Lie symmetries and 2D Material Physics

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Abstract

Inspired from Lie symmetry classification, we establish a correspondence between rank two Lie symmetries and 2D materials physics. The material unit cell is accordingly interpreted as the geometry of a root system. The hexagonal cells, appearing in graphene like models, are analyzed in some details and are found to be associated with $A_2$ and $G_2$ Lie symmetries. This approach can be applied to Lie supersymmetries associated with fermionic degrees of freedom. It has been suggested that these extended symmetries can offer a new way to deal with doping material geometries. Motivated by Lie symmetry applications in high energy physics, we speculate on a possible connection with $(p,q)$ brane networks used in the string theory compactification on singular Calabi-Yau manifolds.

Keywords: Lie symmetries, root systems, supersymmetry, string theory and 2D material physics.
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1 Introduction

Several studies of magnetic physical properties of strongly correlated electron models have been carried out, in connection with the elaboration of nano-materials. The most studied model is the graphene using different calculation methods with appropriate approximations[1, 2]. The material is a monolayer of carbon crystal forming a two dimensional hexagonal geometric lattice [3]. Energy spectrum of this material has a particular structure where the valence and the conduction bands intersect at Dirac points producing a semi-metal. In this way, low-energy excitations are described by a pair of two-component fermions, equivalently, a four-component Dirac fermion [4].

Recently, there have been many attempts to build a bridge between high energy physics and the graphene using different methods including the BTZ black hole physics and the AdS/CFT correspondence explored in string theory and related topics [5, 6]. More precisely, a stringy description in terms of the (D3,D7) brane system embedded in type IIB superstring has been proposed in [6]. In the corresponding brane representation, each D3-D7 pair produces a complex massless two-component spinor living in the three dimensional space-time. In connection with these activities, a brane realization of the quantum Hall effect, based on the Calabi-Yau singularities classified by Lie symmetries, has been proposed in [7]. In particular, it has been suggested a possible link between the graphene and a special class of Lie symmetries called indefinite.

More recently, Lie symmetries has been used to investigate a class of materials engineered from the hexagonal structure. It is recalled that this geometry can be considered as the most stable one in nature which has been explored in many physical applications, including particle physics, string theory and nano-technology. Indeed, an experimental treatment on the hexagonal materials by the scanning tunneling spectroscopy (STS) has been elaborated producing a \((\sqrt{3} \times \sqrt{3})R30^\circ\) supercell configuration on the graphene and the silicene surfaces, in contrast to the usual structure known by the \((1 \times 1)\) geometry [8]. A close inspection in rank two Lie symmetries has showed that the \((\sqrt{3} \times \sqrt{3})R30^\circ\) structure appears naturally in the construction of the root system of the \(G_2\) exceptional Lie symmetry [9, 10]. Based on this observation, a combination of \((\sqrt{3} \times \sqrt{3})R30^\circ\) and \((1 \times 1)\) geometries has been developed to engineer new materials relaying on a double hexagonal structure arising in the root system of the \(G_2\) Lie symmetry [11].

Motivated by the above works, we establish a correspondence between 2D material physics and Lie symmetries. In this way, we interpret the material unit cells as root systems of Lie symmetries. This may offer a new take on the geometrical elaboration of 2D materials. Our focus is on rank two Lie symmetries. In particular, we consider the hexagonal structure, and we find that it is linked to \(A_2\) and \(G_2\) root systems. This method can be applied to Lie
supersymmetries associated with fermionic degrees of freedom. We expect that this class of symmetries can offer a new way to approach doping material geometries. Supported by the role placed by Lie symmetries in high energy physics, we speculate on a possible connection with \((p,q)\) brane webs used in the string theory compactification on toric Calabi-Yau manifolds.

The paper is organized as follows. In section 2, we give a short overview on Lie symmetries. Section 3 concerns a dictionary between the root systems of rank two Lie symmetries and 2D material physics. Extension to Lie supersymmetries is discussed in section 4. Section 5 contains concluding remarks and a speculation from string theory.

