Summer 2023

Quantum Mechanics and Dynamical Models for Finite Unlabeled Simple Graphs

Nathan M. Lewis
San Jose State University

QUANTUM MECHANICS AND DYNAMICAL MODELS FOR FINITE UNLABELED SIMPLE GRAPHS

A Thesis

Presented to

The Faculty of the Department of Physics and Astronomy

San José State University

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

by

Nathan Lewis

August 2023

The Designated Thesis Committee Approves the Thesis Titled

QUANTUM MECHANICS AND DYNAMICAL MODELS FOR FINITE UNLABELED SIMPLE GRAPHS

by

Nathan Lewis

APPROVED FOR THE DEPARTMENT OF PHYSICS AND ASTRONOMY

SAN JOSÉ STATE UNIVERSITY

August 2023

Kassahun Betre, Ph.D.	Department of Physics and Astronomy
Curtis Asplund, Ph.D.	Department of Physics and Astronomy
Christopher Smallwood, Ph.D.	Department of Physics and Astronomy

ABSTRACT

QUANTUM MECHANICS AND DYNAMICAL MODELS FOR FINITE UNLABELED SIMPLE GRAPHS

by Nathan Lewis

This thesis constructs quantum mechanical theories of finite simple graphs for both labeled and unlabeled graphs. These theories may provide a description for discrete spacetime in a quantum gravity theory. Finite simple graphs and their properties are introduced. The first and second quantization of the standard quantum mechanics of particle systems are reviewed. A quantum mechanical theory of graphs similar to first quantization of standard quantum mechanics is developed via a correspondence of graph edges to particles in particle systems. An algorithm for constructing quantum states of graphs which is independent of graph vertex labeling is developed. It builds antisymmetric graph states which describe fermion graphs, the analog of systems of fermions for graphs. A quantum mechanical theory of graphs similar to second quantization of standard quantum mechanics is developed via the same correspondence of graph edges and particles. Edge creation and annihilation operators are defined which insert or delete edges between any pair of graph vertices. The commutation and anticommutation relations of these operators are defined to produce states which are symmetric and antisymmetric upon any vertex label permutation. Operators for certain graph properties and constructions are defined in this theory. Dynamics are then incorporated into the second quantization approach of the quantum mechanical graph theory by developing two model Hamiltonians, in analogy with the Hamiltonians of the Ising and Heisenberg models of ferromagnetism. From these Hamiltonians, statistical mechanics can be used to describe the dynamics of graphs.

DEDICATION

To my parents, who have supported me in my educational journey, and to my Tito Edgar Morada, my role model and mentor.

ACKNOWLEDGEMENTS

I would like to thank my research advisor Dr. Kassahun Betre for giving me the opportunity to work on this project and guiding me through my research and my work on this thesis.

DISCLAIMER

The work presented in this thesis was done in collaboration with my thesis advisor Dr. Kassahun Betre and is to appear in an upcoming publication to be coauthored with him.

TABLE OF CONTENTS

LIST OF FIGURES

I INTRODUCTION

The search for a quantum theory of gravity is one of the most pressing problems in modern physics. The Standard Model of particle physics is currently the best theory of fundamental particles and interactions consistent with quantum mechanics.[1] Although a very effective theory, it leaves many phenomena unexplained, including gravitation. Various approaches have been developed to address this limitation, including the quantization of spacetime. This places gravity on equal mathematical footing with quantum mechanics, where physical observables are quantized. Emergent quantum gravity builds quantized spacetime from simple constituents. For example, the graph emergent quantum gravity approach builds quantized spacetime from finite graphs, which consist of a set of objects and binary relationships between them. Geometrically, they may be represented by a set of vertices and edges connecting them. The vertices may represent constituents of space and the edges may represent binary relationships between these constituents, which encode the structure of space. The time evolution of graphs in a dynamical theory leads to the emergence of spacetime. The graph emergent quantum gravity approach was introduced by Konopka et al., who developed a quantum theory of finite graphs and graph dynamics.[2] Spacetime can then emerge from macroscopic phenomena arising from graph dynamics. One limitation of this theory is its dependence on graph vertex labeling; Konopka builds a quantum theory of graphs with distinguishable vertices. These graphs must be labeled to properly distinguish between their vertices. This is akin to defining a coordinate system on the graph. An emergent quantum gravity theory, however, must be coordinate system independent, as is general relativity, so that the predictions of the theory do not depend on the coordinate system used. This thesis addresses this issue by developing quantum theories of unlabeled finite graphs similar to Konopka's quantum theory of finite graphs. In describing unlabeled graphs, the theory does not depend on a graph's vertex labeling to describe a quantum state of the graph, and so is inherently coordinate system independent. This theory may then be used to derive a coordinate system invariant description of emergent spacetime.

II LITERATURE REVIEW

II.A The Standard Model of Particle Physics and the Quantum Gravity Problem

The Standard Model of particle physics is a quantum field theory which describes fundamental particles and interactions. It is the most accurate and complete theory of fundamental particles and interactions today.[1] It has successfully explained many physical phenomena, such as the anomalous magnetic moment of the muon, whose predicted value from the Standard Model constitutes the most accurate agreement between theory and measurement in all of science.[3] However, it also has many limitations, including its neglect of gravitation, which arises from the background dependence of the theory. The Standard Model assumes a static Minkowskian (flat) spacetime background for particles and their interactions. This contradicts the dynamical spacetime of general relativity, where there is a mutual interaction between spacetime and matter; the former provides a stage for particle dynamics, but can change in response to these dynamics. Quantum gravity is a field of physics which attempts to rectify this problem by incorporating quantum mechanics into gravitational theory.[4]

One important step in developing a quantum gravity theory is the formulation of quantum field theory in curved spacetime.[5] This is a step in the right direction because it generalizes the Minkowskian spacetime background of the Standard Model to general spacetime backgrounds. However, these theories are still limited because the background spacetime is still classical; they do not account for quantum effects. Also, they are not background independent; they still depend on a static spacetime background, so they do not address the considerable challenge of incorporating the mutual interaction of matter and spacetime into gravitational theory.

However, a quantum gravity theory may be well worth the difficulty required to formulate it. It would not only provide a more fundamental description of gravity, but also resolve more pressing issues in physics, such as singularities in general relativity. These singularities signal the mathematical breakdown of the theory, which occurs because it neglects unknown

fundamental principles which govern gravity. A quantum theory of gravity may provide these principles and cure these singularities, which may be useful, for instance, for curing the Big Bang singularity at the beginning of the universe.[6] A quantum theory of gravity may also explain the source of black hole entropy, whose existence is required by the second law of thermodynamics. The required entropy of a black hole is known,[7] but the source of this entropy is unknown. In describing the fundamental constituents of spacetime, quantum gravity theories may account for black hole entropy because they naturally arise from the internal degrees of freedom of spacetime. For example, loop quantum gravity has been used to derive the expected black hole entropy from the internal degrees of freedom the theory associates with spacetime.[8]

Motivated by these promises, many physicists have formulated quantum theories of gravity, but none of them have proven to be complete and accurate. This section will outline some of the progression of quantum gravity theories.

II.B Semiclassical Gravity

A common approach to formulating a quantum gravity theory is to quantize perturbations of a background spacetime. This makes gravitational theory more mathematically consistent with quantum mechanics, since both theories are now premised on discrete mathematical objects. However, we can also keep geometry classical while accounting for the quantization of matter by preserving the Einstein field equations of general relativity and using the quantum expectation value for the energy-momentum tensor in these equations. This is called the semiclassical approach to quantum gravity, since it is a partly classical and partly quantum treatment of gravity.

One clear deficiency of this theory is its use of the quantum expectation value of the energy-momentum tensor, which neglects fluctuations and correlations in this quantity. The stochastic approach to semiclassical gravity addresses this issue by accounting for these correlations and fluctuations.[9] Although this approach may be useful for developing an exact

quantum gravity theory, it is still an approximation which is inaccurate when there are large fluctuations in the energy-momentum tensor. The intractability of these fluctuations calls the semiclassical paradigm into question.[10] In addition, some experiments have revealed mathematical inconsistencies in this approach.[11]

II.C The Quantization of Spacetime

We now discuss quantum gravity theories which quantize spacetime. These theories may be broadly classified as perturbative and nonperturbative theories.

II.C.1 Nonperturbative Theories: Wheeler-DeWitt Canonical Quantization

Wheeler-DeWitt canonical quantization is a nonperturbative theory of quantum gravity which quantizes spacetime by enforcing quantum commutation relations on the Arnowitt-Deser-Misner (ADM) formalism for general relativity, a Hamiltonian (canonical) representation of the theory.[12] In this representation, the metric is defined as a canonical position variable and the Hamiltonian is constructed to yield the Einstein field equations of general relativity from the canonical equations of motion. The theory is quantized by promoting the canonical variables to operators and imposing the appropriate quantum commutation relations between them. The theory thus incorporates quantum effects into the metric, and thus into spacetime.

One of the most notable developments from this approach is loop quantum gravity, one of the mainstream quantum gravity theories today. It arose from a variable change in the ADM formalism to the Ashtekar variables, where the canonical quantization regime yields solutions representable by loops. Consequently, space may be viewed as a web of interlocking loops.[13]

This approach is appealing because it simply extends a known theory, canonical quantization, to quantum gravity. However, the ADM formalism of general relativity contains constraints, which encode the Einstein field equations into the theory.[14] The incorporation of these constraints is difficult and the Wheeler-DeWitt equations have not yet been solved in their

full generality. A more fatal flaw of this approach, however, is the incommensurate treatment of time in canonical quantization and general relativity: the former assumes time monotonically increases, while the latter does not assign time a fixed direction.[15]

II.C.2 Perturbative Theories: Gravitational Perturbative Quantum Field Theory

Quantum gravity has also been formulated as a perturbative quantum field theory, where the fluctuations of the metric tensor of general relativity are treated as a quantized field.[16] This formulation eliminates the specious extension of canonical quantization to general relativity, but is still flawed because it is still background dependent. The theory also has mathematical limitations. Perturbative quantum field theory depends on the existence of a nondynamical field configuration, which is not clearly defined in the gravitational theory.[14] The most significant drawback of the perturbative formulation, however, is that it is nonrenormalizable; it yields nonsensical infinities which cannot be tamed by mathematically modifying the theory.[17]

Neither the perturbative nor nonperturbative approaches to quantum gravity can account for the interaction of matter and spacetime because they are both background dependent. We thus suspect to create a quantum gravity theory by accounting for more fundamental principles of spacetime rather than mathematically modifying current theories. For this purpose, we discuss emergent quantum gravity.

II.D Emergent Quantum Gravity

Emergent quantum gravity does not appeal to previous theories and starts from fundamental principles. Spacetime is derived solely from macroscopic properties emergent from interactions of simple constituents. Thus, these theories are self-referential and provide a fundamental description of spacetime.

We mention two approaches to emergent quantum gravity in passing: quantum gravity built from quantum entanglement and from matrices. Quantum gravity is constructed from quantum entanglement via the AdS/CFT correspondence, which is a duality between a gravity theory

describing spacetime in negatively curved Anti-de Sitter (AdS) space to a conformal quantum field theory defined on the spacetime's boundary. We can thus correspond quantum field states with spacetime geometries in the gravity theory. Additionally, entangling or disentangling quantum field states corresponds to connecting or disconnecting spacetime in the gravity theory.[18] Spacetime can thus be constructed by entangling or disentangling quantum field states. Emergent quantum gravity built from matrices incorporates quantum mechanical non-commutativity into the commutative geometry of general relativity as a result of the non-commutativity of matrices, thus incorporating quantum principles into spacetime.

II.D.1 Quantum Graphity: Emergent Spacetime from Graphs

This thesis considers an approach to emergent quantum gravity which utilizes finite graphs, which consist of sets of objects with binary relationships between their constituent objects. We can represent a graph's objects with vertices and their relationships with edges connecting them. Finite graphs have been used in physics in various contexts, including in the study of crystals and quantum chaos.[19,20] In 2006, Konopka et al. applied finite graphs to emergent quantum gravity, where the graphs describe the structure of space.[2] They developed a quantum theory of graphs which associates graphs with vectors in a Hilbert space. With this association, graphs may time evolve quantum mechanically by a Hamiltonian operator defined in the Hilbert space. The graph state at a fixed time determines the structure of space and its dynamical evolution incorporates time into space. Thus, the graphs and their resulting dynamics may provide a quantum description of spacetime.

One limitation of this approach is that it utilizes labeled graphs. Since vertex labeling defines a coordinate system on a graph, the analog of coordinate system invariance for graphs is the permutation invariance of the vertex labels. Thus, Konopka's theory cannot provide a coordinate system invariant description of spacetime like general relativity. This thesis builds upon Konopka's formalism by similarly developing quantum descriptions for graphs in analogy

with the first and second quantization of quantum mechanics, but with unlabeled graphs instead of labeled graphs. Starting with unlabeled graphs ensures that the theory is coordinate system independent, so that any quantum gravity theory emerging from this theory is also coordinate system independent. It will then incorporate dynamics into the theory to provide a foundation for describing quantized spacetime, as in Konopka's work.

The remainder of this thesis is outlined as follows. Section III will discuss properties of finite graphs relevant to this thesis. Section IV will review the first and second quantization of quantum mechanics, which will be important for constructing a quantum formalism for graphs. Sections V and VI will develop quantum mechanical theories of unlabeled graphs similar to first and second quantization of standard quantum mechanics. In starting with unlabeled graphs, the formalism is coordinate system invariant from the beginning. Section VII will incorporate dynamics into the theory. It will construct Hamiltonians which can model graph state dynamics and explain how quantum gravity may emerge from the quantum graph theory. Section VIII concludes the thesis.

III FINITE GRAPHS

In this section, we introduce properties of finite graphs relevant to this thesis. We first present the formal set definition of graphs and a geometrical representation of them.

III.A Definition of Graphs

Definition 1. *A graph G consists of a vertex set V and an edge set E which is a subset of* $V \times V$.

For example, a graph may consist of a vertex set $V = \{1,2,3,4\}$ and an edge set $E = \{\{1,2\},\{2,3\},\{3,4\},\{1,3\}\}$, as shown in Figure 1. The vertices in this figure correspond to the elements of the vertex set and the edges to the elements of the edge set (hence the names for each set chosen in the definition). We also define vertex degree for each vertex in a graph:

Definition 2. *The degree of a vertex v is the number of vertices adjacent to it.*

The definition of the edge set E in Definition 1 implies that graphs may generally have self-looping edges, which start and terminate at the same vertex. These edges correspond to ordered pairs $(x,y) \in V \times V$ where $x = y$. Also, this definition of edges implies that graphs may have directed edges, which have a sense of pointing from one vertex to another. These edges correspond to the edges $\{(x,y),(y,x)\} \in V \times V$. Note that these two elements describe an edge between the same vertices, but are ordered differently, and so have a sense of being directed differently. We will neglect graphs with self-looping and directed edges in this thesis and instead consider simple graphs, which will constitute the graph analogs of fermions systems later in the thesis. Multigraphs, graphs which can have multiple edges defined between any pair of graph vertices, may constitute the graph analogs of boson systems, but will not be utilized in this thesis. Figure 1 shows an example of a simple graph. The more abstract set definition and the more intuitive geometrical representation of graphs will be used throughout the thesis depending on context.

