On Space-Group-Symmetric Cell Decompositions of Real Space and Momentum Space

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Let G be a space group. We want to construct a space-group-symmetric cell decomposition of real space or momentum space such that every cell is a fundamental domain and no unnecessary subdivision remains. The method below applies both to real space and momentum space. I describe the three-dimensional case, and only record the essential points, omitting implementation details.

A useful fact for numerical computations is that, when searching among cells of the same dimension p, each p-cell is uniquely specified by the coordinates of its midpoint.

Assume that the vertices of a fundamental domain are already known, so that their convex hull is the fundamental domain.[1]

- Search for equivalent 2-cells among the boundary 2-cells of the 3-cell (the fundamental domain).

  Assume each boundary face s^a of the fundamental domain is specified by ordered boundary points $s^a = (p^a_1, p^a_2, \dots, p^a_n)$. First search for faces related by symmetry, $s^a = g(s^b)$ with $g \in G$. It is enough to use the midpoint of the face. Record a representative boundary face s_a and the group element $g \in G$.

- Subdivide the boundary faces.

  Focus on a representative face s. A symmetry may map an interior point of s to another interior point of s. Equivalently, there may be a symmetry point or a symmetry line inside s. For a space-group symmetry, because s is a boundary face of a fundamental domain, such an object is either an inversion center $(x, y, z) \mapsto (-x, -y, -z)$ or a twofold rotation axis $(x, y, z) \mapsto (x, -y, -z)$, where x, y are coordinates in s and z is normal to s. Other cases would imply a mirror plane perpendicular to s.

  Thus a symmetric subdivision of s can be performed as follows.

  - Suppose $s = (p_1, p_2, \dots, p_n)$ is specified by ordered boundary points.
  - Compute the little group G_{GP} of a generic point of s. One may choose a point not lying on a twofold axis, for instance $p = p_1 + 0.1(p_2 - p_1) + 0.01(p_3 - p_1)$, and set $G_{GP} = G_p$.
  - Compute the little group G_{p_M} of the midpoint $p_M = \frac{1}{n}\sum_{i=1}^n p_i$ of the face.
  - If $G_p = G_{p_M}$, then the face s itself is a 2-cell and no subdivision is needed. If $G_p \neq G_{p_M}$, subdivide s according to the following rules.
  - Add the midpoints $(p_i + p_{i+1})/2$ of the edges $p_i p_{i+1}$ to exhaust the possible twofold rotation axes. Write $p'_{2j-1} = p_j$, $p'_{2j} = (p_j + p_{j+1})/2$ with $p_{n+1} = p_1$, producing the set $\{p'_1, \dots, p'_{2n}\}$. For points in the interior of s, on possible twofold axes but not at the midpoint, compute the little groups of $q_j = (p'_j + p_M)/2$.
  - If $G_{q_j} \neq G_{p_M}$ for all $j = 1, \dots, n$, then p_M is an inversion center. Subdivide s into two pieces in an inversion-symmetric way.

[1] For example, see http://www2.yukawa.kyoto-u.ac.jp/~ken.shiozaki/doc/FD.pdf.

– If $G_{q_j} = G_{p_M}$ for some j, subdivide s along the twofold rotation axis containing p'_j.

Applying the group orbit to the resulting 2-cells gives the space-group-symmetric set of 2-cells.

- Search for equivalent 1-cells among the boundary 1-cells of the 2-cells.

  First compute all boundary 1-cells of the 2-cells and remove duplicates. Also remove 1-cells that are subdivided at their midpoint by a pair of other line segments, as in the three line segments $((0, 0, 0), (2, 0, 0))$, $((0, 0, 0), (1, 0, 0))$, and $((2, 0, 0), (1, 0, 0))$.

  Search for 1-cells related by the space-group action, and record a representative 1-cell and the group element $g \in G$.

- Space-group-symmetric subdivision of boundary 1-cells.

  Let a representative boundary 1-cell be $l = (p_1, p_2)$. The segment l may be subdivided into two at an inversion-symmetric point. This can be detected by comparing the little group of the midpoint with that of a generic point, for example $p_1 + 0.1(p_2 - p_1)$. If subdivision is needed, divide the 1-cell into $(p_1, (p_1 + p_2)/2)$ and $(p_2, (p_1 + p_2)/2)$.

  Applying the group orbit to the resulting 1-cells gives the space-group-symmetric set of 1-cells.

- Construction of 0-cells.

  The 0-cells are obtained as the boundaries of the 1-cells.

This construction gives a space-group-symmetric cell decomposition. Each resulting n-cell is specified by $n + 1$ points $(p_1, \ldots, p_{n+1})$, and the ordering of these points is chosen so as to respect the space-group symmetry.