

### Crystallographic restriction theorem

See: [http://en.wikipedia.org/wiki/Crystallographic\\_restriction\\_theorem](http://en.wikipedia.org/wiki/Crystallographic_restriction_theorem)

Problem: Consider rotational symmetry operations of a 2D periodic lattice with the rotation axis perpendicular to the lattice plane. Show that only rotations that are multiples of  $60^\circ$  and  $90^\circ$  can be symmetry operations. Thus, 2, 3, 4, and 6-fold symmetries are allowed, but not 5-fold. This theorem also holds for 3D lattices.

Assume that a 2D lattice is invariant under rotation of angle  $\theta$ . Let  $\mathbf{a}$  be a primitive lattice vector. Rotate  $\mathbf{a}$  by angle  $\theta$  to generate  $\mathbf{a}'$ , and rotate  $\mathbf{a}$  by angle  $-\theta$  to generate  $\mathbf{a}''$ . Both  $\mathbf{a}'$  and  $\mathbf{a}''$  must be lattice vectors, and so is  $\mathbf{a}' + \mathbf{a}''$ , which points in either the same or the opposite direction as  $\mathbf{a}$ . Since  $\mathbf{a}$  is primitive (shortest along its direction),  $\mathbf{a}' + \mathbf{a}'' = n\mathbf{a}$ , where  $n$  is an integer (positive, negative, or zero). Taking the dot product of this equation with  $\mathbf{a}$  yields  $2a^2 \cos \theta = na^2$ . Thus,  $\cos \theta = 0, \pm 1/2$ , or  $\pm 1$ . The only possible values of  $\theta$  are  $0^\circ, 60^\circ, 90^\circ$ , and their multiples.

In 3D, consider an arbitrary lattice vector  $\mathbf{R}$  that is not parallel to the rotation axis. Rotate it by  $\theta$  to generate  $\mathbf{R}'$ ; the difference  $\mathbf{R}' - \mathbf{R}$  is a nonzero lattice vector perpendicular to the rotation axis. It follows that one can always find a line of lattice points perpendicular to the rotation axis; let  $\mathbf{a}$  be the primitive (shortest) lattice vector for this 1D lattice. The rest of the proof is the same as the 2D case.

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