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Introduction

The language of the universe is Mathematics. Quantum mechanics is a branch of theoretical physics that describes the laws of the universe. Ideas from quantum physics play a significant role in multiple facets of modern mathematics. For example, many parts of representation theory, are motivated by quantum mechanics, such as, the quantum groups [Lusztig, 2010]. The Jones polynomial in knot theory is another notable example [Atiyah, 1990]. Quantum information theory [Nielsen and Chuang, 2002] is an application of quantum mechanics to information theory. Graph theory [West, 2001] is a well established branch of mathematics. This thesis is at the interface of these two branches of knowledge.

1.1 THE INTERFACE OF GRAPH THEORY AND QUANTUM MECHANICS

Graph theory provides a backdrop for the exploration of scientific techniques in discrete mathematics and combinatorics. It has utilizations in Physics, Chemistry, Biology, Engineering, Operational Research, Neural network, Social Science, Finance, and Economics. Combinatorial graphs provide a mathematical model for any system involving a binary relation. Mathematically, a graph $G = (V(G), E(G))$ is a combinatorial object consists of a vertex set $V(G)$ and an edge set $E(G) \subset V(G) \times V(G)$. Combinatorial graphs performs a significant role in quantum information theory. Below we discuss a number of ideas generated by this interface.

1.1.1 Quantum graph

The central idea of the quantum graph [Berkolaiko and Kuchment, 2013] is almost eighty years old. It was first developed by Linus Pauling as a simple model to describe a number of organic molecules. It took two decades before the scheme was worked out [Ruedenberg and Scherr, 1953], and it was forgotten, later on. This lack of interest was strange because it has various attractive features. It gathers intuitions from a number of disciplines such as partial differential equation, graph theory, combinatorics, spectral theory, and mathematical physics. From the eighth decade of the last century it started growing up [Roth, 1984] due to its applications to the fabrication techniques in solid state physics, to prepare structures of designed shapes in materiel and semiconductor analysis etc. Quantum graph provides a very suitable model of electron's movement in microscopic "wires".

The idea of quantum graph begins with metric graphs. A metric graph is a collection of intervals joined together at their end-points. These intervals form the edges of a metric graph whose vertices are the joints of these edges. Roughly speaking, a quantum graph is a metric graph along with a differential operator ("Hamiltonian") acting on functions defined on these intervals, and with suitable boundary conditions at the vertices. From geometric perspective, a quantum graph is an one dimensional complex along with a differential operator.

Quantum graphs [Berkolaiko, 2016] provide many non-trivial mathematical challenges. Studying Schrödinger operators on metric graphs is a growing area of mathematical physics. It is motivated by the applications of combinatorial graphs to physical phenomena. The utilization of graphs generates a simpler setting to study complex phenomena of quantum mechanics, for example scattering and resonances, Bose–Einstein condensation, Anderson localization, universality of spectral statistics, nodal statistics, etc. The model of quantum chaos on graphs in another model which utilize the idea of quantum graphs also.

1.1.2 Graph C* algebra

C* algebra [Arveson, 2012] is a subfield of functional analysis. C*-algebras were initially considered for their applications in quantum mechanics to investigate the physical observables. It began with Heisenberg's matrix mechanics. Subsequently, Neumann attempted establishing a general framework for these algebras. He wrote a series of papers on rings generated by operators. These papers are considered a special class of C*-algebras, also familiar as von Neumann algebras. C*-algebras perform a crucial tool in the theory of unitary representations of locally compact groups. It lies at the basis of quantum mechanics.

Graph C* algebra is a fascinating tool at the interface of graph theory and C* algebra. Here, we use directed graphs. A directed graph is a graph consists of oriented edges joining pairs of vertices. That is, there are edges $(u, v) \in E(G)$ such that $(v, u) \notin E(G)$. These graphs are represented by operators on a Hilbert space $\mathcal{H}$. Its vertices correspond to mutually orthogonal closed subspaces of $\mathcal{H}$. Also, the edges stand for the operators between the appropriate subspaces. The graph algebra is the C*-algebra generated by these operators. For a highly connected graph with finite vertices, the graph algebras coincide with a family of C* -algebras first studied by Cuntz and Krieger in 1980 [Cuntz and Krieger, 1980].

