Graphene, Lattice QFT and Symmetries

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Abstract

Borrowing ideas from tight binding model, we propose a board class of Lattice QFT models that are classified by the ADE Lie algebras. In the case of $A_{N-1} \simeq su(N)$ series, we show that the couplings between the quantum states living at the first nearest neighbor sites of the lattice $\mathcal{L}_{su(N)}$ are governed by the complex fundamental representations $\mathbb{N}$ and $\mathbb{N}$ of $su(N)$; and the second nearest neighbor interactions are described by its adjoint $\mathbb{N} \otimes \bar{\mathbb{N}}$. The lattice models associated with the leading $su(2)$, $su(3)$ and $su(4)$ cases are explicitly studied and their fermionic field realizations are given. It is also shown that the $su(2)$ and $su(3)$ models describe respectively the electronic properties of the acetylene chain and the graphene. It is established as well that the energy dispersion of the first nearest neighbor couplings is completely determined by the $A_N$ roots $\alpha$ through the typical dependence $N/2 + \sum_{\alpha} \cos (k \cdot \alpha)$ with $k$ the wave vector. Other features such as DE extension and other applications are also discussed.

Keywords: Tight Binding Model, Graphene, Lattice QFT, ADE Symmetries.

1 Introduction

Tight Binding Model (TBM) \cite{1, 2, 3, 4} is a particular lattice QFT \cite{5, 6, 7, 8} modeling couplings between quantum states living at closed neighboring sites. The interactions are modeled in terms of hops of crystal particles or holes; and brings together issues from High Energy Physics and Condensed Matter \cite{9, 10, 11, 12, 13, 14, 15}. Despite the
restriction to the first nearest neighbor interactions, the studies based on TBM have been shown to capture the main information on the physical properties of lattice systems; like in graphene \cite{16, 17, 18} whose basic physical properties have been related to QED in (2 + 1) dimensions; for reviews see \cite{9, 10}, refs therein and \cite{19, 20}.

In this paper, we use TBM to engineer a board class of lattice QFTs that are based on ADE Lie algebras \cite{21, 22} and their basic representations \cite{23, 24}. These engineered lattice systems classify the electronic properties of acetylene chain as a su(2) model, graphene as a su(3) lattice model and may have application in other fields; in particular in QFT on non commutative geometry \cite{25, 26, 27}, where space time is viewed as a crystal, and in the special subset of conformal field models based on affine Kac-Moody invariance and vertex operators \cite{28, 29, 30}.

To fix the ideas; let us describe briefly the main lines of the construction in the case of the series $A_{N-1} \simeq su(N)$ \cite{31} which is generated by $(N-1)$ commuting Cartan generators $h^i$ and $N (N-1)$ step operators $E_{\pm \beta}$ where the vectors $\beta = (\beta^1, ..., \beta^{N-1})$ stand for the positive roots of $su(N)$. As a QFT on crystal, our $su(N)$ lattice model involves the two basic following:

1. the lattice $L_{su(N)}$:

It is made by the superposition of two sublattices $A_{su(N)}$ and $B_{su(N)}$ generated by the $su(N)$ simple roots as in eqs (2.1). This $(N-1)$- dimensional lattice extends the 1D chain and the well known 2D honeycomb of graphene corresponding to $N = 2$ and $N = 3$ respectively; see figures (2), (3) for illustration.

Each $r_m$ site of $L_{su(N)}$; say $r_m \in A_{su(N)}$, has $N$ first nearest neighbors at $(r_m + v_i) \in B_{su(N)}$ and $N (N-1)$ second nearest neighbors at $(r_m + V_{ij}) \in A_{su(N)}$ with the two remarkable relations

\begin{align}
1\text{st nearest} & : v_0 + v_1 + \ldots + v_{N-1} = 0, \quad (a) \\
2\text{nd nearest} & : V_{ij} = v_i - v_j, \quad (b)
\end{align}

(1.1)

that respectively have interpretation in terms of the vector weights of the fundamental and the adjoint representations of $su(N)$.

Recall that the weight vectors $\mu_i$ (resp. $\beta_{ij} = \mu_i - \mu_j$) of the complex N dimensional fundamental (resp. adjoint) representations of $su(N)$ obey the following relations

\begin{align}
\text{fundamental} & : \mu_0 + \mu_1 + \ldots + \mu_{N-1} = 0, \quad (a) \\
\text{adjoint} & : \beta_{ij} = \mu_i - \mu_j \quad (b)
\end{align}

(1.2)

which are analogous to (1.1) and so solve them by taking $v_i = a \mu_i$ and $V_{ij} = a \beta_{ij}$ with constant $a$ to be interpreted later on.

Notice that the constraint eqs $\mu_0 + \mu_1 + \ldots + \mu_{N-1} = 0$ and similarly $\sum \beta_{ij} = 0$ are also
important from the physical side since they are interpreted in terms of the conservation of total momentum of the outgoing and incoming waves at each site of $\mathcal{L}_{su(N)}$

$$p_1 + \ldots + p_{N-1} + p_0 = 0 \quad .$$

(2) the hamiltonian $\mathcal{H}_{su(N)}$

Denoting by $F_{\mu_i}$ (resp. $G_{\beta_{ij}}$) the field operators generating the hops of the particles/holes between the site $r_m$ and $r_m + v_i$ (resp. $r_m + V_{ij}$), the proposed hamiltonian $\mathcal{H}_{su(N)}$ describing the quantum state couplings up to second nearest neighbors on $\mathcal{L}_{su(N)}$ reads as follows,

$$\mathcal{H}_{su(N)} = -t_1 \left( \sum_{\text{weights of fund of } su(N)} F_{\mu_k} +hc \right) - t_2 \left( \sum_{\text{roots } su(N)} G_{\beta_{ij}} +hc \right)$$

(1.4)

where the $t_1$, $t_2$ are hop energies. The fermionic field realizations of $F_{\mu_k}$, $G_{\beta_{ij}}$ are given by eqs[2.19].