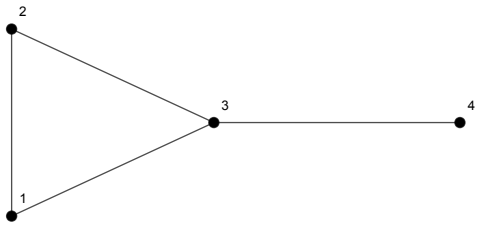

Figure 1: An example of a simple graph.

III.B Constructions on Graphs

In this thesis, we will consider constructions on graphs: the graph complement, induced subgraph, and unit sphere of a graph around a vertex. We first define the graph complement:

Definition 3. *The graph complement G^* of a graph G is the graph produced by defining edges on all non-adjacent vertices of G and deleting edges on all adjacent vertices of G.*

Figure 2 shows two complementary graphs, each composed of black and red edges, which are superimposed to emphasize their complementary relationship. Next, we define the induced subgraph on a subset of vertices of a graph:

Definition 4. *The induced subgraph $G'(H)$ on a subset H of the vertices of a graph G is the graph formed from all the edges defined in G between the vertices in H.*

The unit sphere is a type of induced subgraph considered in this thesis:

Definition 5. *The unit sphere $S(v)$ of a graph G around one of its vertices v is the induced subgraph on the vertices which are unit graph distance from v.*

Note that two vertices are unit graph distance apart if the minimum number of edges separating them is one. Thus, the unit sphere on a graph is clearly an extension of the unit sphere of Euclidean space to graphs. Figure 3 shows an example of the unit sphere of a graph around a vertex. It is defined around vertex 3 of the graph and its edges are shown in red.

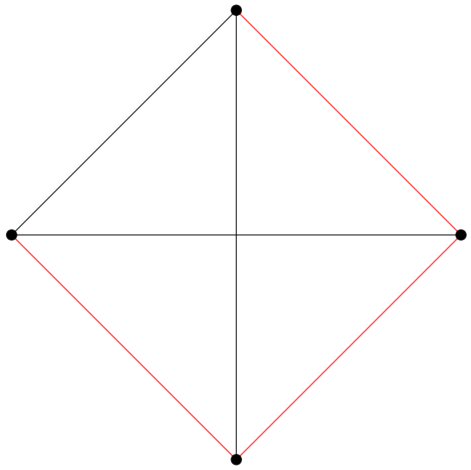

Figure 2: An example of complementary graphs, each shown in black or red. The graphs are superimposed to emphasize the complementary relationship between the graphs.

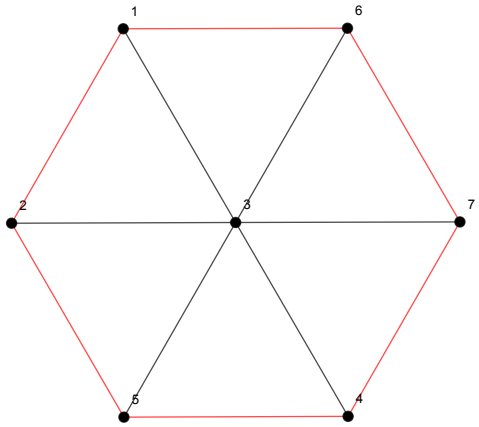

Figure 3: A unit sphere of a graph defined around vertex 3, shown with red edges.

III.C Graph Isomorphism and Automorphism

We conclude this section by introducing equivalence relations for graphs. An equivalence relation is a generalization of equality to general mathematical objects, where the notion of equality is less clear. To define equivalence relations between graphs, we need to specify a graph property which must be the same for a set of graphs if they are to be equivalent. For this purpose, we choose the edge adjacency of graph vertices:

Definition 6. *The edge adjacency of a graph's vertices is a specification of all the vertices*

which are adjacent to each vertex in the graph.

We consider two graphs to be equivalent if the edge adjacency of each of their vertices are identical, in which we call the two graphs isomorphic. Alternatively, we can define an isomorphism of two graphs in terms of mappings between their vertex sets:

Definition 7. *Two graphs G and H are isomorphic if there exists a bijection* Γ *between the vertex sets* $V(G)$ *and* $V(H)$ *of G and H such that if two vertices u and v are adjacent in G,* $\Gamma(u)$ *and* $\Gamma(v)$ *are also adjacent in H.*

We call such a mapping between two isomorphic graphs an isomorphism. This definition of graph isomorphism implies that an isomorphism preserves the edge adjacency of a graph. Figure 4 shows a pair of isomorphic graphs. The right graph is obtained from the left graph by mapping the vertices of the latter as $1 \to A$, $2 \to B$, $3 \to C$, $4 \to D$, $5 \to E$, $6 \to F$, and $7 \to G$. This transformation preserves the edge adjacency of the left graph (this is a trivial example because the isomorphism arises from a simple one-to-one relabeling of vertices).

Finally, we introduce graph automorphism, a special case of graph isomophism relevant to this thesis:

Definition 8. *A graph automorphism is a graph isomorphism which takes a graph G to itself.*

Figure 5 shows an example of two identical graphs related by an automorphism. The right graph is obtained by mapping the vertices of the left graph with $1 \to 4$, $2 \to 1$, $3 \to 2$, and $4 \to 3$. The graphs are automorphic because their edge sets are identical. A graph automorphism is a symmetry transformation of a graph specified by some permutation of the graph vertices. The set of all automorphisms of a graph constitutes a group, a type of axiomatically defined set. We elaborate on groups further in section V.

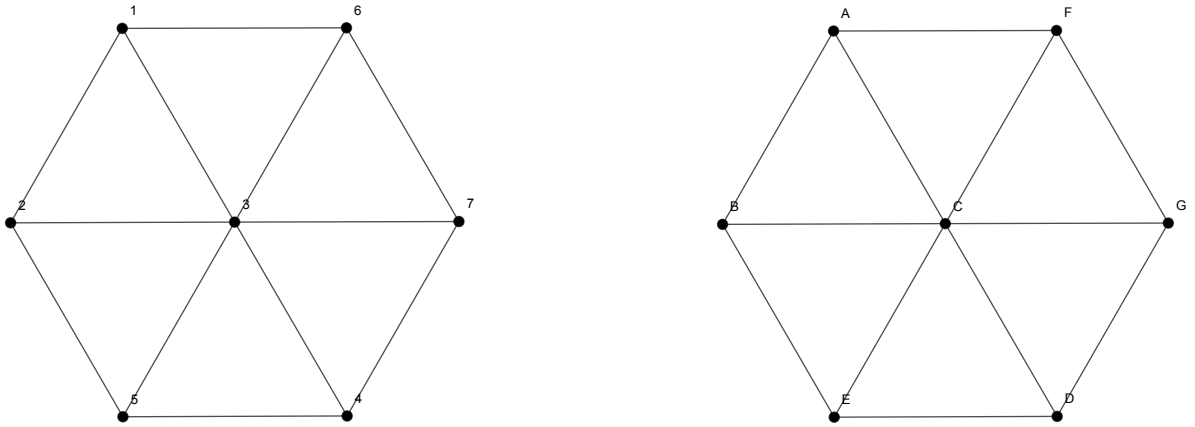

Figure 4: An example of two isomorphic graphs. They are isomorphic because there exists a bijection between their vertex sets which preserves their edge adjacency.

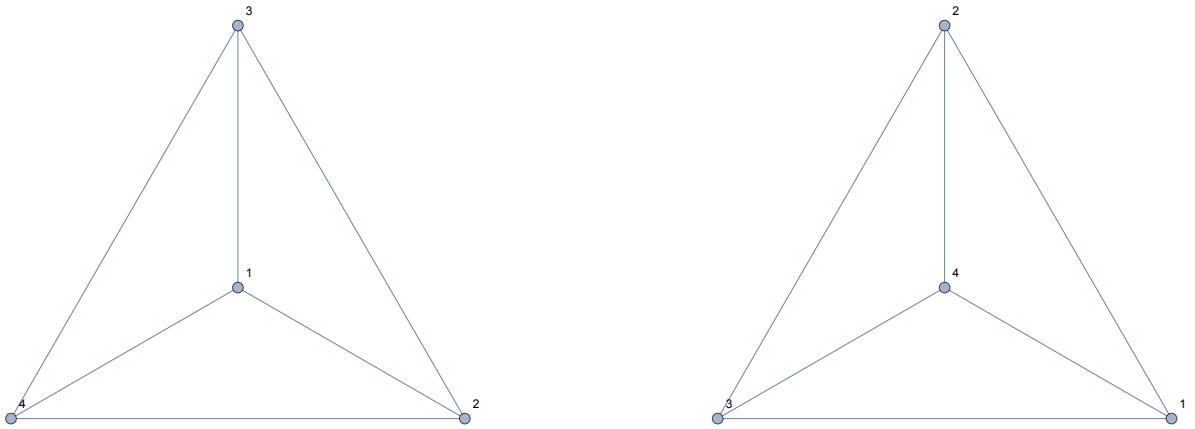

Figure 5: An example of two automorphic graphs. The two graphs are identical and are related by an isomorphism.

IV PARTICLE QUANTUM MECHANICS IN FIRST AND SECOND QUANTIZATION

In this section, we summarize first and second quantization of standard particle quantum mechanics, which will be important for creating a quantum theory of graphs. Quantization of a classical theory must account for the non-commutativity of classical observables such as position and momentum and the quantum statistics of particles. First and second quantization are two methods by which quantum principles can be incorporated into classical theory. First quantization applies to systems of fixed numbers of particles, while second quantization describes quantum mechanics of systems with variable numbers of particles.

IV.A Quantum Statistics of Particles and Symmetries of the Wavefunction

Since we do not assign dynamical variables such as position and momentum to graph states, we focus on incorporating quantum statistics into a quantum theory of graphs. The quantum statistics of particles arise from the indistinguishability of quantum particles and the invariance of the physical predictions of the quantum theory when the wavefunction is multiplied by an overall complex phase $e^{i\theta}$, where $0 \leq \theta < 2\pi$. This invariance arises because the probability distribution of an observable is given by the complex modulus of the wavefunction expressed in the basis of that observable. The invariance then follows because $|e^{i\theta}| = 1$. To begin, we consider a system of N identical particles. Classically, we can distinguish between these particles by tracking their trajectories, since they are deterministic in principle. Quantum mechanically, however, we cannot distinguish between these particles because their trajectories are nondeterministic; we can only specify the probability of a particle following a certain trajectory between two points. Because identical quantum particles are indistinguishable, quantum mechanical predictions of a particle system must be independent of particle labeling. Since physical predictions in quantum theory are determined by the complex modulus of a wavefunction, the wavefunction must only change by a complex phase under any particle label

permutation P:

$$\Psi(x_1, x_2, ..., x_N) = e^{i\theta_P}\Psi(x_{P(1)}, x_{P(2)}, ..., x_{P(N)}), \tag{1}$$

where $P(i)$ denotes the particle label i is permuted to upon action of the permutation P and $0 \leq \theta < 2\pi$ is a complex phase which depends on the permutation P. Although the phase θ_P is any complex phase, wavefunctions for most quantum particle systems transform according the the phases $\theta_P = 0, \pi$ under permutations P of order two (i.e., they only consist of a single interchange of two particle labels. Note that the phases for permutations P of general order are found by applying (1) for each of the order two permutations which compose P). These phases correspond to systems of bosons and fermions, which have wavefunctions which are symmetric or antisymmetric under any permutation of order two, which we call the interchange of a pair of particle labels. The symmetry properties of boson and fermion wavefunctions dictate the statistical properties of boson and fermion systems. The antisymmetry of fermion wavefunctions leads to the Pauli exclusion principle, which restricts occupation of particle states to at most one particle. On the other hand, the symmetry of boson wavefunctions places no such restriction on occupation number of states, so bosons will tend to condense into lower energy states to minimize the system energy.

We now incorporate quantum statistics into a quantum mechanical theory of particles using both first and second quantization.

IV.B Particle Quantum Mechanics in First Quantization

IV.B.1 Quantum Mechanics of a Single Particle in First Quantization

First quantization was the first method used to quantize classical theory of a fixed number of particles. In this approach, system states are promoted to vectors which live in a Hilbert space $\mathscr{H}$, a vector space equipped with an inner product. The inner product is a generalization of the dot product, so it multiplies two vectors to yield a scalar. To define an inner product on a general vector space, we introduce the dual space V^* to a vector space V as the set of all linear maps which take vectors in V to the scalars of V. We take an inner product by acting a dual

vector on a vector to obtain a scalar. The inner product has the same properties as the dot product of Euclidean vector spaces, but its meaning depends on the nature of the vectors in the vector space. Observable quantities are represented by Hermitian operators in the Hilbert space, which we assume are differential operators for this discussion. State vectors in the Hilbert space are then functions of some dynamical variable and the inner product $\langle\phi|\psi\rangle$ of a state vector $|\psi\rangle$ with a dual vector $\langle\phi|$ is then defined in terms of an integral:

$$\langle\phi|\psi\rangle = \int \phi^*(x)\psi(x)dx, \tag{2}$$

where x is some dynamical variable and the integral is taken over all x.

Like any Hermitian operator acting in a vector space, any operator representing an observable in the Hilbert space can be expressed in any basis, but we are most concerned with the basis in which the operator is diagonalized. We find this basis by determining the eigenvalues and eigenvectors of these operators, which comprise the possible measurements of the observable and the quantum states corresponding to these measurements. Because the eigenvalues of a Hermitian operator are real, the operators representing observables in the Hilbert space are guaranteed to give real values for measurements of observables, as expected. The eigenvectors of a Hermitian operator form an orthonormal basis for the Hilbert space, and it is assumed that this basis is complete. We may express these eigenvectors as functions of any dynamical variable to obtain eigenfunctions of the observable represented by the operator. We may then express any wavefunction as a linear combination of these eigenfunctions. If $|\Psi\rangle$ represents a system state and $|\phi\rangle$ is an eigenstate of an observable, the probability of measuring the system in state $|\phi\rangle$ is given by $|\langle\phi|\Psi\rangle|^2$.

