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Toroidal fullerenes with the Cayley graph structures☆

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ABSTRACT

We classify all possible structures of fullerene Cayley graphs. We give each one a geometric model and compute the spectra of its finite quotients. Moreover, we give a quick and simple estimation for a given toroidal fullerene. Finally, we provide a realization of those families in three-dimensional space.

1. Introduction

Since the discovery of the first fullerene, Buckministerfullerene C_{60}, fullerenes have attracted great interest in many scientific disciplines. Many properties of fullerenes can be studied using mathematical tools such as graph theory and group theory. A fullerene can be represented by a trivalent graph on a closed surface with pentagonal and hexagonal faces, such that its vertices are carbon atoms of the molecule; two vertices are adjacent if there is a bond between corresponding atoms. Then fullerenes exist in the sphere, torus, projective plane, and the Klein bottle. In order to realize in the real world, we shall assume that the closed surfaces, on which fullerenes are embedded, are oriented. In this case, a fullerene is called spherical if it lies on the sphere (which is indeed just C_{60}); it is called toroidal if it lies on the torus. Fullerenes with heptagonal faces are called generalized fullerenes, which have to be realized on a high genus surface. (See [6] for constructing of high genus fullerenes.)

According to the Hückel molecular orbital theory, the energy spectrum of π-electrons of the fullerene can be approximated by eigenvalues of the adjacency matrix of the associated graph up to a constant multiple. (For details, see [22].) One of the most important information of this energy spectrum is the HOMO–LUMO gap, which is the difference of energies between the highest occupied molecular orbit and the lowest unoccupied molecular orbit. Some partial results about the HOMO–LUMO gaps of certain families of graphs are known [4,5,10,12,14,17,25]. However, it is in general difficult to construct a molecule with the prescribed HOMO–LUMO gap.

In this paper, we consider a special kind of family of fullerene: those with a Cayley graph structure. A Cayley graph $\mathcal{G}(G, S)$ is a graph that encodes the structure of the group G with a generating set S. It turns out that except for the case of C_{60} which is a Cayley graph on $\mathrm{PSL}_2(\mathbb{F}_5)$ realized on the surface of a sphere, the remaining fullerenes are toroidal provided that they are orientable. In chemistry, there are different techniques to construct a family of toroidal molecules, some are based on combinatorial methods [2,3,16] and some are based on geometric approaches [23]. There are also several articles of hexagonal maps on the torus from mathematical viewpoints [1,8,19,24]. Moreover, the spectra of toroidal fullerenes are well studied in [9,13,15].

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A great advantage of the Cayley graph structure is that all the eigenvalues can be explicitly expressed using representations of the underlying group, which allows us to control the HOMO–LUMO gap by choosing a proper group.

The plan of this paper is as follows. We first classify all possible group structures of fullerenes with the Cayley graph structure (for both orientable and non-orientable cases). Second, we give a geometric model of each group structure and compute the spectra of their finite quotients (for orientable cases only). Third,, we give an estimation of HOMO–LUMO gap via solving the CVP(closest vector problem). As a by-product, we get an infinite family of toroidal fullerenes $\{X_{p,q}\}_{q=1}^{\infty}$ with the same HOMO–LUMO gap of size $\frac{2\pi}{\sqrt{3}p} + O(p^{-2})$ for any natural number p not divisible by three.

In molecular modeling, there are constraints on bond lengths, bond angles, etc. There is an energy function associated to these constraints which measures the stability of molecules. In the end of this paper, we provide an embedding of $X_{p,q}$ into three-dimensional space such that all bonds have almost equal lengths. One can choose this embedding as an initial embedding and minimize the energy function using standard algorithms, which can be realized by chemistry softwares, e.g. ChemOffice.

2. Fullerenes with the Cayley graph structure

In graph theory, a map is an embedding of a graph X on a closed surface Σ. For convenience, we regard X as a subset of Σ. Each connected component of $\Sigma \setminus X$ is called a face and the boundary of a face is a cycle of X. Note that every edge of X lies in the boundaries of exact two faces. Conversely, let C be a set of cycles in a graph X such that every edge of X lies in exact two cycles in C, then there is a unique map up to homeomorphism such that the boundaries of faces of X with respect to the map are elements of C.

Let G be a group generated by a finite set S. Assume that S is symmetric, namely if s lies in S, so does s^{-1}. The Cayley graph $X = \mathcal{G}(G, S)$ is defined as follows. Vertices of X are elements in G and two vertices $g_1, g_2 \in G$ are adjacent if $g_1 = g_2 s$ for some $s \in S$. The group G acts on the graph X by left multiplication. Observe that each vertex has exact $|S|$ neighbors and we call X an $|S|$-regular graph. A graph endowed with a map is called a fullerene (graph) if it is a 3-regular Cayley graph $X = \mathcal{G}(G, S)$ such that the boundary of each face is either a pentagon or a hexagon. Moreover, we also require that the map is compatible with the group action of G. That is if γ is a boundary of a face, then so is $g\gamma$ for all g in G.

A path $\gamma = (g_0, \dots, g_n)$ in X can be represented by a word $s_1 \cdots s_n$ for some s_i in S, such that $g_1 = g_0 s_1, g_2 = g_0 s_1 s_2, \dots,$ and $g_n = g_0 s_1 \cdots s_n$. Especially, when γ is a cycle (, that is $g_n = g_0$), we obtain a relation $s_1 \cdots s_n = id$ on S. Let F_S be the free group with the generating set S. One can recover the group structure of G from X by

$$G \cong F_s/\{\text{all relations arising from cycles in } X\}.$$

The relations arising from null-homotopic cycles in X are called trivial relations, which are generated by the relations of the form $s_i^{-1} = s_j$. We call X a universal fullerene graph if all nontrivial relations on S only arise from the faces of X. It is obvious that every fullerene with the Cayley graph structure is a quotient of some universal fullerene graph.

3. Classification of universal fullerene graphs

Let $X = \mathcal{G}(G, S)$ be a universal fullerene graph. Since the faces of X are preserved under the group action of G, it is enough to study the faces containing the identity of G. Let F be a face containing the identity with the boundary $(id, s_1, s_1 \dots s_n = id)$. If we choose s_1 as the starting vertex, such that the boundary of F is represented by $(s_1, s_1 s_2, \dots, id, s_1)$. If we multiply s_1^{-1} on the left to this boundary, we get $(id, s_2, \dots, s_2 \dots s_n s_1 = id)$ which represents the boundary of another face containing the identity. Thus, each cyclic permutation of $s_1 \cdots s_n = id$ represents a different face containing the identity. On the other hand, there are exact three faces containing the identity such that the cyclic permutations of $s_1 \cdots s_n$ can only contain up to three different elements. We conclude that $s_1 \cdots s_n$ must be equal to one of s_1^5, s_1^6, $(s_1 s_2)^3$, and $(s_1 s_2 s_3)^2$.

Set $S = \{a, b, c\}$ and regard G as a quotient of a free group $F_3 = \langle a, b, c \rangle$ by two kinds of relations: the trivial relations and the relations arising from faces. We distinguish two cases:

Case (1). All generators have order two, say, $a^2 = b^2 = c^2 = id$.