The proposed $\mathcal{H}_{su(N)}$ depends on the $su(N)$ algebra representation quantities namely the weight vectors $\mu_i$ of the fundamental of $su(N)$ and its roots $\beta_{ij}$. This property leads a priori to an energy spectrum of $\mathcal{H}_{su(N)}$ completely characterized by the wave vector $k$, the weights $\mu_i$ and the roots $\beta_{ij}$; but as we will see the $\mu_i$ dependence is implicit and appears only through the roots. Such results are also shown to extend naturally to the $so(2N)$ lattice models.

The presentation is as follows: In section 2, we develop our proposal for the case of lattice models based on $su(N)$ Lie algebras. In section 3, we consider the $su(2)$ and $su(3)$ models describing respectively the electronic properties of the acetylene chain and graphene. In section 4, we deepen the $su(4)$ lattice model and in section 5 we give conclusion and further comments regarding DE extension.

2 The proposal: $su(N)$ model

In this section, we develop our proposal by first building the real lattice $\mathcal{L}_{su(N)}$ that is associated with the hamiltonian (1.4) refered to as the $su(N)$ lattice model. Then, we give a QFT realization of the field operators $F_{\mu_i}$ and $G_{\beta_{ij}}$ using free fermionic fields on $\mathcal{L}_{su(N)}$. We also give the energy dispersion $\varepsilon_{su(N)}(k)$ relation in terms of the wave vector $k$, the weights $\mu_i$ and the roots $\beta_{ij}$.
2.1 Building the lattice \( \mathcal{L}_{su(N)} \)

The lattice \( \mathcal{L}_{su(N)} \) is a real \((N-1)\)-dimensional crystal with two superposed integral sublattices \( A_{su(N)} \) and \( B_{su(N)} \); each site \( r_m \) of these sublattices is generated by the \( su(N) \) simple roots \( \alpha_1, \ldots, \alpha_{N-1} \);

\[
    r_m = \sum_{m_1, \ldots, m_{N-1}} m_1 \alpha_1 + m_2 \alpha_2 + \ldots m_{N-1} \alpha_{N-1},
\]

(2.1)

with \( m_i \) integers; for illustration see the schema (a), (b), (c) of the figure (1) corresponding respectively to \( N = 2, 3, 4 \) and which may be put in one to one with the \( sp^1 \), \( sp^2 \) and \( sp^3 \) hybridization of the carbon atom orbitals 2s and 2p.

![Figure 1: (a) 1A+2B lattice sites of \( \mathcal{L}_{su(2)} \); A-type in blue and B-type in red; the 2B form a \( su(2) \) doublet. (b) 1A+3B sites of \( \mathcal{L}_{su(3)} \); the 3B form a \( su(3) \) triplet. (c) 1A+4B sites of \( \mathcal{L}_{su(4)} \) with 4B sites forming a regular tetrahedron.](image)

On each lattice site \( r_m \) of \( \mathcal{L}_{su(N)} \); say of A-type, lives a quantum state \( A(r_m) \) coupled to the nearest neighbor states; in particular the first nearest states \( B(r_m + v_i) \) and the second nearest ones \( A(r_m + V_{ij}) \). Generally, generic sites in \( \mathcal{L}_{su(N)} \) have the following properties:

(1) \( N \) first nearest neighbors with relative position vectors \( v_i \) constrained as

\[
    v_0 + v_1 + \ldots + v_{N-1} = 0,
\]

(2.2)

or equivalently

\[
    -v_0 - v_1 - \ldots - v_{N-1} = 0,
\]

(2.3)

respectively related with the fundamental \( \mathbf{N} \) and anti-fundamental \( \mathbf{\bar{N}} \) representations of \( su(N) \). Indeed, by using \( (1.2\text{-a}) \), these constraint relations are solved in terms of the \( su(N) \) weight vectors \( \mu_i \) (resp. \( -\mu_i \)) of the fundamental (anti-fundamental) representation as follows

\[
    v_i = a \mu_i \equiv d \frac{\mu_i}{||\mu||},
\]

(2.4)
where $d$ is the relative distance between the closest $\mathcal{L}_{su(N)}$ sites. From the QFT view, this means that the quantum states at $r_m + v_i$ sites are labeled by the $\mu_i$ weights as

$$B(r_m + v_i) \equiv B_{\mu_i}(r_m)$$

and so the multiplet

$$\begin{pmatrix} |B_{\mu_0}> \\ \vdots \\ |B_{\mu_{N-1}}> \end{pmatrix}$$

transform in the fundamental representation of $su(N)$ and its conjugate in the anti-fundamental.

(2) $N(N-1)$ second nearest neighbors of A-type with relative position vectors $V_{ij}$ given by eq(1.1-b) and obeying the constraint relation,

$$\sum_{i,j} V_{ij} = 0$$

This condition is naturally solved by (1.2-a) and (2.4) showing that the relative vectors between second nearest neighbors are proportional to $su(N)$ roots $\beta_{ij}$ like

$$V_{ij} = a\beta_{ij}, \quad \beta_{ij} = \mu_i - \mu_j$$

and so the condition (2.7) turns to a $su(N)$ property on its adjoint representation labeled by the roots.

### 2.2 More on $\mathcal{L}_{su(N)}$

To get more insight into the structure of the lattice $\mathcal{L}_{su(N)}$, it is useful to recall some basic results on $su(N)$ [31].

This algebra has $\frac{N(N-1)}{2}$ positive roots $\beta_{ij}$ with $i > j$, which we denote collectively as $+\beta$, and $\frac{N(N-1)}{2}$ negative ones $-\beta$ so that the sum on the total roots is zero

$$\sum_{\text{positive roots}} \beta + \sum_{\text{negative roots}} \beta = 0$$

This property which captures (2.7) is precisely the analog of eq(1.1-a) for the case of the the adjoint representation of $su(N)$.

