Lee-Yang Tensors in Quantum Information and Algorithms for Local Hamiltonian Problems

by

Benjamin Wong

A thesis
presented to the University of Waterloo
in fulfillment of the
thesis requirement for the degree of
Master of Mathematics
in
Combinatorics and Optimization (Quantum Information)

Waterloo, Ontario, Canada, 2026

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Author's Declaration

This thesis consists of material all of which I authored or co-authored: see Statement of Contributions included in the thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Statement of Contributions

This thesis contains work and verbatim text from a collaboration with Sergey Bravyi, David Gosset, and Yinchen Liu appearing in the preprint [WBGL26] as well as results in Section 3.2, Section 3.3, and Section 3.4 which do not appear there.

- In Chapter 2, Section 2.1 and Section 2.2 contain my own presentation of my coauthors' results with the exception of Theorem 8 to which I contributed. Section 2.3 is my own work except for Sergey Bravyi's Lemma 11.
- In Chapter 3, Section 3.1 contains collaborative work with my coauthors. To this section, I contributed the numerics shown in Figs. 3.1, 3.3 and 3.4 in Numerical study 1, the numerics in Numerical study 2, Conjecture 2, and the evidence for it in Numerical study 3. Section 3.2 is my own work with the exception of Lemma 20 and Theorem 12 which are in collaboration with David Gosset and Yinchen Liu. Section 3.3 is my own work generalizing Sergey Bravyi's calculation in Lemma 14. Section 3.4 is my own work with suggestions from Yinchen Liu.

Abstract

Local Hamiltonian problems are central to both quantum complexity theory and quantum many-body physics: ground state problems are the natural quantum constraint satisfaction problems, and computing the partition function reveals thermal equilibrium properties. A turning point in the theory of local Hamiltonians was Lee and Yang's original study relating roots of the partition function to phase transitions [LY52].

In this thesis, we investigate the role of complex tensors which satisfy a Lee-Yang condition in quantum information theory. We find that the class of Lee-Yang tensors is closed under natural operations such as certain post-selective measurements, tensor products, tensor contraction, and the application of certain single-qubit quantum channels. In analogy with the Perron-Frobenius theorem, we show that Hermitian operators with the Lee-Yang property have simple extremal eigenvalues. We show that there are quasipolynomial-size quantum circuits for preparing Lee-Yang tensors.

Furthermore, we present new algorithms for specific families of quantum many-body systems. The EPR Hamiltonian is a model in which local terms energetically favor EPR states $|00\rangle + |11\rangle$ and which includes quantum Max Cut on bipartite graphs as a special case. We provide numerical evidence for an efficient adiabatic quantum algorithm for preparing the ground state of the EPR Hamiltonian. For the ferromagnetic XY model, we give an efficient quantum algorithm for preparing the Gibbs state, thereby extending a classical algorithm due to Bravyi and Gosset [BG17]. We give an efficient classical algorithm for simulating stoquastic systems when the interaction graph has a sufficiently rich family of automorphisms. For the classical Ising model, we establish that a polynomial built from powers of the Hamiltonian satisfies a zero-freeness condition.

Acknowledgements

Thanks to David Gosset for being an attentive, patient, and generous supervisor throughout my master's degree. This thesis would not have been possible without the support of many families. Thanks to

- David Gosset, Calvin Liu, and Sergey Bravyi, my academic family, for shepherding me into the world of research;
- Debbie Leung and Luke Schaeffer for reading and providing feedback on this thesis,
- Kevin Resch and William Slofstra for supporting my earliest research ambitions and writing many reference letters;
- Eric Culf, Raz Firanko, David Gosset, and Calvin Liu for providing valuable feedback on preliminary versions of this thesis and the associated talk;
- Melissa Quantrill, Gen Belford, and Douglas Stebila for making graduate studies in the Combinatorics & Optimization department joyous;
- Jack, Ben, Chris, Wendy, and Tom Bishop for making me feel at home in Waterloo;
- William, Dillon, and Lai Huong Chan for providing me and my friends with affordable housing and valuable camaraderie;
- Ashley, Sean, Rob, and Lisa Geddes for their weekly doses of life;
- Christine and Werner Rohmann for gathering the family every holiday;
- Alice Bush, Don Murray, and Nicola Murray for generosity that keeps me going;
- my parents Bill and Nancy, and my brother Bart for a lifetime of love.

Dedication

This thesis is dedicated to Christine Rohmann. Your love inspires and lives on.

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Chapter 1

Introduction and preliminaries

Introduction

Local Hamiltonians are mathematical models of quantum spin systems arising in nature. We are interested in computing thermal properties which can be derived from the Hamiltonian including the Gibbs state, partition function, and ground energy. However, the runtime of computing these quantities is prohibitively long in both a practical and formal sense. Indeed, naive simulation methods all appear to take exponential time. Furthermore, these problems are also hard in a complexity-theoretic sense: Kitaev showed that estimating the ground energy of local Hamiltonians is complete for the complexity class QMA, a quantum analog of NP [KSV02]. Although Kitaev's original proof involves rather contrived local Hamiltonians, the result has been refined [KKR06, OT05, BL08, JGL10, CGW15, CM16] to establish hardness even for Hamiltonians with more realistic terms, geometry, and locality. These worst-case hardness results underscore the importance of local Hamiltonian problems as the natural constraint satisfaction problems in quantum complexity theory.

Despite the hardness results above, there are some exceptional families of local Hamiltonians which admit efficient classical simulation [Bra15, BG17, HMS20]. Discovering these remarkable families makes progress on the long-term goal of understanding the classical-quantum hardness landscape by providing many-body physics counterparts to celebrated classical simulation results in quantum computation such as the Gottesman-Knill theorem [Got98, AG04], the simulation of free fermions [Val01, TD02], and the simulation of quantum circuits with low tree-width [MS08].

The existing efficient simulations of quantum spin systems target local Hamiltonians with Gibbs states that are either Lee-Yang tensors or have nonnegative matrix elements in the computational basis. We say that a tensor is a Lee-Yang tensor with radius r if the tensor's generating polynomial does not vanish when each variable lies in the open disk with radius r in the complex plane. This condition permits the use of polynomial interpolation methods in designing algorithms for estimating the partition function [LSS18, HMS20]. We say a Hamiltonian is stoquastic if all of its off-diagonal matrix entries are nonpositive. This constraint on the Hamiltonian characterizes when the Gibbs state has nonnegative matrix

elements and permits the use of quantum Monte Carlo methods for estimating the partition function [Bra15, BG17].

In this thesis, we extend the theory of Lee-Yang tensors and stoquastic Hamiltonians. In Chapter 2, we give applications of Lee-Yang tensors in quantum information theory. First, we review properties of the class of Lee-Yang tensors including closure under tensor products, tensor contraction, and limits. We show that the class of Lee-Yang tensors is also closed under certain post-selective measurements and under the application of certain single-qubit channels. We characterize one and two-qubit Lee-Yang tensors and exhibit several new classes of Lee-Yang tensors. We show that Hermitian operators which are Lee-Yang tensors satisfy a Griffiths inequality. Next, we study tensors with Lee-Yang radius $r > 1$ and find that in this case, Lee-Yang Hermitian operators have simple extremal eigenvalue and that there are quasi-polynomial size quantum circuits for preparing Lee-Yang states. These results suggest that $r = 1$ is a key threshold for Lee-Yang states and observables.

In Chapter 3, we develop classical and quantum algorithms for specific families of stoquastic Hamiltonians. In Section 3.1, we consider the EPR model which energetically favors EPR states $|00\rangle + |11\rangle$. Developing approximation algorithms for the ground energy of the EPR Hamiltonian has attracted considerable attention in recent years [Kin23, JKK+25, JN25, ALM+25b, APS25, ALM+25a]. The EPR problem includes bipartite quantum Max Cut as a special case and has been named as an important open problem [Gha23]. Our contribution is the study of a deformed EPR model which allows us to interpolate between a trivial model and the EPR Hamiltonian by energetically favoring deformed EPR states $|00\rangle + s|11\rangle$ for $0 \leq s \leq 1$. We support several conjectures with numerical experiments and exact solutions in some tractable cases. We conjecture that the deformed EPR Hamiltonian has spectral gap at least $1 - s^2$. This conjecture implies that the quantum adiabatic algorithm which prepares the ground state of the EPR model is efficient, thereby providing the first polynomial time exact algorithm for the EPR problem. We suspect that this bound on the spectral gap holds in the more general setting where the Hamiltonian energetically favors terms $|00\rangle + se^{i\theta}|11\rangle$ where the angle θ can be chosen independently for each term. If this more ambitious conjecture is true, then the same adiabatic algorithm can be used to simulate some Hamiltonians beyond the stoquastic regime. Finally, we conjecture that the ground state of the deformed EPR model has Lee-Yang radius $1/\sqrt{s}$. This conjecture suggests the existence of a family of ground states which have Lee-Yang radius $r > 1$.

In Section 3.2, we consider ferromagnetic Hamiltonians with local terms $-X \otimes X - Y \otimes Y$. For these models, we show that Bravyi and Gosset's classical simulation algorithm [BG17] can be extended to a quantum algorithm for preparing a canonical purification of the Gibbs state by using the Grover-Rudolph state preparation procedure. We also show that the ferromagnetic XY models satisfy a Griffiths inequality.

In Section 3.3, we consider the role of the underlying interaction graph. We show that the ground state properties of stoquastic Hamiltonians can be computed efficiently when the underlying interaction graph supports a sufficiently rich class of automorphisms. In particular, we show how automorphisms of the interaction graph can be used to reduce the size of the matrix implementing the Hamiltonian.

In Section 3.4, we show that a polynomial derived from repeated powers of an Ising model

Hamiltonian satisfies a zero-freeness condition. In particular, the trace of the kth power of a deformed classical Ising model Hamiltonian is shown to converge to $1 + s^k$. However, we see that the same property does not hold for repeated powers of the deformed EPR Hamiltonian by explicit counterexample.

Preliminaries

Notations

Binary strings are denoted by lower case Latin letters as in $x \in \{0,1\}^n$ with ith bit $x_i \in \{0,1\}$. Complex tensors are denoted by lower case Greek letters such as ψ, ϕ with indices labeled by binary strings as in $\psi_x \in \mathbb{C}$. Vectors of real numbers are denoted by boldface Latin letters such as $\mathbf{r}, \mathbf{x}$. Vectors of complex numbers are denoted by kets and bras as in $|\psi\rangle, \langle\phi|$, or by lower case Latin letters at the end of the alphabet such as z, w. Linear operators are denoted by capital Latin letters such as A, H, U, and lower case Latin letters such as h. Density matrices are denoted by lower case Greek letters such as ρ, σ. When we wish to emphasize that a matrix is a projector, we denote it by Π. Quantum channels are denoted by capital calligraphic letters such as $\mathcal{E}$.

Local Hamiltonians

First, we review local Hamiltonians and their thermal properties in the context of algorithms and complexity. Then, we give three examples of efficient algorithms for estimating the partition function. Finally, we review the complexity landscape of the XXZ Heisenberg Hamiltonians. Ref. [GHLS15] contains a more comprehensive review on the complexity of local Hamiltonian problems.

We consider Hermitian operators on the n-qubit Hilbert space $(\mathbb{C}^2)^{\otimes n}$.

Definition 1. *A k-local Hamiltonian is a Hermitian operator of the form*

$$H = \sum_{i=1}^{m} h_i \tag{1.1}$$

where each local term h_i acts nontrivially on only k qubits and $m = \mathsf{poly}(n)$.

Each term in the sum Eq. (1.1) represents an interaction between particles. Local terms can be specified as a tensor product of single-qubit Pauli operators

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{1.2}$$

If P is a single-qubit operator, we use the notation P_i to specify the Hermitian operator where P acts on qubit i, i.e. $P_i = I \otimes I \otimes \cdots \otimes P \otimes \cdots \otimes I$ where P is the ith tensor

factor. For example, the quantum Heisenberg model on the graph $G = (V, E)$ is the local Hamiltonian

$$H = -\sum_{(i,j)\in E} (J_{ij}^X X_i X_j + J_{ij}^Y Y_i Y_j + J_{ij}^Z Z_i Z_j) - \frac{\mu}{2} \sum_{i\in V} (I + Z_i) \tag{1.3}$$

for some real coefficients $J_{ij}^X, J_{ij}^Y, J_{ij}^Z, \mu$. We will see that the complexity of computing thermal properties can vary greatly across different special cases of the Heisenberg model. We will also concern ourselves with a family of Hamiltonians which have Gibbs states with nonnegative matrix entries in the computational basis known as stoquastic Hamiltonians. Stoquastic Hamiltonians were introduced by Bravyi, DiVincenzo, Oliveira, and Terhal [BDOT08] as a physically relevant and expressive, but likely non-universal class of Hamiltonians. Stoquastic Hamiltonians play an important role in complexity theory, often as an intermediate class exhibiting some, but not all of the complexity present in quantum phenomena [BBT06, CM16, BH17].

Definition 2 (Stoquastic Hamiltonian)**.** *A Hamiltonian H is said to be stoquastic if all of its off-diagonal matrix elements are nonpositive in the standard basis. In other words, if $x, y \in \{0,1\}^n$ and $x \neq y$, then*

$$\langle x|H|y\rangle \leq 0. \tag{1.4}$$

We make our algorithmic goals precise by focusing on the ground state energy, the partition function, and the Gibbs state. The ground state energy and ground state of a Hamiltonian is its smallest eigenvalue and a corresponding eigenvector. Estimating the ground state energy is the natural quantum generalization of classical constraint satisfaction problems. In particular, ground state problems capture Max Cut and quantum Max Cut as special cases. Estimating the ground state energy is intractable in the sense that its promise version is a hard problem for a quantum analogue of NP known as QMA [KSV02]. This intractability persists even when restricted to a single 2-local interaction on a 2D lattice [KKR06, OT05, BL08, JGL10, CGW15, CM16].

Problem 1 (Estimating the ground state energy)**.** *Given a local Hamiltonian H and $\varepsilon > 0$, compute an estimate λ' satisfying*

$$|\lambda' - \lambda| \leq \varepsilon \tag{1.5}$$

where λ is the ground energy

$$\lambda = \min_{\|x\|=1} \langle x|H|x\rangle. \tag{1.6}$$

The natural counting problem in thermal physics is estimating the partition function $\mathrm{Tr}(e^{-\beta H})$ at some inverse temperature $\beta > 0$. The partition function is the normalization factor of the Gibbs state and can be used to compute the free energy, entropy, and ground energy. Indeed, estimating the partition function to ε-relative error at $\beta = O(n\varepsilon^{-1})$ is enough to ensure that the free energy $F = -\beta^{-1} \log(\mathrm{Tr}(e^{-\beta H}))$ is an ε-additive error estimate for the ground energy. Hence estimating the partition function is at least as hard as estimating the ground energy.

Problem 2 (Estimating the partition function)**.** *Given a local Hamiltonian H, $\beta > 0$, and $\varepsilon > 0$, compute an estimate α satisfying*

$$(1-\varepsilon)\mathrm{Tr}(e^{-\beta H}) \leq \alpha \leq (1+\varepsilon)\mathrm{Tr}(e^{-\beta H}). \tag{1.7}$$

Systems in thermal equilibrium are said to be in their Gibbs state. We consider the task of preparing a Gibbs state on a quantum computer. As with the free energy, taking β sufficiently large ensures that the Gibbs state approximates the ground state. It is also known that preparing the Gibbs state is sufficient to estimate the partition function by a reduction from estimating Pauli observables of the Gibbs state [BCGW22]. Hence preparing the Gibbs state is at least as hard as estimating the partition function: giving us a trio of problems of increasing difficulty.

Problem 3 (Preparing an approximate Gibbs state)**.** *Given a local Hamiltonian H, $\beta > 0$, and $\varepsilon > 0$, prepare a state ρ' satisfying*

$$\|\rho' - \rho\|_1 \leq \varepsilon \tag{1.8}$$

where ρ is the Gibbs state

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})}. \tag{1.9}$$

Let us briefly review Gibbs state and ground state properties of a stoquastic Hamiltonian. Suppose that H is stoquastic, i.e. all off-diagonal elements are nonpositive. We can show that the Gibbs state $\rho = e^{-\beta H}/\mathrm{Tr}(e^{-\beta H})$ has nonnegative matrix elements in the standard basis. Indeed, observe that

$$\rho \propto e^{-\beta H} \tag{1.10}$$

$$= \lim_{k\to\infty} \left(e^{-\beta H/k}\right)^k \tag{1.11}$$

$$= \lim_{k\to\infty} \left(I - \frac{\beta}{k} H\right)^k. \tag{1.12}$$

Since H is stoquastic, for all k sufficiently large, $I - \beta H/k$ will have nonnegative matrix elements in the computational basis and hence so will ρ by Eq. (1.12). By continuity and taking the limit of large β, the ground state can be chosen to have nonnegative amplitudes as well. This nonnegativity enables the use of quantum Monte Carlo methods for classical simulation and the use of the Grover-Rudolph algorithm [GR02] for quantum state preparation. By the Perron-Frobenius theorem (appearing as Theorem 17 in Appendix A) applied to $I - \beta H/k$, the ground state of H is unique when the underlying interaction graph is connected. Estimating the ground state energy of a stoquastic Hamiltonian is known to be contained in AM [BBT06] suggesting that these Hamiltonians are much more tractable than the general case.

Algorithms for local Hamiltonians

We present three families of local Hamiltonians for which efficient classical algorithms for estimating the partition function are known. We begin with a result of Jerrum and Sinclair for the classical Ising ferromagnet. The classical Ising ferromagnet has 2-local terms proportional to $-Z \otimes Z$ which energetically favour alignment between neighbouring particles and 1-local terms proportional to $-Z$ which energetically favour $|0\rangle$. Accordingly, $|00\rangle$ is the ground state for $Z \otimes Z + Z \otimes I + I \otimes Z$, whereas $|0^n\rangle$ is the ground state of an n-qubit Ising ferromagnet.

Theorem 1 (Classical simulation of classical ferromagnets [JS93])**.** *Let $G = (V, E)$ be a graph and let $\varepsilon > 0$ be given. For $c_{ij}, \mu \in \mathbb{R}$ satisfying the ferromagnetic condition $c_{ij}, \mu \geq 0$ consider the classical ferromagnetic Ising model Hamiltonian*

$$H = -\sum_{(i,j)\in E} c_{ij} Z_i Z_j - \mu \sum_{i \in V} (I + Z_i). \tag{1.13}$$

Then there is a randomized classical algorithm which outputs an ε-relative error estimate of the partition function

$$\mathcal{Z}(\beta) = \mathrm{Tr}(e^{-\beta H}) \tag{1.14}$$

in time $\mathsf{poly}(\beta, \varepsilon^{-1}, n)$.

This algorithm results from a sampling to counting reduction and a Markov chain Monte Carlo algorithm (see Appendix A for more information on Markov chain Monte Carlo methods) which uses the set of spanning subgraphs of the interaction graphs as states. Furthermore, this algorithm can be used to sample from the Gibbs distribution of classical ferromagnetic models. Jerrum and Sinclair [JS93] also show that evaluating the partition function exactly is #P-complete, indicating that approximation is the best we can hope for.