In this case, a relation of faces must have the form $(ab)^3 = id$, $(abc)^2 = id$, or their conjugations by permuting a, b, c. Note that $(ba)^3 = id$ and $(ab)^3 = id$ represent the same boundary of a face with opposite directions. Consequently, there are two subcases:

Case (1a). Three relations from faces are $(abc)^2 = id$, $(bca)^2 = id$ and $(cba)^2 = id$.

Case (1b). Three relations from faces are $(ab)^3 = id$, $(bc)^3 = id$ and $(ac)^3 = id$.

Case (2). One generator has order not equal to two, say, $a^2 = id$, $b^2 \neq id$, $c = b^{-1}$. In this case, a relation of faces must have the form $b^5 = id$, $b^6 = id$, $(ab)^3 = id$ or $(ab^2)^2 = id$. Therefore, there are three subcases:

Case (2a). Three relations from faces are $(ab^2)^2 = id$, $(bab)^2 = id$ and $(b^2a)^2 = id$.

Case (2b). Three relations from faces are $b^6 = id$, $(ab)^3 = id$ and $(ba)^3 = id$.

Case (2c). Three relations from faces are $b^5 = id$, $(ab)^3 = id$ and $(ba)^3 = id$.

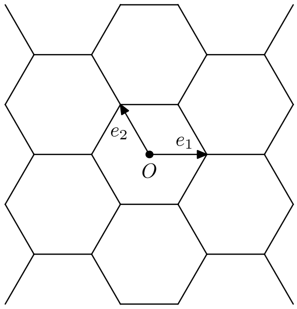

Fig. 1. A hexagonal tiling of $\mathbb{R}^2$.

We conclude that

Theorem 1. *A fullerene with the Cayley graph structure $\mathcal{G}(G, S)$ is isomorphic to a finite quotient of one of the following five graphs described in terms of generators and relations,*

- $G_1 = \langle a, b, c | a^2 = b^2 = c^2 = (abc)^2 = (bca)^2 = (cab)^2 = id \rangle$;
- $G_2 = \langle a, b, c | a^2 = b^2 = c^2 = (ab)^3 = (ac)^3 = (bc)^3 = id \rangle$;
- $G_3 = \langle a, b | a^2 = (ab^2)^2 = (bab)^2 = (b^2a)^2 = id \rangle$;
- $G_4 = \langle a, b | a^2 = b^6 = (ab)^3 = (ba)^3 = id \rangle$;
- $G_5 = \langle a, b | a^2 = b^5 = (ab)^3 = (ba)^3 = id \rangle$.

It is not hard to prove that G_5 is isomorphic to $\mathrm{PSL}_2(\mathbb{F}_5)$ (see [7]) and in this case the graph is the well-known C_{60}. For the first four cases, X contains only hexagonal faces. Let V, E and F be the number of vertices, edges and faces of X, respectively. The Euler characteristic of X is equal to

$$V - E + F = |G| - \frac{3}{2}|G| + \frac{1}{2}|G| = 0.$$

Therefore, X lies on a torus if it is orientable; it lies on a Klein bottle if it is non-orientable.

3.1. Generalized fullerenes

If one allows that fullerene have heptagonal faces (which is called a generalized fullerene), there is one extra universal fullerene graph, whose underlying group is $G_6 = \langle a, b | a^2 = b^7 = (ab)^3 = (ba)^3 = id \rangle$. The group G_6 is the von Dyck group $D(2, 7, 3)$ and it is isomorphic to $\Gamma = \mathrm{PSL}_2(\mathbb{Z})$ modulo E_7, the minimal normal subgroup in $\mathrm{PSL}_2(\mathbb{Z})$ containing $\begin{pmatrix} 1 & 7 \\ 0 & 1 \end{pmatrix}$. Let X be a finite quotient of the universal fullerene graph. The Euler characteristic of X is equal to

$$V - E + F = |G| - \frac{3}{2}|G| + \left(\frac{1}{6} + \frac{1}{6} + \frac{1}{7}\right)|G| = -\frac{1}{42}|G| = 2 - 2g,$$

where g is the genus of the surface which X lies on. Hence we have $|G| = 84(g - 1)$ and $g \geq 2$. A well-known example is that when the underlying group of X is $\Gamma/\Gamma(7) \cong \mathrm{PSL}_2(\mathbb{Z}/7\mathbb{Z})$, X has 168 vertices and it lies on a surface of genus three, called the Klein quartic. (See [11].)

4. Geometric models of universal fullerene graphs

In this section, we will give each G_i a geometric model.

Let Y be the hexagonal tiling of the Euclidean plane $\mathbb{R}^2$ such that the origin O is the center of a hexagon as shown in Fig. 1.

For convenience, we use $\{\vec{e}_1, \vec{e}_2\}$ in Fig. 1 as the basis of $\mathbb{R}^2$ to express linear transformations and translations. The group of affine transformations on $\mathbb{R}^2$ is the semi-direct product $W = \mathbb{R}^2 \rtimes \mathrm{GL}_2(\mathbb{R})$. More precisely, the action of $(\vec{v}, A) \in W$ on $\vec{u} \in \mathbb{R}^2$ is given by

$$(\vec{v}, A)(\vec{u}) = \vec{v} + A\vec{u},$$

and the group law is

$$(\vec{v}_1, A_1) \cdot (\vec{v}_2, A_2) = (\vec{v}_1 + A_1\vec{v}_2, A_1A_2).$$

When A is the identity matrix I_2, $(\vec{v}, I_2)$ is a translation, denoted by $T_{\vec{v}}$. All translations form a subgroup of W, called the translation subgroup, denoted by T. The group W contains four different types of elements: rotations, reflections, translations, and glide reflections. Note that only rotations and reflections have fixed points and may have finite orders.

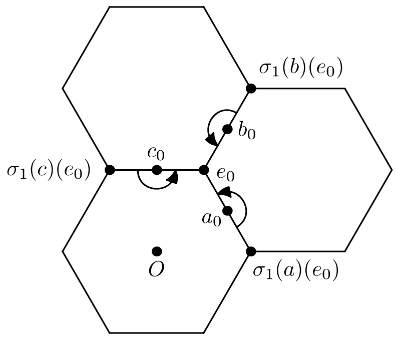

Fig. 2. $\rho \circ \sigma_1(G_1)$.

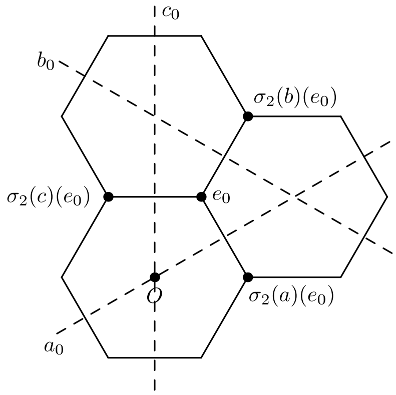

Fig. 3. $\rho \circ \sigma_2(G_2)$.

We shall construct an explicit embedding σ_i of each group G_i into W and show that it induces a graph isomorphism from $\mathcal{G}(G_i, S_i)$ to Y.

Let $\vec{e}_0 = \vec{e}_1 + \vec{e}_2$ and let $\rho : \mathrm{Aut}(Y) \to Y$ be the evaluation map given by $\rho(f) = f(\vec{e}_0)$.

