

3. PHASE TRANSITIONS, TWINNING AND DOMAIN STRUCTURES

symmetry G can be identified with all different orbits of subgroups of G .

In a similar manner, points of the order-parameter space and tensor-parameter space from Examples [sC] 3.2.3.16 and [oT] 3.2.3.21 can be divided into strata which are characterized by the orbits of possible stabilizers.

Next, we formulate three propositions that are essential in the symmetry analysis of domain structures presented in Section 3.4.2.

3.2.3.3.4. Orbits and left cosets

Proposition 3.2.3.23. Let G be a finite group, \mathbf{A} a G -set and $I_G(\mathbf{S}_1) \equiv F_1$ the stabilizer of an object \mathbf{S}_1 of the set \mathbf{A} , $\mathbf{S}_1 \in \mathbf{A}$. The objects of the orbit

$$G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_j, \dots, \mathbf{S}_n\} \quad (3.2.3.67)$$

and the left cosets $g_j F_1$ of the decomposition of G ,

$$G = g_1 F_1 \cup g_2 F_1 \cup \dots \cup g_j F_1 \cup \dots \cup g_n F_1 = \bigcup_{j=1}^n g_j F_1, \quad (3.2.3.68)$$

are in a one-to-one correspondence,

$$\mathbf{S}_j \leftrightarrow g_j F_1, \quad F_1 = I_G(\mathbf{S}_1), \quad j = 1, 2, \dots, n. \quad (3.2.3.69)$$

(See *e.g.* Kerber, 1991, 1999; Kopský, 1983; Lang, 1965.) The derivation of the bijection (3.2.3.69) consists of two parts:

(i) All operations of a left coset $g_j F_1$ transform \mathbf{S}_1 into the same $\mathbf{S}_j = g_j \mathbf{S}_1$, since $g_j \mathbf{S}_1 = g_j (F_1 \mathbf{S}_1) = (g_j F_1) \mathbf{S}_1$, where we use the relation

$$\begin{aligned} F_1 \mathbf{S}_1 &= \{f_1, f_2, \dots, f_q\} \mathbf{S}_1 \\ &= \{f_1 \mathbf{S}_1, f_2 \mathbf{S}_1, \dots, f_q \mathbf{S}_1\} \\ &= \{\mathbf{S}_1, \mathbf{S}_1, \dots, \mathbf{S}_1\} = \{\mathbf{S}_1\} = \mathbf{S}_1, \end{aligned} \quad (3.2.3.70)$$

which in the second line contains a generalization of the group action and in the third line reflects Definition 3.2.3.1 of a set as a collection of distinguishable objects, $\{\mathbf{S}_1, \mathbf{S}_1, \dots, \mathbf{S}_1\} = \mathbf{S}_1 \cup \mathbf{S}_1 \dots \cup \mathbf{S}_1 = \mathbf{S}_1$.

(ii) Any $g_r \in G$ that transforms \mathbf{S}_1 into $\mathbf{S}_j = g_j \mathbf{S}_1$ belongs to the left coset $g_j F_1$, since from $g_j \mathbf{S}_1 = g_r \mathbf{S}_1$ it follows that $g_r^{-1} g_j \mathbf{S}_1 = \mathbf{S}_1$, *i.e.* $g_r^{-1} g_j \in F_1$, which, according to the left coset criterion, holds if and only if g_r and g_j belong to the same left coset $g_j F_1$.

We note that the orbit $G\mathbf{S}_1$ depends on the stabilizer $I_G(\mathbf{S}_1) = F_1$ of the object \mathbf{S}_1 and not on the ‘eigensymmetry’ of \mathbf{S}_1 .

From Proposition 3.2.3.23 follow two corollaries:

Corollary 3.2.3.24. The order n of the orbit $G\mathbf{S}_1$ equals the index of the stabilizer $I_G(\mathbf{S}_1) = F_1$ in G ,

$$n = [G : I_G(\mathbf{S}_1)] = [G : F_1] = |G| : |F_1|, \quad (3.2.3.71)$$

where the last part of the equation applies to point groups only.

