Graph representation of quantum states

Bibhas Adhikari*, Satyabrata Adhikari†, Subhashish Banerjee‡
Centre of Excellence in Systems Science
Indian Institute of Technology Rajasthan, Jodhpur-342011, India

Abstract In this work we propose graphical representation of quantum states. Pure states require weighted digraphs with complex weights, while mixed states need, in general, edge weighted digraphs with loops; constructions which, to the best of our knowledge, are new in the theory of graphs. Both the combinatorial as well as the signless Laplacian are used for graph representation of quantum states. We also provide some interesting analogies between physical processes and graph representations. Entanglement between two qubits is approached by the development of graph operations that simulate quantum operations, resulting in the generation of Bell and Werner states. As a biproduct, the study also leads to separability criteria using graph operations. This paves the way for a study of genuine multipartite correlations using graph operations.

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1 Introduction

Quantum mechanics deals with states living in the Hilbert space, allowing for linear superpositions to be built up, a facility of immmense importance for harnessing the power of quantum mechanics, but at the same time making it computationally a formidable task. This can be most easily appreciated by considering entanglement [1] in higher dimensions as well as in multi-partite systems [2], all mathematically and computationally very formidable tasks. Any tool that would aid in this regard would be very welcome. The theory of graphs [3] is a well-developed mathematical theory that has found many applications in diverse areas such as in network systems [4], optimization [5], algorithms [6]. Graphs have, by their very construction, the inbuilt feature of visualization.

*bibhas@iitj.ac.in
†satya@iitj.ac.in
‡subhashish@iitj.ac.in

A pertinent question to ask is whether a graphical representation of quantum states can be made? This would enable the incorporation of the mathematical machinery of graph states into the problems of quantum mechanics and at the same time bring in the attractive feature of visualization of quantum states.

A number of developments have taken place in this regard over the last decade. One of the key ideas has been the incubation and understanding of graph states: graphical representation of quantum states of a system such as a spin system interacting via an Ising type of interaction. These states have been used successfully to address stabilizer states, cluster states and some multi-partite entangled states, all of which makes them very useful for quantum information. They have been reviewed in [7]. In [8, 9], the question given a graph, what is the corresponding quantum state was posed. Some limitations of these approaches are that they prove to be inadequate to describe a number of general quantum states. Here we pose and try to address the following question: what is the general graphical representation of any quantum state? This task, if accomplished, should lead to a general usage of ideas from graph theory into quantum mechanics and at the same time lead to developments in graph theory itself.

In earlier works, each vertex of a graph is taken to be a quantum state with the edge representing an interaction between them. In contrast to this, in our construction a single quantum system is represented by a graph. In other words, in the earlier constructions a graph with n nodes represent a tensor product of n Hilbert spaces while in our case the entire graph represents a single Hilbert space. Earlier, the graphical construction of a quantum state relied upon undirected unweighted graphs. Our construction proceeds by first considering digraphs with complex edge weights of modulus one. This fails to capture all possible quantum states. This is partially overcome by considering digraphs with complex vertex weights, a construction which allows representation of all pure states and many mixed states, but not all. This is overcome by digraphs with complex edge weights and loops with real positive weights. To the best of our knowledge, a number of these constructions are new. Until now we discussed about the graphical representation of a single quantum system. To discuss the correlation between systems, we need to have at least two of them. Therefore, we attempt to realize the interaction between two quantum states by using graph operations between the corresponding graph representations.

The use of graphs with complex edge weights have been considered in the context of diverse areas such as proteomics [10], the large-scale study of proteins, as well as in neural networks with complex associative memory [11] where it was shown that a complexification of weights results in an increase in the power of the memory by a factor greater than the increase in the degree of freedom.

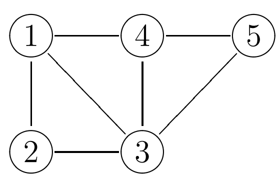
The plan of the paper is as follows. In the next section, an introduction is provided to graphs and specifically the Laplacian of the graph, both the combinatorial as well as the relatively new concept of signless Laplacian [12]. This is followed by a discussion of some interesting analogies between graphs and physical systems. After that we come to the main body of the paper where a construction of graphs corresponding to general quantum states is provided. This leads naturally to a graph-theoretic discussion of some quantum states useful in quantum information as well as the notion of entanglement. The graphical representation of mixed states require an interesting new construction of edge weighted digraphs with loops. The paper ends with our conclusions and some possible future directions.

2 Introduction to Graphs

Graphs represent the essential topological properties of an interconnected system by treating the system as a collection of subsystems and connections between the subsystems. Mathematically, a graph G is a pair of sets (V, E) where V is a finite nonempty set of elements called vertices, and E is a set of unordered pair of distinct vertices called edges [3]. Two vertices are said to be adjacent if they are connected by an edge. The number of edges adjacent to a vertex is called its degree.

Let G be a graph with $V = \{1, 2, \ldots, n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. The adjacency matrix associated with G, denoted by $A(G)$; is the $n \times n$ symmetric matrix defined as follows. The rows and the columns of $A(G)$ are indexed by V. If $i \neq j$ then the (i, j)-entry of $A(G)$ is 0 when vertices i and j are nonadjacent, and the (i, j)-entry is 1 when i and j are adjacent. The (i, i)-entry of $A(G)$ is 0 for $i = 1, \ldots, n$.

Example 2.1. *Consider the graph G :*



Then

$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

A directed graph or digraph G is a graph with a function assigning to each edge an ordered pair of vertices. The first vertex of the ordered pair is called the initial vertex of the edge, and the second is the terminal vertex; together, they are the endpoints. Thus each edge of a digraph is directed; and an undirected edge can be considered as both way directed. An edge-weighted graph G is a graph with a function $w : E \to \mathbb{R}$, defined by $w(e_j) = w_j, j = 1, 2, \ldots, m$. The function w is called an edge-weight function and w_j is called the weight of e_j.

An unweighted graph can be considered as an edge-weighted graph with weight function $w(e_j) = 1$ for all j. Analogously, a vertex-weighted graph G is a graph with a function $w : V \to \mathbb{R}$, defined by $w(i) = w_i, i = 1, 2, \ldots, n$. Then w is called vertex-weight function and w_i is called the weight of the vertex i.

A way of representing a quantum state by a graph; is the graph state [7]. The density matrix of a graph state is identified with the combinatorial Laplacian matrix associated with the graph. The details of such descriptions can be found in for example, [9]. Indeed, the Laplacian matrix associated with a graph G is defined by $L(G) = D(G) - A(G)$ where $D(G) = \text{diag}\{d_1, d_2, \ldots, d_n\}, d_i$ is the degree of vertex i and $A(G)$ is the adjacency matrix associated with the graph G [13]. It is easy to check that $L(G)$ is a symmetric positive semi-definite matrix. The density matrix of a graph state is defined by $\sigma_G = (1/d)L(G)$ where $d = d_1 + d_2 + \ldots + d_n$.

The approach of identifying quantum states by graph states mentioned above has its own limitations. This happens due to the fact that the density matrix defined by Laplacian matrix only produce scalar multiple of symmetric (real) positive semi-definite matrices with entries 0 and 1; although, in general, the density matrix associated with a quantum state is a Hermitian (complex) positive semi-definite matrix. Therefore, graph states constructed by the above procedure represent only a certain class of quantum states.

We overcome this limitation by defining the density matrix as a scalar multiple of combinatorial Laplacian or signless Laplacian matrix associated with edge-weighted and vertex-weighted digraphs with complex weights. Thus we show that this approach of defining the density matrix opens up a new outlook to the graphical representation of a quantum state. Further, we show that any quantum state may not be represented by such a weighted digraph with complex weights. Hence we introduce edge-weighted digraph with loops to represent a quantum state. Below we provide an introduction to edge-weighted digraphs with complex weights of modulus one, vertex-weighted and edge-weighted digraphs with loops, the edge weights being complex but the loops are characterized by real, positive weights.

2.1 Edge-weighted digraphs with complex weights of modulus one

In this section, we analyze the spectral properties of combinatorial Laplacian and signless Laplacian matrices associated with edge-weighted digraphs with complex weights. The combinatorial Laplacian matrix of edge-weighted digraphs with complex unit weights has been introduced by Bapat et al. in [14]. Indeed, the weight function

$$w : E \to \mathbb{S}^1_+ \text{ where } \mathbb{S}^1_+ = \{z = a + \mathrm{i}b \in \mathbb{C} : |z| = 1, b \geq 0\},$$

associated with a digraph $G = (V, E)$ is given by a canonical weight function $w(e_j) = e^{\mathrm{i}\theta_j}, 0 \leq \theta_j \leq 2\pi$ for all $e_j \in E$. The in-degree $p(v)$ and out-degree $q(v)$

of a vertex $v \in V$, respectively, are given by

$$\begin{array}{ll} p(v) = \sum_{e_j \in E} |w(e_j)|, & \text{if } v \text{ is terminal vertex of } e_j \in E \\ q(v) = \sum_{e_j \in E} |w(e_j)|, & \text{if } v \text{ is initial vertex of } e_j \in E. \end{array} \tag{1}$$

Thus the degree $d(v)$ of a vertex v is defined by $p(v) + q(v)$, that is, $d(v)$ is the sum of the modulus of weights of the edges adjacent to the vertex v.