Moreover, the $\pm\beta$ roots have same length $\beta^2 = 2$ and are given by positive/negative integral combinations of the $(N-1)$ simple roots $\alpha_1, ..., \alpha_{n-1}$

$$\pm\beta = \pm \sum_i l_i \alpha_i, \quad l_i \in \mathbb{Z}_+$$
Notice that the simple roots $\alpha_i$ are basic objects in Lie algebras; they capture several information. In particular, they allow to define the fundamental weight vectors $\lambda_i$ obeying
\[ \lambda_i, \alpha_j = \delta_{ij} \] (2.11)
and give as well the intersection matrix
\[ K_{ij} = \frac{2(\alpha_i, \alpha_j)}{(\alpha_i, \alpha_i)} = \alpha_i, \alpha_j \] (2.12)
encoding all data on the Lie algebra properties of $su(N)$. This matrix is real symmetric reading as,
\[
\begin{pmatrix}
2 & -1 & 0 & \cdots & 0 & 0 \\
-1 & 2 & -1 & 0 & 0 \\
0 & -1 & 2 & 0 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & 0 & 2 & -1 \\
0 & 0 & 0 & \cdots & -1 & 2
\end{pmatrix}_{r \times r},
\]
with rank $r = (N - 1)$.
Notice also that $su(N)$ has $(N^2 - 1)$ dimensions generated by $r$ commuting Cartan operators $h^1, ..., h^r$ giving the charge vectors of the $su(N)$ states; and by the step ones $E^{\pm \beta}$ allowing to hop between the states of the representation. These operators obey the commutation relations,
\[
\begin{align*}
[h^i, h^j] &= 0 \\
[h^i, E^\beta] &= \beta^i E^\beta \\
[E^{-\beta}, E^\beta] &= \frac{2}{\beta^2} \beta^i h \\
[E^\alpha, E^\beta] &= \varepsilon_{\alpha \beta} E^{\alpha + \beta} \quad \text{if } \alpha + \beta \text{ is a root}
\end{align*}
\] (2.14)
and are used to construct highest weight state representation (HWR) with highest state $|\phi_\lambda>$ and highest weight vector (dominant weight) $\lambda$ solving the following constraint relations
\[
\begin{align*}
E^{+\beta}|\phi_\lambda> &= 0 \\
h^i|\phi_\lambda> &= \lambda^i|\phi_\lambda>
\end{align*}
\] (2.15)
The other $(N - 1)$ states $|\phi_\mu>$ of the representation are obtained by successive actions on $|\phi_\lambda>$ by the typical monomials $E^{-\beta_m} \cdots E^{-\beta_2} E^{-\beta_1}$.
One of these HWRs is precisely the N dimensional fundamental representation we are interested in here; it has $N$ states,
\[
\begin{pmatrix}
F_{\mu_0} \\
F_{\mu_1} \\
\vdots \\
F_{\mu_{N-1}}
\end{pmatrix},
\] (2.16)
with weight vectors
\[ \mu_i = \lambda - \sum_{l=1}^{i} \beta_l , \] (2.17)
satisfying (1.4a) with \( \mu_0 = \lambda \); and from which we learn that
\[ \mu_{i+1} - \mu_i , \] (2.18)
is indeed an \( su(N) \) root. For an illustration of (2.17); see the explicit analysis regarding the \( su(4) \) lattice model; in particular eq (1.14).

2.3 Fermionic realization of \( \mathcal{H}_{su(N)} \)

Denoting by \( A_{\mathbf{r}_m}^{\pm} \) (resp. \( B_{\mathbf{r}_m + \mathbf{v}_i}^{\pm} \)) the local fermionic creation and annihilation operators satisfying the usual anticommutation relations, the hamiltonian on \( \mathcal{L}_{su(N)} \) reads as in (1.4) with \( F_{\mu_i} \) and \( G_{\beta} \) operators given by
\[
F_{\mu_i} = \sum_{\mathbf{r}_m \in A_{su(N)}} A_{\mathbf{r}_m}^{-} B_{\mathbf{r}_m + a\mu_i}^{+} , \\
G_{\beta} = \sum_{\mathbf{r}_m \in A_{su(N)}} \left( A_{\mathbf{r}_m}^{-} A_{\mathbf{r}_m + b\beta}^{+} + B_{\mathbf{r}_m}^{-} B_{\mathbf{r}_m + b\beta}^{+} \right) ,
\] (2.19)
where \( \mu_i \) are the weight vectors of the fundamental representation of \( su(N) \) and \( \beta \) a generic root. Notice that the operators \( F_{\mu_i} \) and its adjoint \( F_{\mu_i}^\dagger \) transform respectively in the fundamental representation and its complex conjugate
\[
F_{\mu_i} \sim N , \quad F_{\mu_i}^\dagger \sim \bar{N} .
\] (2.20)

By using Fourier transform of the field operators \( A_{\mathbf{r}_m}^{\pm} \) and \( B_{\mathbf{r}_m + \mathbf{v}_i}^{\pm} \) namely,
\[
A_{\mathbf{r}_m}^{\pm} \sim \sum_{\text{wave vectors } \mathbf{k}} e^{\pm i \mathbf{k} \cdot \mathbf{r}_m} \tilde{A}(\mathbf{k}) , \\
B_{\mathbf{r}_m + \mathbf{v}_i}^{\pm} \sim \sum_{\text{wave vectors } \mathbf{k}} e^{\pm i \mathbf{k} \cdot (\mathbf{r}_m + \mathbf{v}_i)} \tilde{B}(\mathbf{k})
\] (2.21)
we can put the hamiltonian \( \mathcal{H}_{su(N)} \) like the sum over the \((N-1)\)-dimensional wave vectors \( \mathbf{k} \) as follows,
\[
\sum_{\text{wave vectors } \mathbf{k}} \tilde{H}_{\mathbf{k}}^{su(N)} ,
\] (2.22)
where \( \tilde{H}_{\mathbf{k}}^{su(N)} \) has dispersion relations depending, in addition to \( \mathbf{k} \), on the weights \( \mu_i \), the roots \( \beta \) and the hop energies \( t_1, t_2 \). In the particular case where \( t_2 \) is set to zero; the hamiltonian (1.4) reduces to the leading term
\[
\mathcal{H}_{su(N)}^1 = -t_1 \left( \sum_{\text{weights } \mu_i} F_{\mu_i} + hc \right) ,
\] (2.23)
and its dual Fourier transform simplifies as follows,

\[ \tilde{H}_k^{su(N)} = (\tilde{A}_k, B_k) \begin{pmatrix} 0 & \varepsilon_{su(N)}(k) \\ \varepsilon_{su(N)}(k) & 0 \end{pmatrix} \begin{pmatrix} A^+ \\ B^+ \end{pmatrix} \]  

