Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 12 June 2012
Accepted 9 October 2012

Topological density of lattice nets

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It was shown in a previous paper [Eon (2004). *Acta Cryst.* A**60**, 7–18] that the topological density of a periodic net can be calculated directly from its cycles figure, a polytope constructed from those cycles of the quotient graph of the net that are associated with its geodesic lines. It may happen that these lines generate a grid pattern forming a supercell, a phenomenon that was not considered in the former derivation of the formula but is common for lattice nets. An adjustment of the expression is proposed to this effect and applied to the square and hexagonal lattice nets as well as to the 13 families of cubic lattice nets.

1. Introduction

The topological density ρ of a p-periodic net is defined as the limit for $k \to \infty$ of the sequence $N(k)/k^p$ where $N(k)$ is the cumulative number of neighbors of a vertex at a distance at most k (O'Keeffe, 1991). A few years ago, the author derived a formula enabling the direct calculation of the topological density of a periodic net, with no need to analyze its full coordination sequence (Eon, 2004). It can be noted, however, that the method fails in the case of the lattice nets defined by Delgado-Friedrichs & O'Keeffe (2009). The aim of this communication is to explain the failure and propose an adjustment to this formula. Because only slight modifications are required in comparison with the original derivation of this expression, the main arguments are quickly sketched below using the case of the square lattice net (1, 2) as an illustration.

2. Grid pattern of geodesic lines and topological density

The method used for the direct determination of the topological density of a periodic net is based on the special nature of its geodesic paths. In any periodic net, there are a small number of preferred directions along which distances increase the fastest, or simply may increase (see also Eon, 2007). A geodesic path between two distant vertices in a 2-periodic net, apart from its two extremities, may be composed of a sequence of paths along at most two of these preferred directions. The set of these directions may be used to construct a polytope that has been called the *cycles figure* of the periodic net in Eon (2004). The value of the topological density of the net derived from an analysis of its cycles figure was shown to be given by

$$\rho = Z \sum_{\sigma} f(\sigma)/p!, \qquad (1)$$

where Z is the number of vertices in the unit cell, p the periodicity of the net and $f(\sigma)$, the *frequency* of the triangular face σ of the cycles figure, is given by the inverse product of the lengths of the cycles associated with preferred (shortest) directions in the respective solid angle. In fact, it was assumed in the proof that only vertices in adjacent cells (in a geometric, Euclidean sense) may be linked, which is not true for lattice nets.

Fig. 1 displays the labelled quotient graph of the square lattice net (u, v) and its cycles figure. The quotient graph is the *bouquet* of four loops with voltages $(\pm u, v)$ and $(\pm v, u)$. To ensure the connectivity of the net, u and v must be co-prime integers with $u + v$ odd and $0 < u < v$. In this case, each loop defines one of these preferred directions; there are altogether eight orientations dividing the plane into eight regions, as shown on the right-hand side of Fig. 1. Geodesic paths between the origin and any vertex localized in some region are composed of a sequence of paths along the two orientations delimiting this angle. Fig. 2 shows the grid pattern of all possible paths starting at the origin in the angle $\{(1, 2), (-1, 2)\}$ and running along lines parallel to 1 2 or −1 2.

It is manifest that not every vertex in the respective angle can be attained by these paths. A geodesic path to any vertex marked in red in Fig. 2 must end by a (limited) sequence of edges along other orientations. We may now associate a supercell with the grid pattern in each angle: that in angle $\{(1, 2), (-1, 2)\}$ contains four vertices. Supercells in the angle $\{(2, 1), (1, 2)\}$ contain three vertices, as may be seen in Fig. 3. Only one vertex per supercell can be reached by a sequence of paths running along lines parallel to the orientations delimiting the respective angle. As a result, the above formula incorrectly predicts a topological density $\rho = 4$.

