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Symmetry group of two special types of carbon nanotori

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This paper studies the symmetry group of two special types of carbon nanotori. The construction is motivated by a group-theoretical result.

1. Introduction

Carbon nanotubes are arrangements of carbon atoms that have the shape of a cylinder (Reich *et al.*, 2004; Iijima, 1992). They have been intensively studied because of their special thermal, mechanical and electrical properties. From a mathematical point of view, the simplest invariant of a nanotube is the group of symmetries of the network formed by the carbon atoms (Damnjanovic & Milosevic, 2010).

Carbon nanotori are of course just arrangements of carbon atoms on a torus (Dienes & Thomas, 2011; Liu *et al.*, 2002). Their group of symmetry was studied in Arezoomand & Taeri (2009) and Yavari & Ashrafi (2009). However, in these papers it was assumed that the meridian of the torus was much smaller than the longitude of the torus.

In this paper we are interested in the group of symmetry of a carbon nanotorus whose meridian and longitude are of comparable size. The examples that we study can be associated in a natural way with a group. More precisely, we consider the Cayley hypergraph associated with a group T_n and show that it can be placed on a torus. Using the notation from Dienes & Thomas (2011), this nanotorus turns out to be the one associated with the pair of vectors $L_1 = n\mathbf{a}_1$ and $L_2 = n\mathbf{a}_1 - n\mathbf{a}_2$.

We also study the Cayley hypergraph associated with the group $SL(2,3)$ and show that it corresponds to the pair of vectors $L_1 = 3\mathbf{a}_1 - \mathbf{a}_2$ and $L_2 = \mathbf{a}_1 - 3\mathbf{a}_2$. The interesting part about this second example is that some of the symmetries of the carbon nanotorus are not induced by symmetries of the graphene sheet.

2. Cayley hypergraph

2.1. The group T_n

Denote by C_n the cyclic group with n elements. It is convenient to see C_n as a subgroup of the complex field $\mathbf{C}$ generated by ζ_n. We denote by ε the generator of C_3.

Definition 2.1. Define the group T_n by

$$T_n = \langle a, b \,|\, a^3 = 1, b^3 = 1, (ab)^3 = 1, (ab^2)^n = 1\rangle.$$

First let us notice that T_n is a finite group.

Lemma 2.2. $|T_n| \le 3n^2$.

Proof. Condition $(ab)^3 = 1$ can be rewritten as $aba = b^2a^2b^2$; since $a^3 = b^3 = 1$ this is equivalent to $(ab^2)(b^2a) = (b^2a)(ab^2)$. We have $\operatorname{ord}(ab^2) = \operatorname{ord}(b^2a) = n$. There exists a morphism $\pi : T_n \to C_3$ such that $a \to \varepsilon$ and $b \to \varepsilon$. Obviously we have $T_n \cong \ker(\pi) \rtimes C_3$. If $x \in \ker(\pi)$ then x can be written as a word of length $3k$ in a and b. Moreover, we can notice that any word of length 3 can be expressed in terms of ab^2 and b^2a. This means that $\ker(\pi)$ is generated by ab^2 and b^2a and so it has at most n^2 elements. In particular $|T_n| \le 3n^2$. □

For all $n \ge 2$ we define an automorphism $u : C_n \times C_n \to C_n \times C_n$ by

$$u(z_1, z_2) = (z_1^{-1}z_2^{-1}, z_1^{-1}).$$

One can easily check that u is an automorphism of $C_n \times C_n$ and that $u^3 = \mathrm{id}$. This allows us to define a homomorphism $\varphi : C_3 \to \operatorname{Aut}(C_n \times C_n)$, by

$$\varphi(\varepsilon) = u.$$

So we can construct the semidirect product of $C_n \times C_n$ by C_3 with respect to φ. Now we have the following result.

Proposition 2.1. $T_n \cong (C_n \times C_n) \rtimes_\varphi C_3$ where φ is the above-defined morphism. In particular $|T_n| = 3n^2$.