(2.24)

with

\[ \varepsilon_{su(N)}(k) = \sum_{\text{weight vectors } \mu_i} e^{iak_i \cdot \mu_i} \]  

(2.25)

From these relations, we can compute the dispersion energies of the "valence" and "conducting" bands by diagonalizing \( \tilde{H}_k^{su(N)} \). These energies are given by

\[ \pm |\varepsilon_{su(N)}(k)| \]  

with

\[ |\varepsilon_{su(N)}(k)| = t_1 \sqrt{N + 2 \sum_{i<j=0}^{N-1} \cos [a \cdot (\mu_i - \mu_j)]} \]  

(2.26)

Notice that \( |\varepsilon_{su(N)}(k)| \) depends remarkably in the difference of the weights \( \mu_i - \mu_j \); which according to (2.10) is just the sum over \( su(N) \) roots \( \sum_{i=1}^j \beta_i \) with \( \beta_i = \mu_i - \mu_{i+1} \). It follows then that dispersion energies for the first nearest neighbors depend on the wave vector \( k \) and the roots of \( su(N) \).

\[ |\varepsilon_{su(N)}(k)| = t_1 \sqrt{N + 2 \sum_{i<j=0}^{N-1} \cos \left( a \sum_{j=1}^N k \cdot \beta_i \right)} \]  

(2.27)

This result is expected from group theory view since \( |\varepsilon_{su(N)}|^2 = \varepsilon_{su(N)} \bar{\varepsilon}_{su(N)} \) should be put in correspondence with the tensor product of the fundamental representation \( N \) and its complex conjugate \( \bar{N} \)

\[ N \otimes \bar{N} = I_{id} \oplus \text{adj}_{SU(N)} \]  

(2.28)

giving the adjoint representation of \( U(N) \simeq U(1) \times SU(N) \).

Notice finally that eq (2.27) may be further explicated by first expressing \( \beta_i \) in terms of simple roots as in (2.10); that is \( \beta_i = \sum_{m=1}^{N-1} M_{ni} \alpha_m \) with \( M_{ni} \) integers. Then expand the wave vector as \( k = \sum_{n=1}^{N-1} q_n \lambda_n \) with \( q_n \) real number; and use (2.11) to put (2.27) in the following handleable form

\[ |\varepsilon_{su(N)}(k)| = t_1 \sqrt{N + 2 \sum_{i<j=0}^{N-1} \cos \left( a \sum_{j=1}^N \sum_{l=1}^{N-1} n q_n M_{nl} \right)} \]  

(2.29)

Below, we consider explicit examples.

### 3 Leading \( su(N) \) lattice models

In this section, we illustrate the above study on the leading examples \( N = 2, 3 \). These two lattice models describe the electronic properties of the delocalized electrons in the infinite acetylene type chain and graphene.
3.1 the $su(2)$ model

In this case, the lattice $L_{su(2)}$ depicted in the figure (2) is a one dimensional chain with coordinate positions $x_m = ma$ where $a$ is the site spacing and $m$ an integer.

![Figure 2](image-url) 

Figure 2: the lattice $L_{su(2)}$ given by the superposition of two sublattices $A_{su(2)}$ (in blue) and $B_{su(2)}$ (in red). The atoms may be thought of as carbons in the $sp^3$ hybridization state.

Each site of $L_{su(2)}$ has two first nearest neighbors forming an $su(2)$ doublet; and two second nearest ones associated with the two roots $\pm \alpha$ of $su(2)$ in agreement with the generic result summarized in the table,

| nearest neighbors | $su(N)$ | $su(2)$ | $su(3)$ | $su(4)$ |
|-------------------|---------|---------|---------|---------|
| first             | $N$     | 2       | 3       | 4       |
| second            | $N(N-1)$| 2       | 6       | 12      |

(3.1)

In this $N = 2$ model, eqs(1.1) read as

$$v_0 + v_1 = 0 \quad , \quad (a)$$
$$V_{01} = v_0 - v_1 \quad , \quad (b)$$

(3.2)

and are solved by the fundamental weights $\mu_0 = +\frac{1}{2}$, $\mu_1 = -\frac{1}{2}$ of the $su(2)$ fundamental representation; i.e the isodoublet.

The hamiltonian $H_{su(2)}$ of this model is given by

$$H_{su(2)} = -t_1 \left( F_{+\frac{1}{2}} + F_{-\frac{1}{2}} + hc \right) - t_2 \left( G_{+1} + G_{-1} + hc \right) .$$

(3.3)

where $t_1$ and $t_2$ are hop energies. The fermionic field realization of the $F_{\pm \frac{1}{2}}$ and $G_{\pm 1}$ operators read in terms of the creation and annihilation $A_{x_m}^\pm, B_{x_m}^\pm$ as follows

$$F_{\pm \frac{1}{2}} = \sum_m A_{x_m}^- B_{x_m, \pm a}^+, \quad G_{\pm 1} = \sum_m \left( A_{x_m, \pm 2a}^- A_{x_m, \pm 2a}^+ + B_{x_m}^- B_{x_m, \pm 2a}^+ \right) .$$

(3.4)

Moreover, substituting $N = 2$ in (2.26), we get the dispersion energy

$$|\varepsilon_{su(2)}(k)| = t_1 \sqrt{2 + 2 \cos(2ak)}$$

(3.5)

which is also equal to $2t_1 \cos(ka)$ and from which we read that the $|\varepsilon_{su(2)}(k)|$ zeros take place for the wave vectors $k_n = \pm \frac{\pi}{2a} \mod \frac{2\pi}{a}$. 

