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Dynamical Generation of Graphene

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Abstract. In recent years, the astonishing physical properties of carbon nanostructures have been discovered and are nowadays being intensively studied. We introduce how to obtain a graphene sheet using group theoretical methods and how to construct a graphene layer using the method of dynamical generation of quasicrystals. Both approaches can be formulated in such a way that the points of an infinite graphene sheet are generated. The main objective is to describe how to generate graphene step by step from a single point of $\mathbb{R}^2$.

Mathematics Subject Classification (2010). Group theory, Mathematical crystallography.

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1. Introduction

Graphene is a two-dimensional Euclidean plane tiled by regular hexagons, these hexagons being all of the same size. The vertices of the hexagons are usually taken as carbon atoms, but other graphene-like structures were also observed [4, 5].

Although the most promising nanomaterials are graphene and carbon nanotubes, their geometrical structures remain so far unexplored. Owing to their exceptional physical, chemical and mechanical properties, they found an increasing variety of applications [6].

The mathematical way to obtain a graphene sheet and the related nanotubes is to use the finite reflection groups. In general, we should use the Lie algebras A_2 and G_2 (or respectively their groups $SU(3)$ and $G(2)$) to construct a layer of graphene, because both of them yield triangular lattices. In this paper, we consider two mathematical methods to construct graphene. Both will provide identical graphene layers.

The first method used to obtain a mathematical model for the graphene is the construction using the simple Lie group $SU(3)$. It gives us an opportunity to define the congruence classes for the points of its weight lattice and, as a result, to

obtain an hexagonal tilling of $\mathbb{R}^2$ by removing the points of one of the congruence classes.

The second method we used is inspired by the process of dynamical generation of quasicrystals [1]. It was shown that, by using the Coxeter groups H_2, H_3 and H_4, quasicrystals can be constructed from a single point of $\mathbb{C}^n$ $(n = 2, 3, 4)$. In our case, we consider the Lie group $SU(3)$ and we define a step-by-step construction of the graphene from a single point of the plane $\mathbb{R}^2$. Furthermore, the method of dynamical generation could be used to obtain any crystallographic structure.

2. Root and weigh lattices of A_n

Let $\Phi = \{\alpha_1, \ldots, \alpha_n\}$ be a root system of rank n of the Lie algebra A_n in real Euclidean space $\mathbb{R}^n$ [2]. It is determined by the Coxeter–Dynkin diagram shown in Figure 1.

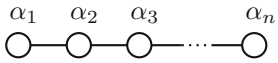

FIGURE 1. Coxeter–Dynkin diagram of the Lie group $SU(n+1)$.

The set of simple roots α_i, $i = 1, \ldots, n$ of the root system Φ of A_n is called an α-basis. Thus, for the Coxeter–Dynkin diagram, there is the corresponding Cartan matrix, which gives the geometry of the α-basis:

$$\mathcal{C}_{jk} = \frac{2\langle \alpha_j, \alpha_k \rangle}{\langle \alpha_k, \alpha_k \rangle}, \quad \text{where} \quad j, k = 1, 2, \ldots, n. \tag{1}$$

The set of ω_k, $k = 1, \ldots, n$ is called the set of fundamental weights and forms the ω-basis (or the basis of fundamental weights). It is convenient to work mostly in the ω-basis. Therefore, we need to convert the α-basis using the duality relation of the bases:

$$\frac{2\langle \alpha_j, \omega_k \rangle}{\langle \alpha_j, \alpha_j \rangle} \equiv \langle \alpha_j^\vee, \omega_k \rangle = \delta_{jk}, \quad \text{where} \quad j, k \in \{1, 2, \ldots, n\}. \tag{2}$$

The link between the α- and ω-bases is also given by the Cartan matrix $\mathcal{C}$ (1) and its inverse $\mathcal{C}^{-1}$:

$$\alpha_j = \sum_{k=1}^{n} \mathcal{C}_{jk}\omega_k \quad \text{and} \quad \omega_j = \sum_{k=1}^{n} (\mathcal{C}_{jk}^{-1})\alpha_k. \tag{3}$$