We have discussed quantum states without showing how they are derived, so we now describe how these states are derived. The Hamiltonian operator of a system specifies its dynamics. The eigenfunctions of this operator are energy eigenfunctions and span the Hilbert

space of the system. The Schrodinger equation determines the wavefunction:

$$\hat{H}\,|\Psi\rangle = \hat{E}\,|\Psi\rangle\,, \tag{3}$$

where $\hat{E}$ is the energy operator:

$$\hat{E} = i\hbar\frac{\partial}{\partial t}. \tag{4}$$

This operator explicitly depends on time, so the Schrodinger equation (3) explicitly depends on time also. We can address the time dependence of this equation with a separable ansatz solution if the Hamiltonian is not explicitly dependent on time. We assume the Hamiltonian is expressed in the position basis and express the state in the position basis $|\psi\rangle \to \Psi(\mathbf{r},t)$. We then substitute the separable ansatz solution $\Psi(\mathbf{r},t) = \psi(\mathbf{r})T(t)$ into (3). This yields a solution of form

$$\Psi(\mathbf{r},t) = e^{-iEt/\hbar}\psi(\mathbf{r}), \tag{5}$$

where the spatial part $\psi(\mathbf{r})$ is governed by the time-independent Schrodinger equation:

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{6}$$

This equation gives the energy eigenvalues and the spatial part of the eigenfunctions of the system. These eigenfunctions can be substituted into the ansatz (5) to yield time dependent energy eigenfunctions for the system. Because the Schrodinger equation (3) is linear, any solution to the system is given by a linear combination of these energy eigenfunctions, which form an orthonormal basis for the system's Hilbert space.

IV.B.2 Quantum Mechanics of Multi-Particle Systems in First Quantization

We now consider the quantum mechanics of systems of identical particles. Consider a system of N identical particles. This system has a Hilbert space $\mathscr{H}_N$ given by the tensor product of N copies of the single-particle Hilbert space $\mathscr{H}$:

$$\mathscr{H}_N = \mathscr{H}^{\otimes N} \tag{7}$$

Because the particles are identical, the predictions of the theory must be invariant upon any permutation of particle labels, so the wavefunction must transform as (1) under such permutations. We only consider the cases where the wavefunction transforms as $\theta_P = 0, \pi$ for any particle interchange, which correspond to bosons and fermions, respectively. Then, (1) implies that the wavefunction must be symmetric or antisymmetric under any particle label interchange for bosons and fermions, respectively. We must restrict the boson Hilbert space to symmetric states in $\mathscr{S}$ under particle label interchange and the fermion Hilbert space to antisymmetric states in $\mathscr{S}$ under particle label interchange. Consider a system of N bosons and let $\Psi_i(x_1, x_2, ..., x_N)$ denote the state of the system. The symmetric states $\Psi_B(x_1, x_2, ..., x_N)$ are

$$\Psi_B(x_1, x_2, ..., x_N) = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_N} \Psi(x_{\sigma(1)}, x_{\sigma(2)}, ..., x_{\sigma(N)}), \tag{8}$$

where S_N is the symmetric group of size N, the group composed of all possible permutations on N elements. It is easy to verify that (8) is symmetric under any particle label interchange. Similarly, the antisymmetrized state of a system of N fermions is

$$\Psi_F(x_1, x_2, ..., x_N) = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_N} \text{sgn}(\sigma) \Psi(x_{\sigma(1)}, x_{\sigma(2)}, ..., x_{\sigma(N)}). \tag{9}$$

The antisymmetrized state is found similarly to the symmetrized state, but with each term weighed by the sign of its corresponding permutation.

The boson and fermion wavefunctions (8) and (9) are cumbersome because there is redundancy in incorporating quantum statistics into quantum theory using first quantization: we must assign assign one particle to each coordinate in each term in (8) and (9). This is not only redundant, but inappropriate: we can only know how many particles occupy each state, or the occupation number of each state. Second quantization remedies this by only specifying the number of particles in each state. This representation of particle states is called the occupation number representation. It not only accounts for the indistinguishability of particles, but also describes systems with a variable number of particles.

IV.C Particle Quantum Mechanics in Second Quantization

Second quantization eliminates the redundancy of first quantization by constructing quantum states from acting creation and annihilation operators on a vacuum state with no particles. These operators add particles to or subtract particles from states and allow them to be specified in the occupation number representation. These operators may be used to construct more complicated operators in the system's Hilbert space. Creation and annihilation operators are mathematically motivated by drawing an analogy between quantum systems of particles and the quantum one-dimensional simple harmonic oscillator, which is described by a Hamiltonian given in the position basis by

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2. \tag{10}$$

Solving the the time-independent Schrodinger equation (6) with this Hamiltonian yields the energy levels of the system:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{11}$$

where $n = 0, 1, 2, ...$ is a non-negative integer. The ground state energy of the system is $\frac{1}{2}\hbar\omega$, and excited states are spaced by $\hbar\omega$. We now consider the operators

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right), \tag{12}$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right). \tag{13}$$

These operators are interpreted as creation and annihilation operators of the quantum of energy $\hbar\omega$, which add or subtract a quantum of energy to or from the system, respectively. To verify this, we act creation and annihilation operators on the energy eigenstates $\psi_n(x)$ of energy E_n of the quantum simple harmonic oscillator, then act the Hamiltonian on this result to measure the energy:

$$\hat{H}\hat{a}^\dagger\psi_n(x) = (E_n + \hbar\omega)\psi_n(x), \tag{14}$$

$$\hat{H}\hat{a}\psi_n(x) = (E_n - \hbar\omega)\psi_n(x). \tag{15}$$

Indeed, the creation and annihilation operators add or subtract the quantum of energy $\hbar\omega$ to or from the system.

We can extend this formulation of creation and annihilation operators to the quantum mechanics of multi-particle systems. The creation and annihilation operators are defined to add or subtract particles to or from the system. We denote creation and annihilation operators for the single-particle state α as $\hat{a}_\alpha^\dagger$ and $\hat{a}_\alpha$, respectively. With these operators, we can "jump" between states of a fixed number of particles in a multi-particle Hilbert space to one corresponding to a different number of particles. Acting on an N-particle state in a tensor product Hilbert space (7) with a creation or annihilation operator yields a state in a tensor product Hilbert space (7) corresponding to $N+1$ or $N-1$ particles, respectively. Thus, second quantization states live in Fock space $\mathscr{F}$, the direct tensor sum of all tensor product powers of the single-particle Hilbert space:

$$\mathscr{F} = \bigoplus_{i=0}^{\infty} \mathscr{H}^{\otimes i}. \tag{16}$$

We must then choose the symmetric and antisymmetric subspaces $\mathscr{H}_+$ and $\mathscr{H}_-$ of the Hilbert space (7) for boson and fermion systems, respectively, to ensure states are consistent with quantum statistics. We then write the Fock spaces $\mathscr{F}_B$ and $\mathscr{F}_F$ for boson and fermion systems as

$$\mathscr{F}_{\mathscr{B}} = \bigoplus_{i=0}^{\infty} \mathscr{H}_+^{\otimes i}, \tag{17}$$

$$\mathscr{F}_{\mathscr{F}} = \bigoplus_{i=0}^{\infty} \mathscr{H}_-^{\otimes i} \tag{18}$$

We now make the second quantization of quantum mechanics consistent with quantum statistics. Since we use creation and annihilation operators to specify states in this formalism, we incorporate quantum statistics into it by fixing commutation and anticommutation relations of the creation and annihilation operators. To distinguish between boson and fermion statistics, we define $\hat{b}_\alpha^\dagger$ and $\hat{b}_\alpha$ to be boson creation and annihilation operators, respectively, and $\hat{c}_\alpha^\dagger$ and

$\hat{c}_\alpha$ to be fermion creation and annihilation operators, respectively. Boson statistics can then be incorporated into the second quantization of quantum mechanics by enforcing the commutation relations

$$[\hat{b}_\alpha^\dagger, \hat{b}_\beta^\dagger] = [\hat{b}_\alpha, \hat{b}_\beta] = 0, \tag{19}$$

$$[\hat{b}_\alpha, \hat{b}_\beta^\dagger] = \delta_{\alpha\beta}. \tag{20}$$

The commutation relation (19) ensures that the boson wavefunctions are symmetrized and (20) ensures the non-commutativity of position and momentum $[\hat{x}, \hat{p}] = i\hbar$.

We must also ensure that states resulting from the action of creation and annihilation operators on other states are normalized. If $|n_\alpha\rangle$ is a boson state with n_α particles in the α'th state, the boson creation and annihilation operators must satisfy

$$\hat{b}_\alpha^\dagger |n_\alpha\rangle = \sqrt{n_\alpha + 1}\, |n_\alpha + 1\rangle\,, \tag{21}$$

$$\hat{b}_\alpha |n_\alpha\rangle = \sqrt{n_\alpha}\, |n_\alpha - 1\rangle\,, \tag{22}$$

to ensure the normalization of boson states which result from action of these operators on other states. We can also construct the number operator, which counts the total number of particles in all one-particle states α. If $|n_1, n_2, ..., n_i\rangle$ denotes the multi-particle state with n_i particles in the ith state, the number operator is defined by

$$\hat{N} |n_1, n_2, ..., n_i\rangle = \left(\sum_\alpha \hat{b}_\alpha^\dagger \hat{b}_\alpha \right) |n_1, n_2, ..., n_i\rangle = \left(\sum_\alpha n_\alpha \right) |n_1, n_2, ..., n_i\rangle\,. \tag{23}$$

Thus, we can determine the particle occupancy of a multi-particle state by finding its eigenvalue under the action of the number operator.

Similarly, fermion particle statistics can be incorporated into the second quantization of quantum mechanics by enforcing the anticommutation relations

$$\{\hat{c}_\alpha, \hat{c}_\beta\} = \{\hat{c}_\alpha^\dagger, \hat{c}_\beta^\dagger\} = 0, \tag{24}$$

$$\{\hat{c}_\alpha, \hat{c}_\beta^\dagger\} = \delta_{\alpha\beta}. \tag{25}$$

Again, (24) ensures that fermion wavefunctions are antisymmetric and (25) ensures the non-commutativity of position and momentum. The fermion creation and annihilation operators also satisfy (21) and (22) (with $\hat{c}_i^\dagger$ and $\hat{c}_i$ in place of $\hat{b}_i^\dagger$ and $\hat{b}_i$, respectively) to ensure the normalization of states which result from action of these operators on other states. A number operator can also be defined as in (23) upon replacement of $\hat{b}_i^\dagger$ and $\hat{b}_i$ with $\hat{c}_i^\dagger$ and $\hat{c}_i$.

The commutation and anticommutation relations of the boson and fermion creation and annihilation operators allow us to create symmetric and antisymmetric boson and fermions states, respectively.

V FIRST QUANTIZATION OF GRAPH QUANTUM MECHANICS

In this section, we develop a quantum theory of finite unlabeled graphs similar to the first quantization of particle quantum mechanics. This quantum formalism for these graphs is similar to that derived by Konopka, but we begin with unlabeled graphs so that the formalism is independent of vertex labeling. We first draw an analogy between multi-particle systems and graphs to connect the quantum mechanics of particles and graphs. In particle quantum mechanics, particles are the dynamical objects, which we may label with one quantum number. In graph quantum mechanics, we consider edges to be the dynamical objects, since graph edges constitute the essential information of a graph. Unlike particles, however, we must label edges with two quantum numbers, since we must specify two vertices to describe an edge. With this correspondence, we can formulate a quantum mechanical theory of unlabeled graphs.

V.A Defining Quantum Graph States

Since we consider edges to be the dynamical objects of graphs, we may define a graph state by specifying its edges. We denote a graph state for a graph with edge set $E = \{\{i_1, j_1\}, ..., \{i_N, j_N\}\}$ as $|i_1 j_1, ..., i_N j_N\rangle$. Note that this notation describes some graphs ambiguously. For instance, $|12\rangle$ and $|21\rangle$ represent the same state, as well as $|12, 34, 56\rangle$ and $|56, 34, 12\rangle$, because these pairs specify the same edges. We will address this ambiguity later in this section.

At this point, we have defined graph states by specifying the presence or absence of an edge between each pair of graph vertices. However, this is overly restrictive. Since we would like to construct a quantum mechanical theory of graphs, we need to incorporate quantum uncertainty into the state of a graph. To do this, we extend the quantization scheme discussed in section IV: we associate a vector with every graph which describes its state. These vectors live in a Hilbert space which contains all vectors describing the quantum state of the graph. Similar to how the Hilbert spaces of multi-particle systems may be decomposed into the tensor product of

single-particle Hilbert spaces, the Hilbert space of a graph of N vertices may be decomposed into a tensor product of edge Hilbert spaces $\mathscr{E}_{ij}$ for each of the $\binom{N}{2}$ pairs of vertices $\{i,j\}$ in the graph:

$$\mathscr{H}(N) = \bigotimes_{j}^{N} \bigotimes_{i<j} \mathscr{E}_{ij}. \tag{26}$$

The edge Hilbert spaces $\mathscr{E}_{ij}$ are spanned by adjacency and non-adjacency states, which we label $|\uparrow\rangle_{ij}$ and $|\downarrow\rangle_{ij}$, respectively:

$$\mathscr{E} = \text{span}\{|\uparrow\rangle, |\downarrow\rangle\}. \tag{27}$$

These states correspond to the presence or absence of an edge between a pair of vertices $\{i,j\}$. A general edge state is thus a linear combination of the $|\uparrow\rangle$ and $|\downarrow\rangle$ states. Note that the single-edge Hilbert space is two-dimensional. Since the graph Hilbert space $\mathscr{H}(N)$ is a tensor product of $\binom{N}{2}$ edge Hilbert spaces $\mathscr{E}_{ij}$, the graph Hilbert space $\mathscr{H}(N)$ has dimension $\dim(\mathscr{H}(N)) = 2^{\binom{N}{2}}$.

V.B Quantum Statistics for Graphs

We would like the predictions of graph quantum mechanics to be independent of the vertex labeling of graphs, similar to how the quantum mechanics of systems of identical particles is particle label invariant. We will see that this leads to quantum statistics of graphs, similar to how the particle label invariance of the quantum mechanics of systems of identical particles leads to quantum particle statistics. As in particle quantum mechanics, we want graph quantum mechanics to make probabilistic predictions via the inner product. Thus, the probabilistic predictions obtained from the quantum theory of graphs should also be invariant under multiplication of a graph wavefunction by an overall complex phase. We can then incorporate the vertex label permutation invariance of the theory by extending (1) to graph states:

$$|i_1 j_1, i_2 j_2, ..., i_n j_n\rangle = e^{i\theta_P} |P(i_1)P(j_1), P(i_2)P(j_2), ..., P(i_n)P(j_n)\rangle, \tag{28}$$

where $P(i)$ is the vertex which results from permuting vertex i with the permutation P. As with (1) θ_P is a phase which depends the permutation P of the vertices. We only consider the phases

$\theta_P = 0, \pi$ in (28) for any permutations P of order 2 (i.e., vertex interchanges). As before, the phase corresponding to a general vertex permutation is found by applying (28) to each of the vertex interchanges which comprise the permutation. The phases $\theta_P = 0$ and $\theta_P = \pi$ correspond to "boson" and "fermion" graphs, the graph analogs of systems of bosons and fermions. Boson and fermion graph states must be symmetric and antisymmetric under any vertex interchange to ensure the theory is independent of vertex labeling. The independence of the theory on vertex labeling can be thought of as making the theory invariant under the action of the symmetric group S_N on the vertices of a graph with N vertices: the theory should yield the same predictions regardless of how we change the vertex labeling. Since these symmetries we would like to incorporate into the graph quantum theory form a mathematical group, we discuss group theory briefly.