9
3.2 the \( su(3) \) model and graphene

The lattice \( \mathcal{L}_{su(3)} \) is precisely the 2D honeycomb of graphene; it is given by the superposition of two sublattices \( \mathcal{A}_{su(3)} \) and \( \mathcal{B}_{su(3)} \) as in the figure (3).

![Image](image_url)

Figure 3: sublattices A (in blue) and B (in red) of the honeycomb. The atoms may be thought of as carbons in the \( sp^2 \) hybridization state.

Each site \( r_m \) in \( \mathcal{L}_{su(3)} \) has 3 first nearest neighbors with relative vectors \( v_i \); and 6 second neighbors \( \pm V_{ij} = \pm \varepsilon_{ijk} V_k \) in one to one correspondence with the vector weights of the \( su(3) \) fundamental representation and its roots. We have

\[
v_i = a \mu_i \quad \text{and} \quad \pm V_i = \pm a \alpha_i,
\]

where \( a = d \sqrt{\frac{3}{2}} \). To fix the ideas, we give below the explicit expressions of the weight vectors \( \mu_1, \mu_2, \mu_0 \) and the roots \( \alpha_1, \alpha_2, \alpha_3 \),

\[
\begin{align*}
\mu_1 &= \left( \frac{\sqrt{2}}{2}, \frac{\sqrt{6}}{2} \right), \\
\mu_2 &= \left( -\frac{\sqrt{2}}{2}, \frac{\sqrt{6}}{2} \right), \\
\mu_0 &= -\left( 0, \frac{\sqrt{6}}{2} \right), \\
\alpha_1 &= \left( \sqrt{\frac{5}{2}}, 0 \right), \\
\alpha_2 &= \left( -\sqrt{\frac{5}{2}}, \frac{\sqrt{6}}{2} \right), \\
\alpha_3 &= \left( \sqrt{\frac{5}{2}}, \frac{\sqrt{6}}{2} \right),
\end{align*}
\]

from which we learn that \( \alpha_3 = \alpha_1 + \alpha_2 \) as it should be. In addition to the feature \( \mu. \alpha \in \mathbb{Z} \), these vectors obey the constraint relations

\[
\sum_{i=0}^{2} v_i = 0 \quad \text{and} \quad \sum_{\text{positive roots}} \alpha + \sum_{\text{negative roots}} \alpha = 0
\]

(3.8)

together with the following remarkable relations

\[
\begin{align*}
\mu_0 - \mu_1 &= \alpha_3, \\
\mu_1 - \mu_2 &= \alpha_1, \\
\mu_2 - \mu_0 &= \alpha_2.
\end{align*}
\]

(3.9)

Substituting \( N = 3 \) in (2.26) and using the above equations, we get the dispersion energy

\[
|\varepsilon_{su(3)}(k)| = t_1 \sqrt{3} + 2 \left[ \cos a k. \alpha_1 + \cos a k. \alpha_2 + \cos a k. \alpha_3 \right],
\]

(3.10)

depending on the wave vector \( k = (k_x, k_y) \) and the \( su(3) \) roots.
4 the \( su(4) \) lattice model

To illustrate the general properties of the \( su(4) \) model; we first give some basic features on the connection between \( L_{su(4)} \), depicted by the figure 4, and the \( su(4) \) representations. Then, we develop a dynamical model based on the crystal \( L_{su(4)} \).

Figure 4: the lattice \( L_{su(4)} \) with sublattices \( A_{su(4)} \) (in blue) and \( B_{su(4)} \) (in red). Each atom has 4 first nearest neighbors, forming a tetrahedron, and 12 second nearest ones.

4.1 structure property of \( L_{su(4)} \)

The lattice \( L_{su(4)} \) is a 3-dimensional crystal; it is made by the superposition of two isomorphic, but shifted, sublattices \( A_{su(4)} \) and \( B_{su(4)} \) following the same logic as in the case of the honeycomb which may be recovered by projection on a 2D plane.

Each site \( r_m \) in \( L_{su(4)} \) has 4 first nearest neighbors at \( (r_m + v_i) \) forming the vertices of a regular tetrahedron. A way to parameterize the relative positions \( v_i \) with respect to the central position at \( r_m \) is to embed the tetrahedron inside a cube; in this case we have:

\[
\begin{align*}
    v_1 &= \frac{d}{\sqrt{3}} (-1, -1, +1) \quad , \quad v_2 = \frac{d}{\sqrt{3}} (-1, +1, -1) \\
    v_3 &= \frac{d}{\sqrt{3}} (+1, -1, -1) \quad , \quad v_0 = \frac{d}{\sqrt{3}} (+1, +1, +1)
\end{align*}
\] (4.1)

Clearly these vectors satisfy the constraint relation (1.1-a). Moreover, having these expressions, we can also build the explicit positions of the 12 second nearest neighbors; these are given by eq(1.1-b); but are completely generated by the following basis vectors

\[
\begin{align*}
    R_1 &= \frac{d}{\sqrt{3}} (2, 2, 0) \quad , \quad R_2 = \frac{d}{\sqrt{3}} (0, -2, 2) \quad , \quad R_3 = \frac{d}{\sqrt{3}} (-2, 2, 0)
\end{align*}
\] (4.2)

that are related to \( V_{ij} \) as follows,

\[
R_i = V_{(i-1)j} \] (4.3)
For later use, it is interesting to notice the two following:

(a) the \( \mathbf{R}_i \) vector basis have the following intersection matrix

\[
\mathbf{R}_i \cdot \mathbf{R}_j = \frac{4d^2}{3} \mathbf{K}_{ij}
\]  

(4.4)

with \( \mathbf{K}_{ij} \) and its inverse as

\[
\mathbf{K}_{ij} = \begin{pmatrix}
2 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 2
\end{pmatrix}, \quad \mathbf{K}_{ij}^{-1} = \frac{1}{4} \begin{pmatrix}
3 & 2 & 1 \\
2 & 4 & 2 \\
1 & 2 & 3
\end{pmatrix}
\]  

(4.5)

(b) using (4.1) and (4.2), it is not difficult to check the following special relation linking the \( \mathbf{R}_i \)'s and \( \mathbf{v}_0 \),

\[
\frac{5}{4} \mathbf{R}_1 + \frac{2}{4} \mathbf{R}_2 + \frac{1}{4} \mathbf{R}_3 = \mathbf{v}_0
\]  

(4.6)

In fact this relation is a \( su(4) \) Lie algebra property following from \( \mathbf{K}_{ij}^{-1} \) and (2.11).