It is important to introduce the root lattice $\mathcal{Q}$ given by the set of all linear combinations of the simple roots α_i:

$$\mathcal{Q} = \Big\{ \sum_{i=1}^{n} a_i\alpha_i \mid a_i \in \mathbb{Z} \Big\} \equiv \bigoplus_i \mathbb{Z}\alpha_i \equiv \mathbb{Z}\alpha_1 + \cdots + \mathbb{Z}\alpha_n. \tag{4}$$

The positive root lattice $\mathcal{Q}_+$ of $\mathcal{Q}$ is defined as:

$$\mathcal{Q}_+ = \Big\{ \sum_{i=1}^{n} a_i \alpha_i \mid a_i = \mathbb{Z}^{\geq 0} \Big\} \equiv a_1\alpha_1 + \cdots + a_n\alpha_n. \tag{5}$$

Likewise, we introduce the weight lattice $\mathcal{P}$ and the cone of dominant weight $\mathcal{P}_+$:

$$\mathcal{P} = \mathbb{Z}\omega_1 + \cdots + \mathbb{Z}\omega_n \quad \text{and} \quad \mathcal{P}_+ = \mathbb{Z}^{\geq 0}\omega_1 + \cdots + \mathbb{Z}^{\geq 0}\omega_n. \tag{6}$$

In general, the points of the weight lattice $\mathcal{P}$ of the Lie group $SU(n+1)$ can be split into $(n+1)$ congruence classes denoted as $\mathcal{K}_k$, $k = \mathbb{Z}^{\geq 0}$ [3]. Each point of $\mathcal{P}$ belongs precisely to one congruence class and the splitting is defined as

$$\begin{aligned} &x = a_1\omega_1 + a_2\omega_2 + \ldots + a_n\omega_n \in K_k, \\ &na_1 + (n-1)a_2 + \cdots + 2a_{n-1} + a_n = k \mod n+1. \end{aligned} \tag{7}$$

3. Construction of the graphene from the Lie algebra A_2

The most appropriate way to construct a mathematical model for the graphene layer is to use the simple Lie algebra A_2. The root system of A_2 and its Coxeter–Dynkin diagram are shown in Figure 2.

FIGURE 2. The root system of Lie algebra A_2 and it's Coxeter–Dynkin diagram are shown from left to right, respectively.

The simple roots α_1 and α_2 span a real Euclidean space $\mathbb{R}^2$. The geometric relations between them are:

$$\langle \alpha_1, \alpha_1 \rangle = \langle \alpha_2, \alpha_2 \rangle = 2, \quad \langle \alpha_1, \alpha_2 \rangle = -1 \quad \text{and} \quad \angle(\alpha_1, \alpha_2) = \frac{2\pi}{3}.$$

The Cartan matrix of A_2 and its inverse are defined from (1) as follows:

$$\mathcal{C}_{A_2} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}, \qquad \mathcal{C}_{A_2}^{-1} = \frac{1}{3}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}. \tag{8}$$

As we mentioned before, the link between α- and ω-bases of A_2 is given by the Cartan matrix (8). Hence, we can write explicitly:

$$\alpha_1 = 2\omega_1 - \omega_2, \quad \alpha_2 = -\omega_1 + 2\omega_2, \quad \omega_1 = \frac{2}{3}\alpha_1 + \frac{1}{3}\alpha_2, \quad \omega_2 = \frac{1}{3}\alpha_1 + \frac{2}{3}\alpha_2.$$

For the A_2 case, the expressions for the root lattice $\mathcal{Q}$ (4) as well as for the weight lattice $\mathcal{P}$ (6) can be simplified:

$$\mathcal{Q}_{A_2} = \mathbb{Z}\alpha_1 + \mathbb{Z}\alpha_2, \quad \mathcal{P}_{A_2} = \mathbb{Z}\omega_1 + \mathbb{Z}\omega_2. \tag{9}$$

From now on, there are two ways to construct a graphene sheet using the Lie algebra A_2. The first one is to consider the root lattice $\mathcal{Q}_{A_2}$ and the second one

is to use the weight lattice $\mathcal{P}_{A_2}$. Both of these lattices are triangular in $\mathbb{R}^2$. Root and weight lattices coincide, but not all the points of $\mathcal{Q}_{A_2}$ belong to $\mathcal{P}_{A_2}$ (Fig. 3).