The adjacency matrix $A = (a_{ij})$ corresponding to an edge-weighted digraph is given by

$$a_{ij} = \begin{cases} w((i,j)), & \text{if } (i,j) \in E; \\ \overline{w((i,j))}, & \text{if } (j,i) \in E; \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

To simplify the edge-weight notation, we write $w_{ij} = w((i,j))$ and $\overline{w}_{ij} = \overline{w((i,j))}$. The combinatorial Laplacian $L(G)$ and signless Laplacian matrix $Q(G)$ associated with an edge-weighted digraph $G = (V, E)$ of order n are given by $L(G) = D(G) - A(G)$ and $Q(G) = D(G) + A(G)$, respectively, where $D = \text{diag}(d_1, d_2, \ldots, d_n)$, d_i denotes the degree of the vertex i. Consider the vertex-edge incidence matrices $M^{\pm}$ given by

$$M^{\pm}_{v,e} = \begin{cases} 1, & \text{if } v \text{ is the initial vertex of } e; \\ \pm\overline{w}_{ij}, & \text{if } v \text{ is the terminal vertex of } e; \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

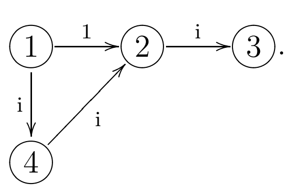
Then it is easy to verify that $L(G) = M^-(M^-)^\dagger$ and $Q(G) = M^+(M^+)^\dagger$ holds and hence $L(G)$ and $Q(G)$ are Hermitian positive semi-definite matrices. In addition to that we have

$$x^\dagger L(G)x = \sum_{(i,j)\in E} |x_i - w_{ij}x_j|^2 \text{ and } x^\dagger Qx = \sum_{(i,j)\in E} |x_i + w_{ij}x_j|^2 \tag{4}$$

for any vector $x = [x_1, x_2, \ldots, x_n]^T$ where ^{T} denotes the transpose of a vector.

The Laplacian eigenvalues of a graph play an important role in the structural analysis of a graph. For example, the multiplicity of combinatorial Laplacian eigenvalue zero is equal to the number of connected components for an undirected unweighted graph. It would be interesting to investigate whether the same is true for edge-weighted digraphs with complex weights. The example given below shows that an edge-weighted digraph may not have a Laplacian eigenvalue zero that contradicts the fact that zero is always a Laplacian eigenvalue for a undirected unweighted graph.

Example 2.2. *Consider the graph G :*



Then

$$L(G) = \begin{bmatrix} 2 & -1 & 0 & -\mathrm{i} \\ -1 & 3 & -\mathrm{i} & \mathrm{i} \\ 0 & \mathrm{i} & 1 & 0 \\ \mathrm{i} & -\mathrm{i} & 0 & 2 \end{bmatrix}$$

and the Laplacian eigenvalues are $0.4384, 1.0000, 2.0000, 4.5616$.

In the following theorem we provide a necessary and sufficient condition for a connected edge-weighted digraph having a Laplacian eigenvalue zero. Recall that, a digraph is said to be connected if it is connected without considering the directions of the edges.

Theorem 2.3. *The least eigenvalue of the signless Laplacian or combinatorial Laplacian of a connected digraph with complex edge-weights of unit modulus is equal to* 0 *if and only if*

$$\begin{cases} W(P) = W(P'), & \textit{if } p - p' \equiv 0 \textit{ mod}(2n) \\ W(P) = -W(P'), & \textit{if } p - p' \equiv 0 \textit{ mod}(2n+1),\ n \in \mathbb{N}. \end{cases}$$

holds for any two paths P, P' *between any fixed two vertices where* $W(P)$ *(resp.* $W(P')$*) is the product of the weights of the edges of* P *(resp.* P'*).*

Proof: We prove the result for signless Laplacian. Similar proof can be given for the combinatorial Laplacian. Assume that 0 is an eigenvalue of the signless Laplacian associated to a connected weighted digraph $G = (V, E)$. Then, by (4) we have $|x_i + w_{ij}x_j|^2 = 0$, for some $0 \neq x = [x_1, \ldots, x_n]^T$ with x_i corresponding to the vertex v_i for all i, for any edge e between vertices v_i and v_j with weight w_{ij}. Let P and P' be two directed paths from u to v. Suppose P and P' are given by

$$(v_{k_1}, v_{k_2}), (v_{k_2}, v_{k_3}), \ldots (v_{k_{p-1}}, v_{k_p}), v_{k_1} = u, v_{k_p} = v$$
$$(v_{l_1}, v_{l_2}, (v_{l_2}, v_{l_3}), \ldots (v_{l_{p'-1}}, v_{l_{p'}}), v_{l_1} = u, v_{l_{p'}} = v.$$

Then we have

$$x_{k_1} = -w_{k_1k_2}x_{k_2}, x_{k_2} = -w_{k_2k_3}x_{k_3}, \ldots, x_{k_{p-1}} = -w_{k_{p-1}k_p}x_{k_p} \tag{5}$$

for the path P, and

$$x_{l_1} = -w_{l_1l_2}x_{l_2}, x_{l_2} = -w_{l_2l_3}x_{l_3}, \ldots, x_{l_{p'-1}} = -w_{l_{p'-1}l_p}x_{l_{p'}} \tag{6}$$

for the path P'. Consequently we have

$$x_u = (-1)^{p-1}W(P)x_v, x_u = (-1)^{p'-1}W(P')x_v \tag{7}$$

$$\Rightarrow \begin{cases} W(P) = W(P'), & \text{if } p \equiv p' \ mod(2n) \\ W(P) = -W(P'), & \text{if } p \equiv p' \ mod(2n+1),\ n \in \mathcal{N}. \end{cases} \tag{8}$$

Note that if $x_i = 0$ for some $i, k_1 \leq i \leq k_p, l_1 \leq i \leq l_{p'}$ then all the x_is are zero.

Conversely, suppose the conditions hold. Then by defining the vector x satisfying (7), (5) and (6), the result follows by (4).

Corollary 2.4. *Let G be a disconnected weighted digraph. The number of connected components of G satisfying the condition given in the above theorem is equal to the multiplicity of combinatorial Laplacian or signless Laplacian eigenvalue* 0.

Proof: Let C_1 be a connected component of G satisfying the condition given in Theorem 2.3. Assume that $x \in \mathbb{C}^n$ is an eigenvector corresponding to the eigenvalue 0 of the signless Laplacian Q_{C_1} of C_1. Then we have

$$Q(G)\begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} Q_{C_1} & 0 \\ 0 & Q_{\widetilde{G}} \end{bmatrix}\begin{bmatrix} x \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \end{bmatrix}$$

where $\widetilde{G}$ is the graph G with C_1 deleted. Thus 0 is a signless Laplacian eigenvalue of G. Similarly it is easy to check that if 0 is a signless Laplacian eigenvalue of any connected component C of G satisfying the condition in the above theorem, then 0 is also a signless Laplacian eigenvalue of G. Thus we obtain the result. Similar proof holds for a combinatorial Laplacian.

2.2 Vertex-weighted digraphs with complex weights

In this section, we introduce vertex-weighted digraphs with complex weights and Laplacian matrices associated with it. Vertex weighted graphs with real weights were considered in [15]. Let $G = (V, E)$ be a digraph without loops and multiple edges. Consider a function $f : V \to \mathbb{C} \setminus \{0\}$ defined by $f(v_i) = w_i$; $v_i \in V$. Then the digraph G along with the function f is called a vertex-weighted digraph. The degree of a vertex v_i is given by $d_i = \sum_{v_i \sim v_j} |w_j|$ where $v_i \sim v_j$ means that there is a directed edge in between v_i and v_j. We denote $w_{ij} = \sqrt{\overline{w}_i w_j}$ and $\overline{w}_{ij} = \sqrt{\overline{w}_j w_i}$. The adjacency matrix $A(G) = (a_{ij})$ corresponding to G is given by

$$a_{ij} = \begin{cases} w_{ij}, & \text{if } i \neq j, (v_i, v_j) \in E \\ \overline{w}_{ij}, & \text{if } i \neq j, (v_j, v_i) \in E \\ 0, & \text{otherwise.} \end{cases}$$

The combinatorial Laplacian matrix $L(G)$ and signless Laplacian matrix $Q(G)$ associated with G are defined in a similar fashion as the edge-weighted digraph.

The vertex-edge incidence matrices are denoted by $N^{\pm}$ where

$$N^{\pm}_{v,e} = \begin{cases} \sqrt{w_j}, & \text{if } v = v_i \text{ is the initial vertex of } e \\ \pm\sqrt{w_i}, & \text{if } v = v_j \text{ is the end vertex of } e \\ 0, & \text{otherwise.} \end{cases}$$

Then, it is easy to verify that $L(G) = N^-(N^-)^\dagger$ and $Q(G) = N^+(N^+)^\dagger$. Thus $L(G)$ and $Q(G)$ are Hermitian positive semi-definite matrices. Further,

$$x^\dagger L(G)x = \sum_{(v_i,v_j)\in E} |x_i\sqrt{\overline{w}_j} - x_j\sqrt{\overline{w}_i}|^2 \tag{9}$$

$$x^\dagger Q(G)x = \sum_{(v_i,v_j)\in E} |x_i\sqrt{\overline{w}_j} + x_j\sqrt{\overline{w}_i}|^2 \tag{10}$$

for any $x = [x_1\, x_2\, \ldots\, x_n]^T \in \mathbb{C}^n$.