Case (a). $G_1 = \langle a, b, c | a^2 = b^2 = c^2 = (abc)^2 = id \rangle$.

Define $\sigma_1 : G_1 \longrightarrow W$ by

$$\sigma_1(a) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \qquad \sigma_1(b) = \left(\begin{bmatrix} 3 \\ 3 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right),$$
$$\sigma_1(c) = \left(\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right).$$

Here $\sigma_1(a)$, $\sigma_1(b)$ and $\sigma_1(c)$ are 180°-rotations centered at a_0, b_0, c_0, respectively, as shown in Fig. 2.

Case (b). $G_2 = \langle a, b, c | a^2 = b^2 = c^2 = (ab)^3 = (ac)^3 = (bc)^3 = id \rangle$.

Define $\sigma_2 : G_2 \longrightarrow W$ by

$$\sigma_2(a) = \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \right), \qquad \sigma_2(b) = \left(\begin{bmatrix} 3 \\ 3 \end{bmatrix}, \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \right),$$
$$\sigma_2(c) = \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -1 & 1 \\ 0 & 1 \end{bmatrix} \right).$$

Here $\sigma_2(a)$, $\sigma_2(b)$ and $\sigma_2(c)$ are reflections with respect to the axes a_0, b_0, c_0, respectively as shown in Fig. 3.

Case (c). $G_3 = \langle a, b | a^2 = (ab^2)^2 = (bab)^2 = (b^2a)^2 = id \rangle$.

Define $\sigma_3 : G_3 \longrightarrow W$ by

$$\sigma_3(a) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \qquad \sigma_3(b) = \left(\begin{bmatrix} 1 \\ 2 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \right).$$

Here $\sigma_3(a)$ is a 180°-rotation around the point a_0 and $\sigma_3(b)$ is a glide reflection with respect to the axis b_0 as shown in Fig. 4.

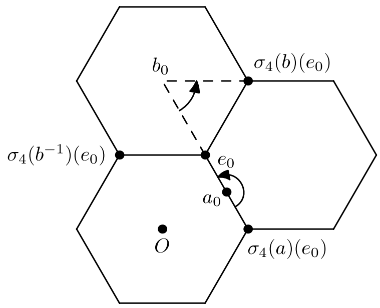

Fig. 4. $\rho \circ \sigma_3(G_3)$.

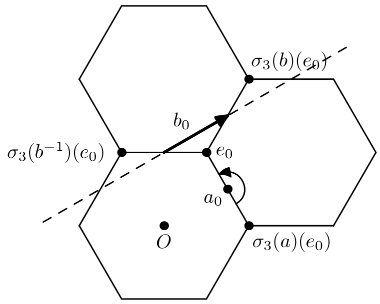

Fig. 5. $\rho \circ \sigma_4(G_4)$.

Case (d). $G_4 = \langle a, b | a^2 = b^6 = (ab)^3 = (ba)^3 = id\rangle$.

Define $\sigma_4 : G_4 \longrightarrow W$ by

$$\sigma_4(a) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right), \qquad \sigma_4(b) = \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 0 \end{bmatrix} \right).$$

Here $\sigma_4(a)$ is a 180°-rotation around the point a_0 and $\sigma_4(b)$ is a 60°-rotation around the point b_0 as shown in Fig. 5.

Observe that ρ induces a graph isomorphism from $\mathcal{G}(\sigma_i(G_i), \sigma_1(S_i))$ to Y for $i = 1, 2, 3, 4$. To show that each σ_i is an isomorphism, we use the following basic propositions in group theory.

Proposition 2. *Let H be a normal subgroup of G and σ be a homomorphism from G to another group G'. If $\sigma|_H$ and the induced map of $\bar{\sigma} : G/H \to \sigma(G)/\sigma(H)$ are both injective, then σ is also injective.*

Proposition 3. *Any surjective homomorphism from $\mathbb{Z}^2$ to $\mathbb{Z}^2$ is an isomorphism.*

Let $\vec{v}_1 = 2\vec{e}_1 + \vec{e}_2$, $\vec{v}_2 = \vec{e}_1 + 2\vec{e}_2$. Recall that $T_{\vec{v}}$ is the translation $\vec{x} \to \vec{x} + \vec{v}$.

Theorem 4. *$\mathcal{G}(G_i, S_i)$ is isomorphic to Y as a graph for $i = 1, 2, 3, 4$.*

Proof. Since $\mathcal{G}(\sigma_i(G_i), \sigma_i(S_i))$ is isomorphic to Y as a graph, we only need to show that σ_i is injective and then it induces a graph isomorphism from $\mathcal{G}(G_i, S_i)$ to $\mathcal{G}(\sigma_i(G_i), \sigma_i(S_i))$. We shall find, for each G_i, the translation subgroups H_i and verify that σ_i is injective on both H_i and G_i/H_i and hence σ_i is injective by Proposition 2.

Case (a). Let $H_1 = \langle bc, ba\rangle$. It is easy to check that H_1 is an abelian normal subgroup of G_1. Since $\sigma_1(H_1) = \langle \sigma_1(bc), \sigma_1(ba)\rangle = \langle T_{\vec{v}_1}, T_{\vec{v}_2}\rangle \cong \mathbb{Z}^2$, we have that H_1 is also isomorphic to $\mathbb{Z}^2$. By Proposition 3, σ_1 is injective on H_1. On the other hand, in G_1/H_1, $c = b^{-1}$, $a = b^{-1}$ and then $G_1/H_1 = \langle b | b^2 = id\rangle$. Since b is not a translation, we have $\sigma(bH_1) \neq \sigma(H_1)$ and so σ_1 is injective on G_1/H_1.

Case (b). Let $H_2 = \langle cbca, abac\rangle$. It is easy to check that H_2 is an abelian normal subgroup of G_2. Since $\sigma_2(H_2) = \langle \sigma_2(abac), \sigma_2(cbca)\rangle = \langle T_{2\vec{v}_1 - \vec{v}_2}, T_{2\vec{v}_2 - \vec{v}_1}\rangle \cong \mathbb{Z}^2$, we have that H_2 is also isomorphic to $\mathbb{Z}^2$. By Proposition 3, σ_2 is injective on H_2. On the other hand, in G_2/H_2, $c = (aba)^{-1}$ and then $G_2/H_2 = \langle a, b | a^2 = b^2 = (ab)^3 = id\rangle$. Thus $G_2 = \coprod gH_2$, where $g = id, a, b, ab, ba, aba$. Since none of a, b, ab, ba, aba is a translation, σ_2 is injective on G_2/H_2.

Case (c). Let $H_3 = \langle b^2, baba\rangle$. It is easy to check that H_3 is an abelian normal subgroup of G_3. Since $\sigma_3(H_3) = \langle \sigma_3(b^2), \sigma_3(baba)\rangle = \langle T_{\vec{v}_1}, T_{2\vec{v}_2 - \vec{v}_1}\rangle \cong \mathbb{Z}^2$, we have that H_3 is also isomorphic to $\mathbb{Z}^2$. By Proposition 3, σ_3 is injective on H_3. On the other hand, $G_3/H_3 = \langle a, b | a^2 = b^2 = (ba)^2 = id\rangle$. Thus $G_3 = \coprod gH_3$, where $g = id, a, b, ab$. Since none of a, b, ab is a translation, σ_3 is injective on G_3/H_3.

