Enumerating tilings of triply-periodic minimal surfaces with rotational symmetries

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Abstract

We present a technique for the enumeration of all isotopically distinct ways of tiling, with disks, a hyperbolic surface of finite genus, possibly nonorientable and with punctures and boundary. This provides a generalization of the enumeration of Delaney-Dress combinatorial tiling theory on the basis of isotopic tiling theory. To accomplish this, we derive representations of the mapping class group of the orbifold associated to the symmetry group of the tiling under consideration as a set of algebraic operations on certain generators of the symmetry group. We derive explicit descriptions of certain subgroups of mapping class groups and of tilings as embedded graphs on orbifolds. We further use this explicit description to present an algorithm that we illustrate by producing an array of examples of isotopically distinct tilings of the hyperbolic plane with symmetries generated by rotations that are commensurate with the prominent Primitive, Diamond and Gyroid triply-periodic minimal surfaces, outlining how the approach yields an unambiguous enumeration. We also present the corresponding 3-periodic graphs on these surfaces.

1 Introduction

Tesselations from repeating motifs have a long and involved history in mathematics, engineering, art and sciences. Most of the literature has focussed on patterns in Euclidean spaces. However, the role of hyperbolic geometry in Euclidean tilings and more generally for the natural sciences is increasingly recognized. More recently, it has been recognized that assemblies of atoms or molecules in crystalline arrangements that are energetically favourable involve (intrinsic) curvature [15]. Many real Zeolite frameworks and metal-organic frameworks were found to reticulate triply-periodic minimal surfaces (TPMS) [13, 14, 15, 4]. TPMS are minimal surfaces, which locally minimize the surface area relative to a boundary curve of a simply connected neighbourhood around any point, which are furthermore invariant under 3 independent translations. These are covered by the hyperbolic plane $\mathbb{H}^2$ [25] in such a way that the symmetries of the surface correspond to hyperbolic symmetries [19].

The above observations and ideas have led to a novel investigation of 3-dimensional Euclidean networks, where TPMS are used as a convenient route to the enumeration of crystallographic nets and polyhedra in $\mathbb{R}^3$ [32, 26, 31, 16, 30, 3]. The aim of the EPINET project [1] is to produce and analyse chemical structures by investigating how graphs embed on TPMS. Most hyperbolic in-surface symmetries of prominent TPMS manifest as ambient Euclidean symmetries of $\mathbb{R}^3$ [29], so that symmetric tilings of TPMS give rise to symmetric graph embeddings in $\mathbb{R}^3$. Not only does knowing the symmetry of a structure in $\mathbb{R}^3$ facilitate further investigations into structural properties, symmetric structures are prominent because they are candidates for structures found in nature as well as for synthesis, and because they favor self-essembly. Structures such as hyperbolic tilings with disks with kaleidoscopic symmetries generated by reflections [20, 30], some simple hyperbolic tilings with slightly more complicated symmetries [28, 27], simple unbounded tiles with a network-like structure [17, 12, 19, 21, 18, 8, 7], and unbounded tiles with totally geodesic boundaries [9]

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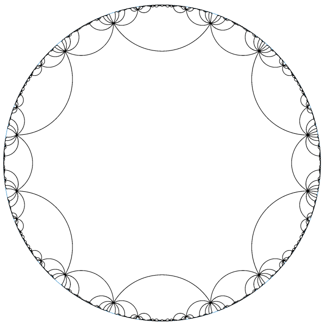
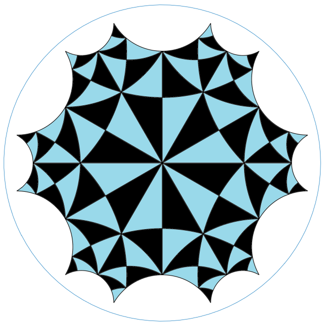
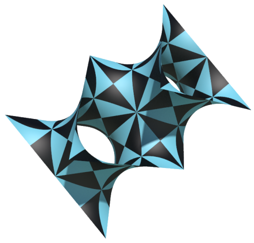


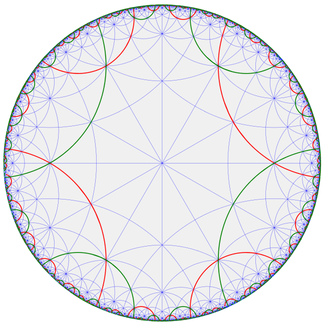
(a) Tesselation of $\mathbb{H}^2$ by dodecagons corresponding to the genus 3 Riemann surface that gives rise to the D-surface.