In the quantum setting, Bravyi extended Jerrum and Sinclair's algorithm for the ferromagnetic Ising model to include a family of stoquastic Hamiltonians known as the ferromagnetic transverse field Ising model [Bra15]. Through a reduction to counting weighted perfect matchings, Bravyi and Gosset generalized Bravyi's algorithm to show that quantum ferromagnetic XY Hamiltonians can be simulated efficiently classically [BG17]. The ferromagnetic XY Hamiltonians have 2-local terms

$$-bX \otimes X + cY \otimes Y = \begin{bmatrix} 0 & 0 & 0 & -b-c \\ 0 & 0 & -b+c & 0 \\ 0 & -b+c & 0 & 0 \\ -b-c & 0 & 0 & 0 \end{bmatrix} \tag{1.15}$$

for parameters $b, c \in \mathbb{R}$ satisfying $|c| \leq b$. Note that these local terms are stoquastic and have ground state $(|00\rangle + |11\rangle)/\sqrt{2}$ or $(|01\rangle + |10\rangle)\sqrt{2}$ depending on the sign of c. This already indicates that finding a ground state for the overall Hamiltonian may be difficult because the monogamy of entanglement [CKW00] ensures that there is no state where each local term is satisfied for a connected interaction graph.

Theorem 2 (Classical simulation of quantum ferromagnets [BG17]). *Let $G = (V, E)$ be a graph and let $\varepsilon > 0$ be given. For $b_{ij}, c_{ij}, d_i \in \mathbb{R}$ satisfying the ferromagnetic condition $|c_{ij}| \leq b_{ij}$ consider the quantum XY ferromagnetic Hamiltonian*

$$H = \sum_{(i,j)\in E} (-b_{ij} X_i X_j + c_{ij} Y_i Y_j) + \sum_{i \in V} d_i (I + Z_i). \tag{1.16}$$

Then there is a randomized classical algorithm which outputs an ε-relative error estimate of the partition function

$$\mathcal{Z}(\beta) = \mathrm{Tr}(e^{-\beta H}) \tag{1.17}$$

in time $\mathsf{poly}(\beta, \varepsilon^{-1}, n)$.

Bravyi and Gosset's algorithm introduces the reduction to perfect matching sums used in our algorithm for preparing the Gibbs state in Section 3.2. The perfect matching sum is not known to be efficiently approximable in general, but the reduction of Bravyi and Gosset always results in graphs possessing a structural property which permits efficient approximation of the perfect matching sum by an algorithm of Jerrum and Sinclair [JS89b]. In Section 3.2, we will consider perfect matching sums of bipartite graphs for which efficient approximation of the perfect matching sum is possible due to an algorithm of Jerrum, Sinclair, and Vigoda [JSV04].

The previous two algorithms both rely on sampling from the Gibbs distribution for stoquastic Hamiltonians. We will now show how a deterministic approximation algorithm can be derived from a zero-free region by surveying an algorithm for the anisotropic XXZ model due to Harrow, Mehraban, and Soleimanifar [HMS20]. In order to give a proof we introduce two results which will be useful in Chapter 2: Barvinok's polynomial interpolation lemma, and a zero-freeness theorem due to Suzuki and Fisher [SF71].

Barvinok polynomial interpolation [Bar16] is a technique used to design efficient deterministic algorithms for approximating the evaluations of polynomials with many terms. This technique requires the target polynomial to have a zero-free region in the complex plane containing the evaluation point as well as a point for which the derivatives are efficiently computable. Typically, the Barvinok method is used to achieve quasipolynomial runtime algorithms for computing relative error estimates to counting problems. However, Patel and Regts show how to achieve a fully polynomial runtime for problems defined on bounded-degree graphs [PR17]. The relation between zero-free regions and polynomial approximation is captured in the following lemma.

Lemma 1 (Barvinok polynomial interpolation [Bar16]). *Let $f(z)$ be a complex polynomial of degree n satisfying*

$$f(z) \neq 0 \text{ for all } |z| \leq r \tag{1.18}$$

for some $r > 1$. Consider $g(z) = \log(f(z))$. If $T_p(z)$ is the degree p Taylor polynomial of $g(z)$ centered at $z = 0$, then we have

$$|g(z) - T_p(z)| \leq \frac{n}{(p+1) r^p (r-1)} \text{ for all } |z| \leq 1. \tag{1.19}$$

Lemma 1 implies that we can choose $p = O(\log(n/\varepsilon))$ so that $\exp(T_p(1))$ is an ε-relative error estimate for $f(1)$. Moreover, this estimate can be computed using derivatives of $g(z)$ at $z = 0$ up to order p. When $f(0)$ and the coefficients of the polynomial f are known up to degree p, these derivatives can be computed by solving a triangular system of linear equations. In particular, letting $f^{(j)}, g^{(j)}$ be the jth derivatives of f, g respectively, evaluated at $z = 0$, we have

$$f^{(m)} = \sum_{j=0}^{m-1} \binom{m-1}{j} f^{(j)} g^{(m-j)} \qquad 1 \leq m \leq p, \tag{1.20}$$

see Ref. [Bar16] for details.

The Suzuki-Fisher theorem gives an easy-to-check sufficient condition for zero-freeness of some quantum Heisenberg models.

Theorem 3 (Suzuki-Fisher [SF71])**.** *Consider the quantum Heisenberg model*

$$H(\mu) = -\sum_{(i,j)\in E} (J_{ij}^X X_i X_j + J_{ij}^Y Y_i Y_j + J_{ij}^Z Z_i Z_j) - \frac{\mu}{2} \sum_{i \in V} (I + Z_i) \tag{1.21}$$

with constants $J_{ij}^X, J_{ij}^Y, J_{ij}^Z \in \mathbb{R}$, $\beta > 0$, and a variable $\mu \in \mathbb{C}$. If the ferromagnetic condition $J_{ij}^Z \geq \max\{|J_{ij}^Y|, |J_{ij}^X|\}$ for each i, j, then the partition function

$$\mathcal{Z}(\mu) = \mathrm{Tr}(e^{-\beta H(\mu)}) \tag{1.22}$$

only vanishes when the real part is zero, i.e. $\mathfrak{Re}(\mu) = 0$.

Although $H(\mu)$ is no longer a Hamiltonian when $\mu \notin \mathbb{R}$, the analyticity of $\log(\mathcal{Z}(\mu))$ on the complex plane constrains the phase transitions of the corresponding spin system. We will see in Chapter 2 that this analyticity also has algorithmic consequences. We will refer to Hamiltonians satisfying these conditions as Suzuki-Fisher Hamiltonians. A slight generalization of the Suzuki-Fisher theorem is stated and proved in Theorem 6. We can now state and prove a result of Harrow, Mehraban, and Soleimanifar [HMS20] which gives a quasi-polynomial time classical algorithm for simulating anisotropic XXZ models. The anisotropic XXZ model has 2-local terms $-(c_{XY}(X \otimes X + Y \otimes Y) + c_Z Z \otimes Z)$ where $c_Z \geq |c_{XY}|$ and 1-local terms proportional to $-Z_i$. The inequality $c_Z \geq |c_{XY}|$ is known as the ferromagnetic condition because it ensures that the $-Z \otimes Z$ terms dominate and that the model favours alignment of the spins and hence has ground state $|0^n\rangle$ for the same reasons as the classical Ising ferromagnet. The "XXZ" part of the name refers to the fact that the $X \otimes X$ and $Y \otimes Y$ terms have the same coefficient, and the "anisotropic" part of the name indicates the presence of 1-local terms.

Theorem 4 (Classical simulation of the anisotropic XXZ model [HMS20])**.** *Let $G = (V, E)$ be a graph and consider the anisotropic XXZ model Hamiltonian*

$$H_{XXZ} = -\sum_{(i,j)\in E} (c_{XY}(X_i X_j + Y_i Y_j) + c_Z Z_i Z_j) - \frac{\mu}{2} \sum_{i \in V} (I + Z_i) \tag{1.23}$$

where the ferromagnetic condition $|c_{XY}| \leq c_Z$ is satisfied. Then the partition function

$$\mathcal{Z}(\beta, \mu) = \mathrm{Tr}(e^{-\beta H_{XXZ}(\mu)}) \tag{1.24}$$

can be estimated to ε-multiplicative error in time $n^{O(\log(n/\varepsilon))}$ on a classical computer for any $\mu > 0$ and $\beta > 0$.

Proof. By Theorem 3, the condition $|c_{XY}| \leq c_Z$, ensures that the partition function

$$\mathcal{Z}(\beta, \mu) = \mathrm{Tr}(e^{-\beta H_{XXZ}(\mu)}) \tag{1.25}$$

has zeros only when μ lies on the imaginary axis for $\beta > 0$. We can compute the partition function as a polynomial in the fugacity variable $z = e^{\beta\mu}$. In terms of z, the partition function only vanishes on the unit circle. The sum $W = \sum_{i \in V}(I + Z_i)/2$ is diagonal in the computational basis with eigenvalues which are the Hamming weight of the corresponding bitstring. Note that each local term $c_{XY}(XX + YY) + c_Z ZZ$ preserves Hamming weight and hence commutes with W so we can compute

$$\begin{aligned}
\mathcal{Z}(\beta, \mu) &= \mathrm{Tr}(e^{-\beta H_{XXZ}(\mu)}) \\
&= \mathrm{Tr}(e^{\beta \sum_{(i,j)\in E} c_{XY}(X_iX_j + Y_iY_j) + c_Z Z_iZ_j} e^{\beta\mu W}) \\
&= \sum_{x \in \{0,1\}^n} \langle x | e^{\beta \sum_{(i,j)\in E} c_{XY}(X_iX_j + Y_iY_j) + c_Z Z_iZ_j} | x \rangle e^{\mu\beta|x|} \\
&= \sum_{k=0}^{n} \mathrm{Tr}_k(e^{\beta \sum_{(i,j)\in E} c_{XY}(X_iX_j + Y_iY_j) + c_Z Z_iZ_j}) z^k.
\end{aligned} \tag{1.26}$$

Hence the partition function is a degree n polynomial in z. Since the dimension of the Hamming weight k subspace of $(\mathbb{C}^2)^{\otimes n}$ has dimension $\binom{n}{k}$, it takes time $O(n^{\log(n/\varepsilon)})$ to compute the coefficients up to Hamming weight $\log(n/\varepsilon)$ by explicit diagonalization. Then by Lemma 1, it takes time $O(n^{\log(n)/\varepsilon})$ to compute estimates of the partition function. □

In light of the fact that Theorem 4 does not cover all of the Suzuki-Fisher models, it is natural to ask whether a zero-free region in the partition function is sufficient to enable efficient approximation. A promising target in this direction is the EPR model which is related to the quantum Max Cut problem in the following sense. Consider the Hamiltonian

$$H = \sum_{\{i,j\}\in E} J_{ij}(X_iX_j + Y_iY_j + Z_iZ_j) \tag{1.27}$$

where $\{J_{ij}\}$ are arbitrary nonnegative coefficients. The problem of estimating the ground energy of this Hamiltonian has known as the "quantum Max Cut" problem. It is known that computing the ground energy to inverse polynomial precision is QMA-hard [PM15], and moreover it remains NP-hard even if we only ask for an approximation to within a certain constant factor [Pid25]. It is therefore extremely unlikely that efficient algorithms exist for the ground energy of this Hamiltonian in the worst case.

However, let us consider the special case of Eq. (1.27) where the graph G is bipartite. This restriction could in principle make the quantum Max Cut problem easier. Indeed,

whether or not the ground energy of Eq. (1.27) for bipartite G can be efficiently approximated is an open question [Gha23] that has attracted considerable attention in the last few years [Kin23, MSS24, TZ25, JN25, ALM+25a, GSS25]. To judge the quality of an algorithm, we will compute the approximation ratio which is the quotient of the algorithm's estimate by the true optimum. The incremental improvements in approximation ratio are summarized in Table 1.1. If $V = AB$ is a bipartition of G and we conjugate Eq. (1.27) by $Y_A = \bigotimes_{i\in A} Y_i$ then we get a Hamiltonian

$$H' = -\sum_{\{i,j\}\in E} J_{ij}(X_iX_j - Y_iY_j + Z_iZ_j)$$

composed of two-qubit interactions $-X\otimes X + Y\otimes Y - Z\otimes Z$ which energetically favor the EPR state $(|00\rangle + |11\rangle)/\sqrt{2}$. For that reason, this model is known as the EPR Hamiltonian [Kin23]. We will refer to the ground state energy problem of this Hamiltonian as the bipartite quantum Max Cut problem. Moreover, the coefficients of the ZZ term dominate, so H' is a Suzuki-Fisher Hamiltonian. In Section 3.1 we will study the EPR problem by investigating a Hamiltonian H_s which energetically favors deformed EPR states $|00\rangle + s|11\rangle$ for $0 \le s \le 1$. We support conjectures regarding the spectral gap of the EPR Hamiltonian and the zero-free region associated with the ground state of the EPR Hamiltonian.

Conjecture 1. *Suppose $n \ge 2$, $s \in [0,1)$, and the interaction graph is connected. Then the spectral gap between the smallest and the second smallest eigenvalues of H_s is at least $1-s^2$. This lower bound is attained on star graphs with $n \ge 3$ vertices.*

Conjecture 2. *Suppose $n \ge 2$, $s \in [0,1)$, and the interaction graph is connected. Let $|\psi\rangle$ be the ground state H_s. Then there exists $r > 1$ such that $|\psi\rangle \in LY(r)$. More ambitiously, $|\psi\rangle \in LY(s^{-1/2})$ and $|\psi\rangle \notin LY(r)$ for any $r > s^{-1/2}$.*

Here $LY(r)$ is a class of tensors to be defined in Chapter 2 with properties similar to the Hamiltonians appearing in Theorem 3.

Suzuki-Fisher Hamiltonians

What is the computational complexity of approximating the ground energy and the partition function of Suzuki-Fisher Hamiltonians? For concreteness, let us discuss the complexity landscape for the Heisenberg XXZ model. Given an interaction graph $G = (V, E)$ with $|V| = n$ and constants $d, f \in [-1, 1]$, consider the Hamiltonian

$$H = -\sum_{(i,j)\in E} w_{ij}h_{ij} \tag{1.28}$$

with nonnegative weights $0 \le w_{ij} \le \mathsf{poly}(n)$ and Heisenberg XXZ local terms

$$h = \frac{1}{2}(f(X\otimes X + Y\otimes Y) + d(I - Z\otimes Z)) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & d & f & 0 \\ 0 & f & d & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{1.29}$$

	QMC	Bip. QMC
Gharibian, Parekh [GHLS15]	0.498	-
Anshu, Gosset, Morenz [AGM20]	0.531	-
Parekh, Thompson [PT21]	0.533	-
King [Kin23]	0.582*	0.707
Lee [Lee22]	0.562	-
Lee, Parekh [LP24]	0.595	-
Joquera, Kolla, et al. [JKK+25]	0.599	0.72
Ju, Nagda [JN25]	-	0.809
Apte, Lee, Marwaha, et al. [ALM+25b]	0.611	0.809
Apte, Parekh, Sud [APS25]	0.614†	0.809†
Gribling, Sinjorgo, Sotirov [GSS25]	0.614*	0.816
Apte, Lee, Marwaha, et al. [ALM+25a]	-	0.8395

Table 1.1: Approximation ratios for (bipartite) quantum Max Cut. A star indicates that the algorithm is only efficient on triangle-free graphs. A dagger indicates that the algorithm analysis relies on a conjecture. Conjecture 1 implies that there is a fully polynomial quantum approximation scheme for bipartite quantum Max Cut.

Note that when $d = f = 1/2$, h is the projector onto $(|01\rangle + |10\rangle)/\sqrt{2}$ and the Hamiltonian is unitarily equivalent to the EPR Hamiltonian via $(SH)^{\otimes n}$ where S and H are the single-qubit unitaries[1]

$$S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, \qquad H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{1.30}$$

We consider several parameter regimes of d and f.

Suppose first that $d \leq 0$ and $|f| \leq |d|$. Then H is a Suzuki-Fisher Hamiltonian since $Z_i Z_j$ terms in H are ferromagnetic and dominating as in Theorem 3. In fact, these 2-local terms are those appearing in the anisotropic XXZ model considered by Harrow, Mehraban, and Soleimanifar [HMS20]. Hence the partition function in the presence of a uniform magnetic field $\mathrm{Tr}(e^{-\beta(H-\mu\sum_i Z_i)})$ can be estimated for any constant $\mu > 0$ in quasi-polynomial time as in Theorem 4.

Suppose now that $f \geq |d|$. Conjugating H by the Clifford gate $e^{i(\pi/4)X}$ on each qubit gives a Suzuki-Fisher Hamiltonian $H' = -\sum_{(i,j)\in E} w_{ij} h'_{ij}$ with the interactions

$$h' = \frac{1}{2}(f(X \otimes X + Z \otimes Z) + d(I - Y \otimes Y)). \tag{1.31}$$

Clearly, the ground energy and the partition function problems for H and H' are equivalent. As commented above, H' coincides with the EPR Hamiltonian if $f = d > 0$. Assuming Conjecture 1 of Section 3.1 is true, the ground energy problem for H' (and thus for H) is contained in the class BQP (for uniform edge weights $w_{ij} = 1$) since one can use the quantum adiabatic evolution algorithm implied by Conjecture 1.

[1]By abuse of notation, we sometimes we use H to denote a the single-qubit Hadamard gate instead of a Hamiltonian. We make note of this when it occurs.

Piddock and Montanaro [PM15] classify the complexity of ground state problems for a wide variety of 2-local terms using perturbative gadgets [KKR06, OT05]. For the Heisenberg XXZ model, they show that if $f < \min\{0, d\}$, then estimating the ground energy of H to within inverse polynomial additive error is QMA-hard. This implies that approximating the partition function to a given relative error is also QMA-hard. Otherwise (for any values of d, f), the Hamiltonian is sign-problem free and the corresponding ground energy problem is contained in StoqMA [BBT06]. In this case (a decision version of) the problem of approximating its partition function is in the complexity class AM [BBT06].

Bravyi and Gosset show that ferromagnetic XY models admit efficient classical simulation by quantum Monte Carlo methods yielding an efficient algorithm for $d = 0$ and $f \geq 0$ as in Theorem 2. These results are summarized in Fig. 1.1.

