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Supplementary Material

Arithmetic proof of multiplicity-weighted Euler characteristic for symmetrically arranged space-filling polyhedra

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Synopsis: A mathematical proof based on arithmetic argument is presented for the modified Euler characteristic $\chi_m = \sum_{i=0}^{N}(-1)^{i} \sum_{j=1}^{n(i)} 1/m(ij) = 0$ (where the first summation runs from 0-dimensional vertices to the *N*-dimensional cell or "interior"), applicable to symmetrically arranged space-filling polytopes in *N*-dimensional space, where the contribution of each j^{th} *i*-dimensional element of the polytope is weighted by a factor inversely proportional to its multiplicity *m*(*ij*).

S1. Coxeter's proof of modified Euler characteristic for translationally arranged polytopes

S2. Examples of modified Euler characteristic calculation in crystallographic 2-D and 3-D space groups

S1. Coxeter's proof of modified Euler characteristic for translationally arranged polytopes

In his book "*Regular Polytopes*", Coxeter (1948) presented an explicit proof of Euler characteristic for 2- and 3-dimensional "honeycombs", *i.e.* infinite sets of identical polyhedra (or polygons in 2-D) filling the space without gaps. He calls this tesselation "a map with infinitely many polytopes".

In 2-D space (Fig. S1a) a finite portion of this map consists of N_2-1 faces (2-D objects), N_1 edges (1-D objects) and N_0 vertices (0-D objects). The exterior of this portion can be treated as one additional face, and the whole diagram can be regarded as a Schlegel diagram of a certain polyhedron (Coxeter, 1948, pp. 10 & 242; https://en.wikipedia.org/wiki/Schlegel_diagram), with all its faces projected onto one selected face. To such a finite map portion, representing a polyhedron, applies the classic Euler's formula:

$$N_0 - N_1 + N_2 = 2$$

If this map is enlarged by inclusion of additional faces, the polyhedron, which can be treated as inscribed into a sphere, enlarges accordingly and the numbers of its bounding elements (N_0, N_1, N_2) increase proportionally to the square of the sphere radius r

$$N_0 = N_0(r) = \nu_0 \cdot r^2 + \cdots$$

$$N_1 = N_1(r) = \nu_1 \cdot r^2 + \cdots$$

$$N_2 = N_2(r) = \nu_2 \cdot r^2 + \cdots$$

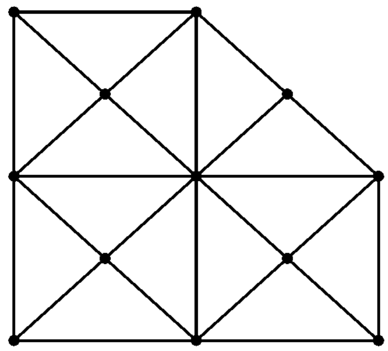
The quantities $N_i(r)$ are proportional to r^2 with non-negative constants v_i and the lower-order terms are smaller in the magnitude than r^2. In the limit, when the size of such a "map" tends to infinity, we obtain the relation

$$\nu_0 - \nu_1 + \nu_2 = 0$$

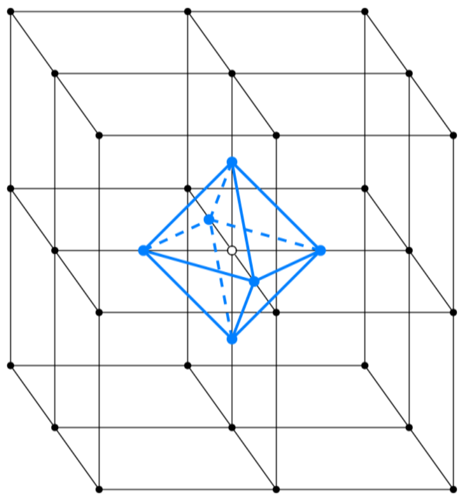
Since all the polygons are identical (have the same numbers of corresponding bounding elements), after normalization to a single polygon ($v_2 = F_m = 1$), the above equation becomes

$$V_m - E_m + F_m = 0$$

i.e. the modified Euler characteristic. This proves the validity of the modified Euler characteristic for any tessellation of 2-D space by identical, plane-filling polygons.



(a)



(b)

Fig. S1. (a) A fragment of 2-D plane filled by symmetrically arranged triangles. (b) A fragment of a 3-D lattice of cubes repeated by translations along the cube edges. A vertex figure (blue) surrounds one (empty circle) of the nodes (vertices) of the original lattice.