V.B.1 Group Theory

Group theory is the mathematical study of groups, a type of axiomatically defined set. Groups are relevant for describing symmetries in physics, including the symmetry of second quantization graph quantum mechanics under any vertex label permutation of graph vertices. We first define a group:

Definition 9. *A group G is a set S and a binary operation $*$ called a group operation with the following properties:*

- *Closure of Group Under Group Operation: For any two elements $A, B \in G$, $A * B$ is also in G:*
$$A * B = C, C \in G. \tag{29}$$
- *Associativity Under Group Operation: For any three elements $A, B, C \in G$,*
$$(A * B) * C = A * (B * C). \tag{30}$$
- *Existence of an Identity Element: There exists an identity element $I \in G$ such that*
$$I * A = A * I = A. \tag{31}$$

- *Existence of Inverse Element: for every $A \in G$, there exists an inverse element A^{-1} which obeys*
$$A * A^{-1} = A^{-1} * A = I. \tag{32}$$

These group axioms define a structure on a set. One way to describe the structure of a group is to decompose it into cosets. Consider a group G and a subgroup H of G. The left and right cosets of H in G are generated by multiplying the subgroup H by each element in G from the left and right:

$$gH = \{gh\}(h \in H, g \in G), \tag{33}$$
$$Hg = \{hg\}(h \in H, g \in G). \tag{34}$$

Finding the cosets of a group with respect to some subgroup generalizes division to groups, as will be verified later in this section. Although we may expect to obtain N unique left or right cosets of H in G, there are actually fewer than N unique cosets because they are either disjoint or identical. Lagrange's theorem gives the size (or index) $[G : H]$ of the set of cosets G/H in terms of the sizes $|G|$ and $|H|$ of G and H:

$$[G : H] = \frac{|G|}{|H|}. \tag{35}$$

The number of cosets of H in G is therefore equal to the quotient of the sizes of G and H, thus verifying the intuition that decomposing a group into cosets is a generalization of division to groups.

Permutation groups consist of sets of permutations which form groups. Since the symmetries we must incorporate into the quantum theory of graphs form permutation groups, they will be relevant to the construction of first quantization graph states. In particular, for a graph of N vertices, we must construct the wavefunction such that it only changes by multiplication of a complex phase under all vertex permutations in the symmetric group S_N. For boson and fermion graphs, this amounts to overall multiplication of the wavefunction by ± 1 under any vertex permutation in S_N

Before doing this, we introduce a notation for representing permutations. We represent a permutation which swaps two objects i and j by (ij). To combine permutations, we place the permutation symbols next to each other, with the permutations placed in the order they are to be applied from right to left. For example, consider a set of objects labeled one through four. To permute objects 1 and 2, then 3 and 4, we write $(34)(12)$. Finally, we represent cyclic permutations, which consist of cyclically permuting a subset of objects in a set while fixing the others. A cyclic permutation of k elements is called a k-cycle. For instance, the set of permutations $(12),(23),(31)$ is a 3-cycle, because it involves taking 1 to 2, 2 to 3, and 3 to 1, so the permutations "close in" on themselves. We can represent a k-cycle consisting of permutations $(12),(23),...,(k-1k),(k1)$ as $(12...k-1k)$ for brevity. For instance, we can represent the permutation $(13)(32)(21)$ as simply (132).

V.C Construction of Antisymmetric Graph States in First Quantization

We now construct antisymmetric graph states in first quantization; we do not address the construction of symmetric states in this thesis. Antisymmetric graph states describe simple finite graphs because at most one edge can be defined between any pair of vertices in the graph as a consequence of the antisymmetry of states upon vertex label interchange (this is similar to how the antisymmetry of multi-particle wavefunctions under particle label interchange prevents more than one particle from occupying a single particle state, which is the Pauli exclusion principle). We first account for the ambiguity in the graph state notation mentioned earlier. We must ensure that the states $|ij\rangle$ and $|ji\rangle$, and $|ij,kl\rangle$ and $|kl,ij\rangle$, are non-distinct, since each of these pairs describes the same graph. To do this, we enforce the antisymmetry of these states under vertex and edge interchange:

$$|ij\rangle = -|ji\rangle\,, \tag{36}$$

$$|ij,kl\rangle = -|kl,ij\rangle\,. \tag{37}$$

This ensures that pairs of states related by vertex or edge interchange are not considered distinct states of the system, similar to how the antisymmetry of fermion wavefunctions prevents

double occupancy of a particle state.

We now conjecture to construct antisymmetrized graph states for a graph of N vertices similarly to how antisymmetrized states are constructed in the first quantization of particle quantum mechanics. We first select a "base state" by arbitrarily labeling the vertices of the graph and writing the resulting state for the graph. We then apply all permutations in S_N onto the base state to produce $N!$ states, multiply each of these state by the sign of the permutation used to produce them from the base state, and sum all the states. To find the antisymmetrized state for the complete graph $K(3)$, for example, we may start with the base state $|12,13,23\rangle$, sum all states resulting from acting all permutations in S_3 to this state, multiply each term by the sign of each state's corresponding permutation, and normalize the result. Doing this gives the antisymmetrized states $|\Psi_-(K(3))\rangle$ for the complete graph $K(3)$:

$$|\Psi_-(K(3))\rangle = \frac{1}{\sqrt{6}}(|12,13,23\rangle - |21,23,13\rangle - |32,31,21\rangle - |13,12,32\rangle + |23,21,31\rangle + |31,32,12\rangle). \tag{38}$$

However, this method for constructing antisymmetrized graph states is flawed. For instance, using (36) and (37) to simplify (38), the graph state is trivially zero.

To rectify this, we note that (38) is anti-symmetric under any permutation of vertex labels if we neglect conditions (36) and (37). It is only when we impose these conditions that the state vanishes because any two kets appearing in the state (38) related by a vertex or edge interchange will cancel. Since all kets in the state (38) are related by some vertex or edge interchange, they all cancel. Thus, there are redundant kets in (38), and we create a non-trivial graph state by deleting these redundant kets. For the complete graph $K(3)$, we only need one ket to specify the state. We choose to keep $|12,13,23\rangle$, so we obtain the new antisymmetrized state

$$|\Psi_-\rangle = |12,13,23\rangle\,. \tag{39}$$

It can easily be shown that the state (39) is antisymmetric upon any vertex permutation in S_3.

Although it is easy to eliminate the redundant kets resulting from the standard anti-symmetrization procedure for the complete graph $K(3)$, it is harder to eliminate redundant kets in more complicated graph states resulting from the standard anti-symmetrization procedure. We thus develop a more systematic way for eliminating redundant kets. The redundancy of kets in a graph state for a graph G is captured in the automorphism group Γ_G of G, which contains the permutations which generate all the graphs automorphic to G. We can thus account for the redundant kets in a graph state of N vertices produced by the standard antisymmetrization procedure by finding the cosets S_N/Γ_G of the automorphism group Γ_G in S_N, which partition the symmetric group S_N according to the symmetries of the graph. Taking the left cosets of Γ_G in S_N, we obtain, from (33),

$$S_N/\Gamma_G = s\Gamma_G = \{s\gamma\}(s \in S_N, \gamma \in \Gamma(G)). \tag{40}$$

According to Lagrange's theorem (35), there are $|S_N|/|\Gamma_G| = N!/|\Gamma_G|$ cosets, each of size $|\Gamma_G|$. They collectively contain all the elements of S_N, since the cosets are disjoint or identical, but these elements are now divided according to the symmetries of the graph. We may obtain a set of permutations which generates the necessary states for constructing the antisymmetrized state by selecting one element from each coset. We call this selection of elements from the cosets a traversal T of the cosets. We then select a base state $|i_1 j_1, i_2 j_2, ..., i_n j_n\rangle$ and act all the permutations in the traversal on this state, multiply each state by the sign of its corresponding permutation, add the resulting states, and normalize the result to obtain an antisymmetrized state $|\Psi_-\rangle$ for the graph. This yields

$$|\Psi_-\rangle = \frac{1}{\sqrt{N!/|\Gamma_G|}} \sum_{P \in T(S_N/\Gamma_G)} \mathrm{sgn}(P)\, |P(i_1)P(j_1), P(i_2)P(j_2), ..., P(i_n)P(j_n)\rangle\,, \tag{41}$$

where the sum is taken over the kets corresponding to each of the $N!/|\Gamma_G|$ permutations P in a traversal of cosets $T(S_N/\Gamma_G)$, $\mathrm{sgn}(P)$ is the sign of permutation P, and the square root factor is a normalization constant. Thus, we have formulated an antisymmetrization procedure to

calculate antisymmetrized states under vertex interchange in the first quantization of graph quantum mechanics:

- Find the automorphism group Γ_G of the graph G.
- Calculate the left cosets S_N/Γ_G.
- Take a traversal $T(S_N/\Gamma_G)$ of the cosets.
- Use (41) to construct the antisymmetrized graph state from the traversal $T(S_N/\Gamma_G)$.

There is freedom in this procedure to choose any traversal $T(S_N/\Gamma_G)$ of the cosets or any base state to construct $|\Psi_-\rangle$. We claim without proof that the antisymmetrization procedure works independently of the traversal of $T(S_N/\Gamma(G))$ taken or base state used.

As an example, we apply this method to find an antisymmetrized state for the complete graph $K(3)$ and check for agreement with our previous result. The automorphism group $\Gamma_{K(3)}$ of $K(3)$ is $\Gamma_{K(3)} = S_3$, and there is only one coset S_3/Γ_G equal to the symmetric group S_3. Thus, we can select any permutation from S_3 to produce the antisymmetrized state. We choose to apply the identity I to the base state $|12,13,23\rangle$, from which we simply obtain (39), as expected.

We also apply the antisymmetrization procedure to a graph G of three vertices and two edges, with vertex and edge sets given by $V = \{1,2,3\},\ E = \{\{1,2\},\{2,3\}\}$. The automorphism group Γ_G of G is

$$\Gamma_G = \{I,(13)\}. \tag{42}$$

The cosets S_3/Γ_G are

$$S_3/\Gamma_G = \{\{I,(13)\},\{(23),(123)\},\{(12),(132)\}. \tag{43}$$

We take the traversal $T(S_3/\Gamma_G)$ to be

$$T(S_3/\Gamma_G) = \{I,(23),(12)\}. \tag{44}$$

Upon applying (41) with the base state $|12,23\rangle$, we obtain for the antisymmetrized state $|\psi_-\rangle$

$$|\psi_-\rangle = \frac{1}{\sqrt{3}}(|12,23\rangle - |13,32\rangle - |21,13\rangle). \tag{45}$$

It can be verified that the state (45) is antisymmetric under any vertex permutation in S_3.

Once symmetric and antisymmetric states can be constructed for graph states, we have completed the construction of first quantization of graph quantum mechanics. We have assigned vectors to graphs which constitute a graph Hilbert space. We may then define operators on this Hilbert space, including a Hamiltonian operator which may describe graph dynamics. However, the construction of operators in first quantization for describing graph properties and graph dynamics is cumbersome because of the way we specify states in this formalism. To understand this, we reconsider the first quantization of particles. As mentioned in section IV, there is redundancy in the first quantization of particles because we inappropriately assign particle labels to indistinguishable particles. Due to this particle label assignment, we had to construct states which are symmetric or antisymmetric under any interchange of these labels. We circumvented this problem by introducing second quantization and the occupation number representation: by only specifying the number of particles in each state, we properly treat the particles as indistinguishable and eliminate the redundancy of particle labels. This allows us to define operators which add or subtract particles from states more naturally than in first quantization. Whereas in first quantization we have to reconstruct the symmetrized or antisymmetrized state for a different number of particles when we change the number of particles in a state, we can simply act creation and annihilation operators on second quantization states to change the number of particles they describe. The commutation and anticommutation relations of these operators are specified so states are consistent with the quantum statistics of first quantization. These operators allow us to more naturally construct Hamiltonians which describe the dynamics of systems with changing numbers of particles.

We may similarly circumvent the construction of symmetrized and antisymmetrized graph

states in first quantization by introducing a quantum theory of graphs similar to the second quantization of standard quantum mechanics. Unlike in the particle theory, we cannot completely eliminate the use of vertex labels because we must assign vertex labels to vertices to specify states. However, we may still define creation and annihilation operators for graph edges, which add edges to or delete edges from pairs of vertices in a graph. We specify the commutation and anticommutation relations of these operators to ensure states are consistent with the quantum statistics of first quantization. With these operators, we may more easily add or delete edges from states by simply acting edge creation and annihilation operators on them. This is especially useful for constructing Hamiltonian operators which may describe graph dynamics. Non-trivial dynamics for unlabeled graphs arise from graphs with variable numbers of edges. If we simply move an edge on a graph to a different pair of vertices, the resulting graph is the same as the original graph because the vertices are indistinguishable. By incorporating operators which allow us to add or subtract edges from graphs more efficiently, we can more easily describe graph state dynamics in a Hamiltonian in a second quantization of graph quantum mechanics. We turn to formulating this theory in the next section.

VI SECOND QUANTIZATION OF GRAPH QUANTUM MECHANICS

In this section, we develop a quantum description of finite unlabeled graphs similar to the second quantization of particle quantum mechanics. We cannot discard vertex labels on graphs as we could eliminate particle labels on particles in systems of particles because vertex labels are required to specify edges on graphs, but we can still avoid constructing symmetric and antisymmetric states by introducing creation and annihilation operators with certain commutation and anticommutation relations.

VI.A Edge Creation and Annihilation Operators

Since edges are analogous to particles in graphs, we first define edge creation and annihilation operators which create or delete edges in a graph, similar to those of the second quantization of particle quantum mechanics. We assume that we can neither add vertices to nor subtract vertices from the graph so that edge states cannot be added or removed. This is in contrast to the creation and annihilation operators of the second quantization of particle quantum mechanics, which can add or subtract particle states to or from the particle system. The graph Hilbert space is therefore not a direct sum of Hilbert spaces of graphs of different numbers of vertices; it consists only of a Hilbert space of a graph with a fixed number of vertices, as in the first quantization of graph quantum mechanics. Although creation and annihilation operators do not allow us to jump between graph states of different numbers of vertices, they do allow us to jump between parts of the graph Hilbert space which correspond to graphs of different numbers of edges.