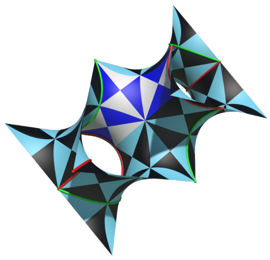
(b) The symmetries of the D-surface within a unit cell in $\mathbb{H}^2$. Each line represents a mirror symmetry.



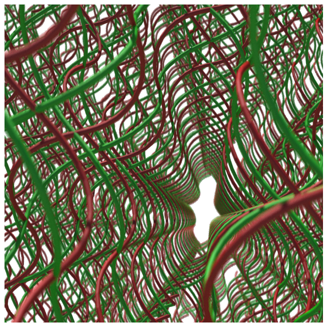
(c) A section of the D-surface in $\mathbb{R}^3$, together with its smallest asymmetric triangle patches.



(d) A tiling of the hyperbolic plane with symmetry group 22222, represented by the green and red edges, with a tiling by triangles with $\star 246$ symmetry shown in blue in the background.



(e) The decoration from (d) and a fundamental domain shown as a decoration of the Diamond triply-periodic minimal surface. The triangles illustrate the symmetries of the surface.



(f) The resulting net in $\mathbb{R}^3$ when the tile boundaries are taken as trajectories in Euclidean 3-space.

Figure 1 (a)-(c) shows symmetries of the D-surface in $\mathbb{R}^3$ and its uniformization in $\mathbb{H}^2$. (d)-(f) shows the progression from a tiling of the hyperbolic plane to a 3-dimensional net via a decoration of the Diamond triply-periodic minimal surface.

have been explored, and resulting structures have been used in analysis in real physical systems [22].

The situation can be summarized as in Figure 1, which shows a hyperbolic tiling that respects the translational symmetries, indicated in (a) and (b), of the covering map of the hyperbolic plane onto a prominent TPMS, the diamond D surface, partly shown in (c). When the tile boundaries are considered as trajectories in 3-dimensional Euclidean space rather than curves on the surface, we obtain a symmetric net in $\mathbb{R}^3$. In (b) and (c), the symmetries of the D surface are illustrated by the tiling by triangles, with each triangle boundary corresponding to a reflection in the surface. This symmetry group can be denoted by $\star 246$, using Conway's notation[5] for 2D orbifold symmetry groups.

1.1 Summary of the problem and results

We summarize the problem as detailed above. The EPINET project produces and analyses chemical structures by investigating how graphs embed symmetrically on triply periodic minimal surfaces (TPMS). The aim of this paper is to introduce techniques to systematically enumerate symmetric embeddings of graphs on the gyroid, primitive, and diamond TPMSs, the most prominent and well understood examples of TPMS in nature. We will concentrate on symmetry groups generated by rotations and graphs which admit a 2-cell embedding into the surface in its smallest translational unit in $\mathbb{R}^3$.

Up until now, this problem has been investigated only for certain classes of simple graphs and attempts to further EPINET have involved ad-hoc ideas with limited applications. To organize the ensuing structures, the problem of a complexity ordering in the enumeration takes up an important role in our investigation and we base our ideas on an intuitive ordering. We seek a systematic approach to investigating graph embeddings on surfaces with a given symmetry group, in an attempt to develop a general framework to tackle similar problems in the future. To achieve these goals, we investigate tilings in $\mathbb{H}^2$ with a given symmetry group will be the focus of our interest.

Our results show that, in theory, the enumeration works. However, some of the algorithms used, for example those of computational group theory cannot easily handle the group presentations we work with.