The construction of the graphene using the root lattice $\mathcal{Q}_{A_2}$ starts from finding the proximity cells, called Voronoi domains or Brillouin zones, for each of the lattice points. In this case, the proximity cells are regular hexagons which tile $\mathbb{R}^2$ (Fig. 3). We obtain the graphene sheet by removing all the points of the lattice $\mathcal{Q}_{A_2}$ while retaining the hexagons of proximity cells.

However, an interesting case appears when we use $\mathcal{P}_{A_2}$. As was defined in the previous section, the points of $\mathcal{P}_{A_2}$ can be split into the three mutually congruent classes $\mathcal{K}_k$, $k = 0, 1, 2$, by applying the rule from Equation (7):

$$x = a_1\omega_1 + a_2\omega_2 \in \mathcal{K}_k, \quad \text{where} \quad 2a_1 + a_2 = k \mod 3 \quad \text{and} \quad k = 0, 1, 2.$$

The result of this splitting is the following: the points of the congruence class $\mathcal{K}_0$ represent the points of $\mathcal{Q}_{A_2}$, the points of $\mathcal{K}_1$ represent the points of $\mathcal{Q}_{A_2} + \omega_1$, and the points of $\mathcal{K}_2$ represent the points of $\mathcal{Q}_{A_2} + \omega_2$ (Fig. 3).

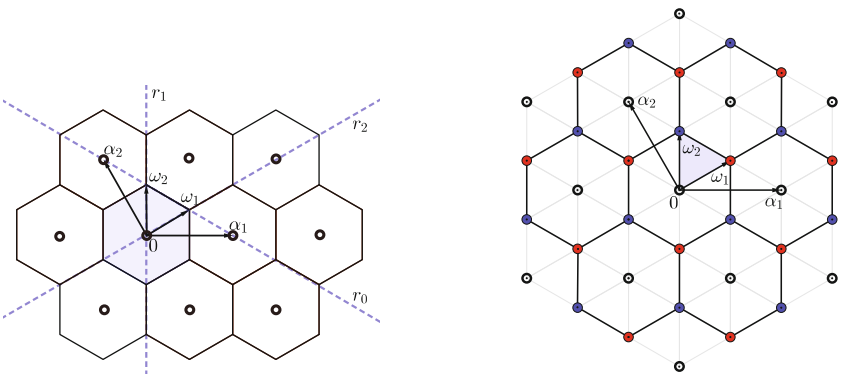

FIGURE 3. On the left, a fragment of the Q_{A_2} is shown. The shaded region stands for the Voronoi domain. On the right, a fragment of the $\mathcal{P}_{A_2}$ is shown. Points marked by white nodes belong to $\mathcal{Q}_{A_2}$ and the congruence class $\mathcal{K}_0$. Points marked by red and blue nodes belong to $\mathcal{P}_{A_2}$ and $\mathcal{K}_1$, $\mathcal{K}_2$, respectively. The shaded region stands for the fundamental domain of $\mathcal{P}_{A_2}$.

Consequently, removing the points of $\mathcal{K}_0$, $\mathcal{K}_1$ or $\mathcal{K}_2$ yields the hexagonal structure which represents a graphene layer. For example, in Figure 3, we disregarded the points of $\mathcal{K}_0$.

Note that even though both constructions start with the triangular lattices, the graphene structure does not form a lattice. A graphene sheet can be refined and the construction will be based on the refinement of the lattices $\mathcal{P}_{A_2}$ and $\mathcal{Q}_{A_2}$.