Case (d). Let $H_4 = \langle b^3a, bab^2\rangle$. It is easy to check that H_4 is an abelian normal subgroup of G_4. Since $\sigma_4(H_4) = \langle \sigma_4(b^2), \sigma_4(baba)\rangle = \langle T_{2\vec{v}_1-\vec{v}_2}, T_{2\vec{v}_2-\vec{v}_1}\rangle \cong \mathbb{Z}^2$, we have that H_4 is also isomorphic to $\mathbb{Z}^2$. By Proposition 3, σ_4 is injective on H_4. On the other hand, in G_4/H_4, $a = b^{-3}$ and then $G_4/H_4 = \langle b | b^6 = id\rangle$. Thus $G_4 = \coprod b^i H_4$, where $0 \le i \le 5$. Since none of b^i is a translation for $1 \le i \le 5$, σ_4 is injective on G_4/H_4. □

For now on, we identify each G_i with $\sigma_i(G_i)$ as a subgroup of W.

5. Non-spherical fullerene

The Cayley graphs discussed in the previous section are infinite graphs and they are all isomorphic to the hexagonal tiling Y as graphs. To obtain finite generalized fullerenes, we shall consider finite quotients of these graphs. Let H be a finite index normal subgroup of G_i, then the Cayley graph $X = \mathcal{G}(G_i/H, S)$ is a finite graph on the surface $S = \mathbb{R}^2/H$. Without changing the local structure of Y, we shall assume that none of two vertices of a hexagon in Y are identified as one vertex in X. Under this assumption, H cannot have any fixed points, so the fundamental group of S is isomorphic to H. In this case, H is torsion-free and $H \cong \mathbb{Z}^2$ if S is a torus; $H \cong \langle s, t | sts^{-1} = t^{-1}\rangle$, if S is a Klein bottle. In the first case, we call X a toroidal fullerene and in the second case, we call X a non-orientable fullerene.

5.1. Toroidal fullerenes

We classify toroidal fullerene in this subsection.

Theorem 5. *Let H be a rank-two free abelian subgroup of G_i, then H is a subgroup of the translation subgroup T.*

Proof. Note that $G_i \cap T$ has finite index in G_i, so $H \cap T$ is a finite index subgroup of H and $H \cap T \cong \mathbb{Z}^2$, a two-dimensional lattice in $\mathbb{R}^2$. Since H is abelian, for any $g = (\vec{v}, A)$ in H, we have $(\vec{v} + A\vec{w}, A) = gT_{\vec{w}} = T_{\vec{w}}g = (\vec{v} + \vec{w}, A)$ for all $T_{\vec{w}} \in H \cap T$. Thus 1 is an eigenvalue of A and its corresponding eigenspace has dimension two. We conclude that A is the identity matrix and H is a subgroup of T. □

Next we shall determine when a subgroup of T is normal in G_i. Observe that $T \subset G_1$ and every subgroup of T is normal in G_1. Moreover, if H is a normal subgroup in both G_i and G_j, then $\mathcal{G}(G_i/H, S_i)$ and $\mathcal{G}(G_j/H, S_j)$ are isomorphic as graphs. Consequently, all finite toroidal fullerenes arise from quotients of $\mathcal{G}(G_1, S_1)$ by its translation subgroups.

Recall that the generators G_1 are

$$a = (\vec{v}_1, -I_2), \qquad b = (\vec{v}_1 + \vec{v}_2, -I_2) \quad \text{and} \quad c = (\vec{v}_2, -I_2).$$

It is easy to see that

$$G_1 = \langle \vec{v}_1, \vec{v}_2\rangle \rtimes \langle -I_2\rangle \cong \mathbb{Z}^2 \rtimes \mathbb{Z}/2\mathbb{Z}.$$

In the rest of the paper, we shall denote $x_1\vec{v}_1 + x_2\vec{v}_2$ by (x_1, x_2). We conclude that.

Theorem 6. *Every toroidal fullerene is isomorphic to some $X_N = \mathcal{G}(G_N, \{a, b, c\})$, where N is a rank-two subgroup of $\mathbb{Z}^2$ and $G_N = \mathbb{Z}^2/N \rtimes \mathbb{Z}/2\mathbb{Z}$.*

Note that when N is generated by $(x_1, 0)$, (x_2, x_3), X_N corresponds to $\mathrm{TPH}(x_1, x_2, x_3)$ in [16] and $\mathrm{H}(x_1, x_3, x_2 - x_3)$ in [18].

5.2. Non-orientable fullerenes

We classify all normal subgroups H of G_i, such that $\mathbb{R}^2/H$ is a Klein bottle in this subsection. Let

$$g = \sigma_3(b) = \left(\begin{bmatrix}1\\2\end{bmatrix}, \begin{bmatrix}1 & 0\\1 & -1\end{bmatrix}\right), \qquad T_1 = T_{\vec{v}_1}, \quad \text{and} \quad T_2 = T_{2\vec{v}_2-v_1},$$

for short.

Theorem 7. *Every non-orientable fullerene is isomorphic to $\mathcal{G}(G_3/H, S)$, where*

$$H = \langle gT_1^m, T_2\rangle, \langle gT_1^m, T_2^2\rangle, \quad \text{or} \quad \langle gT_1^mT_2, T_2^2\rangle.$$

for some $m \in \mathbb{Z}$.

Proof. Let $\mathcal{G}(G_i/H, S)$ be a non-orientable fullerene such that $H \cong \langle s, t | sts^{-1} = t^{-1}\rangle$. In this case, $\langle s^2, t\rangle$ is an index two abelian subgroup of H, which is a subgroup of T by Theorem 5. Write $s = (\vec{v}, A)$ and $t = (\vec{w}, I_2)$. Since s is not a translation and s^2 is a nontrivial translation, we have $A \neq \pm I_2$ and $A^2 = I_2$. From the discussion in Section 4, such A only exists in G_2 and G_3. On the other hand, H is a normal subgroup of G_i, so $\{I_2, A\}$ is a normal subgroup in $G_i/(G_i \bigcap T)$. From the proof of Theorem 4, we have $G_2/(G_2 \bigcap T) \cong S_3$ and $G_3/(G_3 \bigcap T) \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. It is clear that only $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ has an order two normal subgroup. Therefore such normal subgroup H only exists in G_3 and in this case $A = \begin{pmatrix}1 & 0\\1 & -1\end{pmatrix}$. Recall that

$G_3 \bigcap T = \langle T_1, T_2\rangle$. Since $s = \sigma_3(b) = g$ in $G_3/(G_3 \bigcap T)$, write $s = gT_1^m T_2^n$ for some integers m and n. By direct computation, it is easy to see that $sT_1s^{-1} = T_1$ and $sT_2s^{-1} = T_2^{-1}$. Since $sts^{-1} = t^{-1}$, we have $t = T_2^k$ for some k and we may assume $k > 0$. On the other hand, H is normal, so $T_2\, s\, T_2^{-1}\, s^{-1} = T_2^2 \in H$. Hence $k = 1$ or 2. If $k = 1$,

$$H = \langle gT_1^m T_2^n, T_2\rangle = \langle gT_1^m, T_2\rangle.$$

If $k = 2$ and $n = 2n'$, then

$$H = \langle gT_1^m T_2^{2n'}, T_2^2\rangle = \langle gT_1^m, T_2^2\rangle.$$

If $k = 2$ and $n = 2n' + 1$, then

$$H = \langle gT_1^m T_2^{2n'+1}, T_2^2\rangle = \langle gT_1^m T_2, T_2^2\rangle.$$