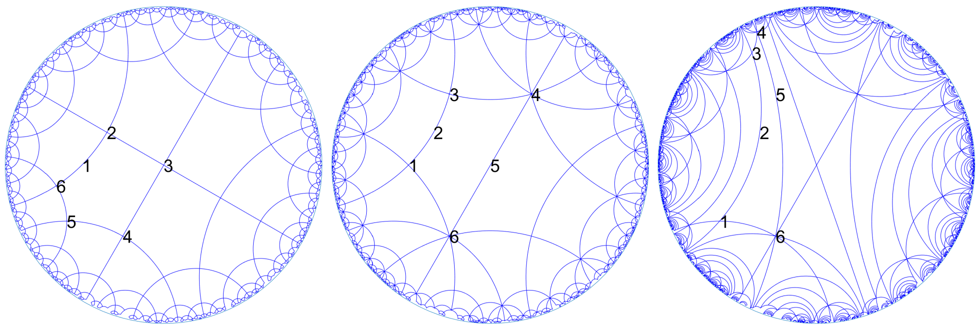
2 Preliminaries and our approach

▶ **Definition 2.1.** A tiling $\mathcal{T}$ of $\mathbb{H}^2$ is a locally finite collection of closed disks in $\mathbb{H}^2$ whose interiors are pairwise disjoint. Let $\mathcal{T}$ be a tiling of $\mathbb{H}^2$ and let Γ be a discrete group of isometries. If $\mathcal{T} = \gamma\mathcal{T} := \{\gamma T \mid T \in \mathcal{T}\}$ for all $\gamma \in \Gamma$ then we call the pair $(\mathcal{T}, \Gamma)$ an *equivariant tiling*. Two tiles $T_1, T_2 \in \mathcal{T}$ are *equivalent* or symmetry-related if there exists $\gamma \in \Gamma$ such that $\gamma T_1 = T_2$. The *orbit* of a tile is the subset of $\mathcal{T}$ given by images of T: $\Gamma.T = \{\gamma T \text{ for } \gamma \in \Gamma\}$. Given a particular tile $T \in \mathcal{T}$, the *stabilizer subgroup* Γ_T is the subgroup of Γ that fixes T, i.e. $\Gamma_T = \{\gamma \in \Gamma \mid \gamma T = T\}$. A tile is called *fundamental* if Γ_T is trivial and we call the whole tiling fundamental if this is true for all tiles. An equivariant tiling is called *tile-k-transitive*, when k is the number of equivalence classes (i.e. distinct orbits) of tile under the action of Γ. Two equivariant tilings $\{(\mathcal{T}_i, \Gamma_i)\}_{i=1}^2$ are **equivariantly equivalent** if there exists a homeomorphism φ such that $\varphi(\mathcal{T}_1) = \mathcal{T}_2$ and $\varphi\Gamma_1\varphi^{-1} = \Gamma_2$.

To simplify the discussion and avoid technical details, we shall assume in this paper that the edge orbits of a tiling are coloured and therefore distinguishable, in the sense that any nontrivial graph isomorphism of the tiling's 1-skeleton changes it. There is a complete invariant for equivariant equivalence classes of tilings, the D-symbol, a weighted graph, whose isomorphism class uniquely determines an equivariant equivalence class of tilings with closed disks in $\mathbb{H}^2$ [11]. There is likewise an algorithm that enumerates all (of the infinitely) possible equivariant equivalence classes of tilings starting from fundamental tile-1-transitive tilings. For a given TPMS, there is a symmetry group S that contains the largest group of translational symmetries T of the TPMS as a subgroup, i.e. $T \subset S$. We call a subgroup H of S satisfying $T \subset H \subset S$ *commensurate* with the symmetries of the TPMS.

▶ **Definition 2.2.** A (hyperbolic) orbifold, for our purposes, is the space $\mathbb{H}^2/\Gamma$, where Γ is a discrete group of isometries of $\mathbb{H}^2$. The orbifold structure is more than the quotient space $\mathbb{H}^2/\Gamma$ with quotient topology in that it keeps track of the data associated to the quotient map $\pi : \mathbb{H}^2 \to \mathbb{H}^2/\Gamma$, so that one can retains the information of how "copies" of $\mathbb{H}^2/\Gamma$ fit together to form $\mathbb{H}^2$. We denote orbifolds by their Conway orbifold symbol [5], a symbol that keeps track of the generators of the symmetry group Γ.

Two main observations lead us to a novel approach to tackle the problem.



(a) A transitive, fundamental equivariant tiling of $\mathbb{H}^2$ with symmetry group 2224.

(b) Another transitive, fundamental equivariant tiling of $\mathbb{H}^2$ with symmetry group 2224.

(c) A different placement of generators, producing a sheared version of the fundamental tiling.

Figure 2 Fundamental tilings with symmetry group 2224.

1. For a given commensurate symmetry group H of a TPMS, two equivariant tilings are equivalent iff they are related by a homeomorphism of $\mathbb{H}^2$ that induces an automorphism of H.
2. Given special sets of geometric generators for H, it is possible to describe graph embeddings in $\mathbb{H}^2$ that give rise to equivariant tilings with symmetry group H as combinatorial descriptions in terms of the generators, see Figure 2. The set of geometric generators we use directly corresponds to a set as given by the orbifold symbol of the symmetry group.

In Figure 2a, consider the rotations corresponding to the generators $r_1, ..., r_4$, with centers $c_1, ..., c_4 \in \mathbb{H}^2$, marked by 1 to 4. It is straightforward to see that the points with rotational symmetry on the polygon's boundary correspond clockwise, starting at c_1, to the points $c_1, c_2, c_3, c_4, r_4(c_3), r_1(c_2)$ and we find similar expressions for other *stellate orbifolds*, i.e. those with only rotations for generators.