In the proof for 3-D space, Coxeter uses the following definitions. For any polytope, the symbol N_{jk} represents the number of k-dimensional elements incident with one j-dimensional element. For example, the cube will have $N_{30} = 8$ since there are 8 corners (0-dimensional elements) at the border of a single cube interior (3-D element), and similarly, $N_{02} = 12$ since there are 12 faces meeting at one vertex, etc.

There are several simple relations (marked by a label above the = sign) involving these values.

$N_{10} \overset{(a)}{=} 2$ each edge has two ends at two vertices

$N_{23} \overset{(b)}{=} 2$ each face always lies between two adjacent 3-cells

$N_{20} \overset{(c)}{=} N_{21}$ each face (polygon) has the same number of edges and vertices

$N_{12} \overset{(d)}{=} N_{13}$ each edge is always common to as many faces as interiors.

In addition

$\sum N_{jk} \overset{(e)}{=} \sum N_{kj}$ where the summations run over the first index.

The last equation expresses the intuitive fact that the sum of all contacts of all *j*-dimensional elements with *k*-dimensional elements is the same as the sum of all contacts of all *k*-dimensional elements with *j*-dimensional elements.

Coxeter also uses the concept of vertex figure attached to a given vertex v. Briefly, a vertex figure is a polyhedron which satisfies the following properties: (i) its vertices belong to the edges incident to vertex v; (ii) its vertices form a convex span of points which is equal to the vertex figure; (iii) each face of the vertex figure is a slice surface of the single 3-cell of the original honeycomb. A vertex figure at a given vertex v is not uniquely characterized by the properties i-iii but the count of *k*-dimensional cells of the figure and their mutual connections and relations are always the same. One can say that two vertex figures are piecewise-linear equivalent. In the particular case of the cubical honeycomb, the vertex figures have identical properties at each vertex and can be identified with the regular octahedron, a figure which is reciprocal to the cube. For general honeycombs this is not always the case and the vertex figures can vary from vertex to vertex. A vertex figure centered at one of the vertices of the original lattice and having its vertices at midpoints of the original edges, is illustrated in Fig. S1b for a 3-D map built from cubes.

The Euler's formula for the original polyhedron is

$$N_{30} - N_{31} + N_{32} \overset{(f)}{=} 2$$

where N_{30}, N_{31}, N_{32} are the numbers of vertices, edges and faces incident with a single 3-D polyhedron (3-D interior).

The Euler's formula for the vertex figure is

$$N_{01} - N_{02} + N_{03} \overset{(g)}{=} 2$$

where N_{01} is its number of vertices, equal to the number of edges meeting at one vertex of the original polyhedron, N_{02} is the number of edges, equal to the number of faces meeting at one vertex of the original polyhedron, and N_{03} is the number of faces equal to the number of cells (interiors) meeting at one vertex of the original polyhedron

We consider the following sum:

$$S = \left(\sum N_{30} - \sum N_{03} \right) - \left(\sum N_{31} - \sum N_{02} \right) + \left(\sum N_{32} - \sum N_{01} \right).$$

On one hand we have

$$S = \sum (N_{30} - N_{31} + N_{32}) - \sum (N_{01} - N_{02} + N_{03})$$

and due to equalities (f) and (g)

$$S = 2N_3 - 2N_0.$$

Notice that $\sum N_{30} - \sum N_{03} \overset{(e)}{=} 0$ and

$$\sum N_{32} - \sum N_{01} \overset{(e)}{=} \sum N_{23} - \sum N_{01} \overset{(a),(b)}{=} 2N_2 - 2N_1.$$

Finally, we observe that

$$\sum N_{31} \overset{(e)}{=} \sum N_{13} \overset{(d)}{=} \sum N_{12} \overset{(e)}{=} \sum N_{21} \overset{(c)}{=} \sum N_{20} \overset{(e)}{=} \sum N_{02}.$$

Finally we obtain

$$S = 2N_2 - 2N_1$$

which matched with the previous expression for S proves

$$N_0 - N_1 + N_2 - N_3 = 0.$$

This equation looks very much like the modified Euler's formula we wish to prove, except that it applies to a finite set of N_3 cells instead of one cell representing an infinite array[1]. However, Coxeter observes again that the chosen portion can be enlarged in such a way that the increasing numbers N_j (equal to $\nu_j \cdot r^3 + \cdots$ when the radius r increases) add up to $(\nu_0 - \nu_1 + \nu_2 - \nu_3)r^3 + \cdots = 0$, so that in conclusion we get

$$\nu_0 - \nu_1 + \nu_2 - \nu_3 = 0$$

[1]Parenthetically Coxeter notes that an alternative proof of this equation was presented by Cauchy (1813) but this seems to be an exaggeration as Cauchy only sketches an argument valid for a single polytope and uses a rather elementary simplices-based approach that lacks proper notation and is quite difficult to follow as a formal proof.

