using eq. (2), identical with the irreducible representations contained in the direct product $D_R^{\mathrm{S}} \times D_R^{\mathrm{V}}$, where R is the point group of the crystal and S is the site symmetry group of one of the atoms. We have tabulated, for all point groups R and site point groups S, the irreducible representations contained in $D_R^{\mathrm{S}} \times D_R^{\mathrm{V}}$[4]).

For example, for $R = D_{4h}$, for $S = D_{2h}^{(z,xy,\bar{x}y)}$ one has

$$D_R^{\mathrm{S}} \times D_R^{\mathrm{V}} = \Gamma_2^- + \Gamma_3^- + 2\Gamma_5^- \tag{3}$$

and for $S = C_{2v}^{(\bar{x}y)}$ one has:

$$D_R^{\mathrm{S}} \times D_R^{\mathrm{V}} = \Gamma_1^+ + \Gamma_2^+ + \Gamma_3^+ + \Gamma_4^+ + \Gamma_5^+ + \Gamma_2^- + \Gamma_3^- + 2\Gamma_5^-. \tag{4}$$

Crystals of the ructile structure of TiO_2 are of space group symmetry $G = D_{4h}^{14}$, with the Ti atoms generated by G from an atom with site point group $S = D_{2h}^{(z,xy,\bar{x}y)}$ and the O atoms generated by G from an atom with site point group $S = C_{2v}^{(\bar{x}y)}$[5]). From eqs. (3) and (4) it follows that the $k=0$ vibrational modes of TiO_2 crystals are associated with the following $k=0$ irreducible representations of the space group D_{4h}^{14}:

$$D_G^{(0,1+)},\ D_G^{(0,2+)},\ D_G^{(0,3+)},\ D_G^{(0,4+)},\ D_G^{(0,5+)},\ 2D_G^{(0,2-)},\ 2D_G^{(0,3-)},\ 4D_G^{(0,5-)}. \qquad (5)$$

Extensive tables of the irreducible representations contained in $D_R^S \times D_R^T$, for all point groups R and site point groups S, and for $D_R^T = D_R^V$, the polar vector representation, D_R^A the axial vector representation, $D_R^V \times D_R^A$, and $[D_G^V]^2$, the symmetrized square of D_G^V, along with applications to magnetic modes in crystals, infrared and Raman active modes, and in testing the validity of the Jahn–Teller theorem in crystals, are to be published elsewhere[4].

3. Tensor field criterion

One of the several group-theoretical criteria used in the Landau theory of continuous phase transitions is the Tensor Field Criterion[6–9]. For equitranslational phase transitions, this criterion can be reformulated as follows[2]: If an equitranslational phase transition is due to a physical property described by a q-component tensor field defined on the atoms of a crystal of space group symmetry G, then the phase transition is associated with a $k=0$ irreducible representation of G contained in the tensor field representation D_G^{TF}.

These $k=0$ irreducible representations contained in the tensor field representation are determined using the method given above. For example, in crystals with the ructile structure, equitranslational phase transitions driven by a vibrational mode are associated with $k=0$ irreducible representations given in eq. (5).

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