Let $\mathcal{H}(V)$ denote the space of functions $f : V \to \mathbb{C}$; which assigns a complex value $f(v)$ to each vertex v. The function f can be represented as a column vector in $\mathbb{C}^{|V|}$ here $|V|$ denotes the number of the vertices in V. Note that $f = 0$ function represents the graph without any edges. The function space $\mathcal{H}(V)$ can be endowed with the usual inner product:

$$\langle f, g \rangle = \sum_v f(v)^\dagger g(v) \tag{11}$$

where $f(v)^\dagger$ denotes the conjugate transpose of $f(v)$. Accordingly, the norm of the function induced from the inner product is $\|f\| = \sqrt{\langle f, f \rangle}$. Thus $\mathcal{H}(V)$ could be considered to be a Hilbert space.

We denote $W^{1/2} = \text{diag}[\sqrt{w_1}, \sqrt{w_2}, \ldots, \sqrt{w_n}]$ and $\mathbf{1}$ is the all-one vector. Then we have the following result.

Theorem 2.5. *Let $L(G)$ be the combinatorial Laplacian matrix associated with a vertex-weighted digraph G. Then $W^{1/2}\mathbf{1}$ is an eigenvector of $L(G)$ corresponding to the Laplacian eigenvalue* 0.

Proof: We know that $L(G) = N^-(N^-)^\dagger$ where N^- is a vertex-edge incidence matrix. Thus 0 is an eigenvalue of $L(G)$ if and only if there is a nonzero vector $x \in \mathbb{C}^n$ such that $(N^-)^\dagger x = 0$. Setting $x = W^{1/2}\mathbf{1}$, the proof follows from the fact that $x^\dagger N^- = 0$.

Theorem 2.6. *A vertex-weighted digraph G is connected if and only if the algebraic multiplicity of combinatorial Laplacian eigenvalue* 0 *is* 1.

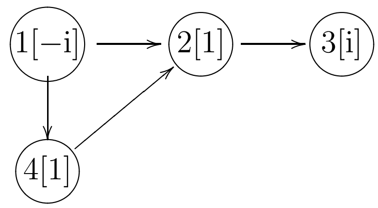
Proof: Let G be a connected vertex-weighted digraph. Then 0 is a Laplacian eigenvalue of $L(G)$ corresponding to the eigenvector $W^{1/2}\mathbf{1}$. Now assume that a nonzero vector $x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{C}^n$ exists such that $x^\dagger N^- = 0$. Suppose $x_j \neq 0$ for some $1 \leq j \leq n$. From the definition of N^- it follows that the jth row of N^- contains a nonzero entry at the junction of some column, say ith column, that is, the column corresponding to the edge e_i. Since G is loopless, there will exist another nonzero entry at the ith column, say at the junction of the kth row. Then we will have $\overline{x}_k\sqrt{w_j} - \overline{x}_j\sqrt{w_k} = 0$ where w_j and w_k denote the weights at the jth and kth vertices, respectively. Thus we have $x_k = (\sqrt{w_k}/\sqrt{w_j})x_j$. Since the graph is connected, by induction process we can show using similar arguments iteratively that x is a multiple of the all one's vector $\mathbf{1}$. (We mention that the other way of proving it by just using (9)). Thus the algebraic multiplicity of 0 is one.

Conversely assume that the algebraic multiplicity of Laplacian eigenvalue 0 is more than one. Then there will exist more than one linearly independent vectors x such that $x^\dagger N^- = 0$. Suppose that G is connected. Then this contradicts the fact that any x satisfying $x^\dagger N^- = 0$ is a multiple of $\mathbf{1}$. Hence G is disconnected. This completes the proof.

Corollary 2.7. *A vertex-weighted digraph G has k connected components if and only if the algebraic multiplicity of Laplacian eigenvalue* 0 *is* k.

Remark 2.8. *Any vertex weighted digraph may not have signless Laplacian eigenvalue* 0. *Consider the following example.*

Example 2.9. *Consider the graph* G :



where $j[z]$ *denotes the vertex* j *with vertex-weight* z. *Then*

$$Q(G) = \begin{bmatrix} 2 & \sqrt{\mathrm{i}} & 0 & \sqrt{\mathrm{i}} \\ \sqrt{-\mathrm{i}} & 3 & \sqrt{\mathrm{i}} & 1 \\ 0 & \sqrt{-\mathrm{i}} & 1 & 0 \\ \sqrt{-\mathrm{i}} & 1 & 0 & 2 \end{bmatrix}$$

and the signless Laplacian eigenvalues are $0.4384, 1.0000, 2.0000, 4.5616$.

Theorem 2.10. *A connected vertex-weighted digraph has a signless Laplacian zero if and only if it does not contain a connected cycle of odd order.*

Proof: Let $G = (V, E)$ be a connected vertex-weighted digraph and 0 a signless Laplacian eigenvalue of G corresponding to the eigenvector $0 \neq x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{C}^n$. Then we have $x_i\sqrt{w_j} = -x_j\sqrt{w_i}$ for any edge $(v_i, v_j) \in E$. Suppose that G contains a cycle C of odd order l. Then for any vertex v_{i_1} of C we have $v_{i_1} \sim v_{i_2}, v_{i_2} \sim v_{i_3}, \ldots, v_{i_{l-1}} \sim v_{i_l}, v_{i_l} \sim v_1$ where $u \sim v$ indicates a directed edge in between the vertices u and v. Consequently we have $x_{i_1}\sqrt{w_{i_2}} = -x_{i_2}\sqrt{w_{i_1}}, x_{i_2}\sqrt{w_{i_3}} = -x_{i_3}\sqrt{w_{i_2}}, \ldots, x_{i_l}\sqrt{w_{i_1}} = -x_{i_1}\sqrt{w_{i_l}}$. This yields $x_{i_1} = -x_{i_1} \Rightarrow x_{i_1} = 0$. This essentially gives $x_i = 0$ for all i since the graph is connected. Thus we arrive at a contradiction. Therefore G does not contain an odd cycle.

Conversely, assume that $G = (V, E)$ is a connected vertex-weighted digraph having no odd cycle. We define a nonzero vector $x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{C}^n$ such that $x_i\sqrt{w_j} = -x_j\sqrt{w_i}$ for any edge $(v_i, v_j) \in E$. Then we have $x^\dagger Q(G)x = 0$ which implies that x is an eigenvector of $Q(G)$ corresponding to the eigenvalue 0. This completes the proof.

2.3 Edge-weighted digraphs with loops

Let $G = (V, E)$ be an edge-weighted digraph with loops (at least one vertex contains a loop) of order n. Let $w : E \to \mathbb{C} \setminus \{0\}$ be the weight function defined by $w((i,j)) = w_{ij}$ if $i \neq j$, and $w((i,j)) = r_i > 0$ if $i = j$. The adjacency matrix $A(G) = (a_{ij})$ associated with G is defined as

$$a_{ij} = \begin{cases} w_{ij}, & \text{if } (i,j) \in E; \\ \overline{w}_{ij}, & \text{if } (j,i) \in E; \\ r_i, & \text{if } (i,i) \in E; \\ 0, & \text{otherwise.} \end{cases}$$

The degree d_i of a vertex $i \in V$ is given by $d_i = \sum_{j=1}^{n} |a_{ij}|$. The Laplacian and the signless Laplacian matrices are defined by

$$L(G) = \text{diag}(\{d_i\}_{i=1}^n) - A \text{ and } Q(G) = \text{diag}(\{d_i\}_{i=1}^n) + A, \tag{12}$$

respectively. Notice that self-loops, even though apparent in the adjacency matrix $A(G)$, do not appear in the Laplacian matrix $L(G)$. The vertex-edge incidence matrix M^- where

$$M^-_{v,e} = \begin{cases} \sqrt{w_{ij}}, & \text{if } v \text{ is initial vertex of nonloop edge } e; \\ -\sqrt{\overline{w}_{ij}}, & \text{if } v \text{ is terminal vertex of nonloop edge } e; \\ 0, & \text{otherwise} \end{cases}$$

gives $L(G) = M^-(M^-)^\dagger$ which implies that $L(G)$ is Hermitian positive semi-definite matrix. The vertex-edge incidence matrix M^+ where

$$M^+_{v,e} = \begin{cases} \sqrt{w_{ij}}, & \text{if } v \text{ is initial vertex of nonloop edge } e; \\ \sqrt{\overline{w}_{ij}}, & \text{if } v \text{ is terminal vertex of nonloop edge } e; \\ \sqrt{r}, & \text{if } e \text{ is a loop with weight } r \text{ at the vertex } v\ ; \\ 0, & \text{otherwise} \end{cases}$$

gives $Q(G) = M^+(M^+)^\dagger$ which implies that $Q(G)$ is Hermitian positive semi-definite matrix. Next we have

$$x^\dagger L(G)x = \sum_{i\neq j,(i,j)\in E} |x_i - \frac{w_{ij}}{|w_{ij}|}x_j|^2 \tag{13}$$

$$x^\dagger Q(G)x = \sum_{i\neq j,(i,j)\in E} |x_i + \frac{w_{ij}}{|w_{ij}|}x_j|^2 + \sum_{(i,i)\in E} r_i|x_i|^2 \tag{14}$$

for any $x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{C}^n$. We call $\widehat{w}_{ij} = w_{ij}/|w_{ij}|$ the normalized weight of the edge (i,j) of an edge-weighted digraph. Then we have the following theorem.