Proof. Consider the elements $A = ((1, \zeta_n), \varepsilon)$ and $B = ((1,1), \varepsilon) \in (C_n \times C_n) \rtimes_\varphi C_3$. One can check that $A^3 = 1$, $B^3 = 1$, $(AB)^3 = 1$ and $(AB^2)^n = 1$. Consequently we have a homomorphism $\Phi : T_n \to (C_n \times C_n) \rtimes_\varphi C_3$ determined by $\Phi(a) = A$ and $\Phi(b) = B$. Since A and B generate $(C_n \times C_n) \rtimes_\varphi C_3$ we have that this morphism is surjective. Finally, because $|T_n| \le 3n^2$, we must have that Φ is an isomorphism. □

2.2. Cayley hypergraph of a group generated by elements of order 3

Hypergraphs are generalizations of the notion of graphs. The main difference is that an edge can connect more than two vertices. Formally, a hypergraph consists of a set of vertices V and a set of hyper-edges E (that is, a collection of subsets in V). A k-hypergraph is a hypergraph with the property that any edge connects exactly k vertices. When $k = 2$ we recover the usual notion of a graph. In this paper we are interested only in the case $k = 3$.

We will assume that each hyper-edge has a cyclic ordering of the vertices (*i.e.* a hyper-edge is a cyclically ordered subset of V). For example if v_0, v_1 and $v_2 \in V$ then $\{v_0, v_1, v_2\}$ is the same hyper-edge as $\{v_1, v_2, v_0\}$ but is different to $\{v_0, v_2, v_1\}$.

It is well known that with a group G and a set of generators S one can associate the so-called Cayley graph $\mathrm{Cay}(G, S)$. A special situation is when all the elements of the set S have order 2. In that case the $\mathrm{Cay}(G, S)$ has the structure of a pre-reflection system (Davis, 2007).

The Cayley graph was generalized to k-hypergraphs by Buratti (1994). When $k = 2$ we recover the classical Cayley graph. In this paper we study groups that are generated by elements of order 3 (they correspond to 3-hypergraphs). We briefly recall from Buratti (1994) the construction of the hypergraph $\mathrm{Cay}_3(G, T)$.

Let G be a group and T a set of generators for G such that every element in T has order 3. Moreover, assume that if $\sigma \in T$ then $\sigma^{-1} = \sigma^2$ is not in T. To construct the 3-hypergraph $\mathrm{Cay}_3(G, T)$ take the set of vertices to be G. A cyclically ordered subset $\{g_1, g_2, g_3\} \subseteq G$ is a hyper-edge if there exists $\sigma \in T$ such that $g_2 = g_1\sigma$ and $g_3 = g_1\sigma^2$. Notice that $g_3 = g_2\sigma$, $g_1 = g_2\sigma^2$ and $g_1 = g_3\sigma$ $g_2 = g_3\sigma^2$ and so each edge has a natural cyclic orientation (we can talk about the 'previous' vertex and the 'next' vertex of an edge).

Just like in the case of the usual Cayley graph, we have an action of the group G on $\mathrm{Cay}_3(G, T)$. The action of G on vertices $G \times V \to V$, where $V = G$, is given by left multiplication: $(g, x) \longmapsto gx$. This is compatible with the hyper-edges in $\mathrm{Cay}_3(G, T)$ and the orientation of hyper-edges.

3. Main result

3.1. First example

Take $G = T_2 (= A_4)$, the alternating group on four letters and $T = \{a, b\}$. In Fig. 1 we draw the hypergraph $\mathrm{Cay}_3(G, T)$. The hypergraph lives in a natural way on a torus, but it is more convenient to draw it in the plane. Of course this will force us to draw some hyper-edges (or part of them) more than once. Let us explain the picture. The vertices of our hypergraph are the small rectangles with a label inside them. A hyper-edge is a Y-shape connector among three vertices. The orientation is induced from the orientation of the plane. Start at the vertex labeled e (in the upper part of the picture); at the first step we get two hyper-edges (e, a, a^2) and (e, b, b^2). We continue this procedure with the new vertices, for example the vertex a is part of two hyper-edges (a, a^2, e) [which is the same as (e, a, a^2)] and the hyper-edge (a, ab, ab^2). Let us see how we get the hexagon in the top-left part of the picture. Our procedure indicates that the vertex labeled by bab should also get the label $a^2b^2a^2$, but these two are equal as elements in T_2. After a few steps, we get the picture in Fig. 1. One can notice that we have several repetitions in our picture. These must be identified as part of the hypergraph $\mathrm{Cay}_3(G, T)$. It means that the three segments on the left labeled with bab, ba and ba^2 are the same as the segments on the right labeled with aba, b^2a^2b and ab^2. Similarly, after making a small twist, the bottom part of the picture can be identified with the top part. In particular, this tells us how to put this hypergraph on a torus.