To illustrate this, note that each term in the Fock space of second quantization of particle quantum mechanics (16) corresponds to a subset of the space which describes states with a fixed number of particles. The creation and annihilation operators in the second quantization of particle quantum mechanics allow us to jump between these subsets of the Fock space. The Hilbert space $\mathscr{H}(N)$ of a graph state with N vertices is given by the tensor product of $\binom{N}{2}$

two-dimensional Hilbert spaces $\mathscr{E}_{ij}$ corresponding to every pair of vertices $\{i,j\}$, but can be decomposed into the tensor sum of $\binom{N}{2}+1$ subspaces $\mathscr{G}(n)$ which comprise Hilbert spaces containing graph states with n edges, for $0 \leq n \leq \binom{N}{2}$. This leads to a decomposition of the graph Hilbert space similar to the Fock space (16):

$$\mathscr{H}(N) = \mathscr{G}(0) \oplus \mathscr{G}(1) \oplus ... \oplus \mathscr{G}\left[\binom{N}{2}\right]. \tag{46}$$

Thus, we expect the dimension of the Hilbert space to be

$$|\mathscr{H}(N)| = 2^{\binom{N}{2}} = |\mathscr{G}(0)| + |\mathscr{G}(1)| + ... + \left|\mathscr{G}\left[\binom{N}{2}\right]\right|. \tag{47}$$

We decompose the graph Hilbert space $\mathscr{H}(3)$, which has dimension $|\mathscr{H}(3)| = 2^{\binom{3}{2}} = 8$, to illustrate. We first determine the dimensions of the component Hilbert spaces $|\mathscr{G}(0)|, |\mathscr{G}(1)|, |\mathscr{G}(2)|$, and $|\mathscr{G}(3)|$ by specifying the states which span each Hilbert space. We assume that the vertices are distinguishable and denote a general graph state as $|s_{12}\rangle \otimes |s_{13}\rangle \otimes |s_{23}\rangle$, where $|s_{ij}\rangle$ specifies the edge state defined between vertices i and j. The Hilbert spaces $\mathscr{G}(0), \mathscr{G}(1), \mathscr{G}(2)$, and $\mathscr{G}(3)$ are then given by

$$\mathscr{G}(0) = \text{span}\{|\downarrow\rangle \otimes |\downarrow\rangle \otimes |\downarrow\rangle\}, \tag{48}$$

$$\mathscr{G}(1) = \text{span}\{|\uparrow\rangle \otimes |\downarrow\rangle \otimes |\downarrow\rangle, |\downarrow\rangle \otimes |\uparrow\rangle \otimes |\downarrow\rangle, |\downarrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle\}, \tag{49}$$

$$\mathscr{G}(2) = \text{span}\{|\uparrow\rangle \otimes |\uparrow\rangle \otimes |\downarrow\rangle, |\downarrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle, |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle\}, \tag{50}$$

$$\mathscr{G}(3) = \text{span}\{|\uparrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle\}. \tag{51}$$

Thus, we see that $|\mathscr{G}(0)| = |\mathscr{G}(3)| = 1$ and $|\mathscr{G}(1)| = |\mathscr{G}(2)| = 3$, and we verify that the dimension of the graph Hilbert space is equal to $8 = 2 \otimes 2 \otimes 2 = 1 \oplus 3 \oplus 3 \oplus 1$, in accordance with (47). This may be extended to an N-vertex graph. Upon working through the possible states in each subset $\mathscr{G}(i)$ of $\mathscr{H}(N)$, we may rewrite (47) as

$$2^{\binom{N}{2}} = \sum_{n=0} \binom{\binom{N}{2}}{n}, \tag{52}$$

where we obtain the sum on the right hand side of (52) because there are $\binom{\binom{N}{2}}{n}$ possible ways to assign states $|\uparrow\rangle$ to n edges out of $\binom{N}{2}$ edges. Note that

$$(x+y)^N = \sum_{n=0} \binom{N}{n} x^n y^{N-n}. \tag{53}$$

Letting $N \to \binom{N}{2}$ and $x = y = 1$, we obtain (47). Thus, any graph Hilbert space for a graph of N vertices may be decomposed into subspaces containing states of fixed numbers of edges. The creation and annihilation operators allow us to jump between these component subspaces.

We now construct the edge creation and annihilation operators $\hat{b}_{ij}^\dagger$ and $\hat{b}_{ij}$ for boson graphs and $\hat{c}_{ij}^\dagger$ and $\hat{c}_{ij}$ for fermion graphs, which add or remove an edge between vertices i and j to or from a graph, respectively. We define a vacuum state $|0\rangle$ which describes an empty graph and construct graph states by acting on this vacuum state with edge creation operators, similar to the creation of second quantization particle states.

To make the second quantization of graph states consistent with quantum statistics, we define commutation and anticommutation relations between the boson and fermion creation and annihilation operators, which ensure that the states they act on are symmetric or antisymmetric, in analogy with the second quantization of particle quantum mechanics. Since the operators are now labeled with two quantum numbers, we must modify equations (19)-(20) and (24)-(25) for bosons and fermions so that the index on the operators contains two vertex labels which specify an edge. The commutation or anticommmutation relations for edge creation and annihilation operators generally depend on all four vertex labels specified in the commutator, but we will consider the two vertex labels of each operator as one unit, so that two creation or annihilation operators labeled with the vertex labels ij and il (i.e., the operators have one common vertex label) will be treated as distinct. We then define the commutation and anticommutation relations for boson and fermion graph edge creation and annihilation operators as

$$[\hat{b}_{ij}^\dagger, \hat{b}_{kl}^\dagger] = [\hat{b}_{ij}, \hat{b}_{kl}] = 0, \tag{54}$$

$$[\hat{b}_{ij}, \hat{b}^{\dagger}_{kl}] = \delta_{\{ij\}\{kl\}}, \tag{55}$$
$$\{\hat{c}^{\dagger}_{ij}, \hat{c}^{\dagger}_{kl}\} = \{\hat{c}_{ij}, \hat{c}_{kl}\} = 0, \tag{56}$$
$$\{\hat{c}_{ij}, \hat{c}^{\dagger}_{kl}\} = \delta_{[ij][kl]}, \tag{57}$$

where

$$\delta_{\{ij\}\{kl\}} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}, \tag{58}$$
$$\delta_{[ij][kl]} = \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}. \tag{59}$$

The properties of the particle creation and annihilation operators carry over to the corresponding graph operators. Since all graph states must be normalized, the boson and fermion graph edge creation and annihilation operators obey (21) and (22). Although we have considered creation and annihilation operators for both boson and fermion graphs, we restrict attention to fermion graphs for the remainder of this thesis. We denote the fermion graph edge creation and annihilation operators $\hat{c}^{\dagger}_{ij}$ and $\hat{c}_{ij}$ as $\hat{a}^{\dagger}_{ij}$ and $\hat{a}_{ij}$, since it is now unnecessary to distinguish between boson and fermion graph creation and annihilation operators.

VI.B Graph Hilbert Space Operators in Second Quantization of Graph Quantum Mechanics

Thus far into the development of graph quantum mechanics, we have associated state vectors with graphs which live in a graph Hilbert space. We may also define Hermitian operators in this Hilbert space which represent graph "observables", which correspond to properties of finite graphs considered in graph theory, similar to how Hermitian operators in particle quantum mechanics represent physical observables of particles. We may construct these observables using the basic edge creation and annihilation operators $\hat{a}^{\dagger}_{ij}$ and $\hat{a}_{ij}$ In this thesis, we build operators for four graph observables, in order of increasing complexity: edge number, vertex degree, graph complement, and unit sphere. To ensure that these operators preserve the norm of states, we also verify that they are unitary.

VI.B.1 Edge Number Operator

We define the edge number of a pair of vertices $\{i, j\}$ on a graph G as the number of edges defined between i and j. For fermion graphs, the edge number associated with any pair of

vertices is either zero or one. The eigenvalue of the edge number operator $\hat{N}_{ij}$ upon acting on a graph state gives the edge number of the graph corresponding to the vertex pair $\{i, j\}$. We construct the edge number operator in analogy with (23), but label each number operator with two labels describing the pair of vertices considered:

$$\hat{N}_{ij} = \hat{a}^{\dagger}_{ij}\hat{a}_{ij}. \tag{60}$$

The unitarity of the edge number operator is verified easily by inspection.

VI.B.2 Vertex Degree Operator

We now construct the vertex degree operators $\hat{d}(i)$ associated with each vertex i in an N-vertex graph. Upon acting on a graph state, the operator $\hat{d}(i)$ should yield an eigenvalue equal to the vertex degree of the vertex i in the graph state.

Note that there are $N-1$ edges definable on any given vertex i of an N-vertex graph, so we want a vertex degree operator for vertex i to check if edges are defined between i and all of the other $N-1$ vertices. It should associate a value of one with any pair of adjacent vertices and zero with any pair of non-adjacent vertices. The sum of the numbers associated with each of the $N-1$ vertex pairs then gives the vertex degree. Since the edge number operator makes this assignment to pairs of vertices on a graph, we sum over edge number operators which contain the vertex label i as one of its indices to construct the vertex degree operator $\hat{d}(i)$:

$$\hat{d}(i) = \sum_{j \neq i} \hat{N}_{ij}, \tag{61}$$

where we take the sum over $j \neq i$ because we want to neglect self-looping edges. The unitarity of the vertex degree operator follows because the operator is a simple sum of number operators, which are unitary.

VI.B.3 Graph Complement Operator

We now construct the graph complement operator $\hat{C}$ which gives the graph complement state of a graph state. This operator must delete edges between adjacent vertices in a graph and

create edges between non-adjacent vertices in a graph, so we decompose $\hat{C}$ into two parts, $\hat{C}_+$ and $\hat{C}_-$, which are subsequently decomposed into a sum of operators $\hat{C}_{ij}^+$ and $\hat{C}_{ij}^-$ over all vertex pairs $\{i, j\}$, with $i < j$. The operator $\hat{C}_{ij}^+$ should create an edge between vertices i and j if they are non-adjacent and delete the state if they are already adjacent, while the operator $\hat{C}_{ij}^-$ should delete the edge defined between vertices i and j if they are adjacent and delete the state if they are non-adjacent. Either $\hat{C}_{ij}^+$ or $\hat{C}_{ij}^-$ are non-zero for any vertex pair $\{i, j\}$, but not both or neither of them, by construction, so they perform complementary functions. To construct $\hat{C}_{ij}^+$, we form the product of a creation operator $\hat{a}_{ij}^\dagger$ and a term which is unity if the vertices i and j are non-adjacent and zero otherwise. We propose the form

$$\hat{C}_{ij}^+ = \hat{a}_{ij}^\dagger (1 - \hat{N}_{ij}). \tag{62}$$

It is easy to verify that this operator functions as expected.

We now construct the operator $\hat{C}_{ij}^-$ by forming the product of an annihilation operator $\hat{a}_{ij}$ and a term which is unity if the vertices are adjacent and zero otherwise. We propose the form

$$\hat{C}_{ij}^- = \hat{a}_{ij} \hat{N}_{ij}. \tag{63}$$

This operator functions as expected because $\hat{N}_{ij}$ is zero if the vertices are non-adjacent and is unity if they are adjacent.

We then add the operators $\hat{C}_{ij}^+$ and $\hat{C}_{ij}^-$ and take the product of the sum over all $i < j$ to create the graph complement operator:

$$\hat{C} = \prod_{i<j} (\hat{C}_{ij}^+ + \hat{C}_{ij}^-) = \prod_{i<j} \left(\hat{a}_{ij} \hat{N}_{ij} + \hat{a}_{ij}^\dagger (1 - \hat{N}_{ij}) \right). \tag{64}$$

To prove the unitarity of the graph complement operator (64), we let $\hat{C}_{ij} = \hat{a}_{ij} \hat{N}_{ij} + \hat{a}_{ij}^\dagger (1 - \hat{N}_{ij})$, so that we may write the graph complement operator as

$\hat{C} = \prod_{i<j} \hat{C}_{ij}$. Calculating $\hat{C}\hat{C}^\dagger$ gives

$$\begin{aligned} \hat{C}\hat{C}^\dagger = \prod_{i<j} \hat{C}_{ij} \left(\prod_{k<l} \hat{C}_{kl} \right)^\dagger &= \hat{C}_{1N}\hat{C}_{2N}...\hat{C}_{N-1,N}(\hat{C}_{1N}\hat{C}_{2N}...\hat{C}_{N-1,N})^\dagger \\ &= \hat{C}_{1N}\hat{C}_{2N}...\hat{C}_{N-1,N}\hat{C}^\dagger_{N-1,N}...\hat{C}^\dagger_{2N}\hat{C}^\dagger_{1N}. \end{aligned} \tag{65}$$

From equation (65), the graph complement operator $\hat{C}$ is unitary if $\hat{C}_{ij}$ is unitary. Calculation of $\hat{C}_{ij}\hat{C}^\dagger_{ij}$ yields

$$\hat{C}_{ij}\hat{C}^\dagger_{ij} = \left(\hat{a}_{ij}\hat{N}_{ij} + \hat{a}^\dagger_{ij}(1-\hat{N}_{ij}) \right) \left(\hat{a}^\dagger_{ij}\hat{N}_{ij} + \hat{a}_{ij}(1-\hat{N}_{ij}) \right) = I. \tag{66}$$

Thus, the operators $\hat{C}_{ij}$, and consequently the graph complement operator $\hat{C}$, are unitary.

VI.B.4 Unit Sphere Operator

We now construct the unit sphere operator, which gives the graph state corresponding to the unit sphere of a graph around a graph vertex. Since the unit sphere of a graph is an induced subgraph, we first define an induced subgraph operator over a subset S of the vertices of a graph G. This operator should delete all edges defined on adjacent vertices i and j which do not both belong to S and preserve any edges defined only on vertices in S. We propose an induced subgraph operator $\hat{I}_G(\{v_1,...,v_N\})$ on the graph G with respect to the vertex set $\{v_1,...,v_N\}$ of the form

$$\hat{I}_G(\{v_1,...,v_N\}) = \prod_{\{j,k\}\subset S} (1-\hat{N}_{jk} + \hat{a}_{jk}\hat{N}_{jk}), \tag{67}$$

where $\{j,k\} \subset V$ indicates the sum over all pairs of vertices $\{j,k\}$ in which j or k do not both belong to the subset S. To verify that this operator gives an induced subgraph, we consider the effect of a term in the product for a general pair of vertices $\{j,k\}$, then consider the operator as a whole. The operator (67) reduces to the annihilation operator $\hat{a}_{jk}$ if vertices j and k are adjacent and to the identity if they are non-adjacent, as expected. Since the product of these operators is taken over vertices j and k which both don't belong to S, the operator has the desired effect of deleting only edges which are not defined between two vertices which both do not belong to S.