Theorem 2.11. *The least eigenvalue of the combinatorial Laplacian of a connected edge-weighted digraph is equal to* 0 *if and only if*

$$\begin{cases} \widehat{W}(P) = \widehat{W}(P'), & \text{if } p - p' \equiv 0 \ mod(2n) \\ \widehat{W}(P) = -\widehat{W}(P'), & \text{if } p - p' \equiv 0 \ mod(2n+1),\ n \in \mathbb{N}, \end{cases}$$

holds for any two paths P, P', which do not contain any loop, between any fixed two vertices where $\widehat{W}(P)$ (resp. $\widehat{W}(P')$) is the product of the normalized weights of the edges of P (resp. P').

Proof: Let $L(G)$ be the combinatorial Laplacian associated to a a connected edge-weighted digraph with edge set E. Then by (39) we have

$$x^{\dagger}L(G)x = \sum_{i\neq j,(i,j)\in E} |x_i - \widehat{w}_{ij}x_j|^2,\ |\widehat{w}_{ij}| = 1$$

for any nonzero $x = [x_1\, x_2\, \ldots\, x_n]^T \in \mathbb{C}^n$. Then the proof follows by applying the similar arguments given in Theorem 2.3.

Corollary 2.12. *Let G be a disconnected edge-weighted digraph. The number of connected components of G satisfying the condition given in the above theorem is equal to the multiplicity of combinatorial Laplacian eigenvalue* 0.

Proof: The proof follows by using similar arguments given in Corollary 2.4.

Remark 2.13. *It is easy to verify that $x^{\dagger}Q(G)x \neq 0$ for any nonzero $x \in \mathbb{C}^n$. Indeed, $r_i|x_i|^2 = 0$ for some loop at the ith vertex if and only if $x_i = 0$ which implies that $x = 0$ for $\sum_{i\neq j,(i,j)\in E} |x_i - \widehat{w}_{ij}x_j|^2$ to be zero as G is connected.*

3 Physical Analogies

Here we present some analogies of graphs to physical systems. The purpose is to highlight the importance of graphs in modelling diverse physical processes.

3.1 Connection to Diffusion and Schrödinger Equation

Consider a situation which models the flow of a system, such as gas, in a network from vertex j to i, of an undirected graph, at a rate $\alpha(\psi_j - \psi_i)$, where ψ_j represents the amount of the quantity at vertex j and α could be thought of as the diffusion constant of the flow. The flow equation would be:

$$\frac{d\psi_i}{dt} = \alpha\Sigma_j A_{ij}(\psi_j - \psi_i). \tag{15}$$

Here A_{ij} is the adjacency matrix that ensures that the only terms appearing in the summation are those vertices that are connected by edges. Using the fact that the degree of a vertex j, k_j, is related to the adjacency matrix by $k_j = \Sigma_i A_{ij}$, the Eq. (15) can be written as:

$$\frac{d\psi_i}{dt} = \alpha\Sigma_j (A_{ij} - \delta_{ij}k_i)\psi_j, \tag{16}$$

which can be formally presented as:

$$\frac{d\psi}{dt} = \alpha(A - D)\psi. \tag{17}$$

Here ψ is a vector with components ψ_j and A, D are the adjacency and diagonal matrices, with vertex degrees along the diagonal, respectively. If we represent the Laplacian of the graph to be $L = A - D$, then Eq. (17) has formal similarity to a diffusion of a free particle or heat equation

$$\frac{\partial \psi}{\partial t} = D_{diff} \bigtriangledown^2 \psi, \tag{18}$$

where $\bigtriangledown^2$ is the Laplacian and D_{diff} is the diffusion constant with $D_{diff} \equiv -\alpha$. An interesting analogy with quantum mechanics emerges if we observe that in Eq. (18), if time t is made imaginary, i.e., if $t = i\tau$, then the equation becomes:

$$\frac{\partial \psi}{\partial \tau} = i D_{diff} \bigtriangledown^2 \psi, \tag{19}$$

which can be formally identified with the Schrödinger equation, of a free particle

$$\frac{\partial \psi}{\partial \tau} = \frac{i\hbar}{2m} \bigtriangledown^2 \psi. \tag{20}$$

Thus the analogy $-\alpha \equiv D_{diff} \equiv \frac{\hbar}{2m}$ provides a formal connection of a simple graph operation to the Schrödinger equation.

3.2 Random Walk On a Weighted Graph

Consider a stochastic evolution modelled by a random walk on a connected, undirected garph with n nodes and weight $w_{ij} \geq 0$ on the edge joining node i to node j. A particle walks randomly from one node to another in this graph. The random walk X_n, $X_n \in 1, 2, ..., n$, is a sequence of vertices of the graph. Given $X_n = i$, the next vertex j is chosen from among the nodes connected to node i with a probability $p_{ij} = \frac{w_{ij}}{\Sigma_k w_{ik}}$, i.e., probability is proportional to the weight of the edge connecting i to j. The stationary distribution γ_j for this random process depends only on the weight of the edges connected to the nodes and the total weight of the edges emanating from a node $w = \Sigma_{i,j:j>i} w_{ij}$ and has the simple form

$$\gamma_j = \frac{w_j}{2w}. \tag{21}$$

From this the entropy rate of the stochastic process can be calculated and shown to be dependent on the entropy of the stationary distribution and the total number of edges of the graph.

3.3 Fock Space

In the wave function representation of Fock space, the antisymmetric wave-function, for fermions, has the form of a determinant, specifically the Slater determinant. Determinants have a very interesting graph theoretic representation [16]. Consider a square $n \times n$ matrix $A = (A_{ij})$ such that the diagonal elements of the matrix A_{ii} represent weights of the directed self-loops at the

ith vertices while the non-diagonal elements A_{ij} represent the weights of the directed edge from ith vertex to jth vertex, of the graph representing the matrix A. This form is called the Coates digraph of A [16]. Some useful terminilogies connected with the Coates digraph are the spanning subgraph, which is the subgraph of a graph such that the vertices of both the graph and subgraph coincide, and the linear subgraph, which is a spanning subgraph such that the incoming degree is equal to the outgoing degree of each vertex and is equal to one. This is illustrated below in the tadpole diagram:

$$\begin{tikzcd} \circ \arrow[loop left, "A_{11}"] \arrow[r, bend left, "A_{12}"] & \circ \arrow[l, bend left, "A_{21}"] \arrow[loop right, "A_{22}"] \end{tikzcd}$$

corresponding to

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \tag{22}$$

Using the concept of the linear subgraph, a graph theoretic representation of the determinant of a matrix A is given by

$$\det(A) = (-1)^n \Sigma_{L\in\mathcal{L}(A)} (-1)^{c(L)} w(L). \tag{23}$$

Here A is a square matrix of order n, L is a linear subgraph of the Coates digraph corresponding to A, $c(L)$ is the number of cycles (loops covering all the vertices) in L, $\mathcal{L}(A)$ corresponds to the set of all linear subgraphs of A and $w(L)$ is the weight of L and is equal to the product of the weights of the edges of L. This formula of the determinant is called the Coates formula [17, 18, 19] and is computationally identical to the standard definition of a determinant. For e.g.: the determinant for the graph drawn in the figure above for A is $\det(A) = A_{11}A_{22} - A_{21}A_{12}$. A point to be noted here is that there is no restriction on the elements of A to be complex, leading to complex weights, a concept we find to be of immense importance in providing a graphical representation of quantum states. In the context of the Slater determinant, the matrix elements A_{ij} would simply be replaced by complex functions corresponding to the n-particle wavefunctions. The Slater determinant would then have a graphical representation in terms of the Coates formula, Eq. (23).

The bosonic wavefunctions, on the other hand, have the form of a permament. Permanents have graph-theoretic interpretations as (a). sum of weights of cycle covers of a digraph, and (b). sum of weights of perfect matchings in a bipartite garph. The class of cycle covers, in the Coates graph, is a subclass of the set of linear subgraphs. Corresponding to an $n \times n$ matrix $A = (A_{ij})$, the permanent is defined as

$$\mathrm{perm}(A) = \Sigma_\sigma \Pi_{i=1}^n a_{i,\sigma(i)}, \tag{24}$$

where σ is a permutation over $(1, 2, ..., n)$. In the case of the figure drawn above, the permanent is $A_{12}A_{21}$.

An interesting consequence of the graphical interpretations of determinant and permanent, as can be seen explicitly from the example of the graph drawn above, is that the determinant, defined from linear subgraphs, is an antisymmetric function and hence can represent Fermions, while permanent, defined from cycle covers, is a symmetric function and can hence be used to represent Bosons. Thus the only class of particles in nature, Bosons or Fermions, have a clear graph theoretic interpretation.

4 Establishing an Isomorphy between Quantum States and Graphs

In this section, we construct an isomorphy between quantum states, both pure as well as mixed, and graphs, that is, we ask the question that given any quantum state what is its corresponding graph representation. Though a number of quantum states, including the ones considered in the literature [7, 8, 9], can be provided with a graph theoretic representation, it is not possible in general, to establish an isomorphy between quantum states and graphs. We, however, find that such a relationship can be established using vertex weighted digraphs with complex weights, as discussed in Sec. (2.2), and edge-weighted digraphs with loops (Sec. (2.3)).

4.1 Pure States and Mixed States

The density matrix representation of a quantum state is a Hermitian positive semi-definite matrix with unit trace. The density matrix ρ corresponding to a state satisfies $\mathrm{Tr}(\rho) = 1$ as well as

$$\begin{cases} \mathrm{Tr}(\rho^2) = 1, & \text{if the state is pure;} \\ \mathrm{Tr}(\rho^2) < 1, & \text{if the state is mixed.} \end{cases} \tag{25}$$

A quantum state, in general, can be represented as

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \tag{26}$$

where $0 \neq |\psi_i\rangle \in \mathbb{C}^2$ with norm one and $\sum_i p_i = 1, 0 \leq p_i \leq 1$. Thus ρ is a convex combination of rank one matrices, in particular, rank one projections. If ρ is just a projection with rank one then ρ is called a pure state, otherwise, a mixed state.