When $f > 0$, the partition function $\mathrm{Tr}(e^{-\beta H})$ can be approximated by the partition function of the classical six-vertex model [Pau35] on a related edge-ordered graph. Assume for simplicity that the edge weights are uniform, $w_{ij} = 1$. The Trotter-Suzuki approximation yields $J = \mathsf{poly}(n, \beta, \varepsilon^{-1})$ and $\delta > 0$ such that the $Z_J = \mathrm{Tr}(G_J \cdots G_2 G_1)$, where each $G_i = e^{\delta h_{e_i}}$, is an ε-relative error estimate for the partition function $\mathrm{Tr}(e^{-\beta H})$. Introducing a parameter $t = e^{\delta d} \sinh(\delta f)$, one gets

$$e^{\delta h} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & t + e^{\delta(d-f)} & t & 0 \\ 0 & t & t + e^{\delta(d-f)} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{1.32}$$

The Trotter circuit $G_J \cdots G_2 G_1$ is comprised entirely of gates which act non-trivially on exactly 2 qubits. In this case, the graph Γ representing the tensor network description of $\mathrm{Tr}(G_J \cdots G_2 G_1)$ is 4-regular. The six-vertex model with parameters $a, b, c \geq 0$ is defined on 4-regular graphs where each vertex has an ordering of its incident edges. On such a graph, an Eulerian orientation is an assignment of each edge to $\{0, 1\}$ (thought of as "incoming" and "outgoing" edges respectively) where each vertex has two incident edges labelled 0 and two incident edges labelled 1. The states of the six-vertex model are the Eulerian orientations of the underlying graph denoted $\mathcal{E}$. Given an Eulerian orientation τ each vertex can be assigned a type based on the direction of the incident edges as shown in Fig. 1.2. Then for each $\tau \in \mathcal{E}$ assign a weight $w(\tau) = a^{n_1} b^{n_2} c^{n_3}$ where n_i denotes the number of vertices of type i in τ. Then the partition function is

$$Z(\Gamma, a, b, c) = \sum_{\tau \in \mathcal{E}} a^{n_1} b^{n_2} c^{n_3}. \tag{1.33}$$

A bit string $x \in \{0, 1\}^{|E(\Gamma)|}$ defines an Eulerian orientation of Γ such that an edge $e \in E(\Gamma)$ is oriented forward in time if $x_e = 0$ and backward in time if $x_e = 1$. Then there is a one-to-one correspondence between the three types of nonzero matrix elements in $e^{\delta h}$ and the three

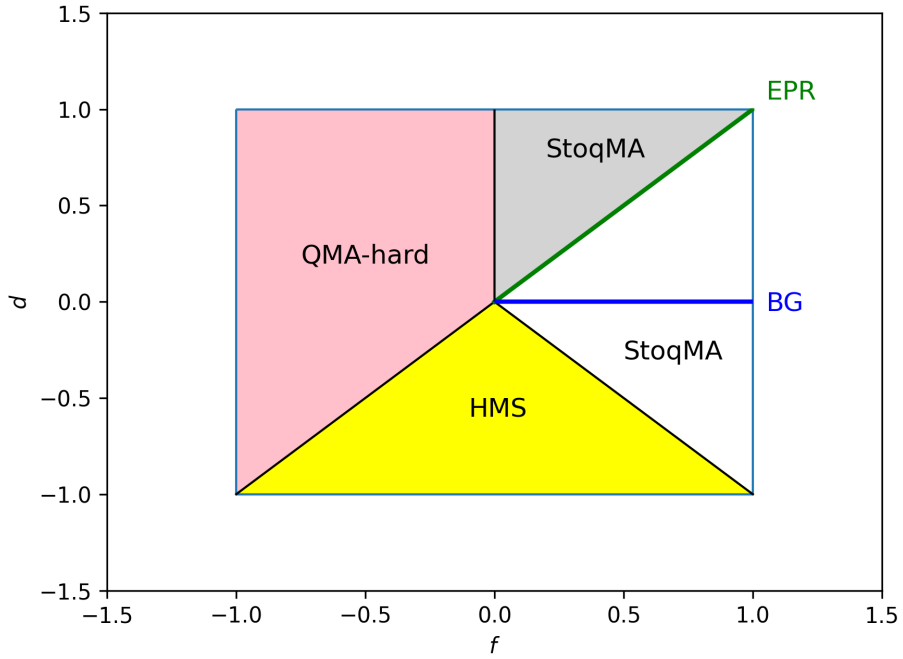


Figure 1.1: Complexity landscape for XXZ Heisenberg Hamiltonians. Ground energy problems for models in the pink region are QMA-hard, while those in the grey and white regions are contained in StoqMA [PM15]. Models in the yellow region have the trivial ground state $|0^n\rangle$ while the partition function admits a quasi-polynomial time approximation algorithm in the presence of a uniform magnetic field [HMS20]. The models on the blue line admit efficient randomized approximation [BG17]. When $f > 0$ the partition functions of these models can be approximated by the partition function of the six-vertex model. On the blue line, one obtains a six-vertex model in a parameter regime where it admits efficient approximation [CLL19]. In contrast, the grey region maps to a six-vertex model in a parameter regime where it is likely intractable to approximate [CLL19]. The white region (including the boundaries shown in black and green) maps to a six-vertex model in a parameter regime where the complexity is a mystery. However, assuming Conjecture 1 is true, the ground energy problem on the green line is in BQP in the uniformly weighted case ($w_{ij} = 1$ for all i, j in Eq. (1.28)). The green line represents EPR Hamiltonians.

vertex types of the six-vertex model. Hence we have agreement of the partition functions

$$Z_J(G_J \dots G_2 G_1) = \sum_{x \in \{0,1\}^{|E(\Gamma)|}} \prod_{u \in V(\Gamma)} \langle x_{e_1(u)} x_{e_2(u)} | G_u | x_{e_3(u)} x_{e_4(u)} \rangle \tag{1.34}$$

$$= \sum_{\tau \in \mathcal{E}} 1^{n_1} t^{n_2} (t + e^{\delta(d-f)})^{n_3} = Z(\Gamma, 1, t, t + e^{\delta(d-f)}) \tag{1.35}$$

where $e_i(u)$ is edge i incident to u as determined by the ordering on Γ. Cai, Lu, and Liu [CLL19] showed that when $a^2 \leq b^2 + c^2$, $b^2 \leq a^2 + c^2$, and $c^2 \leq a^2 + b^2$, the partition function $Z(\Gamma, a, b, c)$ can be estimated efficiently using the Markov chain Monte Carlo

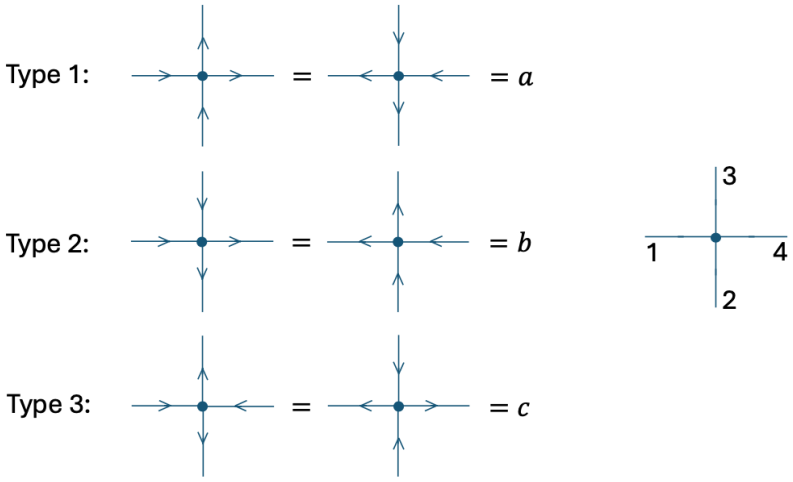


Figure 1.2: Each vertex is assigned a type $1, 2$, or 3 depending the orientation of its incident edges and a fixed ordering (shown on the right). Edges assigned 0 in the orientation are shown as arrows pointing towards the vertex while edges assigned 0 are shown as arrows pointing away from the vertex. The arrows come from the Eulerian orientation and the numbers come from the ordering of the incident edges defined along with the underlying graph.

method for any 4-regular graph Γ. They also showed that when $a > b + c$ or $b > a + c$ or $c > a + b$ the six-vertex model cannot be approximated efficiently unless $\mathsf{RP} = \mathsf{NP}$, which is believed to be extremely unlikely.

This means that when $d = 0$ and $f \geq 0$, the corresponding XXZ Heisenberg models can be simulated classically. In this case, Cai et al. recover the classical simulation of this model demonstrated by Bravyi and Gosset [BG17]. On the other hand, when $d > f > 0$, we are in a parameter regime where $c > a + b$ and the six-vertex model is likely intractable to approximate.

Outlook

The landscape shown in Fig. 1.1 suggests that the complexity of estimating the partition function varies greatly depending on the local terms of the Hamiltonian. In particular, there is a reduction in complexity for some models which satisfy a Lee-Yang condition or which are stoquastic. In Chapter 3, we study both of these special cases in greater depth, giving new algorithms which exploit either the Lee-Yang condition or the stoquastic condition. Before considering specific Hamiltonians though, we investigate applications of the Lee-Yang condition more broadly in quantum information theory in Chapter 2.

Chapter 2

Lee-Yang tensors

In this chapter, we explore the applications of Lee-Yang tensors in quantum information theory. First, we review the class of Lee-Yang tensors. Considering tensors rather than operators allows us to study pure states, density matrices, Hermitian operators, and quantum channels satisfying a Lee-Yang property all at once. We review the closure properties of this class as well as the Suzuki-Fisher theorem, which furnishes a large family of Lee-Yang tensors related to local Hamiltonians. Section 2.1 focuses on applications including closure under certain post-selective measurements and quantum channels. In Section 2.2, we prove that the extremal eigenvalue of Hermitian operators with the Lee-Yang property is simple. In Section 2.3, we show that there are quasi-polynomial sized quantum circuits for preparing Lee-Yang tensors.

Suppose $\psi \in (\mathbb{C}^2)^{\otimes n}$ is a complex tensor with binary indices and entries ψ_x labeled by n-bit strings. Consider the generating polynomial $f_\psi : \mathbb{C}^n \to \mathbb{C}$

$$f_\psi(z) = \sum_{x \in \{0,1\}^n} \psi_x z^x \tag{2.1}$$

where $z^x = \prod_{i:x_i \neq 0} z_i$. For $r > 0$, let

$$\mathbb{D}_r = \{z \in \mathbb{C} : |z| < r\}$$

denote the open zero-centered disk of radius r. If $\mathbf{r} = (r_1, \ldots, r_n) \in \mathbb{R}_+^n$ is a tuple of radii, let

$$\mathbb{D}_{\mathbf{r}} = \mathbb{D}_{r_1} \times \cdots \times \mathbb{D}_{r_n}$$

be the corresponding multi-disk in $\mathbb{C}^n$.

Definition 1 (Lee-Yang tensor)**.** *We say that $\psi \in (\mathbb{C}^2)^{\otimes n}$ is a Lee-Yang tensor with a radius $\mathbf{r} \in \mathbb{R}_+^n$ if the generating polynomial of ψ has no zeros in the open zero-centered multi-disk of radius $\mathbf{r}$, that is,*

$$f_\psi(z) \neq 0 \quad \textit{for all } z \in \mathbb{D}_{\mathbf{r}}. \tag{2.2}$$

Let $LY_n(\mathbf{r})$ be the set of all Lee-Yang tensors $\psi \in (\mathbb{C}^2)^{\otimes n}$ with the radius $\mathbf{r}$. Given a real number $r > 0$, let $LY(r)$ be the set of all Lee-Yang tensors with the radius at least r for each variable:

$$LY(r) = \bigcup_{n \geq 0} LY_n((r, r, \ldots, r)). \tag{2.3}$$

The primary tool for constructing Lee-Yang tensors is the following lemma due to Asano [Asa70], and with refinement by Ruelle [Rue10].

Lemma 2 (Tensor contraction [Asa70, Rue10])**.** *Consider any tensor $\psi \in LY_n(\mathbf{r})$ with $n \geq 2$. Let $\phi \in (\mathbb{C}^2)^{\otimes(n-2)}$ be a tensor obtained from ψ by contracting some pair of indices $i < j$ such that $r_i r_j > 1$. Then $\phi \in LY_{n-2}(\mathbf{r}')$ where $\mathbf{r}'$ is obtained from $\mathbf{r}$ by deleting the components r_i and r_j. Furthemore, if $r_i r_j = 1$ then ϕ is either identically zero or $\phi \in LY_{n-2}(\mathbf{r}')$.*

Before presenting the proof, we note that it is sometimes convenient to consider a sequence of tensors $\{\psi_j\}_{j \geq 1}$ such that $\psi_j \in LY(r)$ for each $j \geq 1$. If the sequence converges to a nonzero tensor ψ, then $\psi \in LY(r)$ as well. As we now explain, this is a simple consequence of Hurwitz's theorem (see, e.g., [COSW04]).

Theorem 5 (Hurwitz's Theorem)**.** *Suppose N is a positive integer, D is a domain in $\mathbb{C}^N$, and $\{f_k\}_{k \in \mathbb{N}}$ is a sequence of non-vanishing analytic functions on D that converges to f uniformly on compact subsets of D. Then f is either non-vanishing or identically zero on D.*

We will use the following corollary to prove Lemma 2.

Corollary 1 (Limit of Lee-Yang tensors)**.** *Let $n \geq 1$ be a positive integer and let $\mathbf{r} \in \mathbb{R}_+^n$. Consider a sequence of tensors $\psi_j \in (\mathbb{C}^2)^{\otimes n}$ for $j \geq 1$. Suppose that for each $x \in \{0,1\}^n$ we have $\langle x|\psi_j\rangle \to \langle x|\psi\rangle$ as $j \to \infty$, for some $\psi \in (\mathbb{C}^2)^{\otimes n}$. If $\psi_j \in LY_n(\mathbf{r})$ for each $j \geq 1$ and ψ is not the zero vector, then $\psi \in LY_n(\mathbf{r})$.*

Proof of Corollary 1. Let $\mathbf{r} = (r_1, r_2, \ldots, r_n)$ and let $R = \max_{1 \leq i \leq n} r_i$. Given $\epsilon > 0$ we can choose $k \in \{1, 2, \ldots\}$ such that $|\langle x|\psi_j\rangle - \langle x|\psi\rangle| \leq (2R)^{-m}\epsilon$ for all $x \in \{0,1\}^m$ and $j \geq k$. Then for $z \in \mathbb{D}_{\mathbf{r}}$ and $j \geq k$ we have

$$|f_{\psi_j}(z) - f_\psi(z)| \leq \sum_{x \in \{0,1\}^n} |\langle x|\psi_j\rangle - \langle x|\psi\rangle| \prod_{a \in \mathrm{supp}(x)} |z_a| \tag{2.4}$$

$$\leq \sum_{x \in \{0,1\}^n} (2R)^{-n} \epsilon R^n \tag{2.5}$$

$$= \epsilon, \tag{2.6}$$

which shows that our sequence of polynomials $\{f_{\psi_j}\}_j$ converges uniformly in $\mathbb{D}_{\mathbf{r}}$ and therefore also on compact subsets of it. Each f_{ψ_j} is non-vanishing on $\mathbb{D}_{\mathbf{r}}$. Since f_ψ is not identically zero on $\mathbb{D}_{\mathbf{r}}$, it follows from Hurwitz's theorem that f_ψ is non-vanishing on $\mathbb{D}_{\mathbf{r}}$, i.e., $\psi \in LY_n(\mathbf{r})$. □

We shall need the following lemma due to Asano [Asa70] and Ruelle [Rue10] to prove Lemma 2.

Lemma 3. *Let K_1 and K_2 be any closed subsets of $\mathbb{C}$ such that $0 \notin K_1 \cup K_2$. Suppose a, b, c, d are complex numbers such that $a + bz_1 + cz_2 + dz_1z_2 \neq 0$ whenever $z_1 \notin K_1$ and $z_2 \notin K_2$. Then $a + dz \neq 0$ whenever $z \notin -K_1K_2$.*

Here $-K_1K_2 = \{-z_1z_2 \,:\, z_1 \in K_1,\ z_2 \in K_2\}$. A proof of Lemma 3 can be found in [Rue10].

Proof of Lemma 2. Assume wlog that ϕ is obtained from ψ by contracting the first two indices (otherwise, permute the indices). Write $z = (z_1, z_2, z') \in \mathbb{C}^n$, where $z' \in \mathbb{C}^{n-2}$. The generating polynomials of ψ and ϕ can be written as

$$f_\psi(z) = g_{00}(z') + z_1 g_{10}(z') + z_2 g_{01}(z') + z_1 z_2 g_{11}(z') \quad \text{and} \quad f_\phi(z') = g_{00}(z') + g_{11}(z') \tag{2.7}$$

for some polynomials $g_{ab} : \mathbb{C}^{n-2} \to \mathbb{C}$.

Suppose $r_1 r_2 > 1$. Let us assume that $f_\phi \notin LY_{n-2}(\mathbf{r}')$ and show that this assumption leads to a contradiction. Indeed, if $f_\phi \notin LY_{n-2}(\mathbf{r}')$ then $f_\phi(z') = 0$ for some $z' \in \mathbb{D}_{\mathbf{r}'}$. By a slight abuse of notation, let us identify the polynomials g_{ab} and their evaluations at the point z'. Then Eq. (2.7) gives

$$g_{00} + g_{11} = 0. \tag{2.8}$$

Condition $\psi \in LY_n(\mathbf{r})$ implies $f_\psi(z) \neq 0$ for $z = (z_1, z_2, z')$ with $z_1 \in \mathbb{D}_{r_1}$, $z_2 \in \mathbb{D}_{r_2}$. From Eqs. (2.7) and (2.8) one gets

$$(1 - z_1z_2)g_{00} + z_1 g_{10} + z_2 g_{01} \neq 0 \quad \text{for all } z_1 \in \mathbb{D}_{r_1} \text{ and } z_2 \in \mathbb{D}_{r_2}. \tag{2.9}$$

Choose K_j as the complement of $\mathbb{D}_{r_j}$ with $j = 1, 2$. Since $r_j > 0$, one has $0 \notin K_1 \cup K_2$. Choose $a = g_{00}$, $b = g_{10}$, $c = g_{01}$, $d = -a$. Then Eq. (2.9) is equivalent to $a + bz_1 + cz_2 + dz_1z_2 \neq 0$ for $z_1 \notin K_1$ and $z_2 \notin K_2$. Lemma 3 then implies $a(1 - z) \neq 0$ for $z \notin -K_1K_2$. Obviously, $-K_1K_2 = K_1K_2$ is the complement of $\mathbb{D}_{r_1r_2}$. From $r_1r_2 > 1$ one gets $1 \in \mathbb{D}_{r_1r_2}$ and thus $1 \notin -K_1K_2$ arriving at a contradiction since $a(1 - z) = 0$ for $z = 1$. This proves $f_\phi \in LY_{n-2}(\mathbf{r}')$.

Suppose now that $r_1r_2 = 1$. Choose an arbitrary sequence $\{s_k\}_{k=1}^\infty$ such that each $s_k \in (0, 1)$ and $\lim_{k\to\infty} s_k = 1$. Consider a sequence of tensors

$$|\psi_k\rangle = (|0\rangle\langle 0| + s_k|1\rangle\langle 1|)^{\otimes n}|\psi\rangle.$$

It follows directly from the definitions that $\psi_k \in LY_n(\mathbf{r}/s_k)$ and $\lim_{k\to\infty} \psi_k = \psi$. Let ϕ_k be the tensor obtained from ψ_k by contracting the first two indices. Clearly, $\lim_{k\to\infty} \phi_k = \phi$. Since $(r_1/s_k)(r_2/s_k) > 1$, we can apply the first part of the lemma to get $\phi_k \in LY_{n-2}(\mathbf{r}'/s_k)$. Since $s_k \in (0, 1)$ we also have $\phi_k \in LY_{n-2}(\mathbf{r}')$ for all $k \geq 1$. From Corollary 1 we infer that either ϕ is identically zero, or $\phi \in LY_{n-2}(\mathbf{r}')$. □

Let us now review a large family of Lee-Yang tensors due to Suzuki and Fisher [SF71]. Not only does this theorem give an easy-to-check sufficient condition for membership in $LY(1)$, but it also chracterizes the Suzuki-Fisher Hamiltonians discussed in Chapter 1.

Theorem 6 (Suzuki-Fisher [SF71]). *Suppose* $\psi \in (\mathbb{C}^2)^{\otimes m}$ *satisfies*

$$X^{\otimes m}|\psi\rangle = \pm|\psi^*\rangle \tag{2.10}$$

where $|\psi^*\rangle$ *is the element-wise complex conjugate of* $|\psi\rangle$ *and*

$$|\langle 0^m|\psi\rangle| \geq \frac{1}{4}\sum_{y\in\{0,1\}^m} |\langle y|\psi\rangle|. \tag{2.11}$$

Then $\psi \in LY(1)$.

One recovers the conditions from Theorem 3 by enforcing the conditions from Theorem 6 on the local operators appearing in the Trotterization of the Gibbs state. For completeness we close this section with a proof of Theorem 6. We follow the strategy from Ref. [SF71]. We shall first establish the result in the special case where Eq. (2.11) holds with a strict inequality, i.e.

$$|\langle 0^m|\psi\rangle| > \frac{1}{4}\sum_{y\in\{0,1\}^m} |\langle y|\psi\rangle|. \tag{2.12}$$

The case where equality holds in Eq. (2.12) then follows via a continuity argument based on Hurwitz's theorem. In particular, if equality holds in Eq. (2.12) for ψ, we can choose a sequence $\{\psi_j\}_{j\geq 1}$ defined by $|\psi_j\rangle = |\psi\rangle + 2^{-j}(|0^m\rangle \pm |1^m\rangle)$. The corresponding vectors all satisfy Eqs. (2.10,2.12) and $\psi_j \to \psi$ entrywise. By Corollary 1, $\psi \in LY(1)$.