In particular, the above equation can be always normalized in such a way that $\nu_3 = I_m = 1$, and in this form it effectively proves our modified Euler's formula (Dauter & Jaskolski, 2020)

$$V_m - E_m + F_m - I_m = 0$$

In a later chapter (IX) of his book, Coxeter (1948) proves a generalization of the formula $N_0 - N_1 + N_2 - N_3 = 0$ to any number of dimensions but still his argument applies strictly only to translational lattices because he assumes that all the vertices are equivalent (transient). The limiting process is related to the realizability of an N-dimensional sphere as a polytope. In two dimensions this is always possible due to the theorem of Steinitz & Rademacher (1934).

S2. Examples of modified Euler characteristic calculation

- 2-D space group *p*4*mm*

A planar lattice built from square unit cells belongs to the *p*4*mm* symmetry group, as illustrated in Fig. S2. The asymmetric unit (ASU) in this group is a triangle with ⅛ of the area of the whole unit cell.

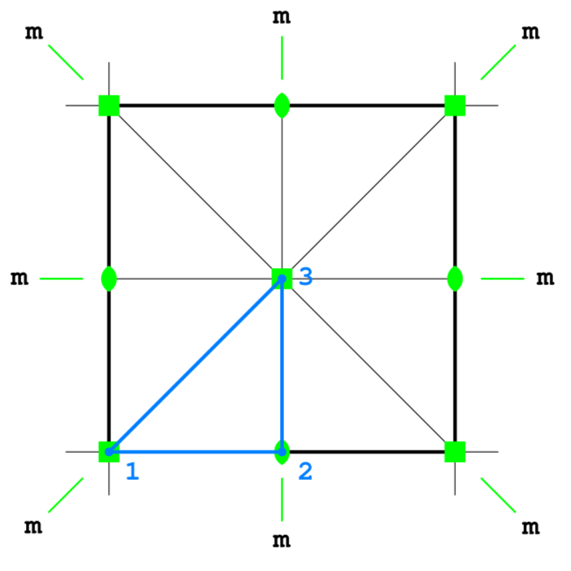


Fig. S2. The unit cell of the planar group *p*4*mm* (black square), with one asymmetric unit shown in blue. Some of the symmetry elements are shown in green. See text for details.

If one triangular ASU is selected (1-2-3, marked in blue in Fig. S2) as a representative polytope, it has the following modified Euler characteristic. Vertices 1 and 3 are shared by eight neighbors each, and vertex 2 is shared by four neighbors, thus $V_m = 2×⅛ + 1×¼ = ½$. All three edges are shared by two neighbors, thus $E_m = 3×½ = 1½$. With one internal face, $F_m = 1$, and the resulting $\chi_m = V_m - E_m + F_m = ½ - 1½ + 1 = 0$.

- 2-D space group *pg*

In some space groups containing symmetry operations with fractional translations, such as screw axes or glide planes, the interpretation involves re-definition of the unit cell. The example of the planar group *pg* is illustrated in Fig. S3. The ASU selected in this group according to the *International Tables for Crystallography*, Vol. A (Aroyo, 2016) corresponds to the rectangle 1-2-3-4-5-6, with an area equal to half of the unit cell, as marked in Fig. S3 in blue.