The vector representation of a pure state is given by $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$.

A combinatorial Laplacian or signless Laplacian matrix associated to a vertex or edge weighted digraph defined in section 2, can be identified with a density matrix. Since the motivation of this paper is to associate a graph with a quantum state described by ρ, we first try to construct a graph representation of a pure state, that is, a graph with rank one Laplacian matrices. Next we do the same for a mixed state. We denote an edge or vertex weighted complete bipartite digraph of order n as K_n. From now onwards we mean vertex or edge weighted graph when we say 'weighted digraphs' unless otherwise stated.

Definition 4.1. *The density matrix σ_G associated to a weighted digraph G is given by*

$$\sigma_G := \frac{1}{d(G)} K(G) \tag{27}$$

where $d(G)$ is the total degree of G and $K(G) \in \{L(G), Q(G)\}$.

It is obvious to see that σ_G is a Hermitian positive semi-definite matrix as $L(G)$ and $Q(G)$ are Hermitian positive semi-definite. Further, we have

$$\lambda_i(\sigma_G) = \frac{1}{d(G)} \lambda_i(K(G)), \tag{28}$$

where $\lambda_i(X)$ denotes the ith eigenvalue of X. We have the following result.

Theorem 4.2. *The density matrix of a weighted digraph G has rank one if and only if the graph is K_2 or $\widehat{K}_2 := K_2 \sqcup v_1 \sqcup v_2 \sqcup \ldots v_{n-2}.$, where $v_1, v_2, \ldots, v_{n-2}$ are isolated vertices.*

Proof: Assume that σ_G has rank one and G contains n vertices. Then σ_G has eigenvalue 1 with multiplicity one (since trace of $\sigma_G = 1$) and 0 is an eigenvalue of multiplicity $n-1$. If $n = 2$ then obviously $G = K_2$. If $n \neq 2$ then by Corollary 2.4 and Corollary 2.7, G contains $n-1$ connected components. Thus $G = \widehat{K}_2$.

Conversely, suppose $G = K_2$ or $\widehat{K}_2$. Then the eigenvalues of σ_G are 0 with multiplicity $n-1$ for $G = \widehat{K}_2$ and multiplicity 1 for $G = K_2$, and 1 with multiplicity one. Hence the result follows.

Remark 4.3. *We mention that the same result has been obtained in [9] for unweighted undirected graphs. Theorem 4.2 generalizes the same result for weighted digraphs.*

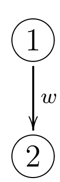
Theorem 4.4. *Let G be a weighted digraph isomorphic to K_2 or $\widehat{K}_2$. Then σ_G represents a pure state.*

Proof: The density matrix σ_G has a simple eigenvalue 1 and other eigenvalues are zeros. Since trace of any matrix is sum of the eigenvalues of the matrix, we have $\mathrm{Tr}(\sigma_G) = 1$ and $\mathrm{Tr}(\sigma_G^2) = 1$. Thus the result follows.

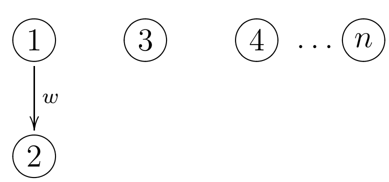
Thus, up to isomorphism, weighted digraph representations of pure states are

1. Edge-weighted digraphs:

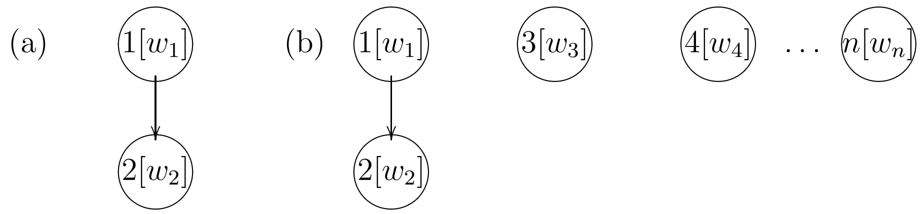
(a)



(b)



2. Vertex-weighted digraphs:



$0 \neq w, w_1, w_2, \ldots, w_n \in \mathbb{C}, n \in \mathbb{N}$.

Theorem 4.5. *Let G be a weighted digraph of order n that is not isomorphic to K_2 and $\widehat{K}_2$. Then G represents a mixed state.*

Proof: Let the eigenvalues of $\sigma(G)$ be $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$. By the definition of σ_G we have $\mathrm{Tr}(\sigma_G) = 1$ as $\sum_{i=1}^n \frac{\lambda_i}{d(G)} = 1$ where $d(G) = \sum_{i=1}^n \lambda_i$. Then the eigenvalues of σ_G^2 are $\frac{\lambda_1^2}{d(G)^2}, \frac{\lambda_2^2}{d(G)^2}, \ldots, \frac{\lambda_n^2}{d(G)^2}$. Thus

$$\mathrm{Tr}(\sigma_G^2) \ = \ \frac{\sum_{i=1}^n \lambda_i^2}{d(G)^2} = \frac{d(G)^2 - 2\sum_{i\neq j, i,j=1}^n \lambda_i \lambda_j}{d(G)^2} < 1.$$

Hence G represents a mixed state.

We recall the spectral value decomposition of any symmetric matrix M. Then M has orthonormal eigenvectors $\psi_1, \psi_2, \ldots, \psi_n$ corresponding to the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, respectively. Then we have $M = X \Sigma X^T$ where $X = [\psi_1, \psi_2, \ldots, \psi_n]$ and $\Sigma = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n]$. Thus the spectral decomposition of

$$M = \lambda_1 |\psi_1\rangle\langle\psi_1| + \lambda_2 |\psi_2\rangle\langle\psi_2| + \ldots + \lambda_n |\psi_n\rangle\langle\psi_n| = \sum_{i=1}^n \lambda_i |\psi_i\rangle\langle\psi_i|. \tag{29}$$

Therefore we have the following result.

Corollary 4.6. *Any pure quantum state is represented by $|\psi\rangle\langle\psi|$ where $|\psi\rangle$ is an eigenvector corresponding to the eigenvalue 1 of σ_{K_2} or $\sigma_{\widehat{K}_2}$.*

Proof: The result follows by (29).

Corollary 4.7. *Any mixed state is represented by*

$$\frac{\lambda_1}{d(G)} |\psi_1\rangle\langle\psi_1| + \frac{\lambda_2}{d(G)} |\psi_2\rangle\langle\psi_2| + \ldots + \frac{\lambda_n}{d(G)} |\psi_n\rangle\langle\psi_n|$$

where G is not isomorphic to K_2 or $\widehat{K}_2$, $d(G) = \sum_{i=1}^n \lambda_i$, λ_i are eigenvalues of σ_G and $|\psi_1\rangle, |\psi_2\rangle, \ldots |\psi_n\rangle$ are the corresponding orthonormal eigenvectors respectively.

Proof: The result follows by (29).

Example 4.8. *Edge weighted digraph representation of pure quantum states:*

Consider graph $G = K_2$ for a pure state with edge weight $w \in \mathbb{S}_1^+$. Then the corresponding density matrix with respect to the Laplacian matrix is given by

$$\sigma_G = \frac{1}{2}L(G) = \frac{1}{2}\begin{bmatrix} 1 & -w \\ -\overline{w} & 1 \end{bmatrix},$$

where $w = e^{i\phi}, 0 \leq \phi \leq 2\pi$. The eigenvalues of σ_G are 0 and 1 corresponding to eigenvectors $|\psi_1\rangle = \frac{1}{\sqrt{2}|z_1|}\begin{bmatrix} z_1 \\ \overline{w}z_1 \end{bmatrix}$ and $|\psi_2\rangle = \frac{1}{\sqrt{2}|z_2|}\begin{bmatrix} z_2 \\ -\overline{w}z_2 \end{bmatrix}$ respectively, where $0 \neq z_1, z_2 \in \mathbb{C}$. Thus the pure state is given by $\rho = |\psi_2\rangle\langle\psi_2|$. Setting $z_2 = re^{i\theta}, |z_2| = r > 0, 0 \leq \theta \leq 2\pi$, the vector representation of the pure state is given by

$$\begin{aligned} |\psi\rangle &= e^{i\theta}(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}e^{-i\phi}|1\rangle), \\ &\equiv \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}e^{-i\phi}|1\rangle. \end{aligned}$$

Further, the density matrix with respect to the signless Laplacian matrix is given by

$$\sigma_G = \frac{1}{2}Q(G) = \frac{1}{2}\begin{bmatrix} 1 & w \\ \overline{w} & 1 \end{bmatrix}.$$

Following a similar approach, as above, the corresponding vector representation of the pure state is given by

$$|\psi\rangle \equiv \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}e^{-i\phi}|1\rangle, 0 \leq \phi \leq 2\pi.$$

The results are similar for $G = \widehat{K}_2$.