Example 3.1. The hypergraph $\mathrm{Cay}_3(T_2, \{a, b\})$ is described in Fig. 1. A similar picture is obtained for the hypergraph $\mathrm{Cay}_3(G, T)$ when $G = T_n$ and $T = \{a, b\}$. In that case we get a tiling of the torus with n^2 hexagons. The corresponding two vectors are $\mathbf{OV}_1 = n\mathbf{a}_1$ and $\mathbf{OV}_2 = n\mathbf{a}_1 - n\mathbf{a}_2$.

Remark 3.2. If one thinks about these hypergraphs as models for nanotori, then the carbon atoms correspond to the joint point of hyper-edges and not to the vertices of the hypergraph.

Next we want to make the identification between the hypergraph and the usual graphene sheet. We consider a tiling with hexagons of the complex plane $\mathbf{C}$ such that $\mathbf{a}_1 = 1$ and $\mathbf{a}_2 = \exp(i5\pi/3)$ (see Fig. 2). Define $\alpha, \beta : \mathbf{C} \to \mathbf{C}$ by

$$\alpha(z) = \exp(i2\pi/3)z,$$

$$\beta(z) = \exp(i2\pi/3)z + 1.$$

One can see that α is the rotation with $2\pi/3$ around O and β is the rotation with $2\pi/3$ around the point B (see Fig. 2). For the second statement, notice that $B = (1/3^{1/2})\exp(i\pi/6)$ and the rotation with angle $2\pi/3$ around B is obtained by first shifting with the vector $\mathbf{BO}$, then making a rotation with angle $2\pi/3$,

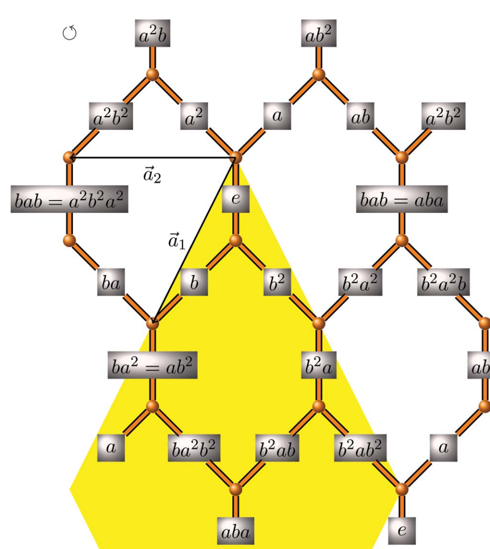

Figure 1
$\mathrm{Cay}_3(T_2, \{a, b\})$.

and finally making a shift back with the vector **OB**. But this corresponds to the function

$$z \rightarrow \exp(i2\pi/3)[z - (1/3^{1/2})\exp(i\pi/6)] + (1/3^{1/2})\exp(i\pi/6)$$
$$= \exp(i2\pi/3)z + (1/3^{1/2})[\exp(i\pi/6) - \exp(i5\pi/6)]$$
$$= \exp(i2\pi/3)z + 1.$$

Also $\alpha\beta^2$ is the translation with minus one unit in the direction of the vector $\mathbf{a}_1 = 1$ and $\alpha\beta$ is a rotation of order 3. In particular we get $\alpha^3 = \mathrm{id}$, $\beta^3 = \mathrm{id}$ and $(\alpha\beta)^3 = \mathrm{id}$. Moreover α and β preserve the tiling with hexagons of $\mathbf{C}$.

To make the identification between Figs. 1 and 2, it is enough to say that the points O and B correspond to the junction points of the hyper-edge (e, a, a^2) and, respectively, (e, b, b^2). We also draw a (shaded) fundamental domain in Fig. 2 and a part of the corresponding fundamental domain in Fig. 1.