2 Lie symmetries

We start by recalling that symmetry is one of the most important ingredient in physics. Precisely, one remarks the crucial role placed by Lie symmetries in standard model and higher dimensional physical models including superstrings, M and F-theories. In this way, the root systems have been explored to partially solve many problems arising in such theories. A particular emphasis put on the hexagonal geometry appearing in Lie symmetries used in string theory compactification. It has been analyzed that many geometrical background relevant to particle physics and string theory are associated with the hexagonal symmetries appearing in the root systems \([12]\).

The hexagonal structure arises also in lower dimensional theories including solid state physics dealing with the graphene-like models. In the investigation of such materials, it has been found the appearance of new structures shearing similarities with the hexagonal root systems of Lie symmetries \([8]\).

Armed by these works, we establish a dictionary between Lie symmetries and 2D material physics. Before going ahead, let us note that the present study assumes some basic knowledge on Lie symmetries and their root systems\([9,12]\). More precisely, we give a flash review on such mathematical backgrounds, used in many physical area including high energy and condensed matter physics. Indeed, a Lie symmetry \(g\) is a vector space together with an antisymmetric bilinear bracket \([,] : g \times g \rightarrow g\) satisfying the Jacobi identity \(([a,[b,c]] + [c,[a,b]] + [b,[c,a]] = 0)\). It is realized that any semi-simple Lie symmetry can be viewed as a direct sum of simple Lie symmetries. The Cartan subalgebra \(H\) is generated by the all semi-simple elements, being the maximal abelian Lie sub-algebra. It is observed that \(g\) may then be written as the direct sum of \(H\) and the subspaces \(g_\alpha\):

\[
g = H \oplus \{ \oplus \alpha g_\alpha \}
\]  \hspace{1cm} (2.1)
where \(\{g_a = x \in g | [h, x] = \alpha (x)x\}\) for \(x \in g\). Here \(\alpha\) ranges over all elements of the dual of \(H\). In Lie theory, these vectors \(\alpha\) are called roots.

Having discussed the Lie structure, we now recall some basic concepts of the root systems which will be explored later on in the discussion of the desired correspondence. Following [9, 10, 12], a root system \(\Delta\) of a Lie symmetry is defined as a subset of an Euclidean space \(E\) satisfying the following constraints:

1. \(\Delta\) is finite and spans \(E\), \(0\) is an element of \(\Delta\)
2. if \(\alpha\) is an element of \(\Delta\), then \(k\alpha\) is also but only for \(k = \pm 1\)
3. for any \(\alpha\) in \(\Delta\), \(\Delta\) is invariant under reflection \(\sigma_\alpha\), where \(\sigma_\alpha(\beta) = \beta - 2\langle \beta, \alpha \rangle \alpha\)
4. if \(\alpha\) et \(\beta\) are two elements of \(\Delta\), the quantity \(\langle \beta, \alpha \rangle = \frac{2(\beta, \alpha)}{\langle \alpha, \alpha \rangle} \in \mathbb{Z}\).

Note by the way that the root system \(\Delta\) contains several information about the associated Lie symmetry structure. These information will be relevant in the present discussion. In Lie theory, it has been shown that there is a nice classification of rank two Lie symmetries. Taking two root elements \(\alpha\) and \(\beta\) of \(\Delta\), it is evident to show the equation

\[
\langle \beta, \alpha \rangle \langle \alpha, \beta \rangle = 4 \cos^2 \theta
\]

where \(\theta\) is the angle between \(\alpha\) and \(\beta\). This leads to the following constraint

\[
0 \leq \langle \beta, \alpha \rangle \langle \alpha, \beta \rangle \leq 4.
\]