Remark 4.9. *From the example above we observe that an edge weighted digraph cannot represent all possible pure quantum states, $\alpha|0\rangle + \beta|1\rangle,\ |\alpha|^2 + |\beta|^2 = 1$. In the next example we consider the vertex weighted digraph.*

Example 4.10. *Vertex weighted digraph representation of pure quantum states:*

Consider the vertex weighted graph $G = K_2$ with nonzero weights $w_1, w_2 \in \mathbb{C}$. The density matrix with respect to the Laplacian matrix $L(G)$ is given by

$$\sigma_G = \frac{1}{|w_1| + |w_2|}\begin{bmatrix} |w_2| & -\sqrt{\overline{w_1}w_2} \\ -\sqrt{\overline{w_2}w_1} & |w_1| \end{bmatrix}.$$

The eigenvalues of σ_G are 0 and 1 corresponding to the eigenvectors $|\psi_1\rangle = \begin{bmatrix} z_1 \\ \frac{\sqrt{\overline{w_2}w_1}}{|w_1|}z_1 \end{bmatrix}$ and $|\psi_2\rangle = \frac{\sqrt{|w_2|}}{|z_2|\sqrt{|w_1|+|w_2|}}\begin{bmatrix} z_2 \\ -\frac{\sqrt{\overline{w_2}w_1}}{|w_2|}z_2 \end{bmatrix}$, respectively. The pure state is *given by* $\rho = |\psi_2\rangle\langle\psi_2|$. *The vector representation of the pure state is:*

$$\begin{aligned} |\psi\rangle &= \frac{z_2\sqrt{|w_2|}}{|z_2|\sqrt{|w_1|+|w_2|}}(|0\rangle - \frac{\sqrt{\overline{w_2}w_1}}{|w_2|}|1\rangle) \\ &= \frac{z_2\sqrt{|w_2|}}{|z_2|\sqrt{|w_1|+|w_2|}}(|0\rangle - \frac{\sqrt{r_1 r_2 e^{i(\phi_1-\phi_2)}}}{r_2}|1\rangle) \\ &= \frac{z_2\sqrt{|w_2|}}{|z_2|\sqrt{|w_1|+|w_2|}}(|0\rangle - \sqrt{\frac{r_1}{r_2}}e^{i(\phi_1-\phi_2)/2}|1\rangle) \\ &\equiv |0\rangle - re^{i\phi}|1\rangle, \end{aligned}$$

where $w_j = r_j e^{i\phi_j}, |w_j| = r_j, 0 \leq \phi_j \leq 2\pi, \phi = (\phi_1 - \phi_2)/2, r = \sqrt{r_1}/\sqrt{r_2}, j = 1, 2$.

Further, the density matrix with respect to the signless Laplacian matrix is given by

$$\sigma_G = \frac{1}{|w_1|+|w_2|}\begin{bmatrix} |w_2| & \sqrt{\overline{w_1}w_2} \\ \sqrt{\overline{w_2}w_1} & |w_1| \end{bmatrix}.$$

Following a similar approach, as above, we obtain the vector representation of the pure state as:

$$|\psi\rangle \equiv |0\rangle + re^{i\phi}|1\rangle,$$

where $w_j = r_j e^{i\phi_j}, |w_j| = r_j, 0 \leq \phi_j \leq 2\pi, \phi = (\phi_1 - \phi_2)/2, r = \sqrt{r_1}/\sqrt{r_2}, j = 1, 2$. *Thus, all possible single-qubit pure states are reproduced.*

Remark 4.11. *We mention that if weights of all the edges in a weighted digraph G are 1, then $L(G)$ coincides with the usual Laplacian matrix of an unweighted undirected graph. This gives the construction of density matrix of a state associated to a Laplacian matrix introduced by Braunstein et. al. in [9]. If weights of the edges in G are ± 1, then (viewing the edges of weight 1 as directed and the edges of weight -1 as undirected) $L(G)$ coincides with the Laplacian matrix of a mixed graph.*

The density matrix $\rho = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ cannot be identified as the Laplacian of a weighted digraph, described above. These leads us to consider edge-weighted digraphs with loops. It follows from the Remark 2.13, that the density matrix $\sigma_G = \frac{1}{d}Q(G), d = \sum_{i=1}^{n} d_i$ does not represent a pure qubit state for any edge-weighted digraph G.

Theorem 4.12. *The density matrix corresponding to the Laplacian matrix associated to an edge weighted digraph with loops G represents a pure state if and only if $G = K_2$ with loops or $G = \widehat{K}_2$ with loops.*

Proof: The proof follows from the proofs of Theorem 4.2 and 4.4.

Theorem 4.13. *If G is an edge weighted digraph with loops not isomorphic to K_2 with loops and $\widehat{K}_2$ with loops then G represents a mixed state.*

Proof: The proof follows from the proof of Theorem 4.5.

5 Generation of Entangled Quantum States

Entanglement is a key resource in quantum information processing [1, 20, 21, 22] and is one of the first quantum correlation measures to be studied in detail. Simply stated, what is not separable is entangled, i.e., if any quantum system cannot be represented as the product of two or more subsystems, then it is entangled. To put our work in the perspective of quantum information processing tasks, a natural question to ask is about the nature of graph operations that could generate entangled quantum states. Let us elaborate on this.

Consider two quantum states described by the density operators $\rho_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and $\rho_2 = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$, respectively. The tensor product of ρ_1 and ρ_2 is given by

$$\rho_1 \otimes \rho_2 = \begin{bmatrix} \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{30}$$

The state $\rho_1 \otimes \rho_2$ is clearly a separable state. We can generate entanglement between ρ_1 and ρ_2 by performing a quantum operation U on $\rho_1 \otimes \rho_2$, the resulting output state being

$$\rho_{12} = U(\rho_1 \otimes \rho_2)U^\dagger = \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{bmatrix}, \tag{31}$$

where $U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$. The state ρ_{12} is now entangled.

We are now in a position to ask the question whether a quantum operation, in particular entanglement, can be realized by a corresponding graph operation? The answer is in affirmative. We address this question by providing a graph operation in an example given below.

Example 5.1. *Let the adjacency matrices of the graphs representing two single qubit states ρ_1 and ρ_2 be*

$$A(G_1) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad A(G_2) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{32}$$

We assume that the adjacency matrix $A(G_1 \otimes G_2)$, corresponding to the tensor *product of single qubit states, is given by*

$$\begin{aligned}A(G_1 \otimes G_2) &= A(G_1)J \otimes A(G_2)P + (A(G_1)J)^\dagger \otimes (A(G_2)+I)P^\dagger \\ &= \begin{bmatrix}0&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{bmatrix},\end{aligned} \tag{33}$$

where $J = \begin{bmatrix}0&0\\0&1\end{bmatrix}$, $P = \begin{bmatrix}0&1\\0&0\end{bmatrix}$. *The degree matrix is given by*

$$D = \begin{bmatrix}1&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&1\end{bmatrix}. \tag{34}$$

Therefore, the Laplacian of a graph $G_1 \otimes G_2$ *is given by*

$$L(G_1 \otimes G_2) = D - A(G_1 \otimes G_2) = \begin{bmatrix}1&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&1\end{bmatrix} \tag{35}$$

The state corresponding to graph $G_1 \otimes G_2$*, that is,* $\sigma_{G_1 \otimes G_2}$*, is given by*

$$\sigma_{G_1 \otimes G_2} = \frac{1}{2}\begin{bmatrix}1&0&0&1\\0&0&0&0\\0&0&0&0\\1&0&0&1\end{bmatrix}. \tag{36}$$

Eq.(36) represents a Bell state.

Given two graphs G and H we can produce a new one by defining a suitable operation on these two graphs. Several ways of defining such an operation are available in the literature [23]. Parsonage *et.al.* [23] have defined a generalized graph product by unifying a number of products, such as, tensor product, strong product, lexicographic product. Given G and H of order n, the generalized graph product is defined as

$$A(G \otimes_{f,g} H) \equiv A_{G*H} := A(G) \otimes f(A(H)) + I_n \otimes g(A(H)), \tag{37}$$

where f and g are defined on the adjacency matrices of the graphs G and H, respectively. Taking suitable f and g one can produce several new graphs.

By considering weighted digraphs G and H as the graph representation of qubits, one can verify that the new graph produced by taking the generalized graph product $G \otimes_{f,g} H$ is always a separable state. We prove this by using the following lemma.