The expression giving the topological density ρ of a periodic net may now be corrected if one takes asymptotic properties into account. It results from the original derivation that one needs only to include the multiplicity N_σ of the supercell of the grid pattern associated with each face σ. This provides the following adjusted expression:

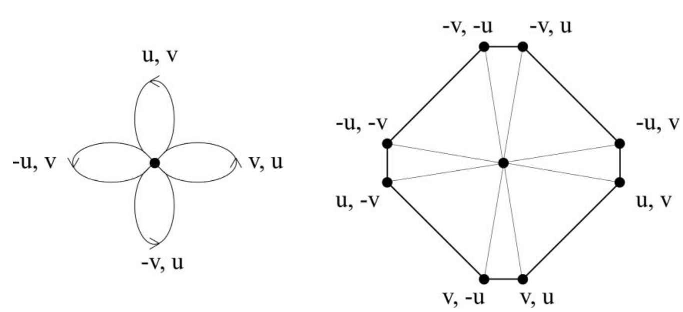

Figure 1
The labelled quotient graph (left) and cycles figure (right) of the square lattice net (u, v).

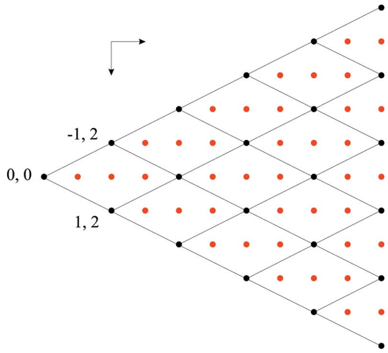

Figure 2
Grid pattern of the square lattice net (1, 2) in the angle {(1, 2), (−1, 2)}.

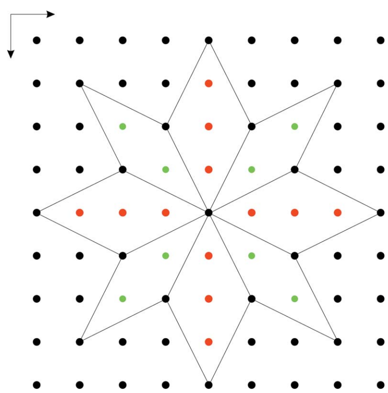

Figure 3
Complete view of supercells in the grid pattern of the square lattice net (1, 2).

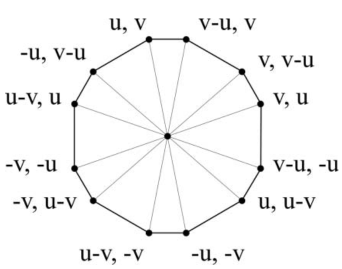

Figure 4
Cycles figure of the hexagonal lattice net (u, v).

$$\rho = Z\sum_{\sigma}[N_{\sigma}f(\sigma)]/p!. \qquad (2)$$

We now apply this expression to lattice nets.

2.1. Topological density of the square lattice net (u, v)

The cycles in the cycles figure of the square lattice nets are all loops, with length 1; hence the frequency of any face is just 1. The multiplicity of supercells is given by the determinant of limiting directions, which are of two kinds:

$$N_1 = \begin{vmatrix} u & -u \\ v & v \end{vmatrix} = 2uv, \quad N_2 = \begin{vmatrix} v & u \\ u & v \end{vmatrix} = v^2 - u^2. \qquad (3)$$

With one vertex per unit cell, we get

$$\rho = [4(2uv) + 4(v^2 - u^2)]/2 = 2(v^2 + 2uv - u^2). \qquad (4)$$

2.2. Topological density of the hexagonal lattice net (u, v)

The hexagonal lattice net admits as its quotient graph the bouquet of six loops with voltages (u, v), $(v-u, -u)$, $(-v, u-v)$, (v, u), $(-u, v-u)$ and $(u-v, -v)$ where the connectivity condition imposes that u and v be co-prime integers with $u + v \neq 3n$ (where n is an integer) and $0 < u < v - u$. Fig. 4 shows the cycles figure of this net.