Combining all together, we prove the theorem. □

Corollary 8. *When $N = \langle 2m\vec{v}_1, 2\vec{v}_2 - \vec{v}_1\rangle$ or $\langle 2m\vec{v}_1, 4\vec{v}_2 - 2\vec{v}_1\rangle$ for some m. The toroidal fullerene X_N is a double covering of a non-orientable fullerene.*

Proof. From the above theorem, we see that

$$H \cap T = \langle s^2, t\rangle = \langle T_1^{2m}, T_2\rangle \quad \text{or} \quad \langle T_1^{2m}, T_2^2\rangle.$$

When $N = \langle s^2, t\rangle$, an index two subgroup of H, X_N is a double covering of $\mathcal{G}(G_3/H, S)$. □

6. Spectra of toroidal fullerenes

In this section, we compute the spectrum of the toroidal fullerene X_N. We do not discuss the spectra of non-orientable fullerenes since they cannot be realized in three-dimensional space. (One can study the spectrum of a non-orientable fullerene through its double covering X_N.) First, we recall some basic facts in representation theory of finite groups.

6.1. Characters, regular representations and induced representations

A group representation of a group G is a homomorphism $\Phi : G \to \mathrm{Aut}(V)$, where V is a finite dimensional vector space over $\mathbb{C}$. When $V = \mathbb{C}$, Φ is called a character of G. When $V = C(G)$, the set of all $\mathbb{C}$-valued functions on G, Φ is called the right regular representation of G provided that for $f(x) \in C(G)$, $\Phi(g)(f)(x) = f(xg)$.

The right regular representation Φ can be decomposed as the direct sum of irreducible representations $\{\Phi_i\}$ of G such that the multiplicity of Φ_i in Φ is equal to the dimension of Φ_i for all Φ_i. If S is a generating set of G, then the adjacency matrix of $\mathcal{G}(G, S)$ can be written as $\sum_{s\in S} \Phi(s)$.

Let ρ be a character of a subgroup H of G. The induced representation $\mathrm{Ind}_H^G\rho$ is the set of functions given by

$$\mathrm{Ind}_H^G\rho = \{f : G \to \mathbb{C} | f(hg) = \rho(h)f(g)\},$$

such that for $f(x) \in \mathrm{Ind}_H^G\rho$, $\mathrm{Ind}_H^G\rho(g)(f)(x) = f(xg)$. Note that $\mathrm{Ind}_H^G\rho$ can be naturally regarded as a subspace of $C(G)$.

6.2. The spectrum of G_N

Let Φ is the right regular representation of G_N, then the adjacent matrix of X_N is equal to $\Phi(a)+\Phi(b)+\Phi(c)$. It suffices to compute the eigenvalues of $\Phi_i(a) + \Phi_i(b) + \Phi_i(c)$ for every irreducible representation Φ_i. Denote by $\hat{A}$ the set of characters of an abelian group A. To find all irreducible representations of G_N, we apply the following theorem [21].

Theorem 9. *Let $G = A \rtimes H$, where H is a subgroup and A is a normal abelian subgroup of G. For $\chi \in \hat{A}$, let $H_\chi = \{h \in H | \chi(h^{-1}ah) = \chi(a), \forall a \in A\}$. Let ρ be an irreducible representation of H_χ. Extend χ and ρ to a representation of AH_χ. Then $\mathrm{Ind}_{AH_\chi}^G(\chi\rho)$ is an irreducible representation of G and all irreducible representations of G come from this construction.*

In our case, $G = G_N$, $H = \mathbb{Z}/2\mathbb{Z} = \langle s\rangle$, $A = \mathbb{Z}^2/N$ and $H_\chi = \{id\}$ or $\langle s\rangle$.

If $H_\chi = \{id\}$, then it has only the trivial representation. In this case, $\mathrm{Ind}_{AH_\chi}^G(\chi\rho) = \mathrm{Ind}_A^G(\chi)$ is a two-dimensional representation, denoted by $\tilde{\chi}$, such that $\tilde{\chi}(a) = \begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)} \\ \chi(\vec{v}_1) & 0 \end{pmatrix}$, $\tilde{\chi}(b) = \begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)\chi(\vec{v}_2)} \\ \chi(\vec{v}_1)\chi(\vec{v}_2) & 0 \end{pmatrix}$ and $\tilde{\chi}(c) = \begin{pmatrix} 0 & \overline{\chi(\vec{v}_2)} \\ \chi(\vec{v}_2) & 0 \end{pmatrix}$. So

$$\tilde{\chi}(a) + \tilde{\chi}(b) + \tilde{\chi}(c) = \begin{pmatrix} 0 & \overline{\chi(\vec{v}_1)} + \overline{\chi(\vec{v}_1)\chi(\vec{v}_2)} + \overline{\chi(\vec{v}_2)} \\ \chi(\vec{v}_1) + \chi(\vec{v}_1)\chi(\vec{v}_2) + \chi(\vec{v}_2) & 0 \end{pmatrix},$$

which has eigenvalues $\pm|\chi(\vec{v}_1) + \chi(\vec{v}_2) + \chi(\vec{v}_1)\chi(\vec{v}_2)|$.

If $H_\chi = \langle s \rangle$, then $\mathrm{Ind}_{AH_\chi}^{G}(\chi\rho) = \chi\rho$. Since $\rho \in \hat{H}$ takes values in $\{1, -1\}$ and eigenvalues of the adjacency matrix are all real, we have

$$\begin{aligned}\rho\chi(a) + \rho\chi(b) + \rho\chi(c) &= \rho(s)(\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2)) \\ &= |\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2)| \quad \text{or} \quad -|\chi(\vec{v}_1) + \chi(\vec{v}_1 + \vec{v}_2) + \chi(\vec{v}_2)|.\end{aligned}$$

We conclude that

Theorem 10. *The spectrum of X_N is $\{\pm|\chi(\vec{v}_1) + \chi(\vec{v}_2) + \chi(\vec{v}_1)\chi(\vec{v}_2)| \mid \chi \in \hat{A}\}$.*

6.3. HOMO and LUMO eigenvalues

For a graph X with $2M$ vertices, the HOMO eigenvalue λ_H is the $(M+1)$-th largest eigenvalue of X; the LUMO eigenvalue λ_L is the M-th largest eigenvalue X. The difference $\lambda_H - \lambda_L$ is called the HOMO–LUMO gap,[1] denoted by Gap(X). If X is bipartite, the spectrum of X is symmetric. In this case, λ_H is equal to the smallest non-negative eigenvalue; λ_L is equal to the largest non-positive eigenvalue and $\lambda_L = -\lambda_H$. Note that G_N can be written as a disjoint union of $(\mathbb{Z}^2/N, I_2)$ and $(\mathbb{Z}^2/N, -I_2)$, which gives a bipartite structure of X_N.

