Weighted Graph Theory Representation of Quantum Information Inspired by Lie Algebras

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Abstract

Borrowing ideas from the relation between simply laced Lie algebras and Dynkin diagrams, a weighted graph theory representation of quantum information is addressed. In this way, the density matrix of a quantum state can be interpreted as a signless Laplacian matrix of an associated graph. Using similarities with root systems of simply laced Lie algebras, one-qubit theory is analyzed in some details and is found to be linked to a non-oriented weighted graph having two vertices. Moreover, this one-qubit theory is generalized to $n$-qubits. In this representation, quantum gates correspond to graph weight operations preserving the probability condition. A speculation from string theory, via D-brane quivers, is also given.

Keywords: Graph Theory; Laplacian Matrix; Density Matrix; Quantum Gates; Dynkin Diagram; Cartan Matrix.
1 Introduction

Quantum information combines computer science and quantum mechanics. It has been remarked that such a combination can be explored to produce computers operating according to quantum mechanics providing fast calculations and simulations using the properties of quantum bits. For these reasons, quantum information theory has been extensively investigated in connections with quantum algorithms and communication protocols [1,2]. This theory is based on quantum systems approached using mathematical backgrounds dealing with density matrices and operators associated with tensor-product of Hilbert vector spaces. These fundamental pieces are quite relevant in the discussion of interesting quantum phenomena including entanglement [3,4].

Recently, qubit systems have been studied using different approaches including string theory and related models [5,6,7,8]. These investigations have brought new understanding of the fundamental physics associated with qubits and their supersymmetric extensions. The latters are connected to many theories including D-branes, toric geometry and supermanifolds. More precisely, a nice interplay between the black holes and qubits have been discussed using higher dimensional supergravity models [5,6,9]. Alternative studies have been conducted using toric geometry and Adinkra graph theory [10,11]. This graph theory has been used in the study of the supersymmetric representation of quantum field theories. The corresponding graphs are formed by nodes associated with bosonic and fermionic degree of freedom. These graphs have been used to classify a class of qubit black holes [12]. Alternatively, a graphic representation has been also explored to approach quantum states using Seidel switching for weighted multidigraphs [13].

The aim of this work is to contribute to these activities by considering a weighted graph theory to represent basic pieces of quantum information. The present proposition can bring more features on quantum information operations. In fact, unitary evolutions will be displayed by modifications over their graph representations. Instead of performing quantum computations, the proposed graph representation allows one to encode qubit physical properties in terms of simple combinatorial data. This realization, which has similarities with quivers used in string theory, may permit to extract the essential on the qubit physics by simply knowing graph vertices and edges. Inspired by the relation between simply laced Lie algebras and Dynkin diagrams, we first interpret the corresponding density matrices as signless Laplacian matrices of weighted graphs. Borrowing ideas from root systems, we discuss one-qubit theory in some details and show that it is linked to two weighted vertices sharing similarities with $A_2$ quivers placed on singularities associated with D-brane physics. This one-qubit theory is generalized to $n$-qubits. Then, we reveal that the quantum gates correspond to graph weight operations preserving the probability condition. We finish with
speculations motivated by string theory and quivers.

The organization of this paper is as follows. In section 2, we present a weighted graph theory of one-qubit systems. Section 3 concerns a general discussion involving higher dimensional qubits. Operations on graph weights are explored in Section 4 to discuss universal quantum gates. Section 5 is devoted to open questions and speculation supported by string theory.

2 Graph theory representation of quantum states

In this section, we establish a rigorous correspondence between quantum states and weighted graph theory. The present approach is firstly inspired by Lie algebra structure and partly by the work given in [13] in which a quantum state is represented by its corresponding and identifying graph. In some related works, every vertex graph is considered to be a quantum state with the edge being the interaction between vertices. However, in the present paper, a quantum system is represented by a graph that is associated with a single element in the Hilbert space. The bridge employed here is the density matrix of a quantum state that is identified with the Signless Laplacian matrix of the corresponding graph.

