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Comments

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Equivalence among isotropy subgroups of space groups

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We discuss the physical interpretation of equivalence among isotropy subgroups of space groups in the context of phase transitions in solids. We give some examples from the literature and point out the different ways in which the question of equivalence has been applied.

The Landau theory[1] of continuous phase transitions provides a powerful tool for understanding transitions between solid phases whose symmetries have a group-subgroup relationship. In the Landau theory, the thermodynamic free energy F of the crystal is written as a function of an order parameter ψ. In the high-symmetry phase, the minimum of F is at $\psi=0$. In the low-symmetry phase, the minimum of F occurs for some nonzero value of ψ. Let G_0 be the space-group symmetry of the high-symmetry phase. The space-group symmetry of the low-symmetry phase must be an isotropy subgroup of G_0. Such subgroups can be obtained by group-theoretical methods.[2] Thus, from a complete list of isotropy subgroups one can obtain *all* possible values of ψ for which the free energy may be at a minimum.

Isotropy subgroups of a space group may be obtained by group-theoretical methods. We have implemented these methods on computer and obtained for all **k** points of symmetry a list of all isotropy subgroups of each of the 230 three-dimensional space groups,[3] as well as each of the 17 two-dimensional space groups[4] and each of the 80 diperiodic space groups.[5]

In generating these lists, we have encountered a problem concerning "equivalent" isotropy subgroups. This question of equivalence has been treated ambiguously in the literature, as we will show below. In this paper, we briefly discuss the physical basis for defining equivalence and then through some specific examples demonstrate an appropriate application of this physical basis.

Consider an isotropy subgroup G of G_0. We can decompose G_0 into left cosets of G,

$$G_0=h_1G+h_2G+h_3G+\cdots+h_nG.$$

The elements h_i are the coset representatives with respect to G, and n is the index of G in G_0. If we apply one of the symmetry operations h_i to the crystal structure of the lower-symmetry phase, we obtain a structure of space-group symmetry $h_iGh_i^{-1}$. Using each of the n coset representatives, we can form n structures. Their space-group symmetries, $h_1Gh_1^{-1}$, $h_2Gh_2^{-1}, \ldots,$ $h_nGh_n^{-1}$, are *distinct but equivalent* subgroups of G_0. (By *distinct*, we mean that their elements differ in orientation and/or location.) The thermodynamic free energy of each of these n structures is identical. Thus, the phase transition $G_0 \rightarrow G$ is equally likely to bring the crystal to any one of these n structures. Often, the low-symmetry phase exhibits domains,[6] so that all n structures are simultaneously present. For the remainder of this paper, we will refer to these n-equivalent structures of the lower-symmetry phase as the n domains of that phase.

If G is an isotropy subgroup of G_0, then the n subgroups $h_iGh_i^{-1}$ are also isotropy subgroups of G_0. However, a list of isotropy subgroups of G_0 needs to contain only one of these n subgroups. The other $n-1$ isotropy subgroups can be generated using the coset representatives as discussed above. All the domains arise from the *same* phase transition. If we intend that a list of isotropy subgroups provides a list of *distinct* possible phase transitions, then there should be only one entry for each group of domains.

In the isotropy subgroup lists we have generated to date, we have taken a different view of equivalence. We used the philosophy that two lower-symmetry structures were *physically* equivalent only if there existed a *physical* operation (rotation, translation, or combination), which left the high-symmetry structure invariant but brought one lower-symmetry structure into the other. Thus we only considered coset representatives h_i which contained *proper* point operations (e.g., rotation). Any pairs of isotropy subgroups which were equivalent only through an element h_i which contained an *improper* point operation (e.g., inversion), were listed as two separate entries. However, we now feel that the "domain" approach described above makes more sense.

Using this approach, we find that in our published list[4] of isotropy subgroups of the two-dimensional space groups there are ten pairs of entries which are physically equivalent in the "domain" approach (Table I). If we want our list to represent only distinct phase transitions, then one of each of these pairs should be omitted from the list.