Firstly note that using the fact that $X^{\otimes m}|\psi\rangle = \pm|\psi^*\rangle$ we have

$$\sum_{y\in\{0,1\}^{m-1}, y\neq 0^m} |\langle 0y|\psi\rangle| = \sum_{y\in\{0,1\}^{m-1}, y\neq 1^m} |\langle 1y|\psi\rangle| \quad \text{and} \quad |\langle 0^m|\psi\rangle| = |\langle 1^m|\psi\rangle|.$$

Plugging into Eq. (2.12) we infer

$$|\langle 0^m|\psi\rangle| > \sum_{y\in\{0,1\}^{m-1}: y\neq 0^m} |\langle 0y|\psi\rangle|. \tag{2.13}$$

Write

$$f_\psi(s_1,\ldots,s_m) = \sum_{x\in\{0,1\}^m} \langle x|\psi\rangle s_1^{x_1}\ldots s_m^{x_m} = s_1 A_1(s_2,\ldots,s_m) + A_0(s_2,\ldots,s_m). \tag{2.14}$$

We first show that

$$A_0(s_2,\ldots,s_m) \neq 0 \quad \text{whenever} \quad |s_2|,|s_3|,\ldots,|s_m| \leq 1. \tag{2.15}$$

To see this note that

$$|A_0(s_2,\ldots,s_m)| = \Big|\sum_{x\in\{0,1\}^{m-1}} \langle 0x|\psi\rangle s_2^{x_2}s_3^{x_3}\ldots s_m^{x_m}\Big| \tag{2.16}$$

$$\geq |\langle 0^m|\psi\rangle| - \sum_{y\in\{0,1\}^{m-1}, y\neq 0^m} |\langle 0y|\psi\rangle| \tag{2.17}$$

$$> 0 \tag{2.18}$$

where in the first inequality we used the fact that $|s_j| \leq 1$ for $j \in \{2, 3, \ldots, m\}$ and in the second inequality we used Eq. (2.13).

Now suppose that $(t_1, t_2, \ldots, t_m)$ is a root of f_ψ and that

$$|t_j| < 1 \quad j \in \{2, 3, \ldots, m\} \tag{2.19}$$

To complete the proof of the theorem it suffices to show that $|t_1| \geq 1$. Firstly, note that

$$A_1(t_2, t_3, \ldots, t_m) \neq 0. \tag{2.20}$$

To see this, note that otherwise we would have $f_\psi(t_1, t_2, \ldots, t_m) = 0 = A_0(t_2, \ldots, t_m)$ which contradicts Eq. (2.15). Using Eqs. (2.14,2.20) and the fact that $f_\psi(t_1, t_2, \ldots, t_m) = 0$ gives

$$|t_1| = \left| \frac{A_0(t_2, t_3, \ldots, t_m)}{A_1(t_2, t_3, \ldots, t_m)} \right| \geq \left(\max_{|s_2|, |s_3|, \ldots, |s_m| \leq 1} \left| \frac{A_1(s_2, s_3, \ldots, s_m)}{A_0(s_2, s_3, \ldots, s_m)} \right| \right)^{-1} = 1,$$

where the last inequality follows from the lemma below.

Lemma 4.

$$\max_{|s_2|, |s_3|, \ldots, |s_m| \leq 1} \left| \frac{A_1(s_2, s_3, \ldots, s_m)}{A_0(s_2, s_3, \ldots, s_m)} \right| = 1 \tag{2.21}$$

Proof. Suppose that $(r_2, r_3, \ldots, r_m)$ maximizes the LHS of Eq. (2.21) and such that $|r_j| < 1$ for some j. In this case one can choose $w_j \in \mathbb{C}$ such that $|w_j| = 1$ and such that the tuple

$$(r_2, \ldots, r_{j-1}, w_j, r_{j+1}, \ldots, r_m)$$

maximizes the LHS of Eq. (2.21). This follows by using the maximum modulus principle from complex analysis, on the univariate function

$$F(w_j) = \frac{A_1(r_2, \ldots, r_{j-1}, w_j, r_{j+1}, \ldots, r_m)}{A_0(r_2, \ldots, r_{j-1}, w_j, r_{j+1}, \ldots, r_m)}$$

from which we infer that the maximum of $|F(w_j)|$ over the unit circle is achieved on its boundary. Applying this fact recursively shows that the maximum is achieved by a vector with all coordinates on the unit circle:

$$\max_{|s_2|, |s_3|, \ldots, |s_m| \leq 1} \left| \frac{A_1(s_2, s_3, \ldots, s_m)}{A_0(s_2, s_3, \ldots, s_m)} \right| = \max_{|s_2|, |s_3|, \ldots, |s_m| = 1} \left| \frac{A_1(s_2, s_3, \ldots, s_m)}{A_0(s_2, s_3, \ldots, s_m)} \right|.$$

Finally, using the symmetry $X^{\otimes m}|\psi\rangle = \pm|\psi^*\rangle$ and Eq. (2.14) we see that

$$\left(\prod_{j=1}^{m} s_j \right) f_{\psi^*}(1/s_1, \ldots, 1/s_m) = \pm f_\psi(s_1, \ldots, s_m)$$

and therefore

$$\left(\prod_{j=2}^{m} s_j \right) (A_1(s_2, \ldots, s_m))^* = \pm A_0(s_2, \ldots, s_m) \qquad \text{whenever} \quad |s_2| = |s_3| = \ldots = |s_m| = 1.$$

This gives

$$\max_{|s_2|, |s_3|, \ldots, |s_m| = 1} \left| \frac{A_1(s_2, s_3, \ldots, s_m)}{A_0(s_2, s_3, \ldots, s_m)} \right| = \max_{|s_2|, |s_3|, \ldots, |s_m| = 1} \left| \pm \frac{(A_0(s_2, s_3, \ldots, s_m))^*}{A_0(s_2, s_3, \ldots, s_m)} \right| = 1.$$

□

2.1 Applications in quantum information

In this section, we establish the use of Lee-Yang tensors in quantum information theory by characterizing $LY(1)$ for few qubits, by proving that $LY(r)$ is closed under post-selection in any equatorial basis, and by providing single-qubit channels which preserve $LY(1)$.

We begin by characterizing the one and two-qubit states in $LY(r)$. Evidently, a single-qubit state $|\psi\rangle = \psi_0|0\rangle + \psi_1|1\rangle$ is contained in $LY(1)$ iff $|\psi_0| \geq |\psi_1|$. The following lemma gives an analogous condition for containment in $LY(1)$ for two-qubit states.

Lemma 5. *A two-qubit state ψ is contained in $LY(1)$ if and only if*

$$|\psi_{10}\psi_{00}^* - \psi_{11}\psi_{01}^*| + |\psi_{11}\psi_{00} - \psi_{10}\psi_{01}| \leq |\psi_{00}|^2 - |\psi_{01}|^2. \tag{2.22}$$

Proof. Let $a = \psi_{11}$, $b = \psi_{10}$, $c = \psi_{01}$, and $d = \psi_{00}$. The generating polynomial of ψ is $f_\psi(z) = cz_2 + d + z_1(az_2 + b)$. Hence $f_\psi(z) \neq 0$ for $z_1, z_2 \in \mathbb{D}_1$ iff $|cz_2 + d| > |az_2 + b|$ for $z_2 \in \mathbb{D}_1$. This is equivalent to $M(\mathbb{D}_1) \subseteq \mathbb{D}_1$ for a Möbius map.

$$M(v) = \frac{av + b}{cv + d}$$

Theorem 1 in [Mar06] asserts that $M(\mathbb{D}_1) \subseteq \mathbb{D}_1$ iff $|b\bar{d} - a\bar{c}| + |ad - bc| \leq |d|^2 - |c|^2$, which is equivalent to Eq. (2.22). □

A striking corollary of Lemma 2 is that the set of multi-qubit states contained in $LY(r)$ is closed under a class of post-selective measurements that includes measurements in the Pauli X or Y basis, provided that $r \geq 1$. To describe this formally, suppose $|\theta\rangle$ is a single-qubit normalized state and let n be the total number of qubits. A post-selective measurement of the i-th qubit is an operator $M_\theta : (\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes(n-1)}$ that applies the projector $|\theta\rangle\langle\theta|$ to the i-th qubit and then discards the i-th qubit. The measurement is called equatorial if

$$|\theta\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\theta}|1\rangle) \tag{2.23}$$

for some angle $\theta \in [0, 2\pi)$. For example, measurements in the Pauli X or Y basis are equatorial.

Lemma 6 (Equatorial post-selection)**.** *Suppose $r \geq 1$ and $|\psi\rangle \in LY(r)$ is an n-qubit state. For any post-selective equatorial measurement M_θ one has $M_\theta|\psi\rangle \in LY(r)$ or $M_\theta|\psi\rangle = 0$.*

Proof. Let $|\theta^*\rangle$ be the complex conjugate of $|\theta\rangle$. The generating polynomial of $|\theta^*\rangle$ is $(1 + e^{-i\theta}z)/\sqrt{2} \neq 0$ for $|z| < 1$. Hence $|\theta^*\rangle \in LY(1)$. Suppose $\psi \in LY_n((r, r, \ldots, r))$ and we measure the i-th qubit of ψ. We have

$$|\psi\rangle \otimes |\theta^*\rangle \in LY_{n+1}((r, r, \ldots, r, 1)).$$

By definition, $M_\theta|\psi\rangle$ is obtained from the tensor $|\psi\rangle \otimes |\theta^*\rangle$ by contracting the i-th and the last index. Lemma 2 then implies that either $M_\theta|\psi\rangle = 0$ or $M_\theta|\psi\rangle \in LY_{n-1}((r, r, \ldots, r))$. The case $M_\theta|\psi\rangle = 0$ can only occur if $r = 1$. Hence M_θ maps $LY(r)$ to $LY(r) \cup \{0\}$. □

Finally, we can use Theorem 6 to construct single-qubit quantum channels that preserve the $LY(1)$. Let us first review some basic facts about quantum channels (see, e.g., [Wat18]). Recall that if $\mathcal{E}$ is a 1-qubit quantum channel, its Choi matrix is a 4×4 complex matrix defined by

$$C(\mathcal{E}) \equiv (\mathcal{E} \otimes I)|\beta\rangle\langle\beta| \qquad |\beta\rangle = |00\rangle + |11\rangle.$$

Moreover, a 4×4 complex matrix is the Choi matrix of a single-qubit quantum channel iff it satisfies

$$C(\mathcal{E}) \geq 0 \quad \text{and} \quad \mathrm{Tr}_1(C(\mathcal{E})) = I.$$

Let us say that a channel $\mathcal{E}$ is in $LY(r)$ iff its Choi matrix satisfies $C(\mathcal{E}) \in LY(r)$. Note that the output of a quantum channel $\mathcal{E}$ on input state ρ can be computed by contracting $C(\mathcal{E})$ with ρ. In particular, suppose ρ is an n-qubit state and $\mathcal{E}$ is a 1-qubit channel. Let $C'(\mathcal{E})$ be the partial transpose of $C(\mathcal{E})$ on the first qubit. Then

$$\mathrm{Tr}_2((C'(\mathcal{E}) \otimes I_{n-1})(I_1 \otimes \rho)) = (\mathcal{E} \otimes I_{n-1})(\rho)$$

Note that $C'(\mathcal{E}) \in LY(1)$ iff $C(\mathcal{E}) \in LY(1)$. From this and Lemma 2 we infer that $\mathcal{E} \in LY(1)$ and $\rho \in LY(1)$ imply that the output state $(\mathcal{E} \otimes I_{n-1})(\rho) \in LY(1)$.

Consider a single-qubit Pauli channel

$$\mathcal{E}_{\vec{p}}(\rho) = p_0\rho + p_1 X\rho X + p_2 Y\rho Y + p_3 Z\rho Z.$$

Here $\vec{p}$ is a probability distribution over $\{0, 1, 2, 3\}$.

Theorem 7. *The set of multi-qubit density matrices contained in $LY(1)$ is closed under single-qubit Pauli channels $\mathcal{E}_{\vec{p}}$ for all $\vec{p}$ satisfying $\min\{p_0, p_3\} \geq \max\{p_1, p_2\}$.*

Proof. The Choi matrix is

$$C(\mathcal{E}_{\vec{p}}) = \begin{pmatrix} p_0 + p_3 & 0 & 0 & p_0 - p_3 \\ 0 & p_1 + p_2 & p_1 - p_2 & 0 \\ 0 & p_1 - p_2 & p_1 + p_2 & 0 \\ p_0 - p_3 & 0 & 0 & p_0 + p_3 \end{pmatrix}$$

It suffices to show that $C(\mathcal{E}_{\vec{p}}) \in LY(1)$. To this end we can vectorize the Choi matrix (i.e., view it as a vector in $\mathbb{C}^{16}$) and verify Eqs. (2.10,2.11) from Theorem 6. Eq. (2.10) is equivalent to $(X \otimes X)C(\mathcal{E}_{\vec{p}})X \otimes X = \pm C(\mathcal{E}_{\vec{p}})^*$, which is satisfied with the + sign.

Eq. (2.11) gives

$$p_0 + p_3 \geq \frac{1}{2}\left(p_0 + p_1 + p_2 + p_3 + |p_0 - p_3| + |p_1 - p_2|\right).$$

Rearranging the above we get

$$\left(p_0 + p_3 - |p_0 - p_3|\right) \geq \left(p_1 + p_2 + |p_1 - p_2|\right),$$

or equivalently $\min\{p_0, p_3\} \geq \max\{p_1, p_2\}$. □

For example, the depolarizing channel with parameter $\lambda \in [0,1]$ corresponds to the case

$$p_0 = (1 - 3\lambda/4) \quad p_1 = p_2 = p_3 = \lambda/4,$$

and we see that it is in $LY(1)$ for all λ. Similarly, the dephasing channel with parameter $q \in [0,1]$ corresponds to the choice $p_1 = p_2 = 0$, $p_0 = 1 - q$, $p_3 = q$, which again is in $LY(1)$ for all q.

2.2 Lee-Yang Hermitian operators

Next let us consider Hermitian operators contained in $LY(1)$. For example, one can easily check that the identity I, Pauli Z operator, SWAP gate, and an operator $|0^n\rangle\langle 0^n| - |x\rangle\langle x|$ with any nonzero $x \in \{0,1\}^n$ are contained in $LY(1)$. The same holds for any tensor product of such operators since $LY(1)$ is closed under tensor products.

The following lemma can be viewed as a generalization of the Griffiths inequality [Gri67] asserting that the expected value of any Z-type Pauli observable on the Gibbs state of the ferromagnetic Ising model is non-negative.

Lemma 7 (Griffiths inequality)**.** *Suppose $P \in LY(1)$ is a Hermitian n-qubit operator such that $\langle 0^n|P|0^n\rangle > 0$. Then for any n-qubit density matrix $\rho \in LY(1)$ one has $\mathrm{Tr}(\rho P) \geq 0$.*

Proof. Let $D_s = |0\rangle\langle 0| + s|1\rangle\langle 1|$. Consider a family of matrices

$$\rho_s = D_s^{\otimes n} \rho D_s^{\otimes n}, \qquad 0 \leq s \leq 1.$$

From $\rho \in LY(1)$ one gets $\rho_s \in LY(1/s)$. Applying Lemma 2 to perform the contraction $P \otimes \rho_s \to \mathrm{Tr}(\rho_s P)$ one concludes that

$$\mathrm{Tr}(\rho_s P) \neq 0 \quad \text{for all } s \in [0,1). \tag{2.24}$$

We have $\langle 0^n|\rho|0^n\rangle > 0$ since $\langle 0^n|\rho|0^n\rangle \geq 0$ and $\langle 0^n|\rho|0^n\rangle \neq 0$ due to the inclusion $\rho \in LY(1)$. By assumption, $\langle 0^n|P|0^n\rangle > 0$. Thus

$$\mathrm{Tr}(\rho_0 P) = \langle 0^n|\rho|0^n\rangle\langle 0^n|P|0^n\rangle > 0. \tag{2.25}$$

From Eqs. (2.24) and (2.25) and continuity of the function $s \to \mathrm{Tr}(\rho_s P)$ one gets $\mathrm{Tr}(\rho P) = \mathrm{Tr}(\rho_1 P) \geq 0$. □

Let us now describe a large family of Hermitian operators in $LY(1)$.

Lemma 8. *Let $|z\rangle = \bigotimes_{a=1}^n (|0\rangle + z_a^*|1\rangle)$ and define an n-qubit Hermitian operator*

$$P = |z\rangle\langle z| - X^{\otimes n}|z^*\rangle\langle z^*|X^{\otimes n}.$$

Then $P \in LY(1)$ whenever $z \in \mathbb{D}_1^n$.

Proof. Consider any complex vectors $u, v \in \mathbb{D}_1^n$. Since $\langle u|P|v\rangle = f_P(v^*, u)$, it suffices to prove that $\langle u|P|v\rangle \neq 0$ to ensure that $P \in LY(1)$. We have

$$\begin{aligned}\langle u|P|v\rangle &= \prod_{a=1}^{n}(1+u_a z_a^*)(1+v_a^* z_a) - \prod_{a=1}^{n}(u_a+z_a)(v_a^*+z_a^*) \\ &= \prod_{a=1}^{n}(1+u_a z_a^*)(1+v_a^* z_a)\left(1 - \prod_{a=1}^{n}\frac{(u_a+z_a)(v_a^*+z_a^*)}{(1+u_a z_a^*)(1+v_a^* z_a)}\right). \end{aligned} \tag{2.26}$$

We claim that

$$\left|\frac{(u_a+z_a)(v_a^*+z_a^*)}{(1+u_a z_a^*)(1+v_a^* z_a)}\right| < 1 \tag{2.27}$$

for all a. Indeed, we have

$$|1+u_a z_a^*|^2 - |u_a+z_a|^2 = 1+|u_a|^2|z_a|^2+2\mathfrak{Re}(u_a z_a^*) - |u_a|^2 - |z_a|^2 - 2\mathfrak{Re}(u_a z_a^*) = (1-|z_a|^2)(1-|u_a|^2) > 0.$$

Thus

$$\left|\frac{u_a+z_a}{1+u_a z_a^*}\right| < 1.$$

The same argument shows that

$$\left|\frac{v_a^*+z_a^*}{1+v_a^* z_a}\right| < 1$$

which proves Eq. (2.27). Substituting Eq. (2.27) into Eq. (2.26) shows that $\langle u|P|v\rangle \neq 0$ for all $u, v \in \mathbb{D}_1^n$, that is, $P \in LY(1)$. □

Next we show that *real-valued* tensors contained in $LY(r)$ for some $r > 1$ are sign-problem-free in the sense that all their entries must have the same sign, up to a simple basis change.

Lemma 9. *Suppose P is an n-qubit operator with real matrix elements in the standard basis. Suppose $P \in LY(r)$ for some $r > 1$ and $\langle 0^n|P|0^n\rangle > 0$. Then P has strictly positive matrix elements in the Pauli X basis.*

Proof. Let H be the Hadamard gate. One can easily check that $H|0\rangle \in LY(1)$ and $H|1\rangle \in LY(1)$. Hence $H^{\otimes n}|x\rangle \in LY(1)$ for all $x \in \{0,1\}^n$. Applying Lemma 2 to perform the contraction

$$P \otimes H^{\otimes n}|x\rangle \to PH^{\otimes n}|x\rangle$$

and using $r > 1$ gives $PH^{\otimes n}|x\rangle \in LY(r)$. Choose any $y \in \{0,1\}^n$. Applying Lemma 2 again to perform the contraction

$$\langle y|H^{\otimes n} \otimes PH^{\otimes n}|x\rangle \to \langle y|H^{\otimes n}PH^{\otimes n}|x\rangle$$

and using $r > 1$ and $H^{\otimes n}|y\rangle \in LY(1)$ gives

$$\langle y|H^{\otimes n}PH^{\otimes n}|x\rangle \neq 0 \tag{2.28}$$

for all $x, y \in \{0,1\}^n$. Accordingly, it suffices to consider two cases.