4. Method of dynamical generation

In this section we describe a step-by-step process to build a graphene sheet starting from a single point of $\mathbb{R}^2$. We consider the weight lattice $\mathcal{P}_{A_2}$. We will be using two different steps, namely $\mathcal{S}_1$ and $\mathcal{S}_2$ (Fig. 4):

$$\mathcal{S}_1 = (\omega_1, -\omega_1 + \omega_2, -\omega_2), \quad \mathcal{S}_2 = (\omega_2, \omega_1 - \omega_2, -\omega_1).$$

The points of $\mathcal{S}_1$ belong to the $\mathcal{K}_1$ and the points of $\mathcal{S}_2$ belong to the $\mathcal{K}_2$.

As the seed point of our construction we can choose any point of $\mathcal{P}_{A_2}$. If the chosen point belongs to the congruence class $\mathcal{K}_0$ then the first step can be either $\mathcal{S}_1$ or $\mathcal{S}_2$. If it belongs to $\mathcal{K}_1$ then the next step should be $\mathcal{S}_1$. Finally, if it belongs to $\mathcal{K}_2$ then the next step should be $\mathcal{S}_2$.

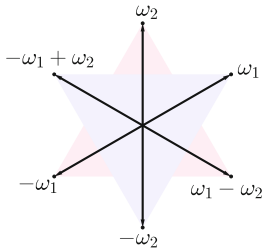

FIGURE 4. The steps of the dynamical generation of the graphene are shown. The blue and red regions correspond to the steps $\mathcal{S}_1$ and $\mathcal{S}_2$, respectively.

By applying this rule to a single point of $\mathbb{R}^2$, we dynamically generate the points of our structure in the following way: three vectors of the starting step define three points of the plane. If any of these points coincides with an already existing point of the graphene structure, we disregard it. If it is a new point, it should be kept. The more steps we do, the bigger the graphene structure gets and after an infinite number of steps the graphene layer is complete.

For example, from Figure 3 we see that adding a point of $\mathcal{K}_1$ to another point of $\mathcal{K}_1$ yields a point of $\mathcal{K}_2$ and adding a point of $\mathcal{K}_2$ to another point of $\mathcal{K}_2$ yields a point of $\mathcal{K}_1$. One should also note that adding a point of $\mathcal{K}_1$ to a point of $\mathcal{K}_2$ yield a point of $\mathcal{K}_0$ which does not belong to the graphene structure. Therefore, such an addition is not allowed.

However, an interesting situation arises when removing one, two, or even three vectors from each of the steps $\mathcal{S}_1$ or $\mathcal{S}_2$. For example, consider the following combinations of the steps:

(a) $\mathcal{S}_1 = (\omega_1, -\omega_1 + \omega_2, -\omega_2)$, $\mathcal{S}_2 = (\omega_2, 0, 0)$;

(b) $\mathcal{S}_1 = (\omega_1, 0, -\omega_2)$, $\mathcal{S}_2 = (\omega_2, 0, -\omega_1)$;

(c) $\mathcal{S}_1 = (\omega_1, -\omega_1 + \omega_2, -\omega_2)$, $\mathcal{S}_2 = (0, 0, 0)$.

This way we can obtain sheets of graphene that will not cover the entire plane $\mathbb{R}^2$. The resulting graphene structures are shown in Figure 5.

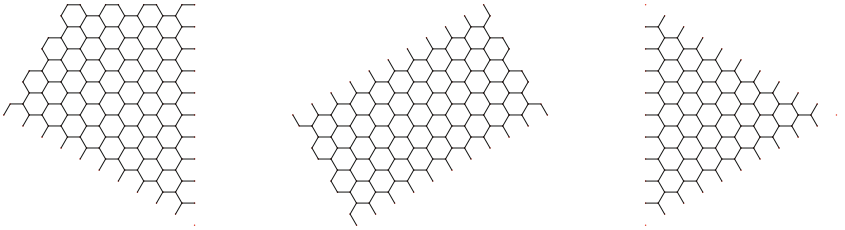

FIGURE 5. The resulting graphene layers are shown for the combinations of steps $\mathcal{S}_1$ and $\mathcal{S}_2$ from (a), (b) and (c) from left to right, respectively.

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