The multiplicity of supercells is given by the determinant of limiting directions, which are again of two kinds:

$$N_1 = \begin{vmatrix} v-u & v \\ -u & u \end{vmatrix} = 2uv - u^2, \quad N_2 = \begin{vmatrix} v & v \\ u & v-u \end{vmatrix} = v^2 - 2uv. \qquad (5)$$

Since the frequency is also 1, we get

$$\rho = [6(2uv - u^2) + 6(v^2 - 2uv)]/2 = 3(v^2 - u^2). \qquad (6)$$

2.3. Topological density of cubic lattice nets

Thirteen families of cubic lattice nets distributed between two point groups have been listed by Delgado-Friedrichs & O'Keeffe (2009). We consider in detail the nets (u, v, w) belonging to point group $m\bar{3}m$. The quotient graph of these nets consists of 24 loops with voltages $(\pm u, \pm v, w)$ and six possible permutations, submitted to the conditions $u < v < w$ with u, v and w co-prime integers. The cycles figure is a truncated cuboctahedron with six equivalent octagonal faces, eight equivalent hexagonal faces and 12 equivalent square faces (vertex symbol 4.6.8). Fig. 5 displays a projection of this cycles figure along the 001 axis.

Fig. 6 shows a possible triangulation of the square and hexagonal faces, respectively, marked with the letters a and b in Fig. 5. Notice the existence of symmetry relations between some triangles. The corresponding multiplicities are obtained as before (N_i is the multiplicity for the triangle i in Fig. 6):

$$N_1 = N_2 = \begin{vmatrix} v & w & w \\ u & -u & u \\ w & v & v \end{vmatrix} = 2u(w^2 - v^2), \qquad (7)$$

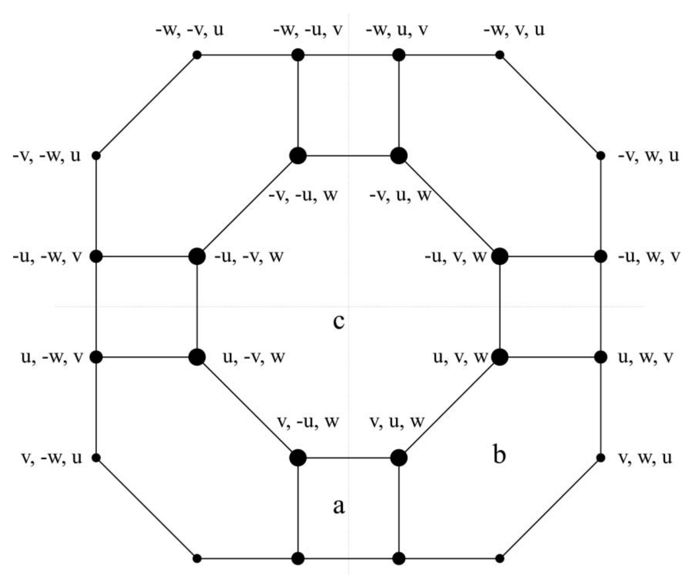

Figure 5
Cycles figure of the cubic lattice net (u, v, w) with point group $m\bar{3}m$ in projection along 001.

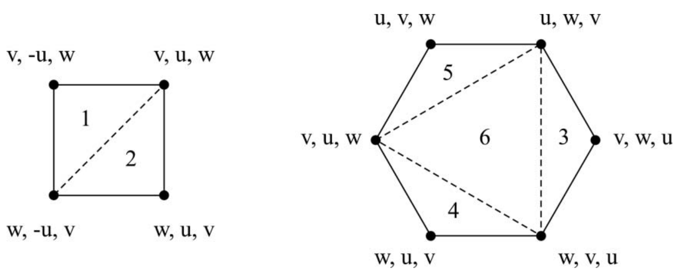

Figure 6
Triangulation of the square and hexagonal faces in the cycles figure of the cubic lattice net (u, v, w) (point group $m\overline{3}m$).

$$N_3 = N_4 = N_5 = \begin{vmatrix} v & u & u \\ u & w & v \\ w & v & w \end{vmatrix} = (u+v+w)(v-u)(w-v), \quad (8)$$

$$N_6 = \begin{vmatrix} u & v & w \\ w & u & v \\ v & w & u \end{vmatrix} = u^3 + v^3 + w^3 - 3uvw. \quad (9)$$

The triangulation of the octagonal face marked c in Fig. 5 is shown in Fig. 7, with the following multiplicities:

$$N_7 = \begin{vmatrix} v & v & u \\ -u & u & v \\ w & w & w \end{vmatrix} = 2uw(v-u), \quad (10)$$

$$N_8 = \begin{vmatrix} u & -v & v \\ v & u & -u \\ w & w & w \end{vmatrix} = 2w(u^2+v^2). \quad (11)$$