In order to describe the arrangement of carbon atoms for a nanotorus, one must know the two vectors that give the identification in the graphene sheet. These two vectors are denoted by $V_1 = m\mathbf{a}_1 + n\mathbf{a}_2$ and $V_2 = p\mathbf{a}_1 + q\mathbf{a}_2$. Without loss of generality we can assume that the angle β between V_1 and a_1 is in the interval $(-\pi/3, \pi/3]$ and the angle θ between V_1 and V_2 is in the interval $(0, \pi/2)$. This will force the quantity $N_{\mathrm{hex}} = np - mq$ to be positive.

With the above convention the tiling of the torus described in Fig. 1 (and Fig. 2) corresponds to the vectors:

$$\mathbf{OV}_1 = 2\mathbf{a}_1,$$

$$\mathbf{OV}_2 = 2\mathbf{a}_1 - 2\mathbf{a}_2.$$

Since the group T_2 acts on $\mathrm{Cay}_3(T_2, \{a, b\})$, this gives an action of the T_2 on the carbon nanotorus corresponding to $\mathbf{OV}_1$ and $\mathbf{OV}_2$. Let Γ be the lattice determined by the vectors $\mathbf{OV}_1$ and $\mathbf{OV}_2$. One can notice that the action of a (respectively, b) on the torus $T^2 = \mathbf{C}/\Gamma$ is induced by the action of α (respectively, β) on $\mathbf{C}$.

More generally one can show that the 3-hypergraph associated with the group T_n gives a tiling of the torus that corresponds to vectors $\mathbf{OV}_1 = n\mathbf{a}_1$ and $\mathbf{OV}_2 = n\mathbf{a}_1 - n\mathbf{a}_2$.

Notice that a and b preserve the orientation of the torus. If we do not need to preserve the orientation of the torus, then we also have the symmetry that corresponds to the reflection in the line determined by the vector $\mathbf{a}_1 - \mathbf{a}_2$ (*i.e.* the line determined by O and B). This generates a subgroup of the group of symmetries which is isomorphic to the semidirect product of Σ_3, the symmetric group on three letters, with $C_n \times C_n$. This group is usually denoted by $G(n, n, 3)$ (Shephard & Todd, 1954; Lehrer & Taylor, 2009). To get all the symmetries that can be extended to symmetries of the torus, one has to consider also the symmetry with respect to the mediator line of the segment OB.

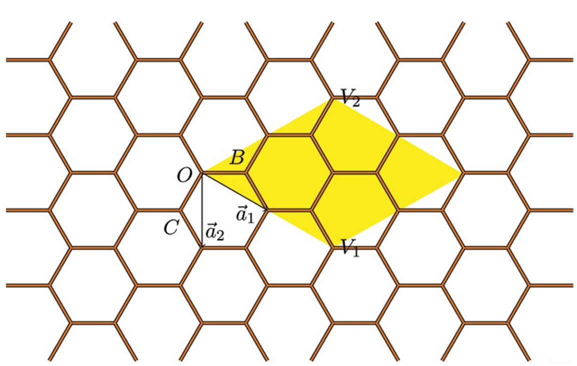

Figure 2
$\mathbf{OV}_1 = 2\mathbf{a}_1$, $\mathbf{OV}_2 = 2\mathbf{a}_1 - 2\mathbf{a}_2$.

3.2. Second example

Consider the group $G = SL(2, 3)$. Using the program *GAP* (http://www.gap-system.org), one can see that G has a presentation with generators and relations as

$$G = \langle x, y \,|\, x^3 = 1, y^3 = 1, xyx = yxy \rangle.$$

We will show that the Cayley hypergraph of G can be placed on the torus T^2; however the orientation of hyper-edges is not going to be induced by the orientation on T^2.

In Fig. 3 we have the hypergraph associated with the above presentation. Notice that the edge (e, y, y^2) has the same orientation as the orientation of the plane (and we label it with an anticlockwise arrow symbol), while the edge (e, x, x^2) has the opposite orientation (and we label it with a clockwise arrow symbol). A similar convention was used for all the other hyper-edges of $\mathrm{Cay}_3(SL(2, 3), \{x, y\})$. In total, we have eight hyper-edges that have the same orientation as T^2 and eight that have the opposite orientation. Just like in the previous example some of the vertices and edges appear more than once in the picture, but after they are identified we get a tiling of the torus.