To describe the characters of $\mathbb{Z}^2/N$, recall that a character χ of $\mathbb{Z}^2$ is uniquely determined by $\chi(\vec{v}_1) = \exp(i\theta_1)$ and $\chi(\vec{v}_2) = \exp(i\theta_2)$, where $\theta_1, \theta_2 \in \mathbb{R}/2\pi\mathbb{Z}$. We identify $\chi \in \hat{\mathbb{Z}}^2$ with $(\theta_1, \theta_2) \in (\mathbb{R}/2\pi\mathbb{Z})^2$. The characters of $\mathbb{Z}^2/N$ are the characters of $\mathbb{Z}^2$ trivial on N, which can be identified with

$$N^\perp = \{(\theta_1, \theta_2) \in (\mathbb{R}/2\pi\mathbb{Z})^2 \mid \exp(i(\theta_1 x + \theta_2 y)) = 1, \text{ for all } (x, y) \in N\}.$$

Consider a function f defined by

$$\begin{aligned}f(\theta_1, \theta_2) &= |\exp(i\theta_1) + \exp(i\theta_2) + \exp(i\theta_1 + i\theta_2)|^2 \\ &= 3 + 2\cos\theta_1 + 2\cos\theta_2 + 2\cos\theta_1\cos\theta_2 + 2\sin\theta_1\sin\theta_2.\end{aligned}$$

By Theorem 10, we have

Corollary 11. $\mathrm{Gap}(X_N) = \min\{2\sqrt{f(\theta_1, \theta_2)} \mid (\theta_1, \theta_2) \in N^\perp\}$.

Observe that $f(\theta_1, \theta_2)$ has the minimum value zero for at $(\pm\frac{2\pi}{3}, \mp\frac{2\pi}{3})$. Suppose N is generated by (a, c) and (b, d) for some integers a, b, c, d. Then $N^\perp$ is generated by $\vec{w}_1 = \frac{2\pi}{ad-bc}(d, -b)$ and $\vec{w}_2 = \frac{2\pi}{ad-bc}(-c, a)$. Solving the equation $x_1\vec{w}_1 + x_2\vec{w}_2 = (\frac{2\pi}{3}, -\frac{2\pi}{3})$, we have $x_1 = \frac{a-c}{3}$ and $x_2 = \frac{b-d}{3}$. We conclude that $\mathrm{Gap}(X_N) = 0$ if and only if $\frac{a-c}{3}$ and $\frac{b-d}{3}$ are integers.

Theorem 12. *The following are equivalent*

(1) $\mathrm{Gap}(X_N) = 0$.
(2) $a - c \equiv b - d \equiv 0 \bmod 3$.
(3) *X_N is a quotient of $\mathcal{G}(G_i, S_i)$ for at least three different i.*

Proof. We have seen that (1) $\Leftrightarrow$ (2), so it suffices to show that (2) $\Leftrightarrow$ (3). Recall that X_N can be realized as a quotient of $\mathcal{G}(G_i, S_i)$ if and only if N is a subgroup of T_i, the translation subgroup of G_i. From the proof of Theorem 4, we see that $T_2 = T_4 = \langle(2, -1), (-1, 2)\rangle$. Hence (3) $\Leftrightarrow N \subseteq \langle(2, -1), (-1, 2)\rangle \Leftrightarrow$ (2). $\square$

7. Closest vector problem

To explicitly find the minimum of f on $N^\perp$, it is enough to consider the values of f around $(\frac{2\pi}{3}, -\frac{2\pi}{3})$. From the Taylor expansion of $f(x, y)$ at $(\frac{2\pi}{3}, -\frac{2\pi}{3})$, we have

$$\begin{aligned}f\left(x - \frac{2\pi}{3}, y + \frac{2\pi}{3}\right) &= 3 - \cos(x) - \cos(x - y) - \cos(y) + \sqrt{3}\,[\sin(x - y) - \sin(x) + \sin(y)] \\ &= x^2 - xy + y^2 + O(|x|^3 + |y|^3).\end{aligned}$$

Note that $x^2 - xy + y^2$ is a positive-definite quadratic form, so we can define a norm as

$$\|(x, y)\|^2 = x^2 - xy + y^2.$$

Let

$$d_N = \min_{(x,y)\in N^\perp} \left\|\left(x - \frac{2\pi}{3}, y + \frac{2\pi}{3}\right)\right\|^2.$$

[1] In terms of eigenvalues of the Laplacian, $3 - \lambda_H$ corresponds to HOMO and $3 - \lambda_L$ corresponds to LUMO.

We can rewrite Corollary 11 as

Theorem 13.

$$\mathrm{Gap}(X_N) = 2\sqrt{d_N} + O(d_N^{3/4}).$$

Note that we can regard $N^{\perp}$ as a lattice in $\mathbb{R}^2$, then to find d_N, it is equivalent to solve a CVP(closest vector problem) on the two-dimensional lattice $N^{\perp}$. Set

$$\epsilon_1 = \frac{a-c}{3} - \left[\frac{a-c}{3}\right] \quad \text{and} \quad \epsilon_2 = \frac{b-d}{3} - \left[\frac{b-d}{3}\right],$$

where $[x]$ is the closest integer to x (which is well defined if x is not a half integer). Note that $\epsilon_1, \epsilon_2 \in \{0, \pm\frac{1}{3}\}$ and we can rewrite d_N as

$$d_N = \min_{(n_1,n_2)\in\mathbb{Z}^2} \|(n_1+\epsilon_1)\vec{w}_1 + (n_2+\epsilon_2)\vec{w}_2\|^2.$$

Recall that the basis $\{\vec{w}_1, \vec{w}_2\}$ is called Gaussian reduced, if

$$\|\vec{w}_1\| \le \|\vec{w}_2\| \quad \text{and} \quad |\langle \vec{w}_1, \vec{w}_2\rangle| \le \frac{1}{2}\|\vec{w}_1\|^2.$$

where $\langle\cdot,\cdot\rangle$ is the inner product on $\mathbb{R}^2$ induced by $\|\cdot\|$. Such basis always exists and can be constructed by the Gaussian reduction algorithm as follows. (For more details, see [20]).

Gaussian reduction algorithm

Given a basis $\{\vec{w}_1, \vec{w}_2\}$ of a two-dimensional lattice with $\|\vec{w}_1\| \le \|\vec{w}_2\|$, let $\mu = \frac{\langle \vec{w}_1, \vec{w}_2\rangle}{\|\vec{w}_1\|^2}$. If $|\mu| \le \frac{1}{2}$, then $\{\vec{w}_1, \vec{w}_2\}$ is already Gaussian reduced; if $|\mu| > \frac{1}{2}$, replace $\vec{w}_2$ by $\vec{w}_2 - [\mu]\vec{w}_1$, then we have $|\mu| \le \frac{1}{2}$. In this case, if $\|\vec{w}_1\|$ is still less than or equal to $\|\vec{w}_2\|$, then $\{\vec{w}_1, \vec{w}_2\}$ is Gaussian reduced; if not, switch $\vec{w}_1$ and $\vec{w}_2$ and repeat the same process.