Concerning the vector positions of the remaining 9 second neighbors, 3 of them are given by \( -\mathbf{R}_1, -\mathbf{R}_2, -\mathbf{R}_3 \) and the other 6 by the linear combinations

\[
+\mathbf{R}_4 = \mathbf{V}_{02} = +\mathbf{R}_1 + \mathbf{R}_2, \quad +\mathbf{R}_5 = \mathbf{V}_{13} = +\mathbf{R}_2 + \mathbf{R}_3 \\
-\mathbf{R}_4 = \mathbf{V}_{20} = -\mathbf{R}_1 - \mathbf{R}_2, \quad -\mathbf{R}_5 = \mathbf{V}_{31} = -\mathbf{R}_2 - \mathbf{R}_3 \\
+\mathbf{R}_6 = \mathbf{V}_{03} = +\mathbf{R}_1 + \mathbf{R}_2 + \mathbf{R}_3, \quad -\mathbf{R}_6 = \mathbf{V}_{30} = -\mathbf{R}_1 - \mathbf{R}_2 - \mathbf{R}_3
\]  

(4.7)

From this construction, it follows that generic positions \( \mathbf{r}_m^A \equiv \mathbf{r}_m \) and \( \mathbf{r}_m^B \) in the \( \mathcal{A}_{su(4)} \) and \( \mathcal{B}_{su(4)} \) sublattices are given by

\[
\mathcal{A}_{su(4)} : \quad \mathbf{r}_m^A = m_1 \mathbf{R}_1 + m_2 \mathbf{R}_2 + m_3 \mathbf{R}_3, \\
\mathcal{B}_{su(4)} : \quad \mathbf{r}_m^B = \mathbf{r}_m + \mathbf{v}
\]  

(4.8)

where \( \mathbf{m} = (m_1, m_2, m_3) \) is an integer vector and where the shift vector \( \mathbf{v} = \mathbf{r}_m^B - \mathbf{r}_m^A \) is one of \( \mathbf{v}_i \)'s in (4.1).

Regarding the connection between \( \mathcal{L}_{su(4)} \) and the \( su(4) \) Lie algebra representations, we distinguish two kinds of relations:

(1) a relation involving the roots

From (4.4), it follows that the basis vectors \( \mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3 \) may be interpreted in terms of the simple roots \( \alpha_1, \alpha_2, \alpha_3 \) of the \( su(4) \) Lie algebra. More precisely, we have

\[
\mathbf{R}_1 = \frac{2d}{\sqrt{3}} \alpha_1, \quad \mathbf{R}_2 = \frac{2d}{\sqrt{3}} \alpha_2, \quad \mathbf{R}_3 = \frac{2d}{\sqrt{3}} \alpha_3
\]  

(4.9)

from which we learn that the matrix \( K_{ij} = \alpha_i \cdot \alpha_j \) is indeed the Cartan matrix of \( su(4) \).

We also have the following relations showing that the position vectors of the second nearest neighbors are indeed in one to one correspondence with the roots of \( su(4) \),

\[
\mathbf{R}_4 = \frac{2d}{\sqrt{3}} (\alpha_1 + \alpha_2), \quad \mathbf{R}_5 = \frac{2d}{\sqrt{3}} (\alpha_2 + \alpha_3), \quad \mathbf{R}_6 = \frac{2d}{\sqrt{3}} (\alpha_3 + \alpha_1)
\]  

(4.10)
together with their opposites.

(1) a relation involving the fundamental representation of \(su(4)\)

As described for the generic \(su(N)\), the four relative vectors \(v_i\) are, up to a global scale factor, nothing but the four weight vectors \(\mu_i\) of the fundamental representation of \(su(4)\). The highest weight \(\lambda\) of this representation, which we set as \(\mu_0\), is precisely given by eq.(4.6). Thus, we have

\[
v_0 = \frac{2d}{\sqrt{3}} \mu_0, \quad v_1 = \frac{2d}{\sqrt{3}} \mu_1, \quad v_2 = \frac{2d}{\sqrt{3}} \mu_2, \quad v_3 = \frac{2d}{\sqrt{3}} \mu_3 \tag{4.11}
\]

that obey obviously the constraint relation

\[
\mu_0 + \mu_1 + \mu_2 + \mu_3 = 0 \tag{4.12}
\]

This constraint equation is a typical vector relation for highest weight representations of Lie algebras; it extends the well known \(su(2)\) ones whose leading terms are

\[
\begin{array}{c|c}
\text{sum over weights} & \text{su(2)} \\
\hline
\text{doublet} & \frac{1}{2} - \frac{1}{2} = 0 \\
\text{triplet} & 1 + 0 - 1 = 0 \\
\text{quartet} & \frac{3}{2} + \frac{1}{2} - \frac{3}{2} - \frac{1}{2} = 0
\end{array}
\tag{4.13}
\]

To exhibit more explicitly the constraint relation \((4.12)\), it is interesting to express the weight vectors \(\mu_i\) in terms of the simple roots of \(su(4)\). We have

\[
\begin{align*}
\mu_0 &= \frac{3}{4} \alpha_1 + \frac{2}{4} \alpha_2 + \frac{1}{4} \alpha_3 \\
\mu_1 &= -\frac{1}{4} \alpha_1 + \frac{2}{4} \alpha_2 + \frac{1}{4} \alpha_3 \\
\mu_2 &= -\frac{1}{4} \alpha_1 - \frac{2}{4} \alpha_2 + \frac{1}{4} \alpha_3 \\
\mu_3 &= -\frac{1}{4} \alpha_1 - \frac{2}{4} \alpha_2 - \frac{3}{4} \alpha_3
\end{align*}
\tag{4.14}
\]

This analysis teaches us as well two basic things:

First the number \(N_1\) of the first nearest neighbors in the lattice \(L_{su(4)}\) is related to the dimension of the fundamental representation of \(su(4)\)

\[
N_1 = \dim (4) = 4 \tag{4.15}
\]

This means that the QFT on this lattice should capture some data on \(su(4)\).