To check the unitarity of the induced subgraph operator, we rewrite it as $\hat{I}_G(\{v_1,...,v_N\}) = \prod_{\{j,k\}\subset V} \hat{I}_{jk}$, where $\hat{I}_{jk} = 1 - \hat{N}_{jk} + \hat{a}_{jk}\hat{N}_{jk}$. Calculating $\hat{I}_{jk}\hat{I}_{jk}^{\dagger}$ directly gives

$$\hat{I}_{jk}\hat{I}_{jk}^{\dagger} = (1 - \hat{N}_{jk} + \hat{a}_{jk}\hat{N}_{jk})(1 - \hat{N}_{jk} + \hat{a}_{jk}\hat{N}_{jk})^{\dagger} = I. \tag{68}$$

Thus, $\hat{I}_{jk}$ is a unitary operator and, since $\hat{I}_G\hat{I}_G^{\dagger} = \hat{I}_{1N}\hat{I}_{2N}...\hat{I}_{N-1,N}\hat{I}_{N-1,N}^{\dagger}...\hat{I}_{2N}^{\dagger}\hat{I}_{1N}^{\dagger}$, $\hat{I}_G(\{v_1,...,v_N\})$ is also a unitary operator.

We can now construct the unit sphere operator around a vertex v using (68), taking the set of all vertices unit graph distance from v as the vertex set V.

With the construction of graph state operators with the edge creation and annihilation operators of the second quantization of graph quantum mechanics, we may now define dynamics on a graph using this formalism by constructing Hamiltonians which describe the quantum time evolution of graphs. We turn to this in the next section.

VII GRAPH DYNAMICS

The graph quantum mechanics theories developed previously cannot describe graph dynamics at this point because they only describe static states, or states which do not time evolve. In this section, we incorporate dynamics into the theory. We construct adjustable model Hamiltonians in the second quantization of graph quantum mechanics, similar to the Hamiltonians in the Ising and Heisenberg models of ferromagnetism, which can describe various kinds of graph dynamics. Before defining graph state Hamiltonians, we first discuss how to describe dynamics from a Hamiltonian using quantum mechanics and statistical mechanics.

VII.A Quantum Mechanical Graph State Evolution

We can use quantum mechanics to describe the time evolution of a graph state given a Hamiltonian. If the Hamiltonian does not explicitly depend on time, we can construct exact time evolved quantum graph states using (5). The state (5) describes the time evolution of an energy eigenstate. Since these energy eigenstates form a complete orthonormal basis for the graph Hilbert space, we can decompose any graph state into linear combinations of these time evolved energy eigenstates. We may write a general graph state $|\Psi\rangle$ as

$$|\Psi\rangle = \sum_i a_i e^{iE_i t/\hbar} |E_i\rangle \,, \tag{69}$$

where $|E_i\rangle$ is an energy eigenstate of the graph with energy E_i and $\{a_i\}$ is a set of complex coefficients which must satisfy $\sum_i a_i^2 = 1$ to ensure that the state $|\Psi\rangle$ is normalized. The decomposition (69) depends on knowledge of the energy eigenstates of the graph with Hamiltonian $\hat{H}$, which can be obtained using the time-independent Schrodinger equation (6).

Although this method for time evolving graph states is exact, it can be intractable for large graphs, where solving (6) and decomposing a graph state into energy eigenstates can be tedious. For this reason, we turn to statistical mechanics to describe graph dynamics.

VII.B Statistical Mechanical Description of Graph State Dynamics

Statistical mechanics provides a statistical description of physics; it describes average or expected states of systems within some uncertainty. This uncertainty is usually negligible if the system is large enough, so statistical mechanics is accurate for large systems. Statistical mechanics is premised on a distinction between a system's microstate and macrostate. The microstates of a system correspond to the exact microscopic configurations of its constituents. For instance, the microstates of a three-dimensional ideal gas consist of the position and momentum of each of its constituent particles. In contrast, the macrostate of a system describes its macroscopic properties which emerge from its microscopic properties. For instance, pressure is a macroscopic property associated with an ideal gas in a container, which arises from the sum of the forces the gas molecules exert on the container. A state with a fixed pressure is a macrostate of the system. We associate with every macrostate all the microstates which result in that macrostate, and we call the number of microstates associated with a macrostate its multiplicity. The probability of measuring a particle in a given macrostate is then the ratio between the multiplicity of the macrostate and the total number of microstates, assuming all the microstates are equally likely (this is referred to as the fundamental assumption of statistical mechanics).

Since probabilities of measuring certain macrostates depend on their multiplicities, we must analyze the microscopic states of a system and their correspondence to macrostates. Although this is often tractable for simple systems, it is impractical to do for most realistic systems. For example, to describe one mole of an ideal gas, we would need to solve for the motions of $\sim 10^{23}$ particles, a very tedious task. For this reason, we consider a macroscopic approach which describes the expected states of the system rather than the exact states of the system. This approximate description of the system is coarse for small systems, but is justified for large enough systems according to the thermodynamic limit: the averaged thermodynamic

description of a system of N particles occupying a volume V becomes exact in the limit $N, V \to \infty$ which preserves the particle density N/V. In this discussion, we only consider systems which are large enough so that the thermodynamic description is justified. These systems are in the state with highest multiplicity with considerable certainty because this is the state with the highest probability of being measured. We find this state by introducing entropy, a quantity related to the multiplicity of a macrostate of a system. For a macrostate Q with multiplicity Ω_Q, the entropy S of the macrostate Q is given by

$$S = k_B \ln \Omega_Q, \tag{70}$$

where k_B is the Boltzmann constant. The most probable state of the system is then the one of maximal entropy. This is the second law of thermodynamics: the entropy of an isolated system cannot decrease, but will tend to evolve to a configuration of maximal entropy.

This analysis still depends on knowledge of the microstates of a system. To rectify this, we introduce temperature, which is usually defined as a macroscopic state variable which is the same for two systems after they have reached thermal equilibrium. There is also a microscopic definition of temperature, which may be derived by finding the most likely system state by maximizing the entropy. Consider two systems, labeled 1 and 2, confined to closed, rigid containers which do not let particles in and out. The systems are in thermal contact and have a fixed total energy E. We maximize the entropy of the system with respect to the energy E_1 of system 1 (we can then specify the energy E_2 of system 2 by calculating $E - E_1$). The total entropy of both systems is

$$S_{tot} = S_1 + S_2 = k_B \ln[\Omega_1(E_1)\Omega_2(E - E_1)]. \tag{71}$$

We maximize the entropy with respect to E_1 by setting $\frac{dS_{tot}}{dE_1} = 0$. This results in the condition

$$\frac{dS_1}{dE_1} = \frac{dS_2}{dE_2}, \tag{72}$$

which determines thermodynamic equilibrium between systems 1 and 2. It implies that there is a quantity that is equal for both systems at thermodynamic equilibrium, which, by definition, is temperature. Thus, we define temperature as

$$\frac{1}{T} = \frac{dS}{dE}. \tag{73}$$

This definition of temperature implies that the temperature gives the "energy cost" of changing the system's entropy. Note that (73) is only valid for systems with fixed volume and particle number because it assumes that energy cannot change due to mechanical work or diffusion of particles into or out of the system.

We now use temperature to find a probability distribution for measuring macrostates of a system which does not depend on knowledge of the system's microstates. This derivation parallels that presented in section 6.1 of Sethna's work.[21] We consider a system with discrete energy levels $\{E_i\}$ which is held at a fixed temperature by being placed in contact with a heat bath. Letting E_s be the energy of the system and E be the total energy of the system and heat bath, the energy of the heat bath is $E_{bath} = E - E_S$. If S_i is the entropy associated with this energy state, then inverting (70) for Ω gives the multiplicity Ω_i of an energy state E_i:

$$\Omega_i = e^{S_i/k_B}. \tag{74}$$

We now consider the ratio of the probability of the heat bath having an energy $E_{ba} = E - E_a$ to having an energy $E_{bb} = E - E_b$. We obtain for this ratio

$$\frac{P(E_{ba})}{P(E_{bb})} = \frac{\Omega_{ba}}{\Omega_{bb}}, \tag{75}$$

where Ω_{ba} and Ω_{bb} are the number of microstates associated with the heat bath at energies E_{ba} and E_{bb}, respectively. Using equation (74), (75) can be rewritten in terms of the entropy:

$$\frac{P(E_{ba})}{P(E_{bb})} = e^{S_{ba} - S_{bb}/k_B} = e^{(\partial S/\partial E)(E_b - E_a)/k_B} = e^{(E_b - E_a)/k_B T} = e^{\beta(E_b - E_a)}, \tag{76}$$

where $\beta = 1/k_B T$. The second equality in this equation follows from assuming the energy fluctuations are small, which is valid for a large heat bath. The factor $e^{-\beta E_a}$ in (76) is related to the probability of finding the heat bath with energy E_{ba} (or, equivalently, the probability of finding the system with energy $E - E_{ba} = E_b$) and the factor $e^{\beta E_b} = \frac{1}{e^{-\beta E_b}}$ is a normalization factor. To find the overall probability of measuring the system in a given energy, we replace the denominator with a normalization factor Z called the partition function, which sums over all factors $e^{-\beta E_i}$ associated with each possible measurement of energy:

$$Z = \sum_i e^{-\beta E_i}. \tag{77}$$

The desired probability distribution is then

$$P(E_i) = \frac{e^{-\beta E_i}}{Z} \tag{78}$$

and is called the Boltzmann distribution. It can be used to calculate expectation values for dynamical variables. The expectation value $\langle A \rangle$ for a dynamical quantity A is the weighted average of the quantity with respect to the Boltzmann probability distribution:

$$\langle A \rangle = \sum_i E_i P(E_i) = \sum_i \frac{A_i e^{-\beta E_i}}{Z}. \tag{79}$$

With the statistical mechanical theory laid out in this section, we may describe the average dynamics of a system.

VII.C Dynamical Models for Ferromagnetism

We now construct graph Hamiltonians from the Ising and Heisenberg models for ferromagnetism, which describe ferromagnetic systems comprised of systems of atoms.[22,23] The nucleus of each of these constituent atoms has intrinsic spin and consequently a spin magnetic moment which can interact with those of other nuclei and with external magnetic fields. Ferromagnetism arises from these interactions of the magnetic moments of the constituent atoms of the system. Because of the dependence of ferromagnetism on intrinsic spin, we briefly discuss intrinsic spin.

VII.C.1 Intrinsic Spin

Intrinsic spin must be treated with quantum mechanics because it is a quantum property of matter. The principles of quantum mechanics of section IV hold: the spin states live in a Hilbert space which is spanned by a basis corresponding to an observable. The difference with spin states is that they live in finite dimensional Hilbert spaces, since particles can only assume a finite number of spin states. The dimension of a particle's spin Hilbert space depends on the particle's spin quantum number, a quantity intrinsic to the particle and related to the magnitude of its intrinsic spin. Thus, the magnitude of a particle's spin is invariant, in contrast to the classical angular momentum of a particle, which can change depending on its motion. Even though a particle's spin is fixed, it has more than one spin state because only the magnitude of spin is specified by the spin quantum number; the direction of the spin may still vary. Due to quantum mechanical uncertainty, there is only a finite number of directions for the spin's orientation and only one component of the spin is completely determined. We label this determined component the z-component of spin. Quantum mechanics then dictates that the possible values of the z-component spin S_z for a particle of spin quantum number $s/2$ are

$$S_z = -\frac{s}{2}\hbar, \left(-\frac{s}{2}+1\right)\hbar, ..., \left(\frac{s}{2}-1\right)\hbar, \frac{s}{2}\hbar. \tag{80}$$

We may write this more compactly by defining the magnetic quantum number m_s, given by

$$m_s = -\frac{s}{2}, -\frac{s}{2}+1, ..., \frac{s}{2}-1, \frac{s}{2}. \tag{81}$$

The z-component spin S_z is then given by

$$S_z = m_s\hbar. \tag{82}$$

According to (80) or (81), the spin states of a spin-s particle live in a $2s+1$-dimensional Hilbert space, so the spin state of a spin-s particle is described by a $2s+1$-component vector. As with any Hilbert space, the spin Hilbert space is equipped with Hermitian operators which represent

observables. These observables are the total spin S and the components of the spin S_1, S_2, S_3 (the components are not labeled with the traditional x, y, and z labels to emphasize that we can describe the three components of spin using any orthogonal coordinate basis). We label one of these axes the z-axis, which points in the direction of the determined component of the spin. We define the x and y axes to define a right-handed coordinate system. A Hermitian operator is associated with each of these quantities, which is represented by a $2s+1$-by-$2s+1$ matrix. Since we may write quantum operators in any basis, we choose to write these operators in terms of the S_z eigenbasis for convenience. We then express the spin state of the particle as a $2s+1$-dimensional vector in the S_z eigenbasis. Each component of the vector describes a spin state with a particular value for S_z. We determine that S_z is a diagonal matrix with entries given by the possible measurements for z-component spin because the z-component of particle spin is well determined and the eigenvalues of the matrix must give the possible measurements for the z-component of spin. To determine the other spin operators, we use the spin commutation relations, which are derived from group theory:

$$[\hat{S}_i, \hat{S}_j] = i\hbar\varepsilon_{lmn}\hat{S}_n, \tag{83}$$

where $i, j, k = 1, 2, 3$ (we let 1,2, and 3 correspond to x, y, and z, respectively) and ε_{lmn} is the Levi-Civita tensor. The spin operators are obtained in any basis by first fixing the operator corresponding to the determined component of spin then requiring that the remaining operators obey (83).

To describe ferromagnetic systems, we specialize the previous discussion to spin-1/2 particles. According to (81), the only two spin states are $m_s = \frac{1}{2}$ and $m_s = -\frac{1}{2}$, which are called spin up and spin down states, respectively. We can then express the spin matrices $\hat{S}_x, \hat{S}_y, \hat{S}_z$ in the S_z eigenbasis. The matrix representation for $\hat{S}_z$ is

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{84}$$

The other matrices $\hat{S}_x$ and $\hat{S}_y$ can be found by requiring that they satisfy the commutation relations (83):

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{85}$$

$$\hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{86}$$

There is an additional structure embedded in the spin-1/2 Hilbert space relevant to this thesis. We define the spin ladder operators $\hat{S}_\pm$ as

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y. \tag{87}$$

These operators raise or lower the spin of a spin state. Calculation of $\hat{S}_z\hat{S}_+$ for a spin-down state $|\downarrow\rangle$ yields

$$\hat{S}_z\hat{S}_+ |\downarrow\rangle = (\hat{S}_+\hat{S}_z + [\hat{S}_z, \hat{S}_+])\,|\downarrow\rangle\,. \tag{88}$$

It can be shown that

$$[\hat{S}_z, \hat{S}_+]\,|\downarrow\rangle = \hbar\hat{S}_+ |\downarrow\rangle\,. \tag{89}$$

Thus,

$$\hat{S}_z\hat{S}_+ |\downarrow\rangle = \frac{\hbar}{2}\hat{S}_+ |\downarrow\rangle\,. \tag{90}$$

Therefore, the operator $\hat{S}_+$ has the effect of raising the spin of a spin down particle. Furthermore,

$$\hat{S}_z\hat{S}_+ |\uparrow\rangle = 0. \tag{91}$$

Thus, the ladder operator $\hat{S}_+$ annihilates the spin up state. Similarly, calculation of $\hat{S}_z\hat{S}_-$ yields

$$\hat{S}_z\hat{S}_- |\uparrow\rangle = -\frac{\hbar}{2}\hat{S}_- |\uparrow\rangle\,, \tag{92}$$

$$\hat{S}_z\hat{S}_- |\downarrow\rangle = 0. \tag{93}$$

We thus see that the ladder operator $\hat{S}_-$ lowers the spin of the spin up state and annihilates a spin down state.