Theorem 14. *If $\{\vec{w}_1, \vec{w}_2\}$ is Gaussian reduced, then $d_N = \|\epsilon_1\vec{w}_1 + \epsilon_2\vec{w}_2\|^2$.*

Proof. Consider

$$\begin{aligned}
&\|(n_1+\epsilon_1)\vec{w}_1 + (n_2+\epsilon_2)\vec{w}_2\|^2 - \|\epsilon_1\vec{w}_1 + \epsilon_2\vec{w}_2\|^2 \\
&\quad = (n_1^2 + 2n_1\epsilon_1)\|\vec{w}_1\|^2 + 2(n_1n_2 + \epsilon_1 n_2 + \epsilon_2 n_1)\langle \vec{w}_1, \vec{w}_2\rangle + (n_2^2 + 2n_2\epsilon_2)\|\vec{w}_2\|^2 \\
&\quad \ge (n_1^2 + 2n_1\epsilon_1)\|\vec{w}_1\|^2 - |n_1n_2 + \epsilon_1 n_2 + \epsilon_2 n_1|\|\vec{w}_1\|^2 + (n_2^2 + 2n_2\epsilon_2)\|\vec{w}_1\|^2 \\
&\quad = (n_1^2 + 2n_1\epsilon_1 - |n_1n_2 + \epsilon_1 n_2 + \epsilon_2 n_1| + n_2^2 + 2n_2\epsilon_2)\|\vec{w}_1\|^2.
\end{aligned}$$

Let

$$\begin{aligned}
F_{\pm}(n_1, n_2) &= n_1^2 + 2n_1\epsilon_1 \pm (n_1n_2 + \epsilon_1 n_2 + \epsilon_2 n_1) + n_2^2 + 2n_2\epsilon_2 \\
&= \left(n_1 + \epsilon_1 \pm \frac{1}{2}(n_2+\epsilon_2)\right)^2 + \frac{3}{4}(n_2+\epsilon_2)^2 - (\epsilon_1^2 \pm \epsilon_1\epsilon_2 + \epsilon_2^2).
\end{aligned}$$

It suffices to prove that $F_{\pm}(n_1, n_2) \ge 0$, for all $n_1, n_2 \in \mathbb{Z}$. Note that $F_{\pm}(0,0) = 0$. Now if $n_1 \ne 0$, we have $|n_1 + \epsilon_1| \ge \frac{2}{3}$ and

$$\begin{aligned}
F_{\pm}(n_1, n_2) &= \frac{3}{4}(n_1+\epsilon_1)^2 + \left(\pm\frac{1}{2}(n_1+\epsilon_1) + n_2 + \epsilon_2\right)^2 - (\epsilon_1^2 \pm \epsilon_1\epsilon_2 + \epsilon_2^2) \\
&\ge \frac{3}{4}\left(\frac{2}{3}\right)^2 + 0 - \left(\frac{1}{9} + \frac{1}{9} + \frac{1}{9}\right) = 0.
\end{aligned}$$

Similarly, if $n_2 \ne 0$, we have $|n_2 + \epsilon_2| \ge \frac{2}{3}$ and

$$\begin{aligned}
F_{\pm}(n_1, n_2) &= \left(n_1 + \epsilon_1 \pm \frac{1}{2}(n_2+\epsilon_2)\right)^2 + \frac{3}{4}(n_2+\epsilon_2)^2 - (\epsilon_1^2 \pm \epsilon_1\epsilon_2 + \epsilon_2^2) \\
&\ge 0 + \frac{3}{4}\left(\frac{2}{3}\right)^2 - \left(\frac{1}{9} + \frac{1}{9} + \frac{1}{9}\right) = 0. \quad \square
\end{aligned}$$

Note that N is a lattice in $\mathbb{R}^2$, which has the standard norm as $\|a\vec{e}_1 + b\vec{e}_2\| = a^2 - ab + b^2$. (See Fig. 1.) Then for $(x, y) \in N$,

$$\|(x, y)\| = \|x\vec{v}_1 + y\vec{v}_2\| = \|x(2\vec{e}_1 + \vec{e}_2) + y(\vec{e}_1 + 2\vec{e}_2)\| = 3(x^2 + xy + y^2).$$

It is easy to see that $\{\frac{2\pi}{ad-bc}(-c, a), \frac{2\pi}{ad-bc}(d, -b)\}$ is a Gaussian reduced basis of $N^{\perp}$ if and only if $\{(a, c), (b, d)\}$ is a Gaussian reduced basis of N.

Consider a function $\epsilon : \mathbb{Z} \to \{-1, 0, 1\}$, such that $\epsilon(x) = x \bmod 3$. Then

$$\epsilon(x) = 3\left(\frac{x}{3} - \left[\frac{x}{3}\right]\right).$$

Combining the above all results, we have

Theorem 15. *Let $\{(a, c), (b, d)\}$ be a Gaussian reduced basis of N, then*

$$\mathrm{Gap}(X_N) \approx \frac{4\pi}{3|ad - bc|}\|\epsilon(a - c)(d, -b) + \epsilon(b - d)(-c, a)\|.$$

Example 1. Suppose $N = \langle(1, 8), (10, 1)\rangle$. By Gaussian reduction algorithm, we have

$$(1, 8), (10, 1) \Rightarrow (1, 8), (9, -7).$$

By Theorem 15, the HOMO–LOMO gap of X_N is approximately equal to

$$\frac{4\pi}{3 \cdot 79}\| - (-7, -9) + (-8, 1)\| = \frac{4\pi}{237}\|(-1, 10)\| = \frac{4\pi}{237}\sqrt{111} = 0.55863\cdots.$$

Remark. The HOMO–LOMO gap of X_N is $0.56311\cdots$.

Example 2. For two positive integers p and q with $3 \nmid p$, let $N_{p,q} = \langle(p, 0), (q, -2q)\rangle$ and denote $X_{N_{p,q}}$ by $X_{p,q}$ for short. Note that $\{p\vec{v}_1, -q\vec{v}_1 + 2q\vec{v}_2\}$ is an orthogonal basis, hence it is Gaussian reduced. By Theorem 15,

$$\mathrm{Gap}(X_{p,q}) \approx \frac{4\pi}{3 \cdot 2pq}\|\epsilon(p)(2q, q)\| = \frac{2\pi}{\sqrt{3}p}.$$

Together with Corollary 11, we have

$$\mathrm{Gap}(X_{p,q}) = \frac{2\pi}{\sqrt{3}p} + O(p^{-\frac{3}{2}}).$$

Remark. In fact, one can show that $\mathrm{Gap}(X_{p,q})$ is independent of q.

From chemical physics' viewpoint, we can regarded $X_{p,q}$ as a finite quotient of the carbon nanotube with the chiral vector $(p, 0)$. It is well known that the nanotube is metallic (with zero gap) if and only if $3|p$, which can be regarded as the special case of Theorem 12.