Frequencies are again 1 and we get the following expression for the topological density, after summing over all faces:

$$\rho = 4Z[(u+v+w)^3 - 3v^3 - 9u(v^2+uw)]/3. \quad (12)$$

Now, three kinds of structures are obtained according to the parities of u, v and w. If one of these figures is odd, the net is primitive and all lattice points are on the structure. If two are odd, it is face centered and only contains half the points of the lattice. If they are all odd, the lattice is body centered and contains but one quarter of the points of the lattice. We may take this into account by using $Z = 1$ for primitive nets, $Z = 1/2$ for face-centered nets and $Z = 1/4$ for body-centered nets.

There exist two degenerate cases of lattice nets (u, v, w), namely the nets $(0, v, w)$ and (u, u, w). In both cases the quotient graph consists of 12 loops and the cycles figure reduces to a truncated octahedron (vertex symbol 4.6^2) in the first case and to a distorted rhombicuboctahedron (vertex symbol 3.4^3) in the second case. It may be verified, however, that the above expression of the topological density also applies to the degenerate cases; this phenomenon is clearly due to the geometric origin of the formula.

The remaining families belong to point group $m\overline{3}$. The quotient graph of the nets (u, v, w) consists of 12 loops with voltages $(\pm u, \pm v, w)$ and circular permutations, submitted to the conditions $u < v < w$ with u, v and w co-prime integers. The cycles figure is also a distorted rhombicuboctahedron and the topological density is given by

$$\rho = 4Z[(u+v+w)^3 - 3w(u+v)^2 - 3uv\{2(u+v) - w\}]/3, \quad (13)$$

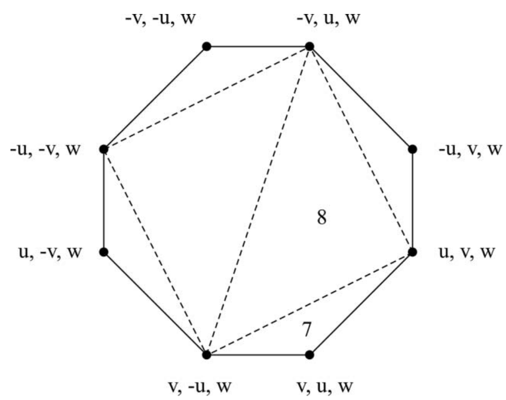

Figure 7
Triangulation of the octagonal face in the cycles figure of the cubic lattice net (u, v, w) (point group $m\overline{3}m$).

where again three kinds of structures are obtained according to the parities of u, v and w as above: the value of Z must be defined in the same way according to the nature of the centering. The only degenerate lattice nets $(0, v, w)$ admit as their quotient graph the bouquet of six loops and the cycles figure reduces to a distorted icosahedron (vertex symbol 3^5). Again, the general expression given above applies to the degenerate case.

The above formulae were verified for all possible cases satisfying $w < 6$. It is worth mentioning that the special cases of **pcu** $(0, 0, 1)$, **fcu** $(0, 1, 1)$ and **bcu** $(1, 1, 1)$ belonging to the class $m\overline{3}m$ equally satisfy the general expression obtained for the topological density of lattice nets in this class.

3. Concluding remarks

Both results for square and hexagonal lattice nets are in agreement with empirical values found by Delgado-Friedrichs & O'Keeffe (2009) for the first members of these series (*i.e.* for relatively small values of u and v). The adjusted formula was applied to obtain an expression of topological densities for the cubic lattice nets (u, v, w) in both classes $m\overline{3}m$ and $m\overline{3}$, which was checked for the first members of both series ($w < 6$). It is worth noting that the topological density in cubic lattice nets is primarily determined by the crystal class of the net and is independent of coordination. It should be emphasized that the adjusted formula yields the same results as were previously obtained for more usual nets because supercell multiplicities are generally equal to one.

The author thanks Michael O'Keeffe for calling his attention to the determination of topological densities in lattice nets and for kindly providing the exact coefficients for the coordination sequences of cubic lattice nets for small values ($w < 6$). CNPq, Conselho Nacional de Desenvolvimento Científico e Tecnológico of Brazil is acknowledged for support during the preparation of this work.

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