Case 1: All matrix elements $\langle y|H^{\otimes n}PH^{\otimes n}|x\rangle$ are strictly positive. Then we are done.

Case 2: At least one matrix element $\langle y|H^{\otimes n}PH^{\otimes n}|x\rangle$ is negative. Consider a function

$$g(s) = \langle y|H^{\otimes n}D_s^{\otimes n}PD_s^{\otimes n}H^{\otimes n}|x\rangle, \qquad D_s = |0\rangle\langle 0| + s|1\rangle\langle 1|$$

with $s \in [0,1]$. From $P \in LY(r)$ one gets $D_s^{\otimes n}PD_s^{\otimes n} \in LY(r/s)$. Hence the same argument as above shows that $g(s) \neq 0$ for all $s \in [0,1]$. Since $g(1) < 0$, continuity argument gives $g(0) < 0$. However, $g(0) = 2^{-n}\langle 0^n|P|0^n\rangle > 0$ which is a contradiction. □

We note that the proof of Lemma 9 can be also applied to operators P that map m qubits to n qubits with $m \neq n$. Choosing $m = 0$ shows that any n-qubit state vector $\psi \in LY(r)$ with $r > 1$, real amplitudes in the standard basis, and $\langle 0^n|\psi\rangle > 0$ must have positive amplitudes in the Pauli-X basis. If the operator P of Lemma 9 is Hermitian, the Perron-Frobenius theorem implies that the maximum eigenvalue of P is simple (has multiplicity one). We now show that any complex-valued Hermitian operator contained in $LY(r)$ for some $r > 1$ must have a simple dominant eigenvalue.

Theorem 8. *Suppose $r > 1$ and $H \in LY(r)$ is an n-qubit Hermitian operator. Then the eigenvalue of H with largest magnitude has multiplicity 1.*

Proof. Suppose $r > 1$ and $H \in LY(r)$ is an n-qubit Hermitian operator. Suppose the eigenvalue of H with largest magnitude has multiplicity $d \in \{1, 2, \ldots\}$. Consider $P \equiv H^2$. P is positive semidefinite and its maximal eigenvalue has multiplicity that is at least d. Moreover, $P \in LY(r)$ using Lemma 2 and the fact that $H \in LY(r)$. To complete the proof, in the following we show that the multiplicity of the largest eigenvalue of P cannot be larger than 1.

Let λ be the maximum eigenvalue of P. From $P \in LY(r)$ one gets $P \neq 0$ and $\lambda > 0$. Define

$$\Pi_m = (P/\lambda)^m \quad \text{and} \quad \Pi = \lim_{m\to\infty} \Pi_m. \tag{2.29}$$

Clearly, Π is a projector and the rank of Π coincides with the multiplicity of λ. Thus we need to show that Π cannot have rank greater than 1. First we claim that

$$\Pi \in LY(r). \tag{2.30}$$

Indeed, Π is the limit of a sequence of tensors $(P/\lambda)^m$ for integers $m \geq 1$. By Lemma 2, each tensor in this sequence is in $LY(r)$. By Corollary 1 and the fact that $\Pi \neq 0$, we get Eq. (2.30).

Lemma 10. *Suppose $r > 1$. There is no n-qubit projector $\Pi \in LY(r)$ with rank ≥ 2.*

Proof. Suppose to reach a contradiction that $\Pi \in LY(r)$ has rank $k \geq 2$. Write

$$\Pi = \sum_{j=1}^{k} |\psi_j\rangle\langle\psi_j|. \tag{2.31}$$

where $\langle\psi_i|\psi_j\rangle = \delta_{ij}$. The set of normalized vectors in the image of Π can be identified with the set of unit vectors in $\mathbb{C}^k$ which we denote

$$S = \{u \in \mathbb{C}^k : \|u\| = 1\}.$$

Define a set

$$T = \{u \in S : \sum_{j=1}^{k} u_j|\psi_j\rangle \in LY(r)\}.$$

Below we show that the set T has the following properties:

1. T is compact.
2. T does not contain two orthogonal vectors.
3. For any vector $v \in S \setminus T$, there is a vector $w \in T$ such that $\langle v|w\rangle = 0$.

Clearly T is a bounded set, so to show it is compact it suffices to show that it is closed. This latter property follows from Corollary 1, which shows that a limit of $LY(r)$ tensors is either the zero tensor or it is in $LY(r)$ (since no sequence of points in S has the zero vector as a limit). To show property 2., suppose to reach a contradiction that $v, w \in T$ satisfy $\langle v|w\rangle = 0$. Then letting

$$|\tilde{v}\rangle = \sum_{j=1}^{k} v_j|\psi_j\rangle \qquad \text{and} \qquad |\tilde{w}\rangle = \sum_{j=1}^{k} w_j|\psi_j\rangle,$$

we have $\langle\tilde{v}|\tilde{w}\rangle = 0$. But $|\tilde{v}\rangle, |\tilde{w}\rangle \in LY(r)$ with $r > 1$ (since $v, w \in T$) and so their inner product is the contraction of two $LY(r)$ tensors which cannot be zero by Lemma 2.

Finally, let us show property 3. To this end, suppose $v \in S \setminus T$. Without loss of generality let us suppose $v = (1, 0, 0, \ldots, 0)$ (if it is not we can simply redefine our choice of orthonormal basis $\psi_1, \psi_2, \ldots, \psi_k$ in Eq. (2.31). Then $|\psi_1\rangle \notin LY(r)$, so there exists $\vec{z} \in \mathbb{D}_r^n$ such that $\langle\vec{z}|\psi_1\rangle = 0$. But then $\Pi|\vec{z}^\star\rangle \in LY(r)$, where

$$\Pi|\vec{z}^\star\rangle = \sum_{j=2}^{k} |\psi_j\rangle\langle\psi_j|\vec{z}^\star\rangle.$$

Letting

$$w = \frac{1}{\sqrt{\sum_{j=2}^{k} |\langle\psi_j|\vec{z}^\star\rangle|^2}}(0, \langle\psi_2|\vec{z}^\star\rangle, \langle\psi_3|\vec{z}^\star\rangle, \ldots, \langle\psi_k|\vec{z}^\star\rangle)$$

we see that $w \in T$ and $\langle v|w\rangle = 0$. We have thus established properties 1-3. above.

To complete the proof of the theorem, we show that there is no set $T \subseteq S$ satisfying properties 1-3. Indeed, suppose to reach a contradiction that T is such a set. From property 3 we infer that T cannot be empty. Let $f : T \times T \to [0, \pi/2]$ be the function

$$f(u, v) = \arccos(|\langle u|v\rangle|)$$

This function defines a distance on the unit sphere and in particular it satisfies the triangle inequality (see, e.g., eq. (9.86) from Ref. [NC10]):

$$f(u,v) \leq f(v,w) + f(w,u) \qquad u,v,w \in S. \tag{2.32}$$

The function f is also continuous and it therefore achieves its maximum value in the compact set $T \times T$. This maximum value $\alpha \equiv \max_{u,v\in T} f(u,v)$ satisfies $\alpha \in [0,\pi/2)$ by property 2.

Now let $x \in T$ be an arbitrary vector and let $y \in S$ be any vector such that $\langle y|x\rangle = 0$. Define

$$r(\theta) = \cos(\theta)|x\rangle + \sin(\theta)|y\rangle \qquad \theta \in [0,\pi/2].$$

Note that $r(0) = x \in T$ and $r(\pi/2) = y \notin T$. Since T is a compact set and r is a continuous function, the image $I \equiv r([0,\pi/2]) \cap T$ is also a compact set. Consider the function $g : I \to [0,\pi/2]$ defined by $g(r(\theta)) = \theta$. Since g is continuous and I is compact, this function achieves its maximum value in I, which is strictly less than $\pi/2$ since $r(\pi/2) \notin T$. Therefore there is some point $\theta_0 \in [0,\pi/2)$ such that

$$r(\theta_0) \in T \qquad \text{and} \qquad r(\phi) \notin T \quad \phi \in (\theta_0, \pi/2]. \tag{2.33}$$

Define a set

$$W(\theta) = \{v \in S : \langle v|r(\theta)\rangle = 0\} \quad \theta \in [0,\pi/2].$$

Now consider the value $\beta = \theta_0 + \epsilon$ for some $\epsilon \in (0, \pi/2 - \theta_0]$ to be chosen later. From Eq. (2.33) we have

$$r(\beta) \in S \setminus T \tag{2.34}$$

Moreover, by the triangle inequality Eq. (2.32)

$$\min_{u\in W(\beta)} f(u, r(\theta_0)) \geq \min_{u\in W(\beta)} \left(f(u, r(\beta)) - f(r(\beta), r(\theta_0))\right) \tag{2.35}$$

$$= \pi/2 - \epsilon. \tag{2.36}$$

Let us now choose ϵ to be a small positive constant such that $\pi/2 - \epsilon > \alpha$. With this choice we have

$$\min_{u\in W(\beta)} f(u, r(\theta_0)) > \alpha = \max_{c,d\in T} f(c,d).$$

Since $r(\theta_0) \in T$ we infer that

$$W(\beta) \cap T = \emptyset. \tag{2.37}$$

Now Eqs. (2.34,2.37) states that all vectors in S that are orthogonal to $r(\beta) \in S \setminus T$ are not in T. This contradicts property 3, completing the proof. □

□

Note that the proof of Theorem 8 also shows that the eigenvector corresponding to the eigenvalue with largest magnitude of H has Lee-Yang radius r by contracting the input indices of the rank 1 projector Π defined in Eq. (2.29).

2.3 Circuits for Lee-Yang tensors

In this section we show that any n-qubit quantum state which is a Lee-Yang tensor with radius $r > 1$ is (quasi)-efficiently describable in the sense that (a) there exists a quasi-polynomial-sized classical circuit that, given any $y \in \{0,1\}^n$, approximates the corresponding X-basis amplitude $\langle y|H^{\otimes n}|\psi\rangle$ of the state to a given relative error, and (b) there exists a quasi-polynomial-sized quantum circuit that approximately prepares the state, to within a given trace distance. An important caveat is that the classical and quantum circuits depend on the state ψ. We also assume that $r > 1$ is a fixed constant independent of n.

The following lemma uses Barvinok's polynomial interpolation to prove that the Lee-Yang radius is robust against small perturbations of a tensor. As a consequence, amplitudes of the target state $\psi \in LY(r)$ to be prepared by a quantum circuit only need to be specified with $\mathsf{poly}(n)$ bits of precision.

Lemma 11. *Suppose $r > 1$ and let $\rho = (1+r)/2$. Let $\psi \in LY(r)$ be a normalized n-qubit state and ϕ be an arbitrary n-qubit state such that*

$$\|\psi - \phi\| \leq 2^{-n/2}(1+\rho^2)^{-n/2} \exp\left[-n\frac{(r+1)}{(r-1)}\right]. \tag{2.38}$$

Then $\phi \in LY(\rho)$.

Proof. Let $\epsilon \equiv \|\psi - \phi\|$. Pick any $z \in \mathbb{C}^n$ such that $|z_j| \leq \rho$ for all j. The triangle inequality and Cauchy–Schwarz give

$$|f_\phi(z) - f_\psi(z)| \leq \sum_{x\in\{0,1\}^n} |\phi_x - \psi_x|\rho^{|x|} \leq \epsilon(1+\rho^2)^{n/2}. \tag{2.39}$$

Thus

$$|f_\phi(z)| \geq |f_\psi(z)| - \epsilon(1+\rho^2)^{n/2} \geq \delta - \epsilon(1+\rho^2)^{n/2}, \tag{2.40}$$

where

$$\delta = \min_{|z_1|,\ldots,|z_n|\leq\rho} |f_\psi(z)|. \tag{2.41}$$

Let us derive a lower bound on δ. Let z be any point such that the minimum in Eq. (2.41) is attained at z. Consider a univariate polynomial $g(t) = f_\psi(tz)$, where $t \in \mathbb{C}$. Clearly, $g(t)$ has degree at most n and $g(t)$ has no zeros if $|t| < R \equiv r/\rho$. Applying the polynomial interpolation lemma (Lemma 1) with the order $p = 0$ one gets

$$|\log g(1) - \log g(0)| \leq \frac{n}{R-1}. \tag{2.42}$$

Taking the real part gives

$$|\mathfrak{Re}(\log g(1)) - \mathfrak{Re}(\log g(0))| \leq \frac{n}{R-1}. \tag{2.43}$$

For any non-zero complex number c one has $\mathrm{Re}(\log c) = \log|c|$. Since $|g(1)| = |f_\psi(z)| = \delta$ and $|g(0)| = |f_\psi(0)| = |\langle 0^n|\psi\rangle|$, one gets

$$|\log\delta - \log|\langle 0^n|\psi\rangle|\,| \le \frac{n}{R-1}. \tag{2.44}$$

Thus $\log\delta \ge \log|\langle 0^n|\psi\rangle| - n/(R-1)$. Exponentiating this inequality gives

$$\delta \ge |\langle 0^n|\psi\rangle| \exp\left[-\frac{n}{R-1}\right]. \tag{2.45}$$

Griffiths inequality (Lemma 7) with the observable $P = |0^n\rangle\langle 0^n| - |x\rangle\langle x| \in LY(1)$ gives $|\langle 0^n|\psi\rangle| \ge |\langle x|\psi\rangle|$ for all $x \in \{0,1\}^n$. Since ψ is normalized, this implies $|\langle 0^n|\psi\rangle| \ge 2^{-n/2}$, that is,

$$\delta \ge 2^{-n/2} \exp\left[-\frac{n}{R-1}\right]. \tag{2.46}$$

Substituting this into Eq. (2.40) gives

$$|f_\phi(z)| \ge 2^{-n/2} \exp\left[-\frac{n}{R-1}\right] - \epsilon(1+\rho^2)^{n/2}. \tag{2.47}$$

Thus $f_\phi(z) \ne 0$ if $|z_j| \le \rho$ for all j provided that

$$\epsilon < 2^{-n/2}(1+\rho^2)^{-n/2} \exp\left[-\frac{n}{(r/\rho)-1}\right]. \tag{2.48}$$

This is equivalent to the statement of the lemma if one substitutes $\rho = (1+r)/2$. □

For simplicity, below we assume that amplitudes of the target state $\psi \in LY(r)$ to be prepared by a quantum circuit are specified exactly. However, if amplitudes of ψ are only specified with $\mathsf{poly}(n)$ bits of precision, one can apply Lemma 11 to replace ψ with the approximating state at the cost of reducing the Lee-Yang radius from r to $r' = (r+1)/2$. Clearly, $r' > 1$ whenever $r > 1$.

The following theorem shows that X-basis amplitudes of states in $LY(r)$ with $r > 1$ can be computed in quasi-polynomial time. We note that the classical circuit described below depends only on the entries $\langle x|\psi\rangle$ with Hamming weight $|x| = O(\log(n/\varepsilon))$.

Theorem 9 (Classical estimation of amplitudes)**.** *Let $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ be in $LY(r)$ for $r > 1$ and $\varepsilon > 0$. There is a classical circuit of size $n^{O(\log(n/\varepsilon))}$ which takes as input $y \in \{0,1\}^n$ and outputs an ε-relative error estimate of the corresponding X-basis amplitude*

$$\langle y|H^{\otimes n}|\psi\rangle.$$

Proof. For any $y \in \{0,1\}^n$, consider the degree-n univariate polynomial

$$F_y(z) = \big(\bigotimes_{i=1}^{n} \frac{1}{\sqrt{2}}(\langle 0| + z(-1)^{y_i}\langle 1|)\big)|\psi\rangle \tag{2.49}$$

Then $F_y(z) \neq 0$ when $|z| < r$, by Lemma 2. The coefficients of F_y are

$$F_y(z) = \sum_{j=0}^{n} c_{y,j} z^j \qquad c_{y,j} = \frac{1}{\sqrt{2^n}} \sum_{\substack{x\in\{0,1\}^n: \\ |x|=j}} \langle x|\psi\rangle (-1)^{x\cdot y}. \tag{2.50}$$

Let $p = C\log(n/\varepsilon)$ for $C = O(1)$ and note that for each $0 \leq j \leq p$ we can compute the function $y \to c_{y,j}$ in quasi-polynomial time using the expression above (this computation also involves the entries $\langle x|\psi\rangle$ for $|x| \leq p$ which can be hardcoded into our circuit). Hence we can compute the coefficients of F_y up to order p in time $n^{O(\log(n/\varepsilon))}$. Also note that $F_y(0) = 2^{-n/2}\langle 0^n|\psi\rangle$ is a constant independent of y. From this data we can then compute the derivatives of $\ln F_y(z)$ up to order p using the triangular linear system Eq. (1.20), as discussed above. Using Lemma 1, we obtain an ε-relative error estimate for

$$F_y(1) = \langle y|H^{\otimes n}|\psi\rangle \tag{2.51}$$

as desired. □

Next we show how to prepare $|\psi\rangle \in LY(r)$ with $r > 1$ in quasi-polynomial time on a quantum computer. We shall use the well-known Grover-Rudolph state preparation technique as a subroutine [GR02]. This is a method of preparing a superposition

$$\sum_{x\in\{0,1\}^n} \sqrt{p(x)}|x\rangle \tag{2.52}$$

corresponding to a classical probability distribution $p(x)$; states of this form where all entries are nonnegative real numbers are sometimes called "quantum samples". The method requires the ability to compute marginal probabilities of the form

$$p_j(y) = \sum_{z\in\{0,1\}^{n-j}} p(yz)$$

where $1 \leq j \leq n$ and $y \in \{0,1\}^j$. A statement of the Grover-Rudolph state preparation technique where the marginals are computed to ε relative error follows.