2.1 Graph theory basics

In this subsection, we give a concise review on graph theory. More details can be found in [14] [15] [16]. Indeed, a graph is mathematically defined by a pair of sets $G = (V(G), E(G))$, where $V(G)$ denotes the vertex set and $E(G)$ corresponds the edge set. Two vertices are said adjacent if they are connected by an edge. For instance, if the vertices $i$ and $j$ are linked, the edge is indexed by $(i, j)$. The number of edges adjacent to a vertex is called its degree, and it is denoted by $d_G(v_i)$ where $v_i$ represents the vertex indexed by $i$. To a graph $G$ we associate a symmetric matrix called an adjacency matrix $M(G) = (m_{ij})$, whose elements are either 0 or 1. The adjacency matrix which provides connections between different vertices encodes all the information residing on the graph. These two different objects share the same data which can explored either in mathematics or physics including string theory and related quiver models. Roughly, the adjacency matrix is defined as follows

$$m_{ij} = \begin{cases} 1, & (i,j) \in E(G), \\ 0, & (i,j) \notin E(G). \end{cases}$$

(2.1)

It is recalled that the adjacency matrix $A(G)$ order is the cardinal of the vertices set $V(G)$ being the number of its elements. Besides the adjacency matrix, we also associate to a graph a diagonal matrix of the same order called the degree matrix $D(G)$. Its $i$-th diagonal element
is the degree of the \( i \)-th vertex of \( G \), with \( i = 1, 2, \ldots, |V| \), where \( |V| \) is the cardinal of the set \( V(G) \). In fact, it is given by

\[
d_{ij} = \begin{cases} 
    d_G(v_i), & \text{if } i = j, \\
    0, & \text{if } i \neq j.
\end{cases}
\]  

(2.2)

In graph theory, one can define the Laplacian matrix \( L(G) \) also called the admittance matrix by combining the degree matrix \( D \) and the adjacency matrix \( M \). It is defined as follows

\[
L(G) = D(G) - M(G).
\]  

(2.3)

In such a literature, we encounter various formulation of Laplacian matrix. For later use, we consider only the signless Laplacian matrix

\[
Q(G) = D(G) + M(G).
\]  

(2.4)

This matrix will be relevant in the forthcoming sections. More precisely, it will play a bridge between quantum information pieces and weighted graph theory.

### 2.2 Weighted graph of the density matrix

The standard formulation of quantum mechanics is based on the Hilbert space structures. Indeed, a quantum system state is an element of a \( r \)-dimensional Hilbert space \( \mathcal{H} \cong \mathbb{C}^r \). For such a state, one defines an \( r \times r \) positive semidefinite, trace-one, hermitian matrix, called density matrix. The latter gives a general description of a quantum state which will be represented by a graph encoding the corresponding quantum information.

Motivated by simply laced Lie algebras and Cartan matrices, the emphasis is put on the signless Laplacian matrix \( Q(G) \) which is positive, semidefinite and Hermitian matrix. It will be scaled by \( tr(Q(G)) \) being defined as follows

\[
\rho = \rho_{Q(G)} = \frac{Q(G)}{tr(Q(G))}.
\]  

(2.5)

### 2.3 Weighted graph theory representation of one-qubit

As claimed above, the description of a quantum state can be made via the density matrix. The corresponding data will be encoded in a graph. Before giving the general statement, we consider examples, through which we will illustrate how practically things work. Indeed, there is no simple example to start with than a one-qubit quantum system. This fundamental piece will play a crucial role in the coming sections and in the graph operations that we will establish later on to deal with quantum gates. This simple example can be considered as
a building block for higher dimensional qubit quantum systems. To start, we illustrate this connection with a two vertex model. Then, one can think of many simple examples involving combinatorial numbers of vertices to build graphs associated with multi-qubits.

It is recalled that a one-qubit is a state of a two dimensional Hilbert space. Employing Dirac notation associated with the basis \( \{|0\>, |1\>\} \), this state can be written, \((i = \{0,1\})\), as follows

\[
|\psi\rangle = a_0|0\rangle + a_1|1\rangle = \sum_{i=0}^{1} a_i|i\rangle
\]  

(2.6)

where \( a_i \) are complex numbers verifying the normalization condition

\[
|a_0|^2 + |a_1|^2 = 1.
\]  

(2.7)

The coefficient \( |a_i|^2 \) corresponds to the probability of measuring the qubit in the state \(|i\rangle\).