Lemma 5.2. *[24] A 2×2 block matrix $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$, $A_{12}^\dagger = A_{21}$, $det(A_{11}) \neq 0$, is Hermitian positive semi-definite if and only if $A_{11} > 0$ and $A_{22} - A_{21}A_{11}^{-1}A_{12} \geq 0$.*

Theorem 5.3. *Let G and H be weighted digraphs which represent single qubit quantum states. The density matrices corresponding to the Laplacian matrices associated with the product graph $G \otimes_{f,g} H$ represent a separable state.*

Proof: Let $A(G) = \begin{bmatrix} 0 & \omega \\ \bar{\omega} & 0 \end{bmatrix}$ for some $0 \neq w \in \mathbb{C}$, $f(A(H)) = \begin{bmatrix} f_{11} & f_{12} \\ \bar{f}_{12} & f_{22} \end{bmatrix}$, $f_{11}, f_{22} \in \mathbb{R}$, and $g(A(H)) = \begin{bmatrix} 0 & g_{12} \\ \bar{g}_{12} & 0 \end{bmatrix}$. Then by (37) we have

$$A_{G*H} = \begin{bmatrix} 0 & g_{12} & \omega f_{11} & \omega f_{12} \\ \bar{g}_{12} & 0 & \omega \bar{f}_{12} & \omega f_{22} \\ \bar{\omega} f_{11} & \bar{\omega} f_{12} & 0 & g_{12} \\ \bar{\omega} \bar{f}_{12} & \bar{\omega} f_{22} & \bar{g}_{12} & 0 \end{bmatrix}.$$

Thus the density matrix σ_{G*H} corresponding to the Laplacian matrix of $G * H$ is given by

$$\sigma_{G*H} = \frac{1}{d_1 + d_2 + d_3 + d_4} \begin{bmatrix} d_1 & g_{12} & \omega f_{11} & \omega f_{12} \\ \bar{g}_{12} & d_2 & \omega \bar{f}_{12} & \omega f_{22} \\ \bar{\omega} f_{11} & \bar{\omega} f_{12} & d_3 & g_{12} \\ \bar{\omega} \bar{f}_{12} & \bar{\omega} f_{22} & \bar{g}_{12} & d_4 \end{bmatrix}, \tag{38}$$

where $d_i, i = 1, 2, 3, 4$ is the sum of modulus of the ith row entries of A_{G*H}. Since $\sigma_{G*H} \geq 0$, by Lemma 5.2 we have

$$\begin{bmatrix} d_1 & g_{12} \\ \bar{g}_{12} & d_2 \end{bmatrix} > 0 \text{ and} \tag{39}$$

$$\begin{bmatrix} d_3 & g_{12} \\ \bar{g}_{12} & d_4 \end{bmatrix} - \frac{1}{d_1 d_2 - |g_{12}|^2} \begin{bmatrix} \bar{\omega} f_{11} & \bar{\omega} f_{12} \\ \bar{\omega} \bar{f}_{12} & \bar{\omega} f_{22} \end{bmatrix} \begin{bmatrix} d_1 & -g_{12} \\ -\bar{g}_{12} & d_2 \end{bmatrix} \begin{bmatrix} \omega f_{11} & \omega f_{12} \\ \omega \bar{f}_{12} & \omega f_{22} \end{bmatrix} \geq 0. \tag{40}$$

The partial transposed state of σ_{G*H} is given by

$$\sigma^{T_B} = \frac{1}{d_1 + d_2 + d_3 + d_4} \begin{bmatrix} d_1 & \bar{g}_{12} & \omega f_{11} & \omega \bar{f}_{12} \\ g_{12} & d_2 & \omega f_{12} & \omega f_{22} \\ \bar{\omega} f_{11} & \bar{\omega} \bar{f}_{12} & d_3 & \bar{g}_{12} \\ \bar{\omega} f_{12} & \bar{\omega} f_{22} & g_{12} & d_4 \end{bmatrix}. \tag{41}$$

Case-I: $det(A_{11}) \neq 0$, where $A_{11} = \begin{bmatrix} d_1 & \bar{g}_{12} \\ g_{12} & d_2 \end{bmatrix}$. Using Eqs. (39), (40), it follows that $\sigma^{T_B} \geq 0$, hence σ_{G*H} represents a separable state [20].
Case-II: If $det(A_{11}) = 0$, then we cannot apply lemma (5.2) to prove the positive semi-definiteness of σ^{T_B}. We overcome this difficulty by considering all possibile cases where $det(A_{11}) = 0$.

From Eq. (38), the degrees d_1 and d_2 are given by

$$d_1 = |\bar{g}_{12}| + |f_{11}| + |f_{12}|, \tag{42}$$
$$d_2 = |\bar{g}_{12}| + |f_{12}| + |f_{22}|. \tag{43}$$

Using (42) and (43), we can re-write the matrix A_{11} as

$$A_{11} = \begin{bmatrix} d_1 & \bar{g}_{12} \\ g_{12} & d_1 - |f_{11}| + |f_{22}| \end{bmatrix}. \tag{44}$$

If $\det(A_{11}) = 0$ then $|g_{12}|\left(|f_{11}| + 2|f_{12}| + |f_{22}|\right) + \left(|f_{11}| + |f_{12}|\right)\left(|f_{12}| + |f_{22}|\right) = 0$ holds. The exhaustive cases which satisfy $\det(A_{11}) = 0$ are given below:

Subcase-I: $d_1 = |g_{12}|$, $|f_{11}| = |f_{22}| = |f_{12}| = 0$. Hence, the matrix $\sigma^{T_B} = \sigma \geq 0$.

Subcase-II: $|g_{12}| = |f_{11}| = |f_{22}| = |f_{12}| = 0$. Thus, the matrix $\sigma^{T_B} = \sigma \geq 0$.

Subcase-III: $d_1 = |f_{11}|$, $|g_{12}| = |f_{22}| = |f_{12}| = 0$. Consequently, $\sigma^{T_B} = \sigma \geq 0$.

Subcase-IV: $|g_{12}| = |f_{11}| = |f_{12}| = 0$. Then, $\sigma^{T_B} = \sigma \geq 0$.

From the above considerations, it can be concluded that the state represented by the density matrix σ_{G*H} is separable. Hence the theorem.

It is evident that the states generated by Eq. (37) are always separable. Thus, to generate entangled states we need to generalize the graph operations. We define

$$A(G * H) := \sum_{i=1}^{k} f_i(A(G)) \otimes g_i(A(H)), \tag{45}$$

where $f_i, g_i, i = 1, \ldots k$, $k \geq 2$, are functions defined on adjacency matrices of the graphs G and H such that $A(G * H)$ is Hermitian and diagonal entries are zeros and $\otimes$ denotes the tensor product. Now by taking suitable choices of these functions we observe that the graphs resulting from the operations (45) could generate entangled states. In particular, we present a graphical construction of all Bell states.

Example 5.4. *Let* $J = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ *and* $X^\dagger$ *be the conjugate transpose of a matrix* X. *The adjacency matrices corresponding to the vertex weighted digraphs* G *with vertex weights* $w_1, w_2 \in \mathbb{C} \setminus \{0\}$, *and* H *with vertex weights* $w_1', w_2' \in \mathbb{C} \setminus \{0\}$, *are given by*

$$A(G) = \begin{bmatrix} 0 & \sqrt{\overline{w_1} w_2} \\ \sqrt{\overline{w_2} w_1} & 0 \end{bmatrix} \text{ and } A(H) = \begin{bmatrix} 0 & \sqrt{\overline{w_1'} w_2'} \\ \sqrt{\overline{w_2'} w_1'} & 0 \end{bmatrix}.$$

1. *Setting the matrix functions* $f_i, g_i, i = 1, 2$ *as*

$$f_1(X) = XJ, f_2(X) = (XJ)^\dagger, g_1 = f_1, g_2 = f_2, \tag{46}$$

we obtain the non-maximally entangled states. For a particular set of values of weights, this construction leads to Bell states. Here G *and* H

represent the qubit pure states and the corresponding density matrices are associated to either Laplacian or signless Laplacian.

Indeed, we have

$$A(G*H) = \begin{bmatrix} 0 & 0 & 0 & \sqrt{\overline{w_1 w_1'} w_2 w_2'} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sqrt{\overline{w_2 w_2'} w_1 w_1'} & 0 & 0 & 0 \end{bmatrix}.$$

The density matrices corresponding to Laplacian and signless Laplacian matrices associated to $G*H$ are given by

$$\sigma_{G*H} = \frac{1}{|w_2 w_2'| + |w_1 w_1'|} \begin{bmatrix} |w_2 w_2'| & 0 & 0 & -\sqrt{\overline{w_1 w_1'} w_2 w_2'} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\sqrt{\overline{w_2 w_2'} w_1 w_1'} & 0 & 0 & |w_1 w_1'| \end{bmatrix} \quad \textit{and}$$

$$\sigma'_{G*H} = \frac{1}{|w_2 w_2'| + |w_1 w_1'|} \begin{bmatrix} |w_2 w_2'| & 0 & 0 & \sqrt{\overline{w_1 w_1'} w_2 w_2'} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sqrt{\overline{w_2 w_2'} w_1 w_1'} & 0 & 0 & |w_1 w_1'| \end{bmatrix},$$

respectively. These density matrices represents non-maximally entangled states.

In particular, setting $w_1 = w_1' = w_2 = w_2' = 1$, that is, by considering simple unweighted undirected graph representations G, H of the pure qubit states we get the Bell states of the form $|\Phi^{\mp}\rangle = \frac{1}{\sqrt{2}}(|00\rangle \mp |11\rangle)$.

2. *Setting the matrix functions $f_i, g_i, i = 1, 2$ as*

$$f_1(X) = XJ, f_2(X) = (XJ)^{\dagger}, g_1 = f_2, g_2 = f_1, \tag{47}$$

we obtain

$$A(G*H) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{\bar{w}_1 w_2 \bar{w}_2' w_1'} & 0 \\ 0 & \sqrt{\bar{w}_1' w_2' \bar{w}_2 w_1} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

The density matrices corresponding to Laplacian and signless Laplacian *matrices associated with $G * H$ are given by*

$$\sigma_{G*H} = \frac{1}{|w_2 w_1'| + |w_1 w_2'|}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & |w_2 w_1'| & -\sqrt{\bar{w}_1 w_2 \bar{w}_2' w_1'} & 0 \\ 0 & -\sqrt{\bar{w}_1' w_2' \bar{w}_2 w_1} & |w_2' w_1| & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and}$$

$$\sigma'_{G*H} = \frac{1}{|w_2 w_1'| + |w_2 w_1'|}\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & |w_2 w_1'| & \sqrt{\bar{w}_1 w_2 \bar{w}_2' w_1'} & 0 \\ 0 & \sqrt{\bar{w}_1' w_2' \bar{w}_2 w_1} & |w_2' w_1| & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

respectively. These density matrices represents non-maximally entangled states.