Lemma 12. *(Grover-Rudolph state preparation [GR02]) Let $p(x)$ be a probability distribution on $\{0,1\}^n$ and $\varepsilon > 0$. Consider the quantum sample*

$$|\psi_p\rangle = \sum_{x\in\{0,1\}^n} \sqrt{p(x)}|x\rangle. \tag{2.53}$$

If the marginal probabilities $p_j(y) = \sum_z p(yz)$ can be computed to δ relative error where $\delta^{-1} = \mathcal{O}(n\varepsilon^{-2})$, then there is an efficient quantum algorithm for preparing a pure state $|\psi'_p\rangle$ satisfying

$$\||\psi'_p\rangle - |\psi_p\rangle\| \leq \varepsilon. \tag{2.54}$$

Proof of Lemma 12. Let $\tilde{p}_j(y)$ denote the δ relative error approximation of $p_j(y)$. That is

$$(1-\delta)p_j(y) \leq \tilde{p}_j(y) \leq (1+\delta)p_j(y). \tag{2.55}$$

First, apply an X-rotation to the initial state $|0\rangle$ to prepare the state

$$|\phi_1\rangle = \sqrt{\frac{\tilde{p}_1(0)}{\tilde{p}_1(0)+\tilde{p}_1(1)}}|0\rangle + \sqrt{\frac{\tilde{p}_1(1)}{\tilde{p}_1(0)+\tilde{p}_1(1)}}|1\rangle. \tag{2.56}$$

For each $1 < j \leq n$, add an ancilla qubit to $|\phi_{j-1}\rangle$ and apply the conditional rotation

$$|y\rangle|0\rangle \mapsto \sqrt{\frac{\tilde{p}_j(y0)}{\tilde{p}_j(y0)+\tilde{p}_j(y1)}}|y\rangle|0\rangle + \sqrt{\frac{\tilde{p}_j(y1)}{\tilde{p}_j(y0)+\tilde{p}_j(y1)}}|y\rangle|1\rangle \tag{2.57}$$

to produce the state

$$|\phi_j\rangle = \sum_{x\in\{0,1\}^j} \left(\prod_{i=1}^{j} \sqrt{\frac{\tilde{p}_i(x^i)}{\tilde{p}_i(x^{i-1}0)+\tilde{p}(x^{i-1}1)}}\right)|x\rangle. \tag{2.58}$$

Let $|\psi'_p\rangle = |\phi_n\rangle$. Because $\tilde{p}_i(x^{i-1}0)+\tilde{p}_i(x^{i-1}1)$ is a relative error δ estimate of $p_{i-1}(x^{i-1})$, the inner product with $|\psi_p\rangle$ is bounded as follows

$$\begin{aligned}
\langle\psi_p|\psi'_p\rangle &= \sum_{x\in\{0,1\}^n} \sqrt{p(x)} \left(\prod_{i=1}^{n} \sqrt{\frac{\tilde{p}_i(x^i)}{\tilde{p}_i(x^{i-1}0)+\tilde{p}_i(x^{i-1}1)}}\right) \\
&\geq \sum_{x\in\{0,1\}^n} \sqrt{p(x)} \left(\prod_{i=1}^{n} \sqrt{\frac{p_i(x^i)(1-\delta)}{p_{i-1}(x^{i-1})(1+\delta)}}\right) \\
&= \sum_{x\in\{0,1\}^n} p(x) \left(\frac{1-\delta}{1+\delta}\right)^{n/2} \\
&= \left(\frac{1-\delta}{1+\delta}\right)^{n/2}
\end{aligned} \tag{2.59}$$

where the second equality follows by simplifying the telescoping product. Taking δ^{-1} to be $\mathcal{O}(n\varepsilon^{-2})$ ensures that $\langle\psi_p|\psi'_p\rangle \geq 1-\varepsilon^2/2$. Hence

$$\||\psi'_p\rangle - |\psi_p\rangle\| \leq \varepsilon. \tag{2.60}$$

□

The following theorem shows that states in $LY(r)$ with $r > 1$ are prepared by quasi-polynomial size quantum circuits.

Theorem 10 (Quantum state preparation). *Let $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ be in $LY(r)$ for $r > 1$ and $\varepsilon > 0$. There is a quantum circuit of size $n^{O(\log(n/\varepsilon))}$ which prepares an n-qubit state $|\psi'\rangle$ satisfying $\||\psi\rangle - |\psi'\rangle\| \leq \varepsilon$.*

Proof. For each $0 \leq k \leq n$ let

$$\rho_k = \mathrm{Tr}_{k+1,\ldots,n}(|\psi\rangle\langle\psi|) \tag{2.61}$$

be the density matrix obtained from $|\psi\rangle$ by tracing out the last $n-k$ qubits. The measured distribution of $H^{\otimes n}|\psi\rangle$ is given by

$$p(x) = |\langle x|H^{\otimes n}|\psi\rangle|^2. \tag{2.62}$$

We also consider marginal probabilities for $0 \leq k \leq n$ defined by

$$p_k(y) = \langle y|H^{\otimes k}\rho_k H^{\otimes k}|y\rangle \qquad y \in \{0,1\}^k. \tag{2.63}$$

The density matrix ρ_k is in $LY(r)$ by Lemma 2 because it is obtained from the tensor $|\psi\rangle\langle\psi|$ by contracting indices corresponding to qubits $k+1,\ldots,n$. Note that we can regard ρ_k as a vector with 4^k entries, so that each marginal $p_k(y)$ is an entry of the vector. We can therefore use Theorem 9 to infer there is a classical circuit with runtime $n^{O(\log(n/\delta))}$ which computes the marginals $y \to p_k(y)$ to within a given relative error δ. Using this subroutine with $\delta = O(\varepsilon^2/n)$ in Lemma 12 gives a quantum algorithm with runtime $n^{O(\log(n/\varepsilon))}$ that prepares a state $|\phi\rangle$ that approximates the quantum sample corresponding to the distribution p:

$$\||\phi\rangle - \sum_{x\in\{0,1\}^x} \sqrt{p(x)}|x\rangle\| \leq \varepsilon/2. \tag{2.64}$$

Next we shall modify this state to ensure that each entry has the correct complex phase. Observe that using Theorem 9 to compute an $O(\varepsilon)$-relative error approximation for $\langle y|H^{\otimes n}|\psi\rangle$, we can infer an $\varepsilon/2$-additive error estimate $\tilde{\theta}_y$ of the phase $\theta_y = \arg(\langle y|H^{\otimes n}|\psi\rangle)$. This approximation to the phase can be computed by a reversible circuit which acts on $n + \log(\varepsilon^{-1})$ qubits as

$$|y\rangle|a\rangle \mapsto |y\rangle|a \oplus \tilde{\theta}_y\rangle. \tag{2.65}$$

With the ancilla register initialized to $|0^{\log(\varepsilon^{-1})}\rangle$, apply a single-qubit diagonal unitary to each ancilla qubit to recover the phase

$$|y\rangle|\tilde{\theta}_y\rangle \mapsto e^{i\tilde{\theta}_y}|y\rangle|\tilde{\theta}_y\rangle. \tag{2.66}$$

Next, uncompute and trace out the ancilla register, resulting in the state

$$|\phi\rangle \mapsto \sum_{x\in\{0,1\}^n} \phi_x e^{i\tilde{\theta}_x}|x\rangle =: |\phi'\rangle, \tag{2.67}$$

which is within $\varepsilon/2$ of the phase-approximate state

$$|\tilde{\psi}\rangle = \sum_{x\in\{0,1\}^n} \sqrt{p(x)}e^{i\tilde{\theta}_x}|x\rangle \tag{2.68}$$

by Eq. (2.64). The state $|\tilde{\psi}\rangle$ is also within $\varepsilon/2$ of $H^{\otimes n}|\psi\rangle$, as can be seen via

$$\begin{aligned} \|H^{\otimes n}|\psi\rangle - |\tilde{\psi}\rangle\|^2 &= \sum_{x\in\{0,1\}^n} p(x)|e^{i\theta_x} - e^{i\tilde{\theta}_x}|^2 \\ &= \sum_{x\in\{0,1\}^n} p(x)(2 - e^{i(\theta_x-\tilde{\theta}_x)} - e^{-i(\theta_x-\tilde{\theta}_x)}) \end{aligned} \tag{2.69}$$

and using the fact that $|\theta_x - \tilde{\theta}_x| < \varepsilon/2$ for all $x \in \{0,1\}^n$. Hence by the triangle inequality we have

$$\|H^{\otimes n}|\psi\rangle - |\phi'\rangle\| \leq \varepsilon \tag{2.70}$$

and the state $|\psi'\rangle = H^{\otimes n}|\phi'\rangle$ satisfies $\||\psi\rangle - |\psi'\rangle\| \leq \varepsilon$ as desired. □

Remark on Lee-Yang radius $r = 1$. Before proceeding, let us briefly comment on the fact that we often discuss states with Lee-Yang radius $r = 1$ (as in the Suzuki-Fisher Theorem 6 for example) whereas we might prefer if the Lee-Yang radius were strictly greater than 1 (for instance to make use of Theorem 10). One way to deal with this is to use the following naive method to increase the Lee-Yang radius of a given state. In particular, if $|\psi\rangle \in LY(1)$ is a normalized n-qubit state then let

$$|\psi(r)\rangle = \frac{1}{\|D_{1/r}^{\otimes n}|\psi\rangle\|} D_{1/r}^{\otimes n}|\psi\rangle$$

where $D_{1/r} = |0\rangle\langle 0| + r^{-1}|1\rangle\langle 1|$. By definition of the Lee-Yang radius, we have $|\psi(r)\rangle \in LY(r)$. Although this transformation with $r > 1$ expands the Lee-Yang radius, it also can drastically change the state; unfortunately $|\psi(r)\rangle$ is not in general close to $|\psi\rangle$ in trace distance. However, the situation is actually not so bad if $|\psi\rangle$ is an eigenstate of a local Hamiltonian H and if we measure closeness with respect to energy rather than trace distance. For example, suppose $H = \sum_{ij} h_{ij}$ is a two-local Hamiltonian such that each term h_{ij} acts nontrivially only on qubits i, j, and that $H|\psi\rangle = \lambda|\psi\rangle$. In that case it is not hard to show that the expected value of H on the state $|\psi(1+\mu)\rangle$ for a small constant $\mu = O(1)$ approximates λ to within an additive term that is bounded as $O(\mu) \cdot \sum_{ij} \|h_{ij}\|$. Hence these perturbed ground states $|\psi(r)\rangle$ have energy which varies from the true ground energy with error scaling in the perturbation and the sum of the norms of the local terms.

To see this note that

$$\langle\psi(r)|H'(r)|\psi(r)\rangle = \lambda, \tag{2.71}$$

where

$$H'(r) = D_{1/r}^{\otimes n} H (D_{1/r}^{-1})^{\otimes n} = \sum_{i,j} D_{1/r}^{\otimes 2} h_{ij} (D_{1/r}^{-1})^{\otimes 2}$$

is in general non-Hermitian. From Eq. (2.71) we have

$$|\langle\psi(r)|H|\psi(r)\rangle - \lambda| = |\langle\psi(r)|H'(r) - H|\psi(r)\rangle| \leq \sum_{i,j} \|D_{1/r}^{\otimes 2} h_{ij} (D_{1/r}^{-1})^{\otimes 2} - h_{ij}\|.$$

Finally, note that if $r = 1 + \mu$ for a small constant μ, then the RHS is upper bounded as $O(\mu) \cdot \sum_{ij} \|h_{ij}\|$.

Chapter 3

Quantum many-body systems

In this chapter, we exhibit or provide evidence for efficient algorithms for local Hamiltonian problems. In Section 3.1, we consider a model with ground states that maximize entanglement known as the EPR Hamiltonians. Estimating the ground state of EPR Hamiltonians includes bipartite quantum Max Cut as a special case. We study the EPR Hamiltonians by considering a family of deformed EPR Hamiltonians with local terms which favor deformed EPR states $|00\rangle + s|11\rangle$ for $0 \leq s \leq 1$. For this deformed EPR model, we give numerical evidence that the spectral gap is bounded below by $1-s^2$ and that the corresponding ground states have Lee-Yang radius $1/\sqrt{s}$. If this bound on the spectral gap is true, then there is an efficient quantum adiabatic algorithm for estimating the ground energy and preparing the ground state of the EPR Hamiltonian.

In Section 3.2, we show that the Gibbs state can be prepared efficiently for a class of ferromagnetic quantum Hamiltonians. Furthermore, we show that the ferromagnetic XY models satisfy a Griffiths inequality. In Section 3.3 we give an efficient classical algorithm for computing the ground energy and ground state of a stoquastic Hamiltonian for which the interaction graph has a sufficiently rich structure of automorphisms. In Section 3.4, we show that polynomials derived from repeated powers of classical Ising model Hamiltonians satisfy a zerofree condition.

3.1 EPR Hamiltonians

The EPR state $(|00\rangle + |11\rangle)/\sqrt{2}$ is the unique ground state of a Hamiltonian $-(X_1X_2 + Z_1Z_2 - Y_1Y_2)$. Given an interaction graph $G = (V, E)$ as above, consider the n-qubit EPR Hamiltonian

$$H = -\sum_{(i,j)\in E} X_iX_j + Z_iZ_j - Y_iY_j. \tag{3.1}$$

As discussed in Chapter 1, the Heisenberg anti-ferromagnetic model on any bipartite graph is equivalent to the EPR Hamiltonian up to a local basis change on each qubit that flips the sign of terms X_iX_j and Z_iZ_j.

Fix a parameter $s \in [0,1]$ and define an EPR-like Hamiltonian

$$H_s = -\sum_{(i,j)\in E} |\phi_s\rangle\langle\phi_s|_{ij} \tag{3.2}$$

where

$$|\phi_s\rangle = |00\rangle + s|11\rangle \tag{3.3}$$

and $|\phi_s\rangle\langle\phi_s|_{ij}$ denotes the operator $|\phi_s\rangle\langle\phi_s|$ applied to qubits i,j tensored with the identity on all other qubits. One can easily check that

$$|\phi_s\rangle\langle\phi_s|_{ij} = \frac{1}{4}\left((1+s^2)I + (1+s^2)Z_iZ_j + (1-s^2)(Z_i+Z_j) + 2sX_iX_j - 2sY_iY_j\right). \tag{3.4}$$

Thus H_1 coincides with the standard EPR Hamiltonian Eq. (3.1) up to rescaling and an energy shift. Since we assumed $s \in [0,1]$, one has $1+s^2 \geq 2s$. Thus H_s has ferromagnetic dominating Z_iZ_j terms and non-negative magnetic Z-fields, that is, H_s is a Suzuki-Fisher Hamiltonian for all $0 \leq s \leq 1$, ignoring an overall energy shift. In particular, $e^{-\beta H_s} \in LY(1)$.

3.1.1 Quantum algorithm for the EPR model

In this section, we consider the quantum adiabatic algorithm which interpolates between H_0 and H_1. To this end, we explore the spectrum of H_s. First we show that the ground states of H_s are unique and structured.

Lemma 13. *Suppose $n \geq 2$, $s \in [0,1)$, and the interaction graph is connected. Then the ground state of H_s is non-degenerate. The ground state can be chosen as a superposition of even-weight bit strings with non-negative amplitudes.*

Proof. Let H be the Hadamard gate. Since $s \in [0,1)$, the state

$$H \otimes H|\phi_s\rangle = (1/2)(1+s)(|00\rangle + |11\rangle) + (1/2)(1-s)(|01\rangle + |10\rangle)$$

has positive amplitudes in the computational basis. It follows that $H^{\otimes 2}|\phi_s\rangle\langle\phi_s|H^{\otimes 2}$ is a matrix with positive entries. Since the interaction graph is connected and $n \geq 2$, each vertex has at least one incident edge. Thus, $-H_s$ is a non-negative irreducible matrix in the Hadamard basis. Perron-Frobenius theorem implies that the smallest eigenvalue of H_s is non-degenerate and the corresponding eigenvector $|\psi\rangle$ has real positive amplitudes in the Hadamard basis. Since the state $|0^n\rangle$ also has real positive amplitudes in the Hadamard basis, one infers that $\langle 0^n|\psi\rangle > 0$. From $H_sZ^{\otimes n} = Z^{\otimes n}H_s$ and the fact that the smallest eigenvalue is non-degenerate one infers that $Z^{\otimes n}|\psi\rangle = \pm|\psi\rangle$. Combining this and $\langle 0^n|\psi\rangle > 0$ gives $Z^{\otimes n}|\psi\rangle = |\psi\rangle$, that is, $|\psi\rangle$ is a superposition of even-weight bit strings with non-negative amplitudes. □

Let λ_j be the j-th smallest eigenvalue of H_s, where $j = 1,\ldots,2^n$. We are interested in the spectral gap $\lambda_2 - \lambda_1$ which controls the cost of preparing the ground state of H_s by quantum adiabatic evolution starting from $s = 0$ (note that H_0 has the unique ground state $|0^n\rangle$).

Since H_s commutes with $Z^{\otimes n}$, eigenvectors of H_s can be chosen such that any eigenvector $|\phi\rangle$ is supported exclusively on the even-weight or the odd-weight subspaces corresponding to $\langle\phi|Z^{\otimes n}|\phi\rangle = 1$ and $\langle\phi|Z^{\otimes n}|\phi\rangle = -1$ respectively. Let λ_j^e and λ_j^o be the j-th smallest eigenvalue of H_s within the even-weight and the odd-weight subspace respectively. Here $j = 1, \ldots, 2^{n-1}$. From Lemma 13 one gets $\lambda_1 = \lambda_1^e < \lambda_1^o$. Thus the spectral gap of H_s is

$$\lambda_2 - \lambda_1 = \min\{\lambda_1^o - \lambda_1^e, \lambda_2^e - \lambda_1^e\}. \tag{3.5}$$

Consider first the simple case when the interaction graph G is a star graph such that

$$H_s = -\sum_{i=2}^{n} |\phi_s\rangle\langle\phi_s|_{1i}.$$

Lemma 14. *Suppose G is the star graph with $n \geq 3$ vertices. Then the EPR-like Hamiltonian H_s has spectral gap $\lambda_2 - \lambda_1 = \lambda_1^o - \lambda_1^e = 1 - s^2$.*

Proof. Let us first compute λ_1^e and λ_1^o. Let H^e and H^o be the restrictions of $-H_s$ onto the even-weight and the odd-weight subspaces. Since H^e and H^o are entry-wise non-negative Hamiltonians, Perron-Frobenius theorem implies that maximum eigenvectors of H^e and H^o can be chosen as real vectors with non-negative amplitudes in the standard basis. Furthermore, since H^e and H^0 are invariant under any permutation of qubits $2, \ldots, n$, one can symmetrize the maximum eigenvectors of H^e and H^o over such permutations (the symmetrization does not annihilate the state since all amplitudes are non-negative). Thus it suffices to compute maximum eigenvalues of H^e and H^o restricted to a subspace

$$\mathcal{H} = \mathbb{C}^2 \otimes \mathcal{S}_{n-1}, \tag{3.6}$$

where $\mathcal{S}_{n-1} \subseteq (\mathbb{C}^2)^{\otimes(n-1)}$ is the symmetric subspace of $n-1$ qubits. By definition, $\mathcal{S}_{n-1}$ is spanned by Dicke states

$$|D_k\rangle = \frac{1}{\sqrt{\binom{n-1}{k}}} \sum_{\substack{x\in\{0,1\}^{n-1} \\ |x|=k}} |x\rangle. \tag{3.7}$$

Straightforward algebra yields

$$-H_s|0\rangle \otimes |D_k\rangle = (n-1-k)|0\rangle \otimes |D_k\rangle + \sqrt{s^2(k+1)(n-k-1)}|1\rangle \otimes |D_{k+1}\rangle \tag{3.8}$$

and

$$-H_s|1\rangle \otimes |D_{k+1}\rangle = s^2(k+1)|1\rangle \otimes |D_{k+1}\rangle + \sqrt{s^2(k+1)(n-k-1)}|0\rangle \otimes |D_k\rangle. \tag{3.9}$$

Hence $-H_s$ preserves the two-dimensional subspace spanned by $|0\rangle \otimes |D_k\rangle$ and $|1\rangle \otimes |D_{k+1}\rangle$. The corresponding 2×2 block of $-H_s$ is a rank-1 matrix

$$\begin{bmatrix} \alpha^2 & \alpha\beta \\ \alpha\beta & \beta^2 \end{bmatrix} \tag{3.10}$$

where $\alpha = \sqrt{n-1-k}$ and $\beta = \sqrt{s^2(k+1)}$. The maximum eigenvalue of this 2×2 matrix coincides with its trace, that is, $\alpha^2 + \beta^2 = n - 1 - k + s^2(k+1)$. Maximizing this expression over even and odd values of $k \geq 0$ and noting that $s \in [0, 1)$ gives

$$-\lambda_1^e = n - 1 + s^2, \quad -\lambda_2^e = n - 3 + 3s^2, \quad -\lambda_1^o = n - 2 + 2s^2.$$

Hence

$$\lambda_1^o - \lambda_1^e = 1 - s^2 \quad \text{and} \quad \lambda_2^e - \lambda_1^e = 2(1 - s^2).$$

The statement of the lemma now follows from Eq. (3.5). □

Numerical experiments support Conjecture 1 and suggest the following conjecture.