The possible values of \(\theta\) are \(30^0, 45^0, 60^0, 90^0, 120^0, 135^0\) and \(150^0\), leading to a nice classification. This generates four different Lie symmetries with the following dimensions

\[
\text{Dim } g = 2 + |\Delta|
\]

where \(|\Delta|\) denotes the number of the roots associated with \(g\). The number 2 is called the rank identified with the number of the simple roots, being the dimension of the corresponding Cartan subalgebra. These four symmetries, classified in terms of the angle between simple roots \(\theta\), are listed in Table 1. More details on this classification and its physical applications can be found in literature. An alternative way to classify these symmetries is to use the Cartan matrices obtained from the scalar product between the simple roots. These matrices \(K = (k_{ij})\) of size 2 take the following general form

\[
K = \langle \alpha_i, \alpha_j \rangle = \begin{pmatrix} 2 & k_{12} \\ k_{21} & 2 \end{pmatrix}
\]
Table 1: Classification of the rank two Lie symmetries in terms of $\theta$ angle

| Lie Symmetry | $\theta$ | $|\Delta|$ |
|--------------|----------|-----------|
| $A_1 \oplus A_1$ | $90^\circ$ | 4 |
| $A_2$ | $120^\circ$ | 6 |
| $B_2$ | $135^\circ$ | 8 |
| $G_2$ | $150^\circ$ | 12 |

where the values of $k_{12}$ and $k_{21}$ are illustrated in table 2. It is recalled that if the Cartan matrix is symmetric, the Lie symmetry is called simply laced ($|\alpha_1| = |\alpha_2|$). Otherwise, it is a non simply laced one ($|\alpha_1| \neq |\alpha_2|$).

Table 2: Classification of rank two Lie symmetries in terms of the Cartan matrices

| Lie Symmetry | $k_{12}$ | $k_{12}$ |
|--------------|----------|----------|
| $A_1 \oplus A_1$ | 0 | 0 |
| $A_2$ | -1 | -1 |
| $B_2$ | -1 | -2 |
| $G_2$ | -1 | -3 |

3 Lie symmetries and pure 2D materials

As mentioned in the introduction, Lie symmetries has been explored to study the physical behaviors of the hexagonal geometries generalizing the structure appearing in the graphene using theoretical and experimental methods. In particular, an experimental treatment on the hexagonal materials by scanning tunneling spectroscopy (STS) has been used to generate a $(\sqrt{3} \times \sqrt{3})R30^\circ$ super cell structure on the graphene like models, in contrast to the usual structure known by $(1 \times 1)$. In fact, the $(\sqrt{3} \times \sqrt{3})R30^\circ$ structure arises naturally in the construction of the $G_2$ root system [9, 10]. Based on this observation, a combination of $(\sqrt{3} \times \sqrt{3})R30^\circ$ and $(1 \times 1)$ supercells has been proposed to model new materials based on such double hexagonal Lie symmetries [11].

Inspired from these activities, we propose a correspondence between the root systems of rank two Lie symmetries and the geometry of 2D material physics. This may offer a novel way to study such materials. Here, thought, we will be concerned with similarities. The link, that we are looking for, can be supported by the interplay between the hexagonal materials and the $A_2$ Lie symmetries.
In order to see this point, let us first consider the hexagonal materials having only the \((1 \times 1)\) structure. The latter appears in valence-four elements. Indeed, there is a similarity between the hexagonal unit cell of such materials and the root system of \(A_2\) Lie symmetry. It is recalled that its dimension reads as

\[
\text{Dim } A_2 = 2 + 6. \tag{3.1}
\]

The corresponding root system is built from two simple roots \(\alpha_1\) and \(\alpha_2\) of unequal length at \(120^\circ\) angle satisfying following constraint

\[
\frac{|\alpha_2|^2}{|\alpha_1|^2} = 1. \tag{3.2}
\]

The six nonzero roots come from these simple ones, with the sum and the opposed, forming the well known hexagon \((A_2\)-hexagon\). In fact, the positions of the six atoms placed on hexagonal unit cell are associated now with these six nonzero roots: \(\{\pm \alpha_1, \pm \alpha_2, \pm (\alpha_1 + \alpha_2)\}\).

An inspection shows that one can elaborate a dictionary between the \(A_2\) root system and the hexagonal materials based on the \((1 \times 1)\) geometry. This can be formulated as follows:

- An atom \(A\) placed on the hexagonal unit cell is associated with a \(A_2\) nonzero root.
- The lattice parameter \(a\), used in the hexagonal material, corresponds to the length of the roots
  \[
a = |\alpha_1| = |\alpha_2|. \tag{3.3}
\]
- The general material configuration with the flat geometry can be obtained by using the fact that the \(A_2\) hexagons tessellate the full plane forming the \((1 \times 1)\) supercell structure.