The concept of equivalence has been applied in different ways in the literature. Zieliński, Cieślewicz, and Marzec[7,8]

TABLE I. Pairs of isotropy subgroups listed in Ref. 4 which are equivalent. We give the space-group symmetry G_0 of the high-symmetry phase, the irreducible representation (irrep), the isotropy subgroups G, the primitive basis vectors of G, and the change in space-group origin (from G_0 to G) in terms of the primitive basis vectors of G_0.

G_0	Irrep	G	Basis vectors		Origin
cm	S_1	*p*1	1,0	0,2	0,0
		*p*1	2,0	0,1	0,0
pmg	X_1	*p*2	2,0	0,1	$\frac{1}{2}$,0
		*p*2	2,0	0,1	0,0
pmg	S_1	*p*2	1,$\bar{1}$	1,1	$\frac{1}{2}$,0
		*p*2	1,$\bar{1}$	1,1	0,0
pgg	X_1	*p*2	2,0	0,1	$\frac{1}{2}$,0
		*p*2	2,0	0,1	0,0
pgg	Y_1	*p*2	1,0	0,2	0,$\frac{1}{2}$
		*p*2	1,0	0,2	0,0
cmm	S_1	*p*2	1,0	0,2	0,0
		*p*2	2,0	0,1	0,0
cmm	S_2	*p*2	1,0	0,2	0,$\frac{1}{2}$
		*p*2	2,0	0,1	$\frac{1}{2}$,0
*p*4*g*	X_1	*p*2	2,0	0,1	$\frac{1}{2}$,0
		*p*2	2,0	0,1	0,0
*p*4*g*	X_1	*p*4	2,0	0,2	$\frac{1}{2}$,$\frac{1}{2}$
		*p*4	2,0	0,2	0,0
*p*4*g*	X_1	*p*2	2,0	0,2	$\frac{1}{2}$,$\frac{1}{2}$
		*p*2	2,0	0,2	0,0
*p*4*g*	M_5	*p*4	1,1	$\bar{1}$,1	$\frac{1}{2}$,$\frac{1}{2}$
		*p*4	1,1	$\bar{1}$,1	0,0
*p*31*m*	$K_3+K_3^*$	*p*3	2,1	$\bar{1}$,1	$\frac{2}{3}$,$\frac{1}{3}$
		*p*3	2,1	$\bar{1}$,1	$\frac{1}{3}$,$\frac{2}{3}$

list the isotropy subgroups of D_{2d}^3, D_{2d}^9, D_{2d}^{10}, D_{2d}^{11}, and D_{2d}^{12}. In their tables, we find a large number of equivalent subgroups listed as separate entries. Some are even equivalent through elements h_i containing a *proper* point operation. For example C_2^3 and C_3^3 are each listed twice as isotropy subgroups of D_{2d}^9 for the 4/5′ representation.[8] The two C_2^3 subgroups are equivalent through the element $h_i=\{\sigma_1|0\}$, and the two C_s^3 subgroups are equivalent through the element $h_i=\{C_2^x|0\}$ (see Table I of Ref. 7 for the representation matrices). The reflection σ_1 is *improper*, and the rotation C_2^x is *proper*.

Jarić and Birman[9] list both D_4^3 and D_4^7 as isotropy subgroups of O_h^3 for the representations $^*\mathbf{X}(3)$ and $^*\mathbf{X}(4)$. The two space groups, D_4^3 and D_4^7 are actually an enantiomorphic pair. They are equivalent to each other via an inversion. But physically they are simply different domains of the *same* lower-symmetry structure of a phase transition.

Similarly, Ghozlen and Mlik[10] list two enantiomorphic pairs, D_4^4, D_4^8 and O^6,O^7, as isotropy subgroups of O_h^5 for the representations A_1^W, A_2^W, B_1^W, and B_2^W. Each of those pairs are also equivalent subgroups via an inversion. Deonarine and Birman[11] list C_4^2 as an isotropy subgroup of C_{4h}^6 for $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Actually C_4^2 and C_4^4 are another enantiomorphic pair, so C_4^4 is *also* an isotropy subgroup of C_{4h}^6. But Deonarine and Birman did not list C_4^4 since it was equivalent to C_4^2 and did not represent a different phase transition.[12] We unjustly indicated this omission in their list.[3]

We feel that the domain approach to equivalence among isotropy subgroups is the best criterion to use and ties directly to the orbit-space description defined by Michel.[13]

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