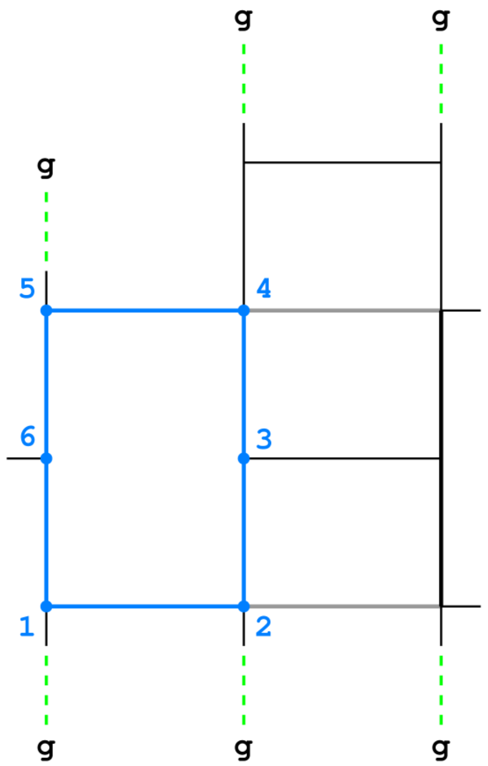


Fig. S3. Interpretation of the asymmetric unit of the planar group *pg*. The glide planes (*g*) are marked in green. The asymmetric unit, shown as a blue rectangle, encompasses half of the unit cell. Two adjacent asymmetric units related by a glide plane are visible, although one of them extends beyond the original unit cell.

In this group, there are glide planes in the vertical direction in Fig. S3, along the edges 1-6, 2-3, 3-4, and 6-5. After application of the glide plane operation, the symmetry equivalent of the asymmetric unit extends beyond the limits of the unit cell. The points 3 and 6, in spite of lying at the straight lines between the corners of the blue rectangle, have to be treated as additional vertices, since they are symmetry-equivalent to the corners of the rectangle. All the ASUs are nevertheless obviously periodically repeated and fill the plane without gaps. The ASU has 6 vertices, each shared by three neighbors, giving $V_m = 6\times⅓ = 2$. There are 6 edges, each shared by two neighbors, giving $E_m = 6\times½ = 3$. With one internal face, $F_m = 1$, the result is $\chi_m = V_m - E_m + F_m = 2 - 3 + 1 = 0$.

- 3-D space group *P*23

Fig. S4 illustrates the three-dimensional cubic space group *P*23. The unit cell is obviously a cube and the asymmetric unit is a tetrahedron marked in the figure in blue.

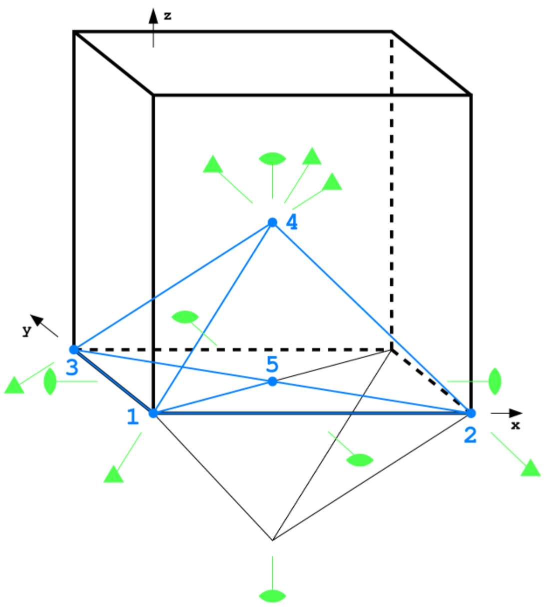


Fig. S4. The unit cell (black) in the cubic space group *P*23 and the ASU in the shape of a tetrahedron shown in blue. The relevant threefold and twofold symmetry axes are shown in green.

As in the previous example, the additional vertex 5 results from the fact that the line 1-5 is symmetry-equivalent to lines 2-5 and 3-5 by the action of the horizontal 2-fold axes. In effect the ASU has five vertices, of which (i) vertices 1, 2 and 3 are common for 36 neighboring ASUs each, (ii) vertex 4 is shared by 12 ASUs, and (iii) vertex 5 is shared by 4 ASUs, so that $V_m = 3\times1/36 + 1/12 + 1/4 = 5/12$.

Out of the eight edges, (i) one (1-4) is shared by 3 ASUs, (ii) two (2-4 and 3-4) are shared by 6 ASUs each, (iii) two (1-2 and 1-3) are shared by 8 ASUs each, and (iv) three (1-5, 2-5, and 3-5) are shared by 3 ASUs each. The contribution of the edges is, therefore, $E_m = \frac{1}{3} + 2\times\frac{1}{6} + 2\times\frac{1}{8} + 3\times\frac{1}{3} = 23/12$. The five faces contribute with $F_m = 5\times\frac{1}{2} = 30/12$, so that with $I_m = 1$ the modified Euler characteristic is

$$\chi_m = V_m - E_m + F_m - I_m = 5/12 - 23/12 + 30/12 - 12/12 = 0.$$

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