Second, the number \(N_2\) of the second nearest neighbors in \(L_{su(4)}\) is also related to a \(su(4)\) quantity namely,

\[
N_2 = \dim [su(4)] - \text{rank } [su(4)] = 15 - 3 \tag{4.16}
\]

These two Lie algebra numbers may be used as an algorithm to extend this construction to the case of the \(so(2N)\) and the \(E_6, E_7, E_8\) exceptional simply laced Lie algebras.

13
4.2 dynamical vacancy on lattice: a toy model

We begin by noting that, as far as the electronic properties are concerned, the schemas (a), (b), (c) of figure (4.1) may be respectively associated with the $sp^1$, $sp^2$ and $sp^3$ hybridizations of the atom orbitals; i.e:

| figures | hybridization | example of molecules |
|---------|---------------|-----------------------|
| (4.1a)  | $sp^1$        | acetylene             |
| (4.1b)  | $sp^2$        | graphene              |
| (4.1c)  | $sp^3$        | diamond               |

In the two first examples, the atoms have delocalized pi-electrons that capture the electronic properties of the lattice atoms and have the following dispersion relation,

$$\left| \varepsilon_{su(N)}(k) \right| = t_1 \sqrt{N + 2 \sum_{i<j} \cos \left[ a \mathbf{k}. (\mu_i - \mu_j) \right]}$$

with $N = 2, 3$.

In the case of $sp^3$, the atoms have no delocalized pi-electrons; they only have strongly correlated sigma-electrons which make the electronic properties of systems based on $L_{su(4)}$ different from those based on $L_{su(3)}$ and $L_{su(2)}$.

However, as far as tight binding model idea is concerned, one may consider other applications; one of which concerns the following toy model describing a system based on the lattice $L_{su(4)}$ with dynamical vacancy sites.

**Toy model**

This is a lattice QFT on the $L_{su(4)}$ with dynamical particles and vacancies. The initial state of the system correspond to the configuration where the sites of the sublattice $A_{su(4)}$ are occupied by particles and those of the sublattice $B_{su(4)}$ are unoccupied.

| sublattice | initial configuration | quantum state |
|------------|-----------------------|---------------|
| $A_{su4}$  | particles at $r_m$    | $A(r_m)$      |
| $B_{su4}$  | vacancy at $r_m + \mathbf{v}$ | $B(r_m + \mathbf{v})$ |

Then, the particles (vacancies) start to move towards the neighboring sites with movement modeled by hop to first nearest neighbors.

Let $A(r_m)$ and $B(r_m + \mathbf{v}_i)$ be the quantum states describing the particle at $r_m$ and the vacancy at $r_m + \mathbf{v}_i$ respectively. Let also $A^\pm_{r_m}$ and $B^\pm_{r_m+\mu_i}$ be the corresponding creation and annihilation operators. The hamiltonian describing the hop of the vacancy/particle to the first nearest neighbors is given by

$$\mathcal{H}_{su4} = -t_1 \left( \sum_{i=0}^{3} A^-_{r_m} B^+_{r_m+\mu_i} + h.c \right)$$

(4.20)
where the \( \mu_i \)'s are the weight vectors of the fundamental of \( su(4) \). By performing Fourier transforms of the \( A^\pm_{r_m}, B^\pm_{r_m+\mu_i} \) field operators, we end with the dispersion energy

\[
|\varepsilon_{su4}(k)| = t_1 \sqrt{4 + 2 \sum_{i<j} \cos (k, \mathbf{V}_{ij})},
\]

with \( \mathbf{V}_{ij} \) as in (4.6-4.7). This relation depends on the wave vector \( k = (k_x, k_y) \) and the \( su(4) \) roots.

5 Conclusion and comments

In the present paper, we have used TBM to engineer a board class of systems that are based on \( su(N) \) Lie algebras and their basic representations. These engineered systems classify the acetylene chain and graphene as \( su(2) \) and \( su(3) \) models respectively. Our construction may have other applications; in particular in QFT on non commutative geometry where space time is a lattice and in lattice QFT for condensed matter as exemplified by the dynamical vacancy/particle toy model introduced in subsection 4.2.

Our \( su(N) \) lattice models relies on the two following basic ingredients:

(1) the \( N \) first nearest neighbors in \( L_{su(N)} \) with positions \( \mathbf{v}_i = a\mu_i \) and wave functions \( \phi_{\mu_i}(r_m) \) transform in the fundamental representation of \( su(N) \). The \( \mathbf{v}_i \)'s and the weight vectors \( \mu_i \) are as in eqs (1.1-a, 1.2-a).

(2) the \( N(N-1) \) second nearest neighbors in \( L_{su(N)} \) with positions \( \mathbf{V}_{ij} = \mathbf{v}_i - \mathbf{v}_j \) are, up to a global scale factor, given by the \( N(N-1) \) roots \( \beta_{ij} \) of \( su(N) \).

Using these features, we have constructed a \( su(N) \) lattice model with hamiltonian \( H_{su(N)} \) (1.4); it involves operator fields \( F_{\mu_i} \) and \( G_{\beta} \) transforming respectively in the fundamental and adjoint representations of \( su(N) \). This symmetry captures basic data on the energy spectrum of \( H_{su(N)} \) as shown by the dispersion energy given by the formulae (2.26-2.27).

