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COPL: program for obtaining a complete list of order parameters for a group-subgroup crystalline phase transition

Harold T. Stokes and Dorian M. Hatch*

Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA. Correspondence e-mail: hatchd@byu.edu

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1. The crystallographic problem

In a crystalline phase transition, the space-group symmetries of the high- and low-symmetry phases often exhibit a group–subgroup relation: $L \subset H$. In the Landau theory of phase transitions, this transition is described by order parameters (OPs). Each such OP is an n-dimensional vector $\boldsymbol{\eta}$ in the space defined by an irreducible representation (IR) of H. The IR maps each operator $h \in H$ onto an $n \times n$ matrix $D(h)$. For a given OP $\boldsymbol{\eta}$, the operators $h \in H$ which satisfy $D(h)\boldsymbol{\eta} = \boldsymbol{\eta}$ form a group L' such that $L \subseteq L' \subseteq H$. The primary OPs are those for which $L' = L$. They determine the symmetry of the low-symmetry phase. The other OPs are secondary OPs. (This situation can become more complex in the case of coupled OPs.) The aim of the program is to generate a complete list of OPs, both primary and secondary, associated with a given group–subgroup pair of space groups $L \subset H$. The generation of this list is a solution to a generalization of the inverse Landau problem (Ascher & Kobayashi, 1977; Ascher, 1977).

2. Method of solution

Consider a phase transition described by a group–subgroup pair of space groups $L \subset H$. We generate a complete list of OPs as follows. (i) Obtain a complete list of vectors $\mathbf{k}$ inside the first Brillouin zone which satisfy $\mathbf{k} \cdot \mathbf{t}$ = integer for every lattice vector $\mathbf{t}$ in L. (ii) Determine which star each $\mathbf{k}$ vector belongs to. (iii) Obtain a list of IRs which are generated by each star of $\mathbf{k}$. We obtain this list from Miller & Love (1967), which is part of the database for our program. (iv) For each IR, determine if there exists a nonzero solution $\boldsymbol{\eta}$ to the simultaneous equations $D(\ell)\boldsymbol{\eta} = \boldsymbol{\eta}$ for every $\ell \in L$. If so, then this IR participates in the phase transition, and the vector $\boldsymbol{\eta}$ is the direction of the associated OP. Note that the matrices D are the matrices of the complete IR, not just the matrices of the IRs of the matrices of the little groups of $\mathbf{k}$. (v) Given the OP, determine which operators $h \in H$ satisfy $D(h)\boldsymbol{\eta} = \boldsymbol{\eta}$. These operators form the group L'. If $L' = L$, the OP is primary, otherwise it is secondary.

3. Software environment

COPL is written in Fortran 90 and has been implemented under the LINUX operating system.

4. Program specification

Input: (i) the space groups H and L in any setting listed in *International Tables for Crystallography* (1995); (ii) the lattice vectors of L in terms of the lattice vectors of H, using the lattice vectors which form the edges of the conventional unit cell as defined in the *International Tables for Crystallography*; (iii) the origin of the space group L with respect to the origin of the space group H in terms of the lattice vectors of H (the origins are also defined in the *International Tables for Crystallography*).

Output: the OPs are listed along with the IR and space group L'. Note that the form of the OP depends on the choice of matrices D of the IR. We use matrices of the complete IR which we have generated using the matrices of the little group of $\mathbf{k}$ listed by Miller & Love (1967). Our choice of matrices can be obtained from Stokes & Hatch (1988) or from the program *ISOTROPY* (http://www.physics.byu.edu/~stokesh/isotropy.html).

5. Documentation and availability

The program can be run over the internet using any computer with an internet browser. The URL of the program is http://www.physics.byu.edu/~stokesh/copl.html. Running the program requires no local installation. Documentation (including an example) is available at this URL. A more complete discussion of the *COPL* program, including additional examples, has been presented by Hatch & Stokes (2002).

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