![Figure 1: \(A_2\) hexagonal materials.](image)
We naturally observe that the $G_2$ Lie symmetry can be also incorporated in the discussion. This may be explored to engineer new 2D hexagonal materials. It is worth noting that $G_2$ is an exceptional Lie symmetry with rank 2 and dimension 14. In this way, eq(2.4) can be written as

$$\text{Dim } G_2 = 2 + 12. \quad (3.4)$$

This symmetry has been extensively studied in the string compactification in connection with a particular seven real dimensional manifold, called $G_2$ manifold. It has been shown that it can play a crucial role in the M-theory compactification generating semi-realistic models with only four supercharges in our universe [13, 14, 15]. Roughly speaking, the root system of $G_2$ symmetry contains a special hexagonal root structure residing on two hexagons of unequal side lengths generated by two simple unequal roots at angle

$$(\alpha_1, \alpha_2) = 150^\circ = 120^\circ + 30^\circ. \quad (3.5)$$

These two simples roots satisfy the constraint

$$\frac{|\alpha_2|^2}{|\alpha_1|^2} = 3, \quad (3.6)$$

leading to the following Cartan matrix

$$\langle \alpha_i, \alpha_j \rangle = K_{ij} = \begin{pmatrix} 2 & -3 \\ -1 & 2 \end{pmatrix}. \quad (3.7)$$

This matrix can be encoded in a geometric graph called Dynkin diagram. It is recalled that, the diagonal elements correspond to two nodes and the non diagonal elements describe the number of the lines between them. In fact, the number of the lines between the node 1 and the node 2 is given by $k_{12}k_{21}$. The Dynkin diagram associated with the $G_2$ Lie symmetry is presented in figure (2). As known, it is obtained from the one of the $D_4 (so(8))$ Lie algebra as illustrated in figure 2.

In fact, each simple root of the $G_2$ Lie symmetry generates a single hexagon. The small one is defined by the root set $\{\pm\alpha_1, \pm(\alpha_1 + \alpha_2), \pm(2\alpha_1 + \alpha_2)\}$ while the second one is rotated by $30^\circ$ and generated by $\{\pm\alpha_2, \pm(3\alpha_1 + \alpha_2), \pm(3\alpha_1 + 2\alpha_2)\}$. In fact, the $G_2$ hexagons can be used to engineer materials with a double honeycomb structure. This involves two hexagons producing materials having the property of being close to usual one with one periodic hexagon associated with the $A_2$ Lie symmetry [19, 21]. It is evident that the above correspondence can be extended to $G_2$ Lie symmetry. It can be organized as follows:
• Each atom placed on the double hexagonal unit cell, involving 12 atoms, is associated with a root of the $G_2$ Lie symmetry.

• The lattices parameters $a_1$ and $a_2$ of this unit cell correspond to the lengths of the two simple roots

$$a_1 = |\alpha_1|, \quad a_2 = |\alpha_2| = \sqrt{3}|\alpha_1|. \quad (3.8)$$

• The general material structure with the flat geometry can be obtained by using the fact that the $G_2$ hexagons tessellate the full plane forming a new supercell crystal structure by mixing the $(1 \times 1)$ and $(\sqrt{3} \times \sqrt{3})R30^\circ$ geometrical configurations. This geometry is illustrated in figure 3.

Inspired from the generalized Pythagorean theorem, the analysis made for the $G_2$ hexagons can be pushed further. In particular, we can do something similar by incorporating the polyvalent geometry generalizing the trivalent and tetravalent geometry appearing in $so(8)$ Lie
symmetry. More precisely, we consider a particular geometry where a central node is connected with \(3N\) legs as illustrated in figure 4. The associated geometry that we are looking for will be obtained by using the standard techniques of folding of the Dynkin nodes which are permuted by an outer-automorphism group leaving the graph invariant. Thus, starting form the polyvalent geometry and folding the nodes that are permuted by \(S_{3N}\) permutation group, we get the graph corresponding to the \(G_2\) extended Lie symmetry. This graph contains two nodes connected by \(3N\) lines as shown in figure 4.