Conjecture 3. *Suppose $n \geq 2$, $s \in [0, 1)$, and the interaction graph is connected. Then the second smallest eigenvalue of H_s coincides with the smallest eigenvalue of H_s restricted to the odd-weight subspace.*

The following summarizes our numerical evidence for Conjecture 1.

Numerical study 1 (Spectral gap of EPR-like Hamiltonians). *We numerically investigated Conjecture 1 and found by exact diagonalization that it holds for 100 uniformly spaced values of $s \in (0, 1)$ for all trees with $n \leq 18$ vertices and all connected graphs with $n \leq 10$ vertices. We also found that it holds for path graphs with $n \leq 100$ vertices and $s \in \{0.9, 0.95, 0.97, 0.99\}$. The spectral gap for path graphs was computed by the exact diagonalization if $n \leq 24$ and using the Matrix Product State library mpnum [ZMP] for larger values of n.*

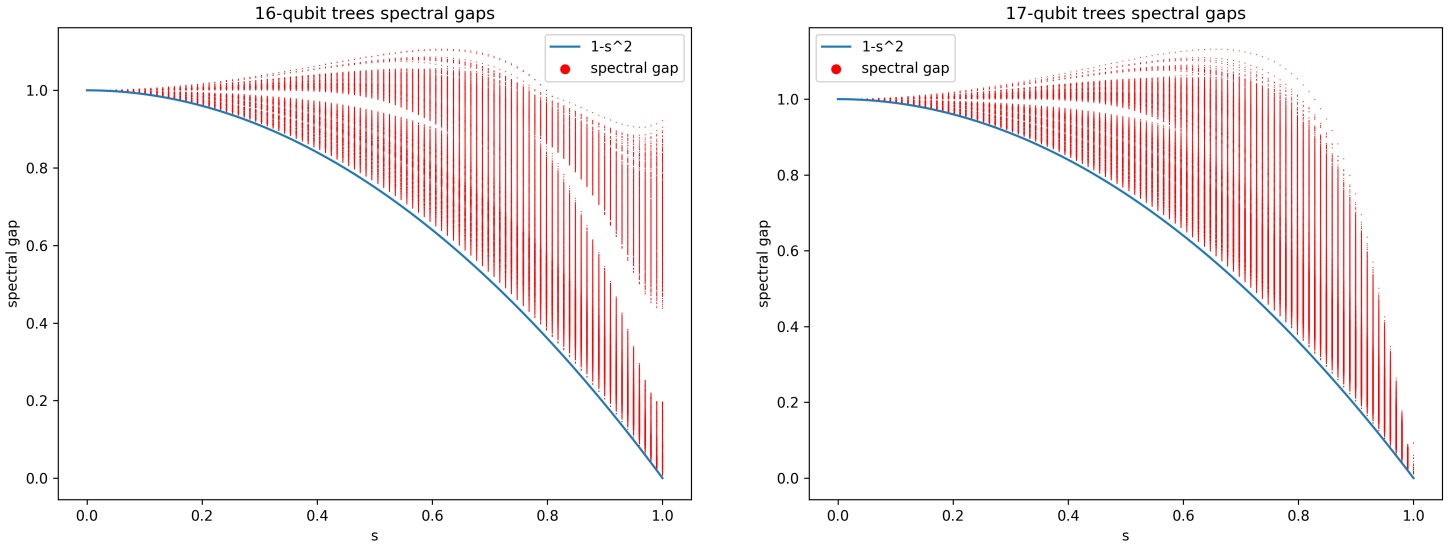


Figure 3.1: Plots from Numerical study 1. For each tree on $n = 16, 17$ vertices, the spectral gap is plotted as a red point for 100 uniformly spaced $s \in (0, 1)$.

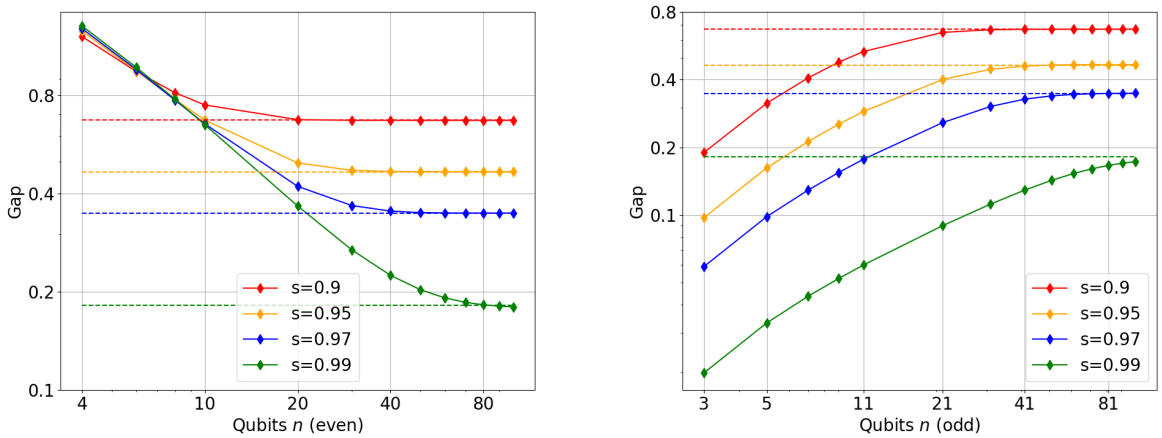


Figure 3.2: Plots from Numerical study 1. Spectral gap of 1D chains with $3 \leq n \leq 100$ qubits and open boundary conditions. The lower bound $1-s^2$ is achieved at $n = 3$ (when the chain is the star graph). Horizontal dashed lines on both plots show a fit $g(s) = 3.03s(1-s)^{0.609}$ which corresponds to the large n limit (parity of n does not matter in this limit).

We note that Conjecture 1 is easy to falsify since it gives a precise bound on the spectral gap for any finite n, as opposed to an asymptotic scaling like $\mathsf{poly}(1/n)$. At the same time, the conjecture is extremely bold. If true, it would imply that the bipartite quantum Max Cut problem is contained in BQP, resolving a long-standing open question. Indeed, the quantum Max Cut problem boils down to approximating the ground energy of the Heisenberg antiferromagnetic Hamiltonian $H_{AF} = \sum_{(i,j)\in E} X_iX_j + Y_iY_j + Z_iZ_j$ on a given graph $G = (V, E)$ within an additive error $\epsilon = \mathsf{poly}(1/n)$. As commented above, H_{AF} coincides with the EPR Hamiltonian H_1 (up to a local basis change on some qubits) whenever the interaction graph is bipartite. Ground energies of H_1 and H_s are related by Weyl's inequality

$$|\lambda_1(H_1) - \lambda_1(H_s)| \leq \|H_1 - H_s\| \leq \sum_{(i,j)\in E} \| \, |\phi_s\rangle\langle\phi_s| - |\phi_1\rangle\langle\phi_1| \, \| \leq 2|E|(1-s).$$

Suppose $s = 1 - \epsilon/(4|E|)$ so that $|\lambda_1(H_1) - \lambda_1(H_s)| \leq \epsilon/2$. Let $\tilde{\lambda}$ be an $(\epsilon/2)$-approximation of the ground energy of H_s found by the quantum adiabatic evolution algorithm. Then $\tilde{\lambda}$ is the desired ϵ-approximation of $\lambda_1(H_1) = \lambda_1(H_{AF})$. Choose the adiabatic path as $\{H_t\}_{0\leq t\leq s}$. Recall that H_0 has the trivial ground state $|0^n\rangle$. Then the quantum runtime scales as $T = \epsilon^{-1} \cdot \mathsf{poly}(g_{min}^{-1}, n)$, where g_{min} is the minimum spectral gap along the chosen adiabatic path, see [BM21] and references therein. Conjecture 1 gives $g_{min} = 1 - s^2 \sim \epsilon/|E|$. Hence $T \leq \mathsf{poly}(n, \epsilon^{-1})$ scales polynomially with all parameters.

We close with some observations on the data from Numerical study 1 presented in Figs. 3.1 to 3.4. Since all trees (as in Fig. 3.1) are bipartite, when $s = 1$, H_1 is unitarily equivalent to the antiferromagnetic Heisenberg model as discussed above and more can be said about the spectral gap. For bipartite graphs with bipartition $V = A \sqcup B$, the Leib-Mattis theorem [LM62] ensures that there is degeneracy if and only if $|A| = |B|$.

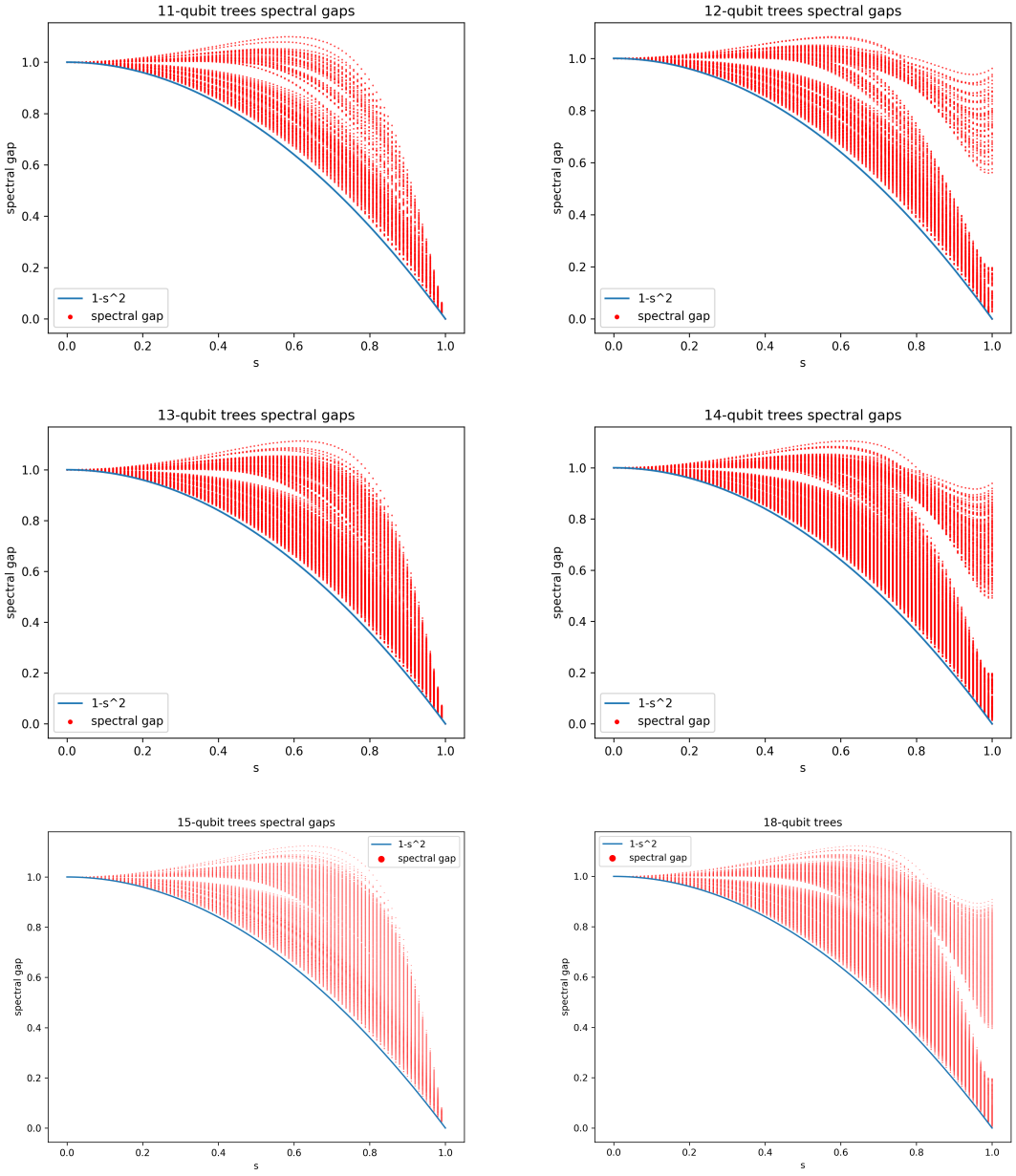


Figure 3.3: More spectral gaps for H_s on trees from Numerical study 1.

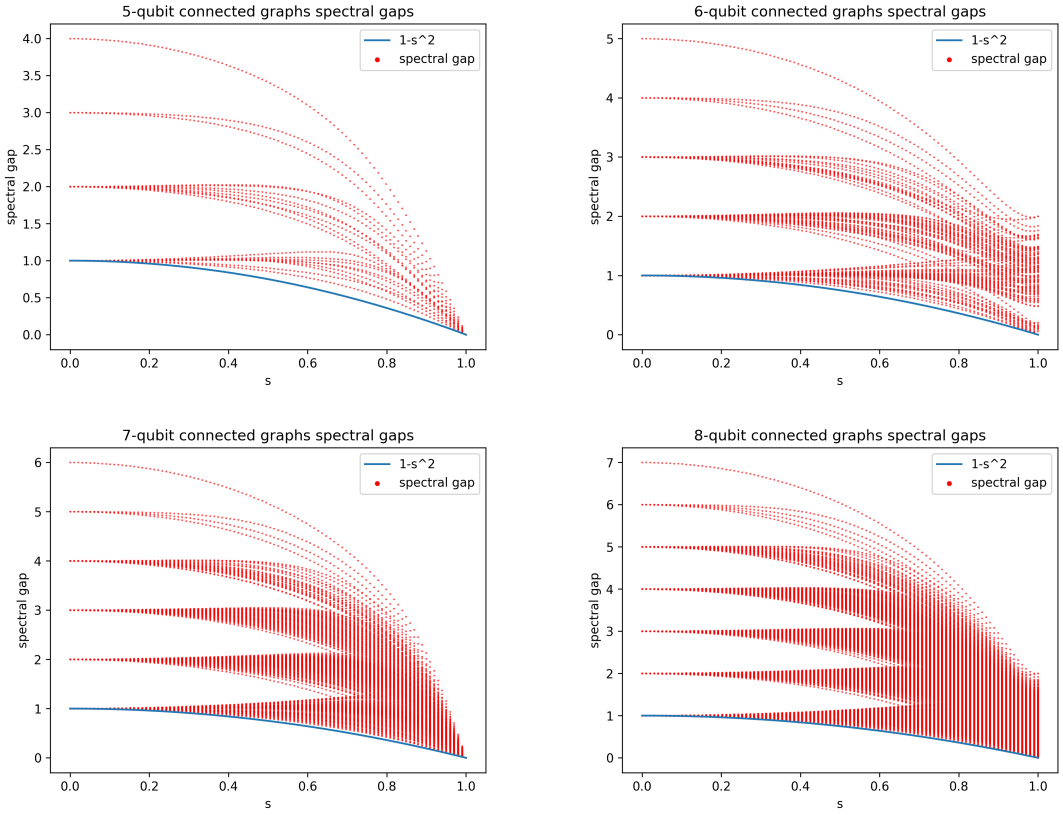


Figure 3.4: Spectral gaps for H_s on connected graphs from Numerical study 1.

For a connected graph G (as in Fig. 3.4), the spectral gap of H_0 is equal to the minimum degree of G denoted $\delta(G)$. At $s = 0$, we have the Hamiltonian

$$H_0 = \sum_{(i,j)\in E} |00\rangle\langle 00|_{ij} \tag{3.11}$$

which is diagonal in the computational basis. For any $S \subseteq [n]$, $X(S)|0^n\rangle$ satisfies all of the terms for which $i, j \in [n] \setminus S$. Hence the eigenvalue of $X(S)|0^n\rangle$ is

$$|E| - |\{(i,j) \in E : i, j \in S\}| \tag{3.12}$$

Hence the spectral gap is $|E| - (|E| - \delta(G)) = \delta(G)$.

3.1.2 Phase-shifted EPR-like Hamiltonians

One limitation of EPR-like Hamiltonians H_s defined in Section 3.1 is that these Hamiltonians are stoquastic (sign-problem-free). One might expect that the ground energy of such Hamiltonians can be estimated for a moderately large number of qubits (say, $n \leq 100$) on a classical computer using quantum Monte Carlo algorithms. In this section we briefly discuss a non-stoquastic version of EPR-like Hamiltonians where local phase shifts are applied on every edge of the graph. Such Hamiltonians may be more suitable for demonstrating a quantum advantage for the ground energy estimation problem. Define a two-qubit operator

$$h(z) = |00\rangle\langle 00| + z|11\rangle\langle 00| + z^*|00\rangle\langle 11| + |z|^2|11\rangle\langle 11|,$$

where $z \in \mathbb{C}$. A phase-shifted EPR-like Hamiltonian is defined as

$$H_s(\theta) = -\sum_{(p,q)\in E} h_{pq}(se^{i\theta_{pq}}), \tag{3.13}$$

where $s \in [0, 1]$ and $\theta_{p,q} \in [0, 2\pi)$ are arbitrary edge-dependent angles (phase shifts). Setting $\theta_{p,q} = 0$ gives the original EPR-like Hamiltonian H_s. If the interaction graph G is a tree, phase shifts do not matter in the sense that $H_s(\theta) = UH_sU^\dagger$, where U is a tensor product of n single-qubit Z-rotations[1]. In particular, the eigenvalue spectrum of $H_s(\theta)$ and the Lee-Yang radius of the Gibbs state $\rho \sim e^{-\beta H_s(\theta)}$ do not depend on θ. However, if the interaction graph contains cycles, phase shifts cannot be generally removed by a global similarity transformation (this is analogous to magnetic fluxes that cannot be removed by a gauge transformation). In this case the eigenvalue spectrum and the Lee-Yang radius of the Gibbs state may depend on θ.