Corollary 3.2.3.25. All objects of the orbit $G\mathbf{S}_1$ can be generated by successive application of representatives of all left cosets $g_j F_1$ in the decomposition of G [see (3.2.3.68)] to the object \mathbf{S}_1 , $\mathbf{S}_j = g_j \mathbf{S}_1$, $j = 1, 2, \dots, n$. The orbit $G\mathbf{S}_1$ can therefore be expressed explicitly as

$$G\mathbf{S}_1 = \{\mathbf{S}_1, g_2 \mathbf{S}_1, \dots, g_j \mathbf{S}_1, \dots, g_n \mathbf{S}_1\}, \quad (3.2.3.72)$$

where the operations $g_1 = e, g_2, \dots, g_j, \dots, g_n$ (left transversal to F_1 in G) are the representatives of left cosets in the decomposition (3.2.3.68).

Example [oP] 3.2.3.26. The number of equivalent points of the point form GX (G orbit of the point X) is called a *multiplicity* $m_G(X)$ of this point,

$$m_G(X) = |G| : |I_G(X)|. \quad (3.2.3.73)$$

The multiplicity of a point of general position equals the order $|G|$ of the group G , since in this case $I_G(X) = e$, a trivial group. Then points of the orbit GX and the operations of G are in a one-to-one correspondence. The multiplicity of a point of special position is smaller than the order $|G|$, $m_G(X) < |G|$, and the operations of G and the points of the orbit GX are in a many-to-one correspondence. Points of a stratum have the same multiplicity; one can, therefore, talk about the multiplicity of the Wyckoff position [see *IT A* (2002)]. If G is a space group, the point orbit has to be confined to the volume of the primitive unit cell (Wondratschek, 1995).

Example [oC] 3.2.3.27. Corollaries 3.2.3.24 and 3.2.3.25 applied to domain states represent the basic relations of domain-structure analysis. According to (3.2.3.71), the index n of the stabilizer $I_G(\mathbf{S}_1)$ in the parent group G gives the number of domain states in the orbit $G\mathbf{S}_1$ and the relations (3.2.3.72) and (3.2.3.68) give a recipe for constructing domain states of this orbit.

Example [oT] 3.2.3.28. If $\mu^{(1)}$ is a principal tensor parameter associated with the symmetry descent $G \supset F_1$, then there is a one-to-one correspondence between the elements of the orbit of single domain states $G\mathbf{S}_1 = \{\mathbf{S}_1, \mathbf{S}_2, \dots, \mathbf{S}_j, \dots, \mathbf{S}_n\}$ and the elements of the orbit of the principal order parameter (points) $G\mu^{(1)} = \{\mu^{(1)}, \mu^{(2)}, \dots, \mu^{(j)}, \dots, \mu^{(n)}\}$ (see Example [oT] 3.2.3.21),

$$\mathbf{S}_j \leftrightarrow g_j F_1 \leftrightarrow \mu^{(j)}, \quad j = 1, 2, \dots, n. \quad (3.2.3.74)$$

Therefore, single domain states of the orbit $G\mathbf{S}_1$ can be represented by the principal tensor parameter of the orbit $G\mu^{(1)}$.

Example [oS] 3.2.3.29. Consider a subgroup F_1 of a group G . Since the stabilizer of F_1 in G is the normalizer $N_G(F_1)$ (see Example [sS] 3.2.3.17), the number m of conjugate subgroups is, according to (3.2.3.71),

$$m = [G : N_G(F_1)] = |G| : |N_G(F_1)|, \quad (3.2.3.75)$$

where the last part of the equation applies to point groups only. The orbit of conjugate subgroups is

$$GF_1 = \{F_1, h_2 F_1 h_2^{-1}, \dots, h_j F_1 h_j^{-1}, \dots, h_m F_1 h_m^{-1}\}, \quad (3.2.3.76)$$

$$j = 1, 2, \dots, m,$$

where the operations $h_1 = e, h_2, \dots, h_j, \dots, h_m$ are the representatives of left cosets in the decomposition

$$G = N_G(F_1) \cup h_2 N_G(F_1) \cup \dots \cup h_j N_G(F_1) \cup \dots \cup h_m N_G(F_1). \quad (3.2.3.77)$$

3.2.3.3.5. Intermediate subgroups and partitions of an orbit into suborbits

Proposition 3.2.3.30. Let $G\mathbf{S}_1$ be a G orbit from Proposition 3.2.3.23 and L_1 an intermediate group,

$$F_1 \subset L_1 \subset G. \quad (3.2.3.78)$$

A successive decomposition of G into left cosets of L_1 and L_1 into left cosets of F_1 [see (3.2.3.25)] introduces a two-indices rela-