Moreover, the state \(|\psi\rangle\), used to describe one-qubit quantum systems, can be associated with a \( 2 \times 2 \) matrix, called the density matrix defined by the following relation

\[
\rho = |\psi\rangle\langle \psi| = \begin{pmatrix} a_0a_0 & a_0a_1 \\ a_1a_0 & a_1a_1 \end{pmatrix}.
\]  

(2.8)

Motivated by physical applications including connection with black holes \([5,6,7,9,10]\), we will consider real density matrices. In this way, they can be written generally as follows

\[
\rho_{ij} = a_ia_j.
\]  

(2.9)

A close inspection shows that this equation can be handled to provide a bridge with graph theory using similarities with Dynkin diagrams of simply laced algebras. To establish such a link, it is useful to recall Lie algebra theory \([17,18]\). Indeed, a Lie algebra is a vector space \( g \) with a bilinear map \([,] : g \times g \rightarrow g \) (i.e. a linear map \([,] : g \otimes g \rightarrow g \)) satisfying the following properties

1. antisymmetry: \([x,y] + [y,x] = 0\),
2. Jacobi identity: \([x,[y,z]] + [y,[z,x]] + [z,[x,y]] = 0\).

A fundamental piece is the Cartan subalgebra \( H \) defined as the maximal abelian Lie subalgebra useful to decompose the root space as follows

\[
g = g_0 \oplus \{ \oplus_{\alpha \neq 0} g_\alpha \}
\]

\[
g = H \oplus \{ \oplus_{\alpha \neq 0} g_\alpha \}.
\]  

(2.10)

where \( g_\alpha = \{ x \in g, \ [h,x] = \alpha(h)x, \forall h \in H \} \). In this way, the vectors \( \alpha \) are called roots. It is
noted that 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 $E$, $0 \not\in \Delta$,
2. if $\alpha$ is an element of $\Delta$, $k\alpha$ is also if $k = \pm 1$,
3. for all $\alpha$ inside $\Delta$, $\Delta$ is invariant under reflections $\sigma_\alpha$,
4. if $\alpha$ and $\beta$ inside $\Delta$, the quantity $\langle \beta, \alpha \rangle = \frac{2(\beta, \alpha)}{(\alpha, \alpha)}$ is an integer.

It has been remarked that $\Delta$ provides connections with matrices and graph theory and can be considered as a strong bridge between simply Lie algebras and modern physics associated with quivers in string theory compactifications. This can be established via the so-called Cartan matrix defined by

$$K_{ij} = \langle \alpha_i, \alpha_j \rangle = 2\frac{\alpha_i, \alpha_j}{\alpha_j, \alpha_j} \tag{2.11}$$

where $\alpha_i$ are simple roots. It has been shown that this matrix can be encoded in a geometric graph called Dynkin diagram where the diagonal elements corresponding to vertices and the non-diagonal ones are associated with edges (links) connecting the vertices.

A close examination shows that one can use such a connection to present a weighted graph representation of qubit physics. Indeed, we explore the connection between Cartan matrices and Dynkin diagrams of simply laced Lie algebras to establish such a correspondence. For such Lie algebras, the Cartan matrices can be reduced to

$$K_{ij} = \langle \alpha_i, \alpha_j \rangle = \alpha_i, \alpha_j \tag{2.12}$$

where $\alpha_j, \alpha_j = 2$ for all simple roots $\alpha_j$.

Replacing the role played by the simple roots $\alpha_i$ with the real numbers $a_i$ appearing in the density matrix, we can interpret the density matrix as a Cartan matrix using the following correspondence

$$\alpha_i \rightarrow a_i$$

$$\alpha_i, \alpha_j \rightarrow a_i a_j \tag{2.13}$$

Of course, there are important differences between the two matrices. Here, though we will not be concerned with them. Our objective is to explore the link between graph theory and simply laced Lie algebras, via Dynkin diagrams.

Roughly speaking, the density matrix $\rho$ can be related to the signless Laplacian matrix $Q(G)$. It is observed that
\[ \rho_{ij} = \begin{cases} a_i^2 D(G)_{ii} & i = j, \\ a_i a_j m_{ij} & i \neq j \end{cases} \] (2.14)

where \( m_{ij} \) are entries of the adjacency matrix of the corresponding graph. In this graph, the vertices \( v_i \) and \( v_j \) are connected if \( a_i a_j \neq 0 \), otherwise they are not linked.

Borrowing the idea of Dynkin diagrams of simply laced algebras, we replace the one-qubit state by a weighted graph formed by two vertices \( v_0 \) and \( v_1 \) labeled by their weights \( a_0^2 \) and \( a_1^2 \), respectively. These two vertices are linked by an edge weighted by \( a_0 a_1 \). Thus, the corresponding graph to this one-qubit is constructed in the figure 1.