VII.C.2 The Ising Model of Ferromagnetism

With this background on intrinsic spin laid out, we turn to the Ising and Heisenberg models of ferromagnetism. The Ising model only considers spin-spin interactions which depend on one spin component (which is conventionally called the z-component) and the interactions of these spins with an external magnetic field. Its Hamiltonian is expressed in terms of the intrinsic spin states σ of the atoms of the atomic system. We may then use statistical mechanics to describe the dynamics of the system. The Ising Hamiltonian $H(\sigma_i)$ is

$$H_I(\sigma_i) = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \mu\sum_j h_j\sigma_j, \tag{94}$$

where σ_i represents the spin of the ith nucleus, and is equal to $+1$ or -1 for spin up and spin down, respectively. Also, J_{ij} represents the spin-spin interaction strength between spins i and j, h_j represents the strength of the magnetic field acting on the spin j, and μ is the magnetic moment of the nuclei. Note that if all $J_{ij} > 0$, the energy is lower when the spins are aligned ($\sigma_i\sigma_j > 0$) rather than anti-aligned ($\sigma_i\sigma_j < 0$), so systems where more of the spins are aligned are more energetically favorable. On the other hand, if all $J_{ij} < 0$, the energy is lower when the spins are anti-aligned ($\sigma_i\sigma_j < 0$) rather than aligned ($\sigma_i\sigma_j > 0$), so systems where more of the spins are anti-aligned are more energetically favorable (this scenario describes antiferromagnetic systems) . Also, the energy is lowered when the spins align with the magnetic field because $h_j\sigma_j > 0$. Because the Hamiltonian sensibly describes the spin-spin interactions and the spin interactions with the external magnetic field, the Ising Hamiltonian accurately describes the ferromagnetic system.

The general Ising Hamiltonian is cumbersome. If the system has N atomic nuclei, we need to specify $\frac{1}{2}N(N-1)$ parameters J_{ij} and N parameters h_j to construct the Hamiltonian. To simplify this Hamiltonian, we assume the nearest neighbor interaction approximation, where we only consider the interactions of nearest neighboring nuclei. We also assume all such interactions are all equal in strength ($J_{ij} = J$). We will also only consider a uniform external

magnetic field so that $h_j = h$. Under these assumptions, the Ising Hamiltonian (94) becomes

$$H_I(\sigma_i) = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - \mu h\sum_i \sigma_i, \tag{95}$$

where $\langle ij\rangle$ denotes a sum over neighboring spins i and j.

The Ising Hamiltonian (95) assumes spins are either in a spin up or spin down state. However, since intrinsic spin is an inherently quantum property of matter, we must consider the spins as assuming quantum states which generally comprise a superposition of spin up and spin down states. The state of an N nuclei system is described by a state vector in a 2^N-dimensional Hilbert space, given by the tensor product of N spin-1/2 Hilbert spaces. The Ising Hamiltonian is then promoted to a quantum operator by promoting the variables σ_i to spin-1/2 operators. For the ith spin of the system, we make the correspondence

$$\sigma_i \to \hat{I}^{\otimes i-1}\otimes\hat{\sigma}_z\otimes\hat{I}^{\otimes N-i}, \tag{96}$$

where $\hat{\sigma}_z$ is the z-component spin-1/2 matrix operator. The spin operator lies in the ith component of the tensor product in the operator and all other components of the operator are equal to the identity so that the action of the operator on a state only depends on the ith spin of the state. Upon promoting the variables σ_i to operators in the Ising Hamiltonian (95) according to (96), we obtain

$$\hat{H}_I = -J\sum_{\langle ij\rangle}\hat{\sigma}_i\hat{\sigma}_j - \mu h\sum_i \hat{\sigma}_i. \tag{97}$$

This quantum generalization of the Ising Hamiltonian will become important later in this section, where we use it to construct a graph Hamiltonian.

VII.C.3 The Heisenberg Model of Ferromagnetism

The Heisenberg model of ferromagnetism generalizes the Ising model by incorporating spin-spin interactions which generally depend on all spin components. It does this by adding terms into the Ising Hamiltonian (97) which account for spin-spin interactions dependent on the x and y spin components. We define constants J_x, J_y, and J_z to denote the strengths of the

couplings of the x, y, and z components of the nuclear spins, respectively, and we define the operators $\hat{\sigma}_i^x, \hat{\sigma}_i^y, \hat{\sigma}_i^z$ as

$$\hat{\sigma}_i^x = \hat{I}^{\otimes i-1} \otimes \hat{\sigma}_x \otimes \hat{I}^{\otimes N-i}, \tag{98}$$

$$\hat{\sigma}_i^y = \hat{I}^{\otimes i-1} \otimes \hat{\sigma}_y \otimes \hat{I}^{\otimes N-i}, \tag{99}$$

$$\hat{\sigma}_i^z = \hat{I}^{\otimes i-1} \otimes \hat{\sigma}_z \otimes \hat{I}^{\otimes N-i}. \tag{100}$$

Note that (100) is the same as $\hat{\sigma}_i$ defined before, when we only considered interactions depending only on the z-component of spin. We then obtain the Heisenberg Hamiltonian:

$$\hat{H}_H = -\sum_{\langle ij \rangle} (J_x \hat{\sigma}_i^x \hat{\sigma}_j^x + J_y \hat{\sigma}_i^y \hat{\sigma}_j^y + J_z \hat{\sigma}_i^z \hat{\sigma}_j^z) - \mu h \sum_i \hat{\sigma}_i^z. \tag{101}$$

Note the presence of additional spin-spin interaction terms which depend on the x and y components of spin. With the quantum Ising and Heisenberg Hamiltonians (97) and (101), we now construct model graph state Hamiltonians by drawing an analogy between magnetic systems and quantum graphs.

VII.D Model Graph State Hamiltonians

In this section, we define dynamical evolution on graph states by constructing model Hamiltonians for graph states from the Ising and Heisenberg Hamiltonians of ferromagnetism.

VII.D.1 Analogy Between Spin and Graph Systems

To construct graph Hamiltonians from the Hamiltonians of the Ising and Heisenberg models of ferromagnetism, we first draw an analogy between magnetic systems and graphs. Consider a spin-1/2 particle and a graph with two vertices, which has one edge state. The Hilbert spaces of these systems are both two-dimensional, so we may correspond adjacency and non-adjacency of any pair of graph vertices with spin up and spin down states in the spin system, respectively. If $|\uparrow\rangle$ and $|\downarrow\rangle$ correspond to spin up and spin down states, respectively, we can make the correspondence between particle and graph states

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow |\text{edge}\rangle, \tag{102}$$

$$|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow |\text{no edge}\rangle\,, \tag{103}$$

where $|\text{edge}\rangle$ and $|\text{no edge}\rangle$ represent states with vertex adjacency and non-adjacency states, respectively. We thus describe adjacency and non-adjancency states of any pair of graph vertices by vectors.

We extend this analogy to general graph and spin systems: a graph with N vertices corresponds to a spin system with $\binom{N}{2}$ spins, since a graph with N vertices has $\binom{N}{2}$ edges. The Hilbert space is a tensor product of $\binom{N}{2}$ edge Hilbert spaces, and thus has dimension $2^{\binom{N}{2}}$, but we now associate a spin-1/2 structure with each component of the Hilbert space. Although this seems arbitrary, this assignment allows us to define graph state Hamiltonians in analogy with the Ising and Heisenberg Hamiltonians, which are defined in terms of spin-1/2 operators. We can now express the Hilbert space $\mathscr{H}(N)$ of a graph with N vertices as the tensor product of spin-1/2 like edge Hilbert spaces $\mathscr{H}_{ij}$:

$$H(N) = \bigotimes_{i<j} \mathscr{H}_{ij}. \tag{104}$$

We emphasize that the edge Hilbert spaces $\mathscr{H}_{ij}$ are different from the previously defined edge Hilbert spaces $\mathscr{S}_{ij}$ because the former is equipped with a spin-1/2 Hilbert space structure.

We can now create graph state operators in analogy with the spin-1/2 operators by defining the edge operators $\hat{E}^x, \hat{E}^y, \hat{E}^z$:

$$\hat{E}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{105}$$

$$\hat{E}^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{106}$$

$$\hat{E}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{107}$$

where we choose a unit normalization for simplicity. These operators are the graph analogs of the spin operators $\hat{S}_x, \hat{S}_y$, and $\hat{S}_z$. The operator $\hat{E}^z$ has a clear interpretation in terms of the graph

state it acts on: it determines the adjacency of any pair of vertices in the graph. On the other hand, $\hat{E}^x$ and $\hat{E}^y$ do not have a clear interpretation in terms of the graph state at present.

We may now define edge operators $\hat{E}^x_{ij}, \hat{E}^y_{ij}$, and $\hat{E}^z_{ij}$ in analogy with (98)-(100):

$$\hat{E}^x_{ij} = \hat{I}^{\otimes i-1} \otimes \hat{E}^x \otimes \hat{I}^{\otimes N-i}, \tag{108}$$

$$\hat{E}^y_{ij} = \hat{I}^{\otimes i-1} \otimes \hat{E}^y \otimes \hat{I}^{\otimes N-i}, \tag{109}$$

$$\hat{E}^z_{ij} = \hat{I}^{\otimes i-1} \otimes \hat{E}^z \otimes \hat{I}^{\otimes N-i}. \tag{110}$$

VII.D.2 Construction of Graph Ising and Heisenberg Hamiltonians

We now construct graph state Hamiltonians in analogy with the Hamiltonians of the Ising and Heisenberg models using the previous correspondence of spin and graph Hilbert spaces. We make the correspondence $\hat{E}^i \to \hat{S}_i$ (with $i = x, y, z$) between operators and ignore normalization constants because they can be absorbed into the coefficients in the graph Hamiltonians. The graph Hamiltonians $\hat{H}_I$ and $\hat{H}_H$ corresponding to the Hamiltonians of the Ising and Heisenberg models of ferromagnetism (97) and (101) are then

$$\hat{H}_I = -\sum_{ij,kl} J_{ij,kl} \hat{E}^z_{ij} \hat{E}^z_{kl} - \mu \sum_{ij} h_{ij} \hat{E}^z_{ij}, \tag{111}$$

$$\hat{H}_H = -\sum_{ij,kl} (J^x_{ij,kl} \hat{E}^x_{ij} \hat{E}^x_{kl} + J^y_{ij,kl} \hat{E}^y_{ij} \hat{E}^y_{kl} + J^z_{ij,kl} \hat{E}^z_{ij} \hat{E}^z_{kl}) - \mu \sum_{ij} h_{ij} \hat{E}^z_{ij}. \tag{112}$$

Assuming that only adjacent edges can interact, in analogy with the nearest neighbor interaction approximation we adopted in the Ising and Heisenberg models of ferromagnetism, we may rewrite the sum over adjacent edges ij and jk, which yields

$$\hat{H}_I = -\sum_{ij,jk} J_{ij,jk} \hat{E}^z_{ij} \hat{E}^z_{jk} - \mu \sum_{ij} h_{ij} \hat{E}^z_{ij}, \tag{113}$$

$$\hat{H}_H = -\sum_{ij,jk} (J^x_{ij,jk} \hat{E}^x_{ij} \hat{E}^x_{jk} + J^y_{ij,jk} \hat{E}^y_{ij} \hat{E}^y_{jk} + J^z_{ij,jk} \hat{E}^z_{ij} \hat{E}^z_{jk}) - \mu \sum_{ij} h_{ij} \hat{E}^z_{ij}. \tag{114}$$

At this point, the Hamiltonians (113) and (114) are not written in terms of the edge creation and annihilation operators $\hat{a}^\dagger_{ij}$ and $\hat{a}_{ij}$ defined in section VI. We must now relate the edge

operators $\hat{E}^x_{ij}, \hat{E}^y_{ij}$, and $\hat{E}^z_{ij}$ to the edge creation and annihilation operators. We do this by developing edge ladder operators $\hat{E}^{\pm}_{ij}$ in analogy with the spin ladder operators $\hat{S}_{\pm}$. Extending the definition of the spin ladder operator (87) to the edge operators, we obtain

$$\hat{E}^{\pm}_{ij} = \hat{E}^x_{ij} \pm i\hat{E}^y_{ij}. \tag{115}$$

The ladder operator $\hat{E}^+_{ij}$ creates an edge between vertices i and j if they are non-adjacent and otherwise deletes the edge state, and the ladder operator $\hat{E}^-_{ij}$ deletes an edge between vertices i and j if they are adjacent and otherwise deletes the edge state. This suggests an association between the ladder operators $\hat{E}^+_{ij}$ and $hat E^-_{ij}$ and the edge creation and annihilation operators $\hat{a}^\dagger_{ij}$ and $\hat{a}_{ij}$:

$$\hat{a}^\dagger_{ij} \to \hat{E}^+_{ij} = \hat{E}^x_{ij} + i\hat{E}^y_{ij}, \tag{116}$$

$$\hat{a}_{ij} \to \hat{E}^-_{ij} = \hat{E}^x_{ij} - i\hat{E}^y_{ij}. \tag{117}$$

Solving the simultaneous equations (116) and (117) for $\hat{E}^x_{ij}$ and $\hat{E}^y_{ij}$ yields

$$\hat{E}^x_{ij} = \frac{\hat{a}^\dagger_{ij} + \hat{a}_{ij}}{2}, \tag{118}$$

$$\hat{E}^y_{ij} = \frac{\hat{a}^\dagger_{ij} - \hat{a}_{ij}}{2i}. \tag{119}$$

We may then write $\hat{E}^z_{ij}$ using the commutation relation $[\hat{E}_x, \hat{E}_y] = i\hat{E}_z$ (we extend the spin commutation relations directly to the edge operators via the correspondence of spin and edge Hilbert spaces), (118), and (119):

$$\hat{E}^z_{ij} = \frac{[\hat{a}^\dagger_{ij}, \hat{a}_{ij}]}{2}. \tag{120}$$

We also rewrite the edge operators $\hat{E}_x$ and $\hat{E}_y$ by multiplying (118) and (119) by $\{a^\dagger_{ij}, a_{ij}\} = a^\dagger_{ij}a_{ij} + a_{ij}a^\dagger_{ij} = 1$ (see (57)), which yields

$$\hat{E}^x_{ij} = \frac{\hat{N}_{ij}\hat{a}^\dagger_{ij} + \hat{a}_{ij}\hat{N}_{ij}}{2}, \tag{121}$$

$$\hat{E}^y_{ij} = \frac{i(\hat{a}_{ij}\hat{N}_{ij} - \hat{N}_{ij}\hat{a}^\dagger_{ij})}{2}. \tag{122}$$