8. Embedding graphs into three-dimensional space

In this section, we discuss how to realize the graph $X_{p,q}$ in three-dimensional space with almost equal lengths. Note that the lattice $N'_{p,q} = N_{p,q}(\vec{e}_0)$ on $\mathbb{R}^2$ has a fundamental domain $\mathcal{D}$ spanned by the orthogonal basis $p\vec{v}_1$ and $-q\vec{v}_1 + 2q\vec{v}_2$ as shown in Fig. 6. Choose the length of $\vec{v}_1$ as the unit of length. The width of $\mathcal{D}$ equals p; its length equals $2\sqrt{3}q$. The toroidal fullerene $X_{p,q}$ is obtained from the hexagon tiling Y quotient by the lattice $N'_{p,q}$, so it suffices to find a map from $\mathbb{R}^2/N'_{p,q}$ to three-dimensional space, which induces an embedding of $X_{p,q}$ to three-dimensional space (see Fig. 7). Consider the standard map $F(u, v) = (x(u, v), y(u, v), z(u, v))$ from $\mathcal{D}$ to a torus, where

$$\begin{cases} x(u, v) = \left(R + r\cos\left(\frac{2\pi u}{p}\right)\right)\cos\left(\frac{\pi v}{\sqrt{3}q}\right), \\ y(u, v) = \left(R + r\cos\left(\frac{2\pi u}{p}\right)\right)\sin\left(\frac{\pi v}{\sqrt{3}q}\right), \\ z(u, v) = r\sin\left(\frac{2\pi u}{p}\right), \end{cases}$$

and R and r are some constants.

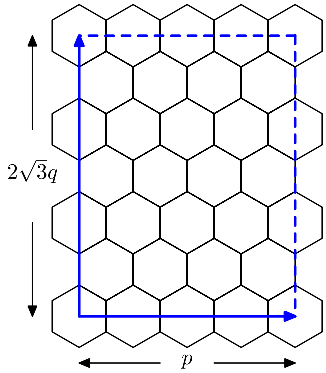

Fig. 6. The fundamental domain $\mathcal{D}$.

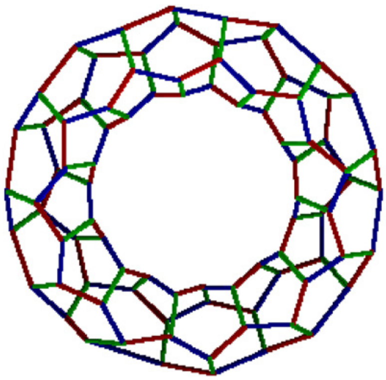

Fig. 7. An embedding of $X_{p,q}$ in $\mathbb{R}^3$.

In order to make all edges of the above embedding of $X_{p,q}$ have the same length, we shall require F to be an isometry. Therefore, F should satisfy $\langle F_u, F_v\rangle = 0$, $\langle F_u, F_u\rangle = \frac{4\pi^2r^2}{p^2} = 1$ and $\langle F_v, F_v\rangle = \frac{\pi^2R^2}{3q^2}|1+\frac{r}{R}\cos(\frac{2\pi u}{p})|^2 = 1$, which is impossible. However, if we let $r = \frac{p}{2\pi}$ and $R = \frac{\sqrt{3}q}{\pi}$, then $\langle F_u, F_u\rangle = 1$ and $\langle F_v, F_v\rangle = |1+\frac{p}{2\sqrt{3}q}\cos(\frac{2\pi u}{p})|^2$ and F is close to an isometry when $\frac{p}{q}$ is small. Thus with p fixed and q increasing, we can increase the stability of the embedding without changing the HOMO–LUMO gap.

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References

[1] A. Altshuler, Construction and enumeration of regular maps on the torus, Discrete Math. 4 (1973) 201–217.
[2] J.E. Avron, J. Berger, Tiling rules for toroidal molecules, Phys. Rev. A 51 (2) (1955) 1146–1149.
[3] J. Berger, J.E. Avron, Classification scheme for toroidal molecules, J. Chem. Soc. Faraday Trans. 91 (22) (1955) 4037–4045.
[4] S.A. Bovin, L.F. Chibotaru, A. Ceulemans, The quantum structure of carbon tori, J. Molecular Catalysis A: Chem. 166 (2001) 47–52.
[5] A. Ceulemans, L.F. Chibotaru, S.A. Bovin, P.W. Fowler, The electronic structure of polyhex carbon tori, J. Chem. Phys. 11 (9) (2000) 4271–4278.
[6] C. Chuang, B.-Y. Jin, Systematics of High-Genus Fullerenes, J. Chem. Inf. Model. 49 (7) (2009) 1664–1668.
[7] F.R.K. Chung, B. Kostant, S. Sternberg, Groups and the Buckyball, Lie Theory and Geometry: In honor of Bertram Kostant, 1994, pp. 97–126.
[8] H.S.M. Coxeter, W.O.J Moser, Generators and Relations for Discrete Groups, 4th ed., Springer-Verlag, New York, 1980.
[9] M. DeVos, L. Goddyn, B. Mohar, R. Samal, Cayley sum graphs and eigenvalues of (3, 6)-fullerenes, J. Comb. Theory Series B 99 (2) (2009) 358–369.
[10] M.V. Diudea, P.E. John, A. Graovac, M. Primorac, T. Pisanskie, Leapfrog and related operations on toroidal fullerenes, Croatica Chemica Acta 76 (2) (2003) 153–159.
[11] N. Elkies, Shimura curve computations, in: Algorithmic Number Theory, in: Lecture Notes in Computer Science, 1998, pp. 1–47.
[12] W. Fowler, P. Hansen, G. Caporossi, A. Soncini, Poylynes with maximal HOMO-LUMO gap, Chem. Phys. Lett. 342 (2001) 105–112.
[13] P.W. Fowler, P.E. John, H. Sachs, (3, 6)-cages, hexagonal toroidal cages, and their spectra, DIMACS Ser. Discrete Math. Theoret. Comput. Sci. 51 (2000) 139–174.
[14] W. Fowler, I. Steer, The leapfrog principle: a rule for electron counts of carbon clusters, J. Chem. Soc., Chem. Commun. 52 (1987) 1403–1405.
[15] P.E. John, H. Sach, Spectra of toroidal graphs, Discrete Math. 309 (9) (2009) 2663–2681.
[16] E.C. Kirby, R.B. Mallion, P. Pollak, Toroidal polyhexes, J. Chem. Soc. Faraday Trans. 89 (12) (1993) 1945–1953.

[17] E. Manolopoulus, R. Woodall, W. Fowler, Electronic stability of fullerenes: eigenvalue theorems for leapfrog carbon clusters, J. Chem. Soc. Faraday Trans. 88 (17) (1992) 2427–2435.
[18] D. Marušič, T. Pisanski, Symmetries of hexagonal molecular graphs on the torus, Croatica Chemica Acta 73 (2000) 969–981.
[19] Seiya Negami, Uniqueness and faithfulness of embedding of toroidal graphs, Discrete Math. 44 (2) (1983) 161–180.
[20] P. Nguyen, D. Stehlé, Low-dimensional lattice basis reduction revisited, Trans. Algorithms 5 (4) (2009).
[21] J.-P. Serre, Linear Representations of Finite Groups, Springer-Verlag, 1997.
[22] W.B. Smith, Introduction to Theoretical Organic Chemistry and Molecular Modelling, Wiley-VCH, 1996.
[23] R. Tamura, M. Ikuta, T. Hirahara, M. Tsukada, Positive magnetic susceptibility in polygonal nanotube tori, Phys. Rev. B 74 (4) (2005) 45418–45424.
[24] C. Thomassen, Tilings of the torus and the klein bottle and vertex-transitive graphs on a fixed surface, Trans. Am. Math. Soc. 323 (1993) 605–635.
[25] F. Zhang, C. An, Acyclic molecules with greatest HOMO-LUMO separation, Discrete Appl. Math. 98 (1999) 165–171.