The graph C* algebras are recognised for providing a rich supply of examples in operator theory. It also provides a number of unexpected mathematical situations. It is also utilised in commutative algebras, non-commutative geometry, and as models for the classification of C* algebras. Graph algebras are attractive due to its structure theory involving the algebraic properties related to combinatorial paths in the underlined directed graph. This area is full of challenging mathematical problems, but like many other branches of mathematics its applications in other fields of science and technology is not clear yet.

1.1.3 Quantum walk and state transfer

The quantum walk and state transfer on graphs [Konno, 2008] has significant applications in quantum information and computation. In quantum information theory, quantum walk is crucial as it generates high speed up in the quantum mechanical analogue of a number of classical algorithms. From mathematical perspective, it is fascinating due to a number of mathematical challenges involving the applications of spectral graph theory and special functions on graphs. In spectral graph theory, we investigate characteristics of combinatorial graphs in terms of the eigenvalues of a number of matrices related to it. The Ihara zeta function [Terras, 2010] of graph has an interesting connection to the discrete time quantum walk on graphs.

Quantum walk is the quantum mechanical analogue of classical random walk on graphs. There are two types of quantum walks: continuous time quantum walk, and discrete time quantum walk. A relationship with the Ihara Zeta function and discrete time quantum walk is studied via the relationship of edge transition matrix and Grover unitary matrix [Konno and Sato, 2012]. The quantum state transfer is a continuous time quantum walk on graph G [Coutinho, 2014]. There are two models of perfect state transfer: XY model and XYZ model. Let $A(G)$, and $L(G)$ be an adjacency matrix, and Laplacian matrix, respectively, of a graph G, defined later. Then the XY model is governed by a Hamiltonian operator $\exp(itA(G))$, with $t \in \mathbb{R}^+$. The graph G admits a perfect state transfer from the vertex u to v if there is a time τ such that $|\exp(i\tau A(G))_{uv}| = 1$. In the XYZ model, we consider the Laplacian matrix instead of adjacency matrix $A(G)$. Therefore, the graph G admits a perfect state transfer from vertex u to vertex v if there is a time τ such that $|\exp(i\tau L(G))_{uv}| = 1$.

Research on quantum walk and state transfer has attracted by Mathematicians, Physicists, Computer scientists and Engineers. It is one of the rapidly growing topics at the interface of graph theory and quantum.

1.1.4 Graph theory in quantum error correcting codes

Analysing quantum error correcting codes is a crucial task in quantum information and communication. One may consider it as a quantum mechanical counterpart of error correcting codes [Huffman and Pless, 2010] in classical information theory. A classical linear code is a subspace of a vector space which is represented by a generator matrix or a parity check matrix. The standard forms of these matrices provide a scope to use matrices related to graphs in it. [Tonchev, 2002]. For instance, the binary matrix $[I|A(G)]$ can be considered as a generator matrix of some code, where $A(G)$ is the adjacency matrix of a graph G.

The idea of quantum CSS code utilises the classical error correcting codes. Let $\mathcal{C}_1$ and $\mathcal{C}_2$ be two classical error correcting codes such that $\{0\} \subset \mathcal{C}_1 \subset \mathcal{C}_2$. Then, the quantum CSS code with codewords $|0\rangle_L$ and $|1\rangle_L$ which are defined by,

$$\begin{aligned} |0\rangle_L &= \frac{1}{\sqrt{|\mathcal{C}_1|}} \sum_{v \in \mathcal{C}_2} |u+v\rangle \text{ where } u \in \mathcal{C}_1, \text{ and} \\ |1\rangle_L &= \frac{1}{\sqrt{|\mathcal{C}_1|}} \sum_{v \in \mathcal{C}_2} |u'+v\rangle \text{ where } u' \in \mathcal{C}_2 - \mathcal{C}_1. \end{aligned} \tag{1.1}$$

Graphs influence the CSS code when the underlined classical codes are related to graphs [MacKay et al., 2004; Schlingemann and Werner, 2001]. Studying quantum codes in terms of graphs is also an interesting topic at the interface of quantum information and graph theory that has attracted mathematicians, physicists, and computer scientists.

1.1.5 Graph states

Graph states [Hein et al., 2004; Anders and Briegel, 2006] are multipartite entangled states. They are defined on graphs where the vertices represent quantum spin systems and edges take the role of their interactions. They are particularly important in quantum computation within the framework of the one-way quantum computer associated with the quantum Fourier transform. For graph states we investigate properties of quantum states in terms of graph theoretical terms. Graph states are utilised in quantum error correction schemas, such as the concatenated CSS code, and the stabilizer code. Graph states are interesting in quantum information and computation as graphs generate an easier interface to describe very large multipartite quantum states.