Example 3.3. $\mathrm{Cay}_3(SL(2, 3), \{x, y\})$ gives a tiling of the torus with eight hexagons. The corresponding two vectors are $\mathbf{OV}_1 = 3\mathbf{a}_1 - \mathbf{a}_2$ and $\mathbf{OV}_2 = \mathbf{a}_1 - 3\mathbf{a}_2$ (see Fig. 4).

The orientation of hyper-edges is not induced by the orientation of T^2, so it is reasonable to expect that some of the symmetries of the hypergraph $\mathrm{Cay}_3(SL(2, 3), \{x, y\})$ do not come from symmetries of the plane. In Fig. 5 we illustrate that

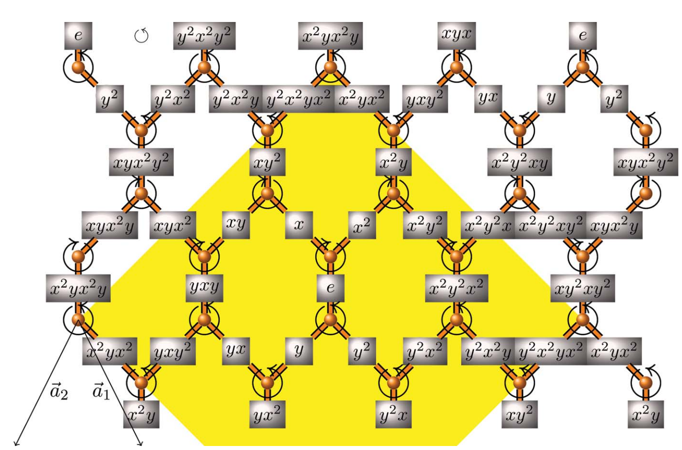

Figure 3
$\mathrm{Cay}_3(SL(2, 3), \{x, y\})$.

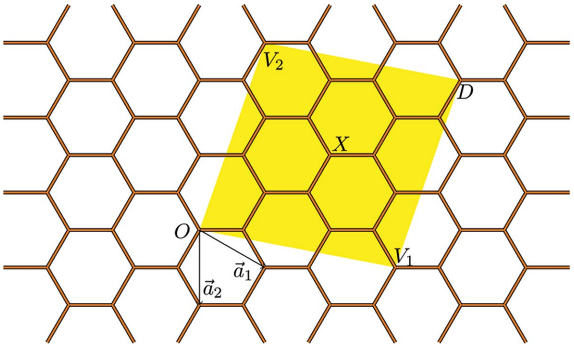

Figure 4
$\mathbf{OV}_1 = 3\mathbf{a}_1 - \mathbf{a}_2$, $\mathbf{OV}_2 = \mathbf{a}_1 - 3\mathbf{a}_2$.

this is indeed the case. More precisely, we present the action of x on $\mathrm{Cay}_3(SL(2, 3), \{x, y\})$. To make the action easier to visualize we divide the elements of G in three orbits a_i, b_i and c_i where $1 \le i \le 8$. The action of x is determined by $xa_i = b_i$, $xb_i = c_i$ and $xc_i = a_i$.

Remark 3.4. The hyper-edges are preserved but they are twisted by the action of x (just like in a Transformers toy). However, the hexagonal faces of the tiling are not preserved by the action of G. For example, the hexagon with vertices a_1, a_2, a_4, b_4, b_2, b_1 is transformed in the loop b_1, b_2, b_4, c_4, c_2, c_1 that is homotopical nontrivial as a loop on the torus.

4. Isospectral equivalence

The models that we described in the previous section have the property that the meridian and the longitude are equal (the T_n case) or of comparable size [the $SL(2, 3)$ case]. This creates a problem when we want to get physical nanotori with that prescribed crystallographic structure (since the bond among carbon atoms is curled).

In Dienes & Thomas (2011), a certain equivalence relation among physically distinct tori is discussed. The equivalence relation is generated by modular symmetries which can change the physical structure of the torus but preserve the band structure, energy spectra, electrical conductivity and number of hexagons. In each equivalence class there exists an element with minimal twist on the bond. This is of course the most likely to exist in a physical shape.