Substitution of (120)-(122) into the Hamiltonians (113) and (114) gives the graph Ising and Heisenberg Hamiltonians:

$$\hat{H}_I = -\sum_{ij,jk} J_{ij,jk}(\hat{N}_{ij}\hat{N}_{jk} - \hat{N}_{ij}(1-\hat{N}_{jk}) - (1-\hat{N}_{ij})\hat{N}_{jk} + (1-\hat{N}_{ij})(1-\hat{N}_{jk})) \\ -\mu\sum_{ij} h_{ij}(2\hat{N}_{ij}-1), \tag{123}$$

$$\hat{H}_H = -\sum_{ij,jk} J^x_{ij,jk}(\hat{a}^\dagger_{ij}(1-\hat{N}_{ij})\hat{N}_{jk}\hat{a}^\dagger_{jk} + \hat{a}^\dagger_{ij}(1-\hat{N}_{ij})(1-\hat{N}_{jk})\hat{a}_{jk} + \hat{a}_{ij}\hat{N}_{ij}\hat{N}_{jk}\hat{a}^\dagger_{jk} \\ + \hat{a}_{ij}(\hat{N}_{ij}(1-\hat{N}_{jk})\hat{a}_{jk}) + J^y_{ij,jk}(\hat{a}_{ij}\hat{N}_{ij}\hat{N}_{jk}\hat{a}^\dagger_{jk} + \hat{a}^\dagger_{ij}(1-\hat{N}_{ij})(1-\hat{N}_{jk})\hat{a}_{jk} - \hat{a}_{ij}\hat{N}_{ij}(1-\hat{N}_{jk})\hat{a}_{jk} \\ - \hat{a}^\dagger_{ij}(1-\hat{N}_{ij})\hat{N}_{jk}\hat{a}^\dagger_{jk} + J^z_{ij,jk}(\hat{N}_{ij}\hat{N}_{jk} - \hat{N}_{ij}(1-\hat{N}_{jk}) - (1-\hat{N}_{ij})\hat{N}_{jk} + (1-\hat{N}_{ij})(1-\hat{N}_{jk})) \\ -\mu\sum_{ij} h_{ij}(2\hat{N}_{ij}-1). \tag{124}$$

VII.E Application of Graph Quantum Mechanics to Quantum Gravity

Now that we have developed a description of quantum dynamics of graphs with the second quantization of graph quantum mechanics, we now discuss how the quantum graph theory may be applied to quantum gravity and cosmology. We summarize and elaborate on the discussion provided in Konopka's work.[24] This work considers a quantum graph of some number of vertices N whose dynamics may describe the discrete spacetime of the universe. We quantize spacetime by embedding this graph into a spacetime manifold. The work specifies a quantum Hamiltonian for this graph which can be adjusted so that it favors a ground state for the graph with specific graph properties. Statistical mechanics can be used to describe the dynamics described by this Hamiltonian. The work discusses two dominant thermodynamic phases of the graph, a high temperature and low temperature phase. In the high temperature phase, the graph is highly connected; most or all of the pairs of vertices on the graph are adjacent. In the extremely high temperature limit, the graph is a complete graph $K(N)$. Recall that the vertices of a graph represent the constituents of space and edges represent relationships between them. In this context, we consider two vertices connected by an edge to be separated by the

fundamental quantum of distance set in the discrete spacetime. Thus, the points of space are highly connected to each other and there is no notion of locality in space. In addition, the graph contains a large number of degrees of freedom due to the high connectivity of its vertices. The large number of degrees of freedom of the graph makes it more difficult to embed these graphs into lower-dimensional spaces. For the same reason, it is more difficult to integrate known physics theories (which have much fewer degrees of freedom than typical high-temperature graphs which describe spacetime) into the discrete spacetime these graphs describe. This is important because other physics theories allow us to integrate physical properties into the discrete spacetime. For instance, quantum field theory describes matter as the excitations of fields which permeate spacetime. We would like to integrate field excitations into the discrete spacetime emerging from the graph quantum theory. In Konopka's work,[24] a dynamical quantum graph theory is developed which associates a spin-1-like edge Hilbert space with every pair of vertices in a graph. In this Hilbert space, there are three possible states for edges, which are analogous to the spin-1 triplet spin states. The dynamical evolution of the graph allows this degree of freedom in edges to constitute a matter field excitation on a lattice, akin to one seen in a lattice quantum field theory, leading to a potentially viable description of matter in discrete spacetime.

In the low temperature phase, the graph approaches a ground state where only a small subset of edges are defined on the graph. Thus, the graph is less connected than it is in the high temperature phase, and locality emerges in space. In addition, it becomes easier to embed these graphs into lower dimensional space and integrate known physics theories into the resulting discrete spacetime. In Konopka's work,[24] a Hamiltonian is constructed which admits dynamical degrees of freedom which yield a simple gauge theory on the discrete spacetime. This gauge theory can constitute matter field excitations on the spacetime and thus integrate matter into discrete spacetime.

It is clear that the description of graph dynamics presented in Konopka's paper[24] may provide a description of the emergence of discrete spacetime in the early universe. The universe was extremely hot in its early stages. The model predicts that there was no meaningful notion of spacetime geometry in the early universe because the high temperature phase of graphs do not admit a description of spacetime with its expected properties, such as locality. However, as the universe cooled, the model predicts that the low temperature phase of graphs is more ordered than the high temperature one, and typical notions associated with spacetime emerge. In addition, the smaller number of degrees of freedom in the space may cause physics described by current physics theories to arise. For example, quantum field theories such as the Standard Model may now arise in the low temperature phase of spacetime, leading to the emergence of matter.

There are two noteworthy advantages of applying the quantum mechanical graph formalism for describing the evolution of the universe. First, the highly connected graph which describes the early universe may provide an alternative to cosmological inflation for resolving the horizon problem which is less fine-tuned. The horizon problem is concerned with explaining the homogeneity of the universe. This is difficult because distant parts of the universe could never have come into contact with each other, given the current age of the universe. Cosmological inflation may provide an explanation for the homogeneity of the universe, but it requires unnatural initial conditions for the universe. On the other hand, the graph theory explains the homogeneity of the universe by the high interconnection of the complete graph describing the early universe; all points in the universe were in causal contact near the beginning of the universe because all points in the complete graph describing spacetime in the early universe are connected to every other point. Thus, when the universe cooled, all points were already in contact and could reach thermal equilibrium, explaining the homogeneity of the universe.[24]

In addition, the graph emergent quantum gravity paradigm offers great flexibility in tuning

the description of the early universe. The graph Hamiltonians presented in Konopka's work[24] and in this thesis have parameters which may be adjusted so that the universe evolves in a very specific way as it cools. This flexibility is important for tuning the theory to experimental input.

The graph quantum theory developed in this thesis builds on the previously discussed developments because it ensures that any quantum gravity or cosmology theory arising from the graph quantum theory is coordinate system independent, as an emergent quantum gravity theory should be. By starting with unlabeled graphs in constructing the quantum theory, coordinate system independence is incorporated into the theory from the start. In addition, the Ising and Heisenberg Hamiltonians presented in this thesis provide another possibility for graph state dynamics which may be used to construct an emergent quantum gravity theory.

VIII CONCLUSION

This thesis developed two quantum mechanical theories of finite graphs similar to those derived in Konopka's work [2] which account for the vertex permutation invariance of graphs. These quantum theories may be used to model discrete spacetime in quantum gravity. Properties of finite graphs relevant to the quantum mechanics of graphs were introduced, and the first and second quantization of quantum mechanics were reviewed. The first quantization of graph quantum mechanics was developed. It was found that the antisymmetrization of graph states is complicated by the requirement that edge states be described by two quantum numbers. It was shown that the sum of states produced by acting all vertex permutations in a traversal of the cosets S_N/Γ_G on a base state and subsequently multiplying by the sign of the permutation applied gives the antisymmetrized graph state. The second quantization of graph quantum mechanics was also developed. Edge creation and annihilation operators were defined in analogy to particle creation and annihilation operators. Second quantization operators for edge number, vertex degree, graph complement, and graph unit sphere were developed in terms of the edge creation and annihilation operators. Finally, a method for describing graph state dynamics in the second quantization of graph quantum mechanics was developed by drawing an analogy to the Ising and Heisenberg models for magnetic systems. These models were introduced then connected to the quantum theory of graphs. Two model Hamiltonians describing graph state dynamics were then derived in analogy with the Ising and Heisenberg Hamiltonians.

We propose four routes for future work on the graph quantum mechanical formalism. First, we would like to elaborate on graph state dynamics. In this thesis, we derived two graph Hamiltonians which describe dynamics in the second quantization quantum graph formalism without actually applying them to make dynamical predictions about graphs. We hope that future work will explore the consequences of the Ising and Heisenberg Hamiltonians. This will

allow us to test the viability of the graph dynamics under these Hamiltonians for describing discrete spacetime. In addition, we would like to construct additional graph state Hamiltonians, including those which live in different graph Hilbert spaces. In this thesis, we drew an analogy between the spin-1/2 Hilbert space and the edge state Hilbert space and corresponded spin up and down states with vertex adjacency and nonadjacency states. However, we may also draw analogies between higher spin Hilbert spaces and edge states. In Konopka's work,[24] a spin-1 Hilbert space is associated with an edge Hilbert space, where the spin-0 state corresponds to a non-adjacency state and the three spin-1 states correspond to three distinct adjacency states. This is unlike the spin-1/2-like edge Hilbert space considered in this thesis, which only has one possible edge state. Constructing edge Hilbert spaces in analogy with other finite-dimensional Hilbert spaces (e.g. spin Hilbert spaces) may provide a means for incorporating additional degrees of freedom in the discrete spacetime emergent from graphs in the quantum graph theory not considered in this thesis. It is hoped that more complex edge Hilbert spaces may be formulated and Hamiltonian operators may be defined on them to explore different kinds of emergence of discrete spacetime from the quantum graph theory. We would also like to elaborate more on how graph quantum statistics manifest themselves in graphs. In particle quantum mechanics, the symmetry of the boson wavefunction leads to Bose-Einstein condensation of bosons and the anti-symmetry of the fermion wavefunction leads to Pauli exclusion. We expect that the symmetry and antisymmetry of boson and fermion graph wavefunctions will lead to some observable consequence on graph states similar to Bose-Einstein condensation and Pauli exclusion. We hope that future work may elucidate how graph statistics manifest themselves in the observable properties of graphs. Finally, we would like to evaluate the credibility of the graph quantum mechanics paradigm for constructing emergent spacetime. In this thesis, we have used graphs as objects with which spacetime may dynamically emerge. However, we have not considered if the emergent phenomena arising from these graphs may lead to a viable description of discrete spacetime from which a quantum

gravity theory may be based. We hope that future work may assess the viability of the graph emergent paradigm for constructing discrete spacetime and, more generally, for constructing a quantum gravity theory.

LIST OF REFERENCES

[1] Mark K. Gaillard, Paul D. Grannis, and Frank J. Sciulli, ‘‘The Standard Model of Particle Physics," Rev. Mod. Phys. **71**, S96-S111 (1999).

[2] Tomasz Konopka, Fotini Markopoulou, and Simone Severini,‘‘Quantum Graphity: a model of emergent locality," Phys. Rev. D **77**, 104029 (2008).

[3] X. Fan et al., ‘‘Measurement of the Electron Magnetic Moment," Phys. Rev. Lett. **130**, 071801 (2023).

[4] C. Keifer, ‘‘Quantum gravity: general introduction and recent developments," Annalen Phys. **15**, 129-148 (2005).

[5] Stefan Hollands, Robert M. Wald, ‘‘Quantum fields in curved spacetime," Physics Reports **574**, 1-35 (2015).

[6] Martin Bojowald, ‘‘Singularities and Quantum Gravity," AIP Conf. Proc. **910** (1), 294-333 (2007).

[7] Jacob D. Bekestein, ‘‘Black Holes and Entropy," **7** (8), 2333-2346 (1973).

[8] Carlo Rovelli, ‘‘Black Hole Entropy from Loop Quantum Gravity," Phys. Rev. Lett. **77** (16), 3288-3291 (1996).

[9] B.L. Hu, ‘‘Stochastic Gravity," Int. J. Theor. Phys. **38** (11), 2987-3037 (1999).

[10] Chung-I Kuo, L.H. Ford ‘‘Semiclassical Gravity Theory and Quantum Fluctuations," Phys. Rev. D. **47** (10), 4510-4519 (1993).

[11] Don N. Page, C.D. Geilker, ‘‘Indirect Evidence of Quantum Gravity," Phys. Rev. Lett. **47** (14), 979-982 (1981).

[12] Bryce S. DeWitt, ‘‘Quantum Theory of Gravity. I. The Canonical Theory," Phys. Rev. **160**, 1113 (1967).

[13] Carlo Rovelli, ‘‘Loop Quantum Gravity," Living Rev. Rel. **1966**, 1.

[14] A. Ashtekar, R. Geroch, ‘‘Quantum theory of gravitation," Rep. Prog. Phys. **37** (10), 1211 (1974).

[15] Chris J. Isham, ‘‘Canonical Quantum Gravity and the Problem of Time," NATO Sci. Ser. C 409, 157-287 (1993).

[16] G.U. Jakobsen, M.S. thesis, Neils Bohr International Academy, 2020.

[17] Assaf Shomer, ‘‘A Pedagogical explanation for the non-renormalizability of gravity," arXiv:0709.3555 [hep-th].

[18] Mark Van Raamsdonk, ‘‘Building up spacetime with quantum entanglement," Int. J. Mod. Phys. D **19** (14), 2429-2435 (2010).

[19] Tsapikos Kottos and Uzy Smilansky, ‘‘Quantum Chaos on Graphs," Phys. Rev. Lett. **79**, 4794 (1997).

[20] P. Kuchment and L. Kunyansky, ‘‘Differential Operators on Graphs and Photonic Crystals," Adv. Comp. Math. **16**, 263-290 (2002).

[21] James P. Sethna, "Statistical Mechanics: Entropy, Order Parameters, and Complexity," 2nd ed. (Oxford University Press, 2022), p. 142.

[22] Barry A. Cipra, ‘‘An Introduction to the Ising Model," **94** (10), 937-959 (1987).

[23] F Bonechi et. al., ‘‘Heisenberg XXZ Model and Quantum Galilei Group," J. Phys. A **25** (15), L939 (1992).

[24] Tomasz Konopka, Fotini Markoupoulou, Lee Smolin, "Quantum Graphity," arXiv:hep-th/0611197v1.