1.1.6 Tensor network

Tensor network provides a scope of practical application of mathematical category theory in quantum information and computation [Biamonte et al., 2011]. Graph theory is heavily used in its foundation. Apart form its beautiful mathematical constructions, it has significant applications in geometrization of biological systems. This geometrization furnish meaningful explanation of functions of brain, and analysis of DNA structure. Also in Physics, it is utilised in the geometrization of gravitation, which was a major achievement in general relativity.

Tensor Network methods [Orús, 2014] have become very popular in recent years because of their capability in simulating strongly correlated systems. Roughly, a tensor is a higher dimensional generalization of a matrix. Intuitively, the interconnection between two tensors is generated by entanglement in quantum states represented by tensors. From another perspective, the tensor is the DNA of the wave-function. The whole wave-function of the system can be reconstructed from this fundamental piece. In this way, Tensor Network offers an efficient description of quantum many-body states. This description is based on the entanglement contained in the wave functions. Mathematically, the quantity and structure of entanglement is a consequence of the given pattern of network or graph, and the number of parameters in the tensor. The density matrix renormalization group [White, 1992], is one of the famous-most example of a tensor network.

We have briefly discussed a number of bridges between quantum mechanics, and graph theory. There are many other such connections not listed above. In fact, new developments, particularly in tensor network, are developing at a very fast pace. Quantum probability has deep connection with spectra of graphs [Hora and Obata, 2007]. Combinatorics plays a significant role in addressing a number of unsolved problems in quantum unitary symmetry [Louck, 2008]. It is our hope that the above collection of topics helps the reader to realise the importance of growing research interest in the intersection of quantum mechanics and graph theory.

1.2 A BRIEF OVERVIEW ON OUR CONTRIBUTIONS

The present work could be said to have its roots in Braunstein et al. [2006b]. Given any graph there are a number of positive semidefinite Hermitian matrices, for example, the Laplacian matrix, and the signless Laplacian matrix. If $K(G)$ is a Laplacian matrix of the graph G, then there is a density matrix defined by, $\rho(G) = \frac{1}{\text{trace}(K(G))}K(G)$. A density matrix represents a quantum state. Therefore, properties of the quantum state can be investigated in terms of the corresponding graph. In later years, a sequence of papers explored this field [Braunstein et al., 2006a; Wu, 2006a; Hildebrand et al., 2008; Wang and Wang, 2007; Wu, 2010, 2009; Hassan and Joag, 2007, 2008; Xie et al., 2013; Rahiminia and Amini, 2008; Hassan and Joag, 2008; Hui and Jiao, 2013; Li et al., 2015; Adhikari et al., 2017; Lockhart and Severini, 2016; Belhaj et al., 2016; Zhao et al., 2017; Simmons et al., 2017].

This thesis is distributed into seven chapters. The essence this work include both graph theory and quantum information theory. Most mathematicians are already familiar with combinatorial graphs. For non-mathematicians we introduce nomenclatures of graph theory whenever we need them for an application. Also, for mathematicians we discuss terminologies of quantum information theory where they are particularly involved. In Chapter 2, we have minimally introduced graph theory and quantum information which are mandatory for understanding the remaining thesis. Constructions in this chapter will be recalled whenever required. We have included a number of well-known quantum states whose density matrices are represented by the Laplacian matrices of graphs. Chapter 3 contains graph theoretic interpretation of quantum gates and a number of local unitary operations. Bell states are very useful in quantum information. We have illustrated a graph theoretic procedure for generating Bell states. This opens up the use of graph theory in quantum computation in future. We have discussed quantum entanglement in Chapter 4. Quantum entanglement is a class of quantum correlation used as a resource in quantum information theory. The idea of entanglement comes from the separability problem. We have found out a class of graphs which corresponds to separable quantum states in higher dimensions. Another class of quantum correlation is quantum discord, discussed in chapter 5. We have found out conditions for zero and non-zero discord states. A graph theoretic measure of quantum discord is also proposed. Constructing non-isomorphic cospectral graphs is one of the oldest problems in spectral graph theory. Here, we have employed tools of quantum information theory in generating non-isomorphic cospectral graphs. It is developed in chapter 6. We draw conclusions in chapter 7. At the end of every chapter, there is a list of open problems.