Since $H_s(\theta)$ is obtained from the Suzuki-Fisher Hamiltonian H_s by conjugating each local term in H_s with single-qubit Z-rotations, one concludes that

$$e^{-\beta H_s(\theta)} \in LY(1) \tag{3.14}$$

[1]This can be proved using the identity $h(se^{i\varphi}) = (R_z \otimes I)h(s)(R_z^\dagger \otimes I)$ with $R_z = e^{-i(\varphi/2)Z}$ and removing phase shifts by a sequence of R_z rotations starting from root of the tree towards the leaves.

for any angles θ from Theorem 6. Taking the limit $\beta \to \infty$ one concludes that the ground state projector for $H_s(\theta)$ is a tensor in $LY(1)$ and thus at least one ground state of $H_s(\theta)$ has a non-zero overlap with $|0^n\rangle$. As a consequence, one can choose a ground state of $H_s(\theta)$ as

$$|\psi\rangle = \lim_{\beta\to\infty} \frac{e^{-\beta H_s(\theta)}|0^n\rangle}{\|e^{-\beta H_s(\theta)}|0^n\rangle\|}.$$

Furthermore, the proof of Lemma 15 works for any phase shift implying that $e^{-\beta H_s(\theta)} \in LY(r)$ for $n = 2$, where the radius r is given by Eq. (3.15). We leave as an open question whether Conjectures 3,1, 2 hold for phase-shifted EPR-like Hamiltonians. If this is the case, Theorem 8 implies that the ground state of $H_s(\theta)$ is non-degenerate and the adiabatic path connecting H_0 with $H_s(\theta)$ has the minimum spectral gap $1 - s^2$. Accordingly, the problem of estimating the ground energy of $H_1(\theta)$ is contained in BQP, see the discussion at the end of Section 3.1

Numerical study 2 (Spectral gap of phase-shifted EPR-like Hamiltonians). *For each connected graph with $n \leq 10$ vertices we selected phase shifts θ_{pq} uniformly and independently at random to construct a Hamiltonian $H_s(\theta)$. We computed the spectral gap of $H_s(\theta)$ using exact diagonalization and found that it is lower bounded by $1 - s^2$, see Fig. 3.5.*

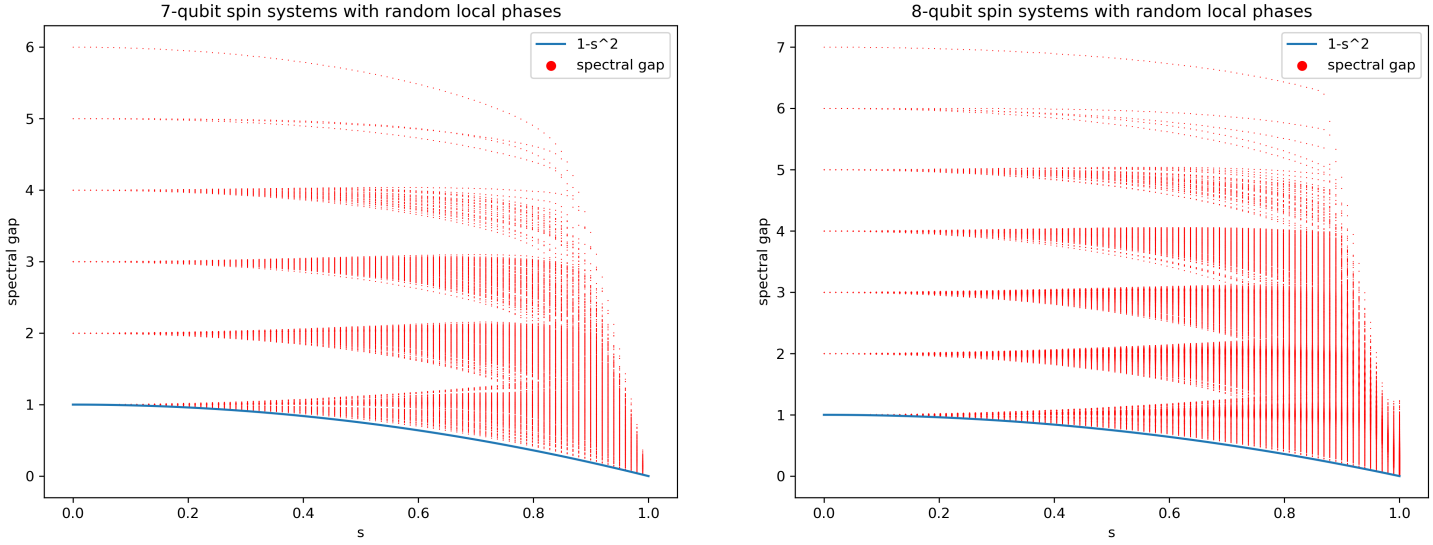


Figure 3.5: Plots from Numerical study 2. For each connected graph on $7, 8$ vertices, random phase shifts θ_{pq} are sampled and the spectral gap of $H_s(\theta)$ is plotted as a red dot for 100 uniformly spaced $s \in (0, 1)$.

3.1.3 Lee-Yang radius of deformed EPR model

From now on we assume that $0 \leq s < 1$ and G is a connected graph. Is it true that $e^{-\beta H_s} \in LY(r)$ for some $r > 1$? Consider first the simplest case when $n = 2$.

Lemma 15. *Suppose $n = 2$ and the graph G is a single edge. Then $e^{-\beta H_s} \in LY(r)$ where*

$$r = \frac{1}{\sqrt{s}} \left(\frac{1 + s^2 e^{-\beta(1+s^2)}}{1 + s^{-2} e^{-\beta(1+s^2)}} \right)^{1/4}. \tag{3.15}$$

Note that $r > 1$ for any $s \in [0, 1)$ and $\beta > 0$. Furthermore, $e^{-\beta H_s} \notin LY(r')$ for any $r' > r$.

Proof. We have

$$e^{-\beta H_s} = I + \epsilon |\phi_s\rangle\langle\phi_s|, \qquad \epsilon = \frac{e^{\beta(1+s^2)} - 1}{1 + s^2}.$$

Note that $\epsilon \geq 0$. The generating polynomial of $e^{-\beta H_s}$ is

$$f(z) = \langle z_1^*, z_2^* | e^{-\beta H_s} | z_3, z_4 \rangle = (1 + z_1 z_3)(1 + z_2 z_4) + \epsilon(1 + s z_1 z_2)(1 + s z_3 z_4).$$

Write $f(z) = \det M(z)$, where

$$M(z) = \begin{bmatrix} 1 + z_1 z_3 & -\epsilon^{1/2}(1 + s z_1 z_2) \\ \epsilon^{1/2}(1 + s z_3 z_4) & 1 + z_2 z_4 \end{bmatrix}. \tag{3.16}$$

We have

$$M(z) = \begin{bmatrix} 1 & -\epsilon^{1/2} \\ \epsilon^{1/2} & 1 \end{bmatrix} + \begin{bmatrix} z_1 & 0 \\ 0 & z_4 \end{bmatrix} \cdot \begin{bmatrix} 1 & -s\epsilon^{1/2} \\ s\epsilon^{1/2} & 1 \end{bmatrix} \cdot \begin{bmatrix} z_3 & 0 \\ 0 & z_2 \end{bmatrix}.$$

Clearly,

$$\begin{bmatrix} 1 & -\epsilon^{1/2} \\ \epsilon^{1/2} & 1 \end{bmatrix} = I - i\epsilon^{1/2} Y = (1 + \epsilon)^{1/2} e^{-i\theta Y}$$

where $\cos\theta = (1 + \epsilon)^{-1/2}$. We arrive at

$$\det M(z) = (1 + \epsilon) \det (I + K(z)),$$

where

$$K(z) = (1 + \epsilon)^{-1/2} e^{i\theta Y} \begin{bmatrix} z_1 & 0 \\ 0 & z_4 \end{bmatrix} \cdot \begin{bmatrix} 1 & -s\epsilon^{1/2} \\ s\epsilon^{1/2} & 1 \end{bmatrix} \cdot \begin{bmatrix} z_3 & 0 \\ 0 & z_2 \end{bmatrix}.$$

Let $r > 0$ be a radius to be defined later. For any $z_1, z_2, z_3, z_4 \in \mathbb{D}_r$ one has

$$\left\| \begin{bmatrix} z_1 & 0 \\ 0 & z_4 \end{bmatrix} \right\| < r, \quad \left\| \begin{bmatrix} z_3 & 0 \\ 0 & z_2 \end{bmatrix} \right\| < r, \quad \left\| \begin{bmatrix} 1 & -s\epsilon^{1/2} \\ s\epsilon^{1/2} & 1 \end{bmatrix} \right\| = \sqrt{1 + s^2 \epsilon}.$$

Sub-multiplicativity of the norm implies that

$$\|K(z)\| < r^2 \left(\frac{1 + s^2 \epsilon}{1 + \epsilon} \right)^{1/2} \leq 1$$

if we choose

$$r = \left(\frac{1 + \epsilon}{1 + s^2 \epsilon} \right)^{1/4}. \tag{3.17}$$

From $\|K(z)\| < 1$ one gets $\det M(z) \neq 0$ and thus $f(z) \neq 0$ for all $z_1, z_2, z_3, z_4 \in \mathbb{D}_r$. Substituting the definition of ϵ into Eq. (3.17) gives Eq. (3.15).

The last statement of the lemma follows from

$$f(r, -r, -r, -r) = (1 - r^2)(1 + r^2) + \epsilon(1 - sr^2)(1 + sr^2) = 1 + \epsilon - r^4(1 + \epsilon s^2) = 0.$$

□

Numerical experiments for small ($n \leq 6$) random examples suggest that the first part of Lemma 15 might hold for all connected graphs, that is, $e^{-\beta H_s} \in LY(r)$, where r is determined by Eq. (3.15) for all $\beta \geq 0$, $s \in [0, 1]$, and all connected graphs G.

Let $|\psi\rangle$ be the ground state of H_s. In Section 3.1, we showed H_s has a non-degenerate ground state whenever $n \geq 2$ and the interaction graph G is connected. Taking the limit $\beta \to \infty$ in Lemma 15 gives $\psi \in LY(r)$ with $r = 1/\sqrt{s}$ for $n = 2$. Numerical experiments suggest that the Lee-Yang radius of these states may be strictly larger than 1 as in Conjecture 2.

Numerical study 3 (Lee-Yang radius of EPR-like Hamiltonians). *For each connected graph with $3 \leq n \leq 8$ vertices and trees with $3 \leq n \leq 13$ vertices, we sampled 10 random values of $s \in (0, 1)$ and computed the roots of the univariate polynomials associated with equatorial postselection*

$$f_y(z) = \bigotimes_{i=1}^{n} (\langle 0| + (-1)^{y_i} z \langle 1|)|\psi\rangle \tag{3.18}$$

for each $y \in \{0, 1\}^n$. We found that none of the sampled polynomials have roots z with $|z| < s^{-1/2}$.

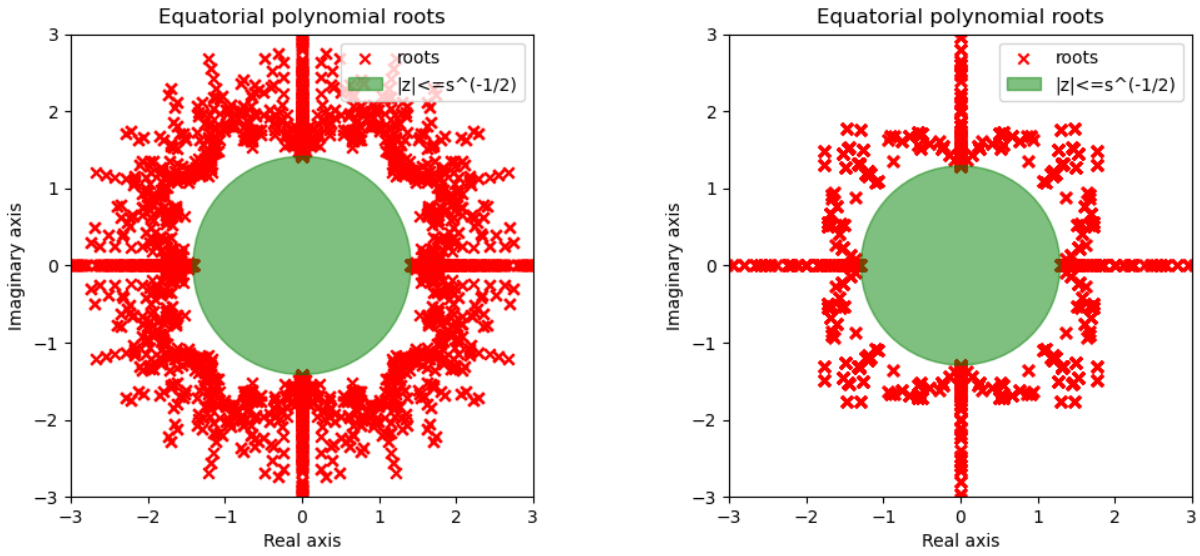


Figure 3.6: Plots from Numerical study 3. Zeros of equatorial polynomials which lie near the disk $\mathbb{D}_{s^{-1/2}}$ for a path and cycle with 10 vertices and $s = 0.5, 0.6$ respectively.

We close the section by analytically computing the LY-radius of the EPR-like Hamiltonian ground states on disjoint edges and star graphs.

Lemma 16. *Consider a graph G which is either n disjoint edges or which is a star graph. Then the ground state of the EPR-like Hamiltonian with interaction graph G has LY-radius $1/\sqrt{s}$ for $s \in [0, 1)$.*

Proof. First consider the graph D_n with n disjoint edges, i.e. with vertices labeled by $[2n]$ with an edge (u, v) if and only if $u = v \mod n$. Since the edges are disjoint, we can minimize the energy of each term and compute the ground state

$$|D_n\rangle = \frac{1}{\sqrt{(1+s^2)^n}} \left(|00\rangle + s|11\rangle\right)^{\otimes n} \tag{3.19}$$

which has generating polynomial

$$F_{D_n}(z_1, z_2, \ldots, z_{2n}) = \frac{1}{\sqrt{(1+s^2)^n}} \prod_{j=1}^{n} (1 + s z_j z_{j+n}). \tag{3.20}$$

If $|z_j| < 1/\sqrt{s}$ for each $j \in [2n]$, then each factor of F_{D_n} has positive real part and hence F_{D_n} does not vanish. Furthermore, if for each j we have $z_j = i/\sqrt{s}$ then F_{D_n} vanishes. Hence $|D_n\rangle$ has LY-radius $1/\sqrt{s}$. Next consider the star graph S_n with n vertices and edges $(1, j)$ for $2 \leq j \leq n$. Then the ground state is

$$|S_n\rangle = ((n-1)(n-1+s^2))^{-1/2} \left((n-1)|0^n\rangle + s \sum_{\substack{x \in \{0,1\}^{n-1} \\ |x|=1}} |1x\rangle \right) \tag{3.21}$$

as in the proof of Lemma 14, which has generating polynomial

$$F_{S_n} \propto n - 1 + \sum_{j=2}^{n} s z_1 z_j. \tag{3.22}$$

If $|z_j| < 1/\sqrt{s}$ for each $j \in [n]$, then F_{S_n} has positive real part and hence F_{Z_n} does not vanish. Furthermore, if for each j we have $z_j = i/\sqrt{s}$ then F_{S_n} vanishes. Hence $|S_n\rangle$ has LY-radius $1/\sqrt{s}$. □

3.2 Ferromagnetic XY Hamiltonians

In this section, we consider ferromagnetic XY Hamiltonians with local terms $-X \otimes X - Y \otimes Y$. We show that the ground state of these Hamiltonians can be prepared efficiently on a quantum computer. This algorithm can be extended to prepare a canonical purification of the Gibbs state as well. Finally, we show that all ferromagnetic XY Hamiltonians satisfy a Griffiths inequality.

3.2.1 State preparation for the XY model

Let us introduce the local Hamiltonians of interest. Suppose that $G = (V, E)$ is a graph with n vertices and a qubit associated with each vertex. Let $0 \leq w_e \leq 1$ be the weight of an edge $e \in E$. Then the Hamiltonian

$$H = \sum_{(i,j)\in E} w_{ij}(-X_iX_j - Y_iY_j) \tag{3.23}$$

is a ferromagnetic XY Hamiltonian with ground state

$$\rho = \lim_{\beta\to\infty} \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})} \tag{3.24}$$

and ground energy

$$\lambda = \mathrm{Tr}(H\rho). \tag{3.25}$$

We first show how to prepare the ground state of H and then observe that this algorithm can be extended to prepare purifications of the Gibbs state as well as ground states of antiferromagnetic XY Hamiltonians on bipartite graphs.

Theorem 11. *For any $\varepsilon > 0$, there is a quantum algorithm with runtime $\mathsf{poly}(n, \varepsilon^{-1})$ which prepares a state $|\tilde{\psi}\rangle$ satisfying*

$$|\langle\tilde{\psi}|H|\tilde{\psi}\rangle - \lambda| \leq \varepsilon \tag{3.26}$$

with probability $3/4$.

Before proving Theorem 11, we review the Trotter-Suzuki formula and the Markov chain Monte Carlo algorithm for counting perfect matchings. The high-level proof strategy is to use Markov chain Monte Carlo to estimate the marginals required for the Grover-Rudolph state preparation procedure in order to prepare the ground state distribution. Since H is stoquastic it is known that the ground state has nonnegative amplitudes and hence can be realized as a quantum sample.

The Trotter-Suzuki formula permits us to study a sequence of local operators instead of the full Hamiltonian. Consider the two-qubit non-unitary operator

$$h(t) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1+t^2 & t & 0 \\ 0 & t & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{3.27}$$

which is derived from the second-order Taylor approximation for $\exp(t(XX + YY))$.

Lemma 17. *(Trotter-Suzuki) For any $\varepsilon, \beta > 0$, there is an efficiently computable sequence of $J = \mathcal{O}((1+\beta^2)n^5\varepsilon^{-1})$ operators G_i such that*

$$G_J \ldots G_2 G_1 = e^{-\beta H + Q} \tag{3.28}$$

for Hermitian Q satisfying $||Q|| \leq \varepsilon/8$. Here each G_i is of the form $h(t)$ for $t > 0$ acting on two qubits in G. A proof can be found in the Supplementary Material of [BG17].

We now consider the Monte Carlo estimation of the perfect matching sum. For a weighted graph Γ with $2N$ vertices, edge weights given by ω, and $1 \leq m \leq N$, let $M_m(\Gamma)$ be the set of matchings with m edges. Then the perfect matching sum is the quantity

$$\mathrm{PM}(\Gamma) = \sum_{M \in M_N(\Gamma)} \prod_{e \in M} \omega(e). \tag{3.29}$$

Jerrum, Sinclair, and Vigoda famously showed how to estimate the perfect matching sum in polynomial time using Markov chain Monte Carlo methods. More information on Markov chain methods can be found in Appendix A.

Lemma 18. *(Bipartite Perfect Matching Sum [JSV04]). Let Γ be a bipartite graph with $2N$ vertices and nonnegative edge weights given by ω. Let $\varepsilon > 0$. Then the perfect matching sum $PM(\Gamma)$ can be approximated to ε relative error with probability at least $3/4$ in time $\mathcal{O}(\varepsilon^{-2} N^{11} (\log N)^3)$. A proof can be found in [JSV04].*

For a bitstring y, the quantities $\mathrm{Tr}(|y\rangle\langle y| G_J \dots G_2 G_1)$ will be important for estimating the marginals required for the proof of Theorem 11. We show that these quantities can be estimated by reducing them to perfect matching sums.

Lemma 19. *Fix a sequence of operators $G_J \dots G_2 G_1$ each of the form $h(t)$ on some qubits in G. Then there is a randomized classical algorithm with runtime $\mathcal{O}(\varepsilon^{-2} J^{11} (\log J)^3)$ which takes as input a bitstring y of length at most n and error tolerance $\varepsilon > 0$ and returns a relative error ε approximation for*

$$\mathrm{Tr}(|y\rangle\langle y| G_J \dots G_2 G_1) \tag{3.30}$$

with probability at least $3/4$. This probability can be boosted to $(1-\delta)$ by taking the median of $\mathcal{O}(\log(\delta^{-1}))$ independent runs of the algorithm.

Proof of Lemma 19. We modify the algorithm of [BG17]. We reduce the problem of approximating $\mathrm{Tr}(|y\rangle\langle y| G_J \dots G_2 G_1)$ to the problem of approximating the perfect matching sum of a weighted bipartite graph. We consider graphs constructed by connecting gadgets shown in Fig. 3.7.



(a) Gadget for $h(t)$ (b) Gadget for $|1\rangle\langle 1|$ (c) Gadget for $|0\rangle\langle 0|$

Figure 3.7: Gadgets for elementary operators. Unlabeled edges have weight 1. The dotted lines are input and output edges.

We consider gadget graphs Θ with k input vertices and k output vertices labels v_i for $1 \leq i \leq 2k$. For each $x \in \{0,1\}^{2k}$ let Θ_x denote the induced subgraph where vertices v_i with $x_i = 1$ are removed. We say that Θ implements a k qubit operator g when

$$\langle x_{2k} \dots x_{k+2} x_{k+1} | g | x_k \dots x_2 x_1 \rangle = \mathrm{PM}(\Theta_x) \tag{3.31}$$

for all $x \in \{0,1\}^{2k}$. Then the gadgets in Fig. 3.7 implement the operators $h(t), |0\rangle\langle 0|$, and $|1\rangle\langle 1|$. Since $|y\rangle\langle y|G_J \dots G_2 G_1$ is a product of operators implemented by the gadgets in Fig. 3.7, the weighted graph $\Gamma = (V_\Gamma, E_\Gamma, w)$ formed by replacing each operator in the product by the corresponding gadget