![Figure 1: One-qubit graph representation.](image)

This graph can be considered as a weighted graph of two vertices with a weight function \( \omega \) satisfying

\[ \omega(v_i, v_j) = \omega(v_j, v_i) = a_i a_j. \] (2.15)

In this way, the edges correspond to \( a_i a_j \neq 0 \) and the non-edges are associated with \( a_i a_j = 0 \).

It is recalled that a simple graph is defined by

\[ \omega(v_i, v_j) = 0, 1 \]
\[ \omega(v_i, v_i) = 0. \] (2.16)

Note in passing that signless Laplacian of a weighted graph can be considered as a weighted adjacency matrix associated with a quiver which has two nodes and a single edge carrying some physical information. If we forget about the normalization condition, we can associate this quiver to a gauge field theory. The vertices \( a_i^2 \) correspond to the adjoint representation of \( \prod U(a_i^2) \), providing a \( G = U(a_0^2) \times U(a_1^2) \) gauge group. The link \( a_0 a_1 \) is associated the the Fermi field bi-fundamental matter. In type II superstrings, this field theory can be obtained when considering D-branes located the near orbifold points of the \( A_2 \) singularity associated with \( \text{su}(3) \) Lie algebra [19, 20].
3 Graph theory representation of multi-qubits

Having constructed the graph associated to one-qubit, we move now to the next model associated with two-qubit quantum systems defined in a 4 dimensional Hilbert space. Then, we give the general statement associated with \( n \)-qubit systems. In the basis \( \{ |ij >, \ i,j = 0,1 \} \), a two-qubit is written as follows

\[
|\psi > = a_{00}|00 > + a_{01}|01 > + a_{10}|10 > + a_{11}|11 > .
\]  (3.1)

Up to a scale factor, the signless Laplacian matrix can be identified with the density matrix. To make contact with graph theory, it is convenient to consider a binary index notation

\[
p = 2^1i + 2^0j,
q = 2^1i' + 2^0j',
\]  (3.2)

where \((i,j,i',j') = 0,1\). For the two-qubit, the density matrix can be written as follows

\[
\rho_{pq} = a_{ij}a_{i'j'}.
\]  (3.3)

This matrix is represented by a graph having four vertices weighted \( a_{ij}^2 \) and linked by edges whose weights depend on the values \( a_{ij}a_{i'j'} \). In this way, the two-qubit is illustrated in the figure 2.

![Two-qubit graph representation.](image)

As in the case of one-qubit, this graph shares similarities with quivers having four vertices and links associated with Fermi field representations.

This analysis can be extended to \( n \)-qubits associated with \( 2^n \)-dimensional Hilbert spaces. In this way, the general state reads as

\[
|\psi > = \sum_{i_1...i_n=0,1} a_{i_1...i_n}|i_1 ... i_n >,
\]  (3.4)
where $a_{i_1...i_n}$ verify the real normalization condition

$$\sum_{i_1,...,i_n=0,1} a_{i_1...i_n}^2 = 1.$$  
(3.5)

Roughly, the qubit systems can be represented by a complete weighted graph of $2^n$ vertices. This graph can be obtained from the corresponding density matrix. As in the two-qubit example, this matrix can be written in terms of the binary indices. A close examination shows that we can use the following index notation

$$p = \sum_{k=0}^{n-1} 2^k i_k$$

$$q = \sum_{k=0}^{n-1} 2^k i'_k$$  
(3.6)

where $(i_k, i'_k) = 0, 1$. In this way, the matrix density takes the following general form

$$\rho_{pq} = a_{i_1...i_n} a_{i'_1...i'_n},$$  
(3.7)

which can be associated with the signless Laplacian matrices of graphs having $2^n$ weighted vertices and $2^{n-1}(2^n - 1)$ weighted edges. In this way, the weight function $\omega$ can be written as

$$\omega(v_p, v_q) = a_{i_1...i_n} a_{i'_1...i'_n}.$$  
(3.8)

## 4 Unitary operations over graph state weights

Having built the graph theory of qubits, we move now to discuss the corresponding quantum gates in the graph theory language. We consider, first, lower dimensional gates, then we propose a general statement. It is noticed that the classical gates can be obtained by combining Boolean operations as AND, OR, XOR, NOT and NAND. In fact, these operations act on classical input bits, taking two values 0 and 1, to produce new bits as output results. However in quantum physics, gates are unitary operators acting in $2^n$-dimensional Hilbert spaces \[21, 22\]. They are considered as simple quantum circuits. Indeed, the simplest quantum gate performs a unitary transformation on single-qubit states. Such a quantum gate is called a single qubit gate. For the 2-dimensional Hilbert space representing single-qubit states, the unitary transformation of a single-qubit gate is given by a $2 \times 2$ unitary matrix. Examples of single qubit gates are the Pauli X and Z gates given, respectively, by
\[
X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\] (4.1)