![Figure 4: \(G_2\) extended Dynkin diagram.](image)

Using the relation between the Dynkin diagrams and the Cartan matrices, this generalized version of the \(G_2\) Lie symmetry should have the following Cartan matrix

\[
K_{ij} = \begin{pmatrix} 2 & -3N \\ -1 & 2 \end{pmatrix}.
\]  
(3.9)

This matrix should be associated with two simple roots constrained by

\[
\frac{|\alpha_2|^2}{|\alpha_1|^2} = 3N.
\]  
(3.10)

It is obvious from this equation that we can build up a double hexagonal geometry based on the generalized \(G_2\) symmetry. It is governed by the following points

- As in the case of \(G_2\), the lattices parameters \(a_1\) and \(a_2\) are linked to the lengths of the simple roots. Correspondingly, we end up with the following relations

\[
a_1 = |\alpha_1|, \quad a_2 = |\alpha_2| = \sqrt{3N}|\alpha_1|
\]  
(3.11)

- The supercell crystal geometry should involve a combined geometry given \((1 \times 1)\) and \((\sqrt{3N} \times \sqrt{3N})R30^\circ\) supercell structures.
To compute the discussion on rank two Lie symmetries, we incorporate the remaining symmetries associated with $B_2$ and $A_1 \oplus A_1$. In fact, the unit cell of the decorated square lattice material can be linked with the root system of the $B_2$ Lie symmetry generated by two simple roots and of unequal length at 135 angle. In this representation, each principal cell is formed by eight atoms. This double geometry contains two squares of unequal side length at angle 45°. Each simple root of the $B_2$ symmetry generates a square. The small one is generated by the root set $\{\pm \alpha_1, \pm (\alpha_1 + \alpha_2)\}$ describing a material with only one square geometry. It is worth noting that the geometry should be associated with $A_1 \oplus A_1$ Lie symmetry. The big square is generated by the following equal side length $\{\pm \alpha_2, \pm (2\alpha_1 + \alpha_2)\}$ describing also a square geometry in material physics.

A close inspection reveals that there is a dictionary between two rank Lie symmetries and 2D material physics. This can be organized in Table 3.

| Lie symmetries | Materials |
|----------------|-----------|
| Root systems   | Unit cells|
| Non zero roots | Atom positions |
| $|\Delta|$   | Number of atoms in the material unit cells |
| Dimension of Cartan Sup-algebras | Dimension of material spaces |
| Simply laced Lie symmetries | Materials with single geometry |
| Non simply laced Lie symmetries | Materials with double geometry |

Table 3: Correspondence between Lie symmetries and 2D material physics.

4 Lie supersymmetries and doping material geometries

On the basis of the above correspondence, it is natural to think about models based on other Lie symmetries. In this section, we consider the Lie supersymmetries associated with fermionic degrees of freedom. These symmetries have been explored in many context in physics and can be thought as a possible extension of the one discussed in the previous section [16, 17, 18, 19]. In fact, we expect that Lie supersymmetries can be used to engineer a new class of materials. This may support the physical application of these symmetries not only in string theory and related models but also in nano-science technology.