In what follows we will recall the equivalence relation from Dienes & Thomas (2011), and show that the vectors $\mathbf{OV}_1$ and $\mathbf{OV}_2$ presented above give that minimal twist.

The arrangement of the carbon atoms of a nanotorus is determined by two vectors $V_1 = m\mathbf{a}_1 + n\mathbf{a}_2$ and $V_2 = p\mathbf{a}_1 + q\mathbf{a}_2$. We associate with the above pair of vectors an element $u = (m + in, p + iq) \in \mathbf{Z}[\mathbf{i}]^2$. Two elements in $\mathbf{Z}[\mathbf{i}]^2$ are equivalent if they are related by compositions of the following maps: $S(m + in, p + iq) = (-(p + iq), m + in)$ and $T(m + in, p + iq) = (m + in, m + p + i(n + q))$. Notice that S and T correspond to the multiplication with

$$S = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in SL_2(\mathbf{Z})$$

and

$$T = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \in SL_2(\mathbf{Z}),$$

respectively. Also S and T do not change $N_{\rm hex} = np - mq$ (the number of hexagons on the torus), but they change the angles β and θ. Also the group of symmetry is not changed, but the embedding in $\mathbf{R}^3$ is different (Dienes & Thomas, 2011). Of course one prefers the embedding that gives the minimal twist (minimal tension on the bond among carbon atoms).

With the element $(m + in, p + iq)$ one can associate the complex number

$$\tau = \frac{p^2 + pq + q^2}{m^2 + mn + n^2} \exp(i\theta).$$

We want τ to be in the fundamental domain (Dienes & Thomas, 2011),

$$\mathcal{F} = \{\tau | \frac{-1}{2} < \mathrm{Re}(\tau) \le \frac{1}{2}, \quad \mathrm{Im}(\tau) > 0, \ |\tau| \ge 1\}.$$

In Example 3.1 we have $\mathbf{OV}_1 = n\mathbf{a}_1$ and $\mathbf{OV}_2 = n\mathbf{a}_1 - n\mathbf{a}_2$ and so

$$\tau = \frac{n^2 - n^2 + n^2}{n^2} \exp[i(\pi/3)] = \frac{1}{2} + i\frac{3^{1/2}}{2} \in \mathcal{F}.$$

In Example 3.3 we have $\mathbf{OV}_1 = 3\mathbf{a}_1 - \mathbf{a}_2$ and $\mathbf{OV}_2 = \mathbf{a}_1 - 3\mathbf{a}_2$ and so

$$\tau = \frac{1 - 3 + 9}{9 - 3 + 1} \exp(i\theta) = \frac{1}{7} + i\frac{4(3^{1/2})}{7} \in \mathcal{F}.$$

Here we are using the fact that in Fig. 4 we have $OX = 2$, $XV_1 = 3^{1/2}$ and so $OV_1 = 7^{1/2}$. From the triangle OV_1V_2 we have

$$\cos(\theta) = \frac{V_1V_2^2 - OV_1^2 - OV_2^2}{-2OV_1OV_2} = \frac{12 - 7 - 7}{-2(7^{1/2})(7^{1/2})} = \frac{2}{14} = \frac{1}{7}.$$

Notice that the rhombus OV_1DV_2 has the property that, relative to the distance induced by the hypergraph, the two diagonals are of equal length 8, *i.e.* the shortest path between

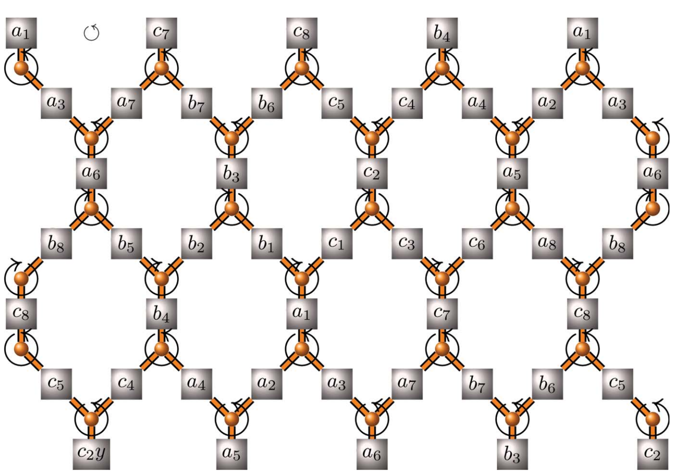

Figure 5
Action of x on $\mathrm{Cay}_3(SL(2, 3), \{x, y\})$.