Our proposal may be extended to the other DE simply laced Lie algebras. In the case of \( D_N \sim so(2N) \) for instance, the lattice \( L_{so(2N)} \) is N-dimensional generated by the simple roots \( \alpha_1, \ldots, \alpha_N \) with matrix intersection

\[
\alpha_i \cdot \alpha_j = \begin{pmatrix}
2 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\
-1 & 2 & -1 & \cdots & 0 & 0 & 0 & 0 \\
0 & -1 & 2 & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 2 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 2 & -1 & -1 & 0 \\
0 & 0 & 0 & \cdots & 0 & -1 & 2 & -1 \\
0 & 0 & 0 & \cdots & 0 & -1 & -1 & 2
\end{pmatrix}
\] (5.1)
Here also, the $L_{\text{so}(2N)}$ lattice is made by the superposition of two sublattices $A_{\text{so}(2N)}$ and $B_{\text{so}(2N)}$. For each site at $r_m$, we have $2N$ first nearest neighbors at $r_m + v_I$ with relative vectors $v_I$, which may be split as,

$$v_i, \quad v_{i+N} = -v_i, \quad 1 \leq i \leq N,$$

satisfying the following constraint relation

$$\sum_{I=1}^{2N} v_I = N \sum_{i=1}^{N} (v_i + v_{i+N}) = 0$$

which extend the su($N$) one given by (1.1-a). In the example of so(6), the first nearest neighbors form an octahedron as depicted in figure (5).

Figure 5: the lattice $L_{\text{so}(6)}$; each (blue) atom has 6 first nearest neighbors constituting an octahedron and transforming in the vector representation of so(6).

The relative vectors $v_I$ transform in the $2N$ vector representation of so(2N); they allow to define the second nearest neighbors by help of (1.1-b) which reads in the so(2N) case as follows

$$V_{IJ} = \begin{cases} \pm (v_i - v_j) \\ \pm (v_i + v_j) \end{cases}$$

These $V_{IJ}$’s should be put in one to one correspondence with the $2N (N-1)$ roots of so(2N). Recall that so(2N) is $N (2N -1)$- dimensional and has rank $N$; that is $N$ simple roots $\alpha_i$ which read in terms of the weight vectors of the $2N$ representation like $\alpha_i = \mu_i - \mu_{i+1}$ and $\alpha_N = \mu_{N-1} + \mu_N$. The generic roots are given by $\pm (\mu_i \pm \mu_j)$ with $1 \leq i, j \leq N$ and should be compared with (5.4). In the end notice that the dispersion energy for the first nearest couplings reads as

$$\varepsilon_{\text{so}(2N)}(k) = t_1 \sqrt{2N + 2 \sum_{i<j=0}^{N} \cos [ak \cdot (\mu_i - \mu_j)] + 2 \sum_{i<j=0}^{N} \cos [ak \cdot (\mu_i + \mu_j)]}$$
and, like in the $su(N)$ case (2.20), it also depends on the $so(2N)$ roots $\beta_{ij} = \mu_i \pm \mu_j$.

We end this conclusion by making one more comment concerning some related works on fermions living on a 4d hyperdiamond lattice $\mathcal{H}_4$ which has been used in lattice QCD [32]; see also [33]-[36] for extensions. It is interesting to note that the 4d hyperdiamond lattice $\mathcal{H}_4$ used in [32] is precisely $L_{su(5)}$; and the higher dimensional diamonds $\mathcal{H}_N$ given in [33] are exactly the $L_{su(N+1)}$ lattices we have discussed in section 2. Moreover, several features obtained for the $N$-dimensional hyperdiamond $\mathcal{H}_N$ with $N \geq 2$ are just algebraic relations on the weight and root systems of the $su(N+1)$ Lie algebra with discrete symmetries generated by Weyl group transformations given by the $S_{N+1}$ permutation group. This is the case for instance of the remarkable relation,

$$\cos \vartheta_{ij} = \frac{\langle \hat{a}_i, a_j \rangle}{\|a_i\| \|a_j\|} = \frac{1}{2}, \quad i \neq j = 1, ..., N,$$

(5.6)

derived in [33] where $\vartheta_{ij} = \langle \hat{a}_i, a_j \rangle$ are the angles between the primitive vectors $a_i = e_i - e_5$ of the lattice $\mathcal{H}_N$ and where the $a_i$'s stand for the generators of the sublattices $A_N$ (resp. $B_N$) of the $N$-dimensional hyperdiamond $\mathcal{H}_N$. Notice that eq(5.6) is independent on lattice dimension and on the orientation of the primitive vectors. A way to prove the universality of this relation is to relate it with basic relations of Lie algebras. A lengthy, but straightforward, analysis shows that the 5 bond vectors $e_i$ and the 4 primitive $a_i$ used in [32] are respectively related to the 5 weight vectors $\mu_i$ of the fundamental representation of $su(5)$ and its 4 simple roots $\alpha_i$ as follows

$$e_i = \frac{\sqrt{5}}{2} \mu_i, \quad \mu_i \cdot \mu_i = \frac{4}{5}, \quad \mu_i \cdot \mu_j = -\frac{1}{5},$$

(5.7)

and

$$a_1 = -\frac{\sqrt{5}}{2} \alpha_1$$
$$a_2 = -\frac{\sqrt{5}}{2} (\alpha_1 + \alpha_2)$$
$$a_3 = -\frac{\sqrt{5}}{2} (\alpha_1 + \alpha_2 + \alpha_3)$$
$$a_4 = -\frac{\sqrt{5}}{2} (\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4)$$

(5.8)

From these realizations, the constraint equation $\sum e_i = 0$ corresponds to the property $\sum \mu_i = 0$; see also (1.2). Moreover eq(5.6) can be read in terms of the $su(5)$ Cartan matrix $K_{ij} = \frac{2\alpha_i \alpha_j}{\alpha_i \alpha_j}$.

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