In higher dimensional theories, there are many examples of such Lie symmetries. The general study is beyond the scope of the present work, though we will consider an explicit example $A(1,0)$ which can be thought of as a particular extension of the $A_2$ Lie bosonic symmetry. This symmetry which has been developed to study aspects of supersymmetric
integrable conformal models is quite similar to $A_2$ but with some differences. It is an eight dimensional Lie symmetry with rank 2. The corresponding root system has been extensively studied involving fermionic and bosonic roots. In fact, it is shown that this symmetry involves two different root systems. The first one has two fermionic nonzero roots $\alpha_1$ and $\alpha_2$ having a length square zero, and a normalized bosonic nonzero root $(\alpha_1 + \alpha_2)$ with a length square 2. In this case, the total root system is given by $\{\pm \alpha_1, \pm \alpha_2, \pm (\alpha_1 + \alpha_1)\}$. The second root system involves one fermionic simple nonzero root $\alpha_1$ having length square zero and a simple bosonic root $\alpha_2$ with length square 2. The normalized fermionic one nonzero root with length square 0 is $(a_2 - a_1)$. The total root system is given by $\{\pm \alpha_1, \pm \alpha_2, \pm (a_2 - a_1)\}$. It has been shown that both of them has a hexagonal geometry involving fermionic and bosonic roots. This indicates that the theory of Lie superalgebras differs from the theory of Lie symmetries. This difference in nature of roots drives us to think that such symmetries could be associated with magnetic doping hexagonal materials. In the study graphene interacting with metal atoms, it has been observed that there are three adsorption sites named by hollow H, bridge B and top T. In fact, the hollow H site is placed at the center of a hexagon. In connection with Lie symmetries, these sites should be associated with zero roots corresponding to the Cartan sub-algebras. The bridge B site is located at the midpoint of a carbon-carbon bond. Indeed, this can be associated with the length of simple roots via the the generalized Pythagorean theorem. However, the top T site is placed directly above a carbon atom. Considering atoms preferring the T sites, the corresponding structures could be interpreted as geometries of the root system. This is motivated by the fact that in the hexagonal unit cell material contains atoms with different nature. In this way, the metal atom positions could be associated with fermionic roots, while the ordinary atoms are associated with the bosonic roots. This observation could be explored further to give a complete picture of the dictionary presented in Table 3.

5 Speculations from string theory

In this paper, we have developed a new method to approach to 2D material physics. In particular, we have presented a dictionary between rank two Lie symmetries and the geometry of 2D material physics. In this way, the material unit cell has been interpreted as a root system. More precisely, we have analyzed in some details the $A_2$ and $G_2$ Lie symmetries and found they are linked to hexagonal materials. This approach could be applied to Lie supersymmetries corresponding to fermionic degrees of freedom providing a new way to investigate doping material geometries. We intend to investigated elsewhere other symmetries to complete the Table 3 by introducing other Lie symmetries used in modern physics.

This work comes up with the opening of many windows. We would like to stress that a
possible connection with string theory can be given. In fact, the correspondence presented here shears many similarities with the link between singularity theory and Lie symmetries. This link based on a correspondence between the ADE roots and the two-cycles used in in the deformation of ADE singularities of ALE spaces considered as local versions of the K3 surface. In fact, to each simple root one associates a complex projective space $\mathbb{CP}^1$ used in the blowing up of singular points. This connection has been considered as an important development in the string theory compactification supported by the string-string duality in six dimensions and D-brane configurations on which gauge theories live. This has been controlled by the root systems including the hexagonal one explored in particle physics[20].

Inspired from these connections, one can speculate on string theory interpretation in terms of $(p,q)$ string junctions associated with root systems of simply and non simply laved Lie symmetries developed in [21, 22]. In this picture, we anticipate that the material physics can be studied using brane physics. It is recalled that a brane is an extended object upon which open strings can end with appropriate boundary conditions. In fact, the $A_2$ material unit cell can be represented by open strings stretched on branes with similar behaviors. Indeed, writing the two simple roots in terms of a real basis $\{e_i, i = 1, 2, 3\}$ of the orthonormal vectors of $\mathbb{R}^3$

$$\alpha_i = e_i - e_{i+1}, \quad i = 1, 2$$

it is possible to give an interpretation in terms of three branes associated with the basis $\{e_i\}$. The corresponding $(p_i, q_i)$ brane charge webs should satisfy the vanishing charge condition

$$p_1 + p_2 + p_3 = 0$$
$$q_1 + q_2 + q_3 = 0$$

required by the $A_2$ root system. The total six $(p_i, q_i)$ open strings can be obtained from the mirror branes with the opposed charges. A possible charge vector can given by solving the above equations. We expect that the corresponding physics content can be determined explicitly from the geometry of the $(p,q)$ networks. This formulation is quite similar to toric realization of the $\mathbb{CP}^2$ projective space [23]. It is a complex two dimensional manifold having an $U(1)^2$ toric action exhibiting three fixed points associated with an equation similar to (5.2). It would therefore be of interest to try to extract information on material physics based on such mathematical backgrounds. We believe that these questions deserve to be investigated further.
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