Given any generators $r_1, ..., r_4$ for the discrete group of isometries 2224, this description of edges defines a fundamental tiling, in this case with geodesic edges, regardless of the generators placement in $\mathbb{H}^2$. For example, for the fundamental tiling of Figure 2b, the edges are given by hyperbolic lines connecting the points marked 1 to 6 in cyclic order, which correspond to the points $c_1, c_2, r_2(c_1), r_3^{-1}(c_4), c_3, c_4$, respectively. Figure 2c illustrates that this relation for the edges still holds in a sheared version of the fundamental tiling with symmetry group. Here, the sheared fundamental domain exhibits less symmetries of the other two tilings. Note that the symmetry group of all tilings in Figure 2 is identical, namely 2224.

It turns out that the generators of the symmetry group H that give rise to isotopically distinct tilings, in the sense that there is no deformation of one tiling that leads to the other while preserving the symmetries of H at every step, are in one-to-one correspondence with special automorphisms of H. These, on the other hand, are in one-to-one correspondence with the orbifold mapping class group MCG. For our purposes we can briefly define the MCG as follows. Consider the set of homeomorphisms $\{\varphi\}$ of $\mathbb{H}^2$ that satisfy $\varphi^{-1}H\varphi = H$, endow this set with the compact-open topology, and identify those that can be connected through a path of such homeomorphisms. It turns out that the MCG of an orbifold is exactly in one-to-one correspondence to the automorphisms that lead to isotopically distinct tilings. For stellate orbifolds, this is proven in [23]. For more general orbifolds, the statement can also be made precise and generalized, but this lies outside the scope of the this paper.

All in all, by the above, we transfer a problem in graph enumeration to the problem of

(a) Curves representing group elements and the half-twist, indicated in red.

(b) The resulting curves after twisting.

Figure 3 Half-twists

enumerating elements of the MCG. An enumeration of tilings with a given symmetry group follows the following steps. First, we find a commensurate symmetry group of a TPMS of interest. Then, we use the complexity ordering of D-symbols [6] to construct a representative of each equivariant tiling class. Subsequently, using a presentation of the MCG and an action on the generators of the symmetry group, we obtain a list of generators that give rise to an enumeration of distinct isotopy classes of these tilings with the same symmetry group. Using the Weierstrass parametrization for minimal surface along with Schwarz-Christoffel maps to deform hyperbolic polygonal domains into spherical ones one can, with analytic continuation, construct a direct map from $\mathbb{H}^2$ to the TPMS of interest. We briefly explain the MCG approach in the next sections.

3 The mapping class group and its action on sets of generators

To investigate the action of mapping class group elements on sets of generators, we use the following idea. Similarly to the classical setting for surfaces, it is possible to interpret group elements of symmetry groups as special curves in the underlying topological space of the orbifold. Given a representative homeomorphism of an element of the MCG, we apply it to the curves representing the generators of the symmetry group and read off the new curves, which in turn designate new group elements. We focus on the action of well-known generators for the MCG with geometric interpretations.

We consider an example. Figure 3 shows the derivation of the representation of a half-twist around two marked points, corresponding to two rotational center for rotations of the same order, in the orbifold's underlying topological space, with Figure 3b giving the result of the twist indicated in Figure 3a. In formulas, Figure 3 translates to the half twists around S_1 and S_2 taking the form

$$\begin{cases} S_1 \mapsto S_1 S_2 S_1^{-1}, \\ S_2 \mapsto S_1. \end{cases} \tag{1}$$

It is straightforward to check that the transformation (1) leaves the global group relation $S_1 S_2 \cdots S_n$ invariant.

One can draw similar pictures for more complicated symmetry groups, their MCGs and their generators. Using presentations of the mixed braid group [24] and exploiting the relationship between braid groups and MCGs [2, 10], one can derive a (lengthy) presentation of MCGs for stellate orbifolds. Using GAP(Groups, Algorithms, Programming) and the package KBMag, one can use this presentation to enumerate elements of the MCG, which together with the action on generators of the symmetry group and the description of the tilings in terms of these generators yields an enumeration of isotopy classes of (coloured) tilings of $\mathbb{H}^2$ with the given symmetry group.

4 Conclusion and open problems

By using MCGs of orbifolds, we were able to significantly generalize known results on the enumeration of hyperbolic tilings that fit onto hyperbolic surfaces. While we only showed how to proceed in case the orbifold is stellate, our methods remain valid in much more general settings. This work provides the basis for a major extension of the EPINET project and associated databases. The methods of this paper open up the possibility for automated searches for 3-periodic graphs in $\mathbb{R}^3$ with given topological properties that embed on TPMS.

Main difficulties in generalizing our approach lie within the fact that (semi-)algorithms like KBMag are not guaranteed to find an enumeration of MCG elements, and they are very sensitive to parameters. Furthermore, for general TPMS, for our methods to work, one first has to investigate commensurate symmetry groups, find a parametrization of the TPMS and lifts of in-surface symmetries and find the description of edges in terms of generators.

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