O and D (along the edges of the tiling with hexagons) has the same length as the shortest path between V_1 and V_2. This partially explains why we have more symmetry than one normally expects.

5. Some remarks

5.1. Map automorphisms

After this paper was written, it was pointed out to us by the referee that there might be some connections with the article by Senechal (1988). We will recall and discuss the results from Senechal (1988).

Let Γ be the standard hexagonal tiling in the Euclidean plane E^2. Let F be a discrete subgroup of E^2 that acts freely on E^2 such that for each element $f \in F$ we have $f\Gamma \subseteq \Gamma$. Suppose that E^2/F is a torus and the graph $\gamma = \Gamma/F$ gives a tiling with hexagons for this torus. We say that an automorphism $\alpha : \gamma \to \gamma$ is a map automorphism if α can be extended to an automorphism of the torus E^2/F. It was proved in Senechal (1988) that the group of map automorphisms of the graph γ is isomorphic with $N_{\mathrm{Aut}(\Gamma)}(F)/F$ [where $N_{\mathrm{Aut}(\Gamma)}(F)$ is the normalizer of the group F in Aut(Γ)].

The group of automorphisms of Γ is generated by the translations $u_1(z) = z + 1$, $u_2(z) = z - \varepsilon$, together with the symmetries $s(z) = -\varepsilon\overline{z}$ (with respect to the vector $\mathbf{a}_1 + \mathbf{a}_2$), and $t(z) = \overline{z} - (i/3^{1/2})$ (with respect to the mediator line of the segment OC), see Fig. 2. One can see that the group generated by u_1 and u_2 is isomorphic with $\mathbf{Z} \times \mathbf{Z}$. The subgroup generated by s and t is isomorphic with D_{12}. Moreover, Aut(Γ) is isomorphic with the semidirect product of $\mathbf{Z} \times \mathbf{Z}$ and D_{12}, where the action of the group D_{12} on $\mathbf{Z} \times \mathbf{Z}$ is given by

$$s(u_1, u_2) = (u_2, u_1),$$
$$t(u_1, u_2) = (u_1, u_1 - u_2).$$

Notice that in general F does not have to be a normal subgroup of Aut(Γ). With the above notations, the nanotorus from Example 3.1 is obtained when F is generated by nu_1 and nu_2. This group is a normal subgroup of Aut(Γ) and so the group of map automorphism of γ is

$$(\mathbf{Z} \times \mathbf{Z}) \rtimes D_{12}/(n\mathbf{Z} \times n\mathbf{Z}) \cong (\mathbf{Z}_n \times \mathbf{Z}_n) \rtimes D_{12}.$$

Regarding Example 3.3, one can notice that x gives an automorphism of the graph of the nanotorus that does not extend to an automorphism of the torus surface (see Remark 3.4). And so, that example is not covered by the results in Senechal (1988). Also notice that neither of these two examples are covered by the results in Damnjanovic & Milosevic (2010), since the automorphisms of the nanotorus that we described cannot be lifted to automorphisms of an appropriate nanotube.

The fact that the two nanotori we constructed are naturally associated with groups makes them intriguing. The above remarks confirm that they are of a special type.

5.2. Final remarks

As we noticed above, the meridian and longitude curves of the torus have the same length relative to the distance function on the hypergraph. This means that these models do not fit in the examples discussed in Arezoomand & Taeri (2009) and Yavari & Ashrafi (2009). If there exists a nanotorus with the above structure, then the bond between the atoms must be curled. This suggests that such nanostructures would need to have a very strong bonding.

Even if the high symmetry of these models makes them interesting to study, they are rather exotic cases which might not have a physical realization. However, we hope that the approach from this paper can be used to study the group of symmetry of other families of carbon nanotori (for example finite covers of the models described here). We intend to approach this problem in a follow-up paper.

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