Setting $w_1 = w_1' = w_2 = w_2' = 1$, we get the Bell states of the form $|\Psi^{\mp}\rangle = \frac{1}{\sqrt{2}}(|01\rangle \mp |10\rangle)$.

For different choices of f_i's and g_i's we get a variety of entangled states and separable states. A detailed study on these issues is being considered in [25].

It is obvious from the above examples that simple weighted digraphs with complex weights represent a large class of quantum states. However, from Sec. IV, it is clear that they fail to provide a graphical representation of all the quantum states. A very important class of mixed states, Werner states, cannot be represented by simple weighted digraphs. This phenomenon motivates us to consider edge weighted digraphs with loops (at least one vertex contains a loop). The corresponding density matrix with respect to the signless Laplacian provides a graphical representation of Werner states.

Using the graph operation $G * H$ defined in (45) for the edge weighted digraphs with loops, G and H, we can obtain graphs which represent entangled pure and mixed states.

Example 5.5. *Consider G and H to be edge weighted digraphs with loop at one vertex of each of the graphs. Then we have*

$$A(G) = \begin{bmatrix} r_1 & w \\ \overline{w} & 0 \end{bmatrix} \text{ and } A(H) = \begin{bmatrix} 0 & w' \\ \overline{w'} & r_2 \end{bmatrix}$$

and corresponding (signless) Laplacian matrices are given by

$$L(G) = \begin{bmatrix} 1 & -w \\ -\overline{w} & 1 \end{bmatrix},\ L(H) = \begin{bmatrix} 1 & -w' \\ -\overline{w'} & 1 \end{bmatrix},$$

$$Q(G) = \begin{bmatrix} 2r_1 + 1 & -w \\ -\overline{w} & 1 \end{bmatrix},\ Q(H) = \begin{bmatrix} 1 & -w' \\ -\overline{w'} & 2r_2 + 1 \end{bmatrix}$$

where $r_1 > 0$ in the diagonal of $A(G)$ is the weight of the loop at the 1st vertex of G, with edge weight $w \in \mathbb{S}^1_+$ and $r_2 > 0$ in the diagonal of $A(H)$ is the weight of the loop at the 2nd vertex of H with edge weight $w' \in \mathbb{S}^1_+$.

Let $J = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, K = \begin{bmatrix} 0 & \overline{w} \\ 0 & 0 \end{bmatrix}, K' = \begin{bmatrix} 0 & \overline{w'} \\ 0 & 0 \end{bmatrix}, Z = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$. *Then setting*

$$f_1(X) = XJ, f_2(X) = JX, f_3(X) = XK^\dagger, f_4(X) = (ZX^\dagger Z)J,$$
$$g_1(X) = f_2(X), g_2(X) = f_1(X), g_3(X) = XK'^\dagger, g_4(X) = f_4(X)$$

and defining

$$G * H = \sum_{i=1}^{4} f_i(A(G)) \otimes g_i(A(H))$$

we have

$$A(G * H) = \begin{bmatrix} r_1 & 0 & 0 & 0 \\ 0 & 0 & w\overline{w'} & 0 \\ 0 & \overline{w}w' & 0 & 0 \\ 0 & 0 & 0 & r_2 \end{bmatrix}.$$

Then the density matrices corresponding to the Laplacian and signless Laplacian matrices are given by

$$\sigma_{G*H} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -w\overline{w'} & 0 \\ 0 & -\overline{w}w' & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{48}$$

and

$$\sigma'_{G*H} = \frac{1}{2(1 + r_1 + r_2)} \begin{bmatrix} 2r_1 & 0 & 0 & 0 \\ 0 & 1 & w\overline{w'} & 0 \\ 0 & \overline{w}w' & 1 & 0 \\ 0 & 0 & 0 & 2r_2 \end{bmatrix}, \tag{49}$$

respectively.

Setting $w = w'$ *in Eq. (48), and since their modulus is one, we get the Bell states of the form* $|\Psi^-\rangle$, *while Eq. (49) represents a Werner state.*

6 Conclusions and Future Directions

In this work we have attempted to provide a graph theoretic representation of arbitrary quantum states. We work with both the usual combinatorial as well as the relatively new signless Laplacian. While the combinatorial Laplacian can be used to represent both pure as well as mixed states, the signless Laplacian only represents mixed states for edge weighted digraphs with loops. We also found some interesting analogies between a number of physical processes and graph representations. In contrast to some of the earlier works on related issues, here the entire graph represents a quantum state. The establishment of an isomorphy between quantum states and graphs led to the use of complex vertex weighted digraphs, in contrast to the earlier usage of unweighted undirected graphs. This construction is able to represent all possible single qubit pure states. The representation of mixed states, in general, envisaged the introduction of a novel graph theoretic construction, viz., complex edge weighted digraphs with loops on the vertex having real weight. This thus incorporates an essentially complex network approach into quantum information, and by doing so also leads to developments in graph theory.

With a view of understanding multiqubit entanglement, we developed a graph theoretic method for generation of entangled two-qubit states, pure as well as mixed, such as Bell and Werner states. The key to this was the identification of graph operations that lead to the development of entangled state. As a byproduct, we also developed graph operations that generate separable states. The classification and study of generalized graph operations, an ongoing project [25], would hopefully yield to an improvement in the understanding of the separability and entanglement issues, both pure as well as mixed, in multipartite systems. In other words, a correspondence between quantum and graph operations is envisaged. This should open up many applications involving bipartite and multipartite entangled states in quantum information processing.

References

[1] W. K. Wootters, *Entanglement of Formation of an Arbitrary State of Two Qubits* Phys. Rev. Lett. 80 (1998) pp. 2245-2248.

[2] A. Miyake, *Classification of multipartite entangled states by multidimensional determinants*, Phys. Rev. A 67 (2003) pp. 012108: 1-10.

[3] R. B. Bapat, *Graphs and Matrices*, Hindustan Book Agency, New Delhi, India, Ist Edition (2011).

[4] M. E. J. Newman, *Networks, An Introduction*, Oxford University Press, New York.

[5] W. Kocay and D. L. Kreher, *Graphs, Algorithms and Optimization*, CRC Press (2005).

[6] Shimon Even and Guy Even, *Graph Algorithms, 2nd Edition*, Cambridge University Press, Cambridge.

[7] M. Hein, W. Dur, J. Eisert, R. Raussendorf, M. V. D. Nest, H. J. Briegel, *Entanglement in Graph States and its Applications*, arXiv:quant-ph/0602096.

[8] R. Idnicioiu and T. P, Spiller, *Encoding graphs into quantum states: an axiomatic approach*, arXiv:1105.5681.

[9] S. L. Braunstein, S. Ghosh and S. Severini, *The Laplacian of a Graph as a Density Matrix: A Basic Combinatorial Approach to Separability of Mixed States,* Annals of Combinatorics 10 (2006) pp. 291-317.

[10] K. Balasubramanian, K. Khokhani and S. C. Basak, *Complex Graph Matrix Representations and Characterizations of Proteomic Maps and Chemically Induced Changes to Proteomes,* Journal of Proteome Research 5 (2006) pp. 1133-1425.

[11] I. Nemoto and M. Kubono, *Complex Associative Memory*, Neural Networks 9 (1996) pp. 253-261.

[12] D. Cvetkovic, P. Rowlinson, S. K. Simic, *Signless Laplacians of finite graphs,* Linear Algebra and Appl.423 (2007) pp. 155 - 171.

[13] R. Grone, R. Merris AND V. S. Sunder, *The Laplacian spectrum of a graph* SIAM J. Matrix Anal. Appl. 11(1990) pp. 218-238.

[14] R. B. Bapat, D. Kalita and S. Pati, *On weighted directed graphs,* submitted.

[15] F. R. K. Chung and R. P. Langlands, *A Combinatorial Laplacian with Vertex Weights,* J. Combinatorial Theory, Series A 75 (1996), pp. 316 - 327.

[16] R. A. Brualdi and D. Cvetkovic, *A Combinatorial Approach To Matrix Theory and Its Applications,* CRC Press, Taylor and Francis Group, London.

[17] C. L. Coates, *Flow Graph Solutions of Linear Algebraic Equations,* IRE Trans. Circuit Theory, CT-6 (1959), pp. 170 - 187.

[18] F. Harary, *The Determinant of the Adjacency Matrix of a Graph,* SIAM Rev., 4 (1962), pp. 202 - 210.

[19] B. Liu and H. J. Lai, *Matrices in combinatorics and graph theory,* Kluwer Academic Publishers, London.

[20] A. Peres, *Separability Criterion for Density Matrices,* Phys. Rev. Lett. 77 (1996) pp. 1413-1415.

[21] W. K. Wootters, *Entanglement of Formation and Concurrence*, Quant. Inf. Comp. 1 (2001) pp. 27-44.

[22] Horodecki , *Quantum Entanglement,* Rev. Mod. Phys. 81 (2009) pp. 865-942.

[23] E. Parsonage, H. X. Nguyen, R. Bowden, S. Knight, N. Falkner, M. Roughan, *Generalized Graph Products for Network Design and Analysis*, IEEE International Conference on Network Protocols, 2011.

[24] F. Zhang, *The Schur Complement and Its Applications*, Springer Science, 2005.

[25] B. Adhikari, S. Adhikari and S. Banerjee, *Graph representations of entangled and separable states,* in preparation.