It is recalled that the \(X\) quantum gate acts as follows

\[
X : \begin{cases} 
|0> \rightarrow |1> \\
|1> \rightarrow |0>
\end{cases}.
\] (4.2)

A close examination shows that one-qubit gates can be considered as transformations on the graph weights preserving the real probability condition, required by black hole applications

\[
a_0^2 + a_1^2 = 1.
\] (4.3)

The \(X\) gate action can be reduced to the following transformation on the weights

\[
a_i \rightarrow a_{i+1}, \quad i = 0, 1.
\] (4.4)

In the weighted graph theory, this action can be interpreted as a permutation operation over the weighted graph associated to one-qubit. This operation permutes the vertex weights and leaves the edge invariant. This can be illustrated in the figure 3.

![Figure 3: X gate action on one-qubit.](image)

However with the \(Z\) gate, the operation can be understood as

\[
a_i \rightarrow (-1)^i a_i, \quad i = 0, 1.
\] (4.5)

This graph operation is illustrated in the figure 4.

![Figure 4: Z gate action on one-qubit.](image)
As we have seen, the unitary operations corresponding to the gates of one-qubit can be reduced to actions over the vertex and edge weights. We have seen how the simple quantum gate acts on a simple qubit, let us see the action over a two-qubit system. For these cases, there are two important universal gates known as CNOT and SWAP gates. In this graph theory language, the CNOT gate defined by

\[
CNOT = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]  

(4.6)
can be obtained by using the following graph weight actions

\[
a_{ij} \rightarrow a_{i,i+j}, \quad i, j = 0, 1.
\]  

(4.7)

This operation acts on the corresponding matrix density as follows

\[
2^1i + 2^0j \rightarrow 2^1i + 2^0(i+j)
\]
\[
2^1i' + 2^0j' \rightarrow 2^1i' + 2^0(i' + j').
\]  

(4.8)

A close inspection shows that the SWAP gate

\[
SWAP = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]  

(4.9)
can be derived from the following permutation action

\[
a_{ij} \rightarrow a_{ji}, \quad i = 0, 1.
\]  

(4.10)

For \(n\)-qubits, the gates are represented by \(2^n \times 2^n\) matrices. In weighted graph theory, they can be replaced by actions preserving the real probability condition (3.5). A simple gate can be obtained by the following index transformation acting on the graph weights \(a_{i_1...i_n}\)

\[
i_n \rightarrow i_1 + \ldots + i_n, \quad i_k = 0, 1.
\]  

(4.11)

This can be considered as a higher dimensional CNOT gate. More generally, we expect that this analysis can be pushed further to deal with other non trivial gates to construct non trivial
quantum circuits.

5 Concluding remarks and speculations from quiver string theory

Using the relation between simply laced Lie algebras and Dynkin diagrams, we have suggested a new graph theory representation of quantum states. Using similarities with root systems of such Lie symmetries, we first have discussed one-qubit theory in terms of a weighted graph having two vertices. Then, we have given a general statement. In this representation, we have shown that quantum gates correspond to graph weight actions.

This work comes up with many open directions and speculations. The intersecting problem is the discussion of the separability problems using graph theory methods. This will be addressed elsewhere. Another connection concerns quiver gauge theories. As in the one-qubit, the weighted graph presented here can be considered as a quiver graph which has two nodes and a single edge carrying some physical information correspond to two factor quiver gauge theory with Fermi field matter representations. This quiver could be obtained by considering D-branes located on the $A_2$ like geometries associated with $\text{su}(3)$ Lie algebra. In this direction, the Cartan matrices can be replaced with the density matrix providing a new way to approach the cohomology class of two dimensional complex surfaces. This link should be explored to make contact with quivers associated with type II superstrings on local Calabi-Yau manifolds. In fact, we expect that the present weighted graphs can be explored to build a new class of local Calabi-manifolds by gluing several non trivial 2-cycles. These geometries can be motivated from results based on the blowing up of ADE singularities used in geometric engineering method of quantum field theories[23, 24]. Similarly as in the ADE cases, one can build new geometries using such a qubit graph theory to deal with black holes in type superstrings. We believe this study deserves more deep reflections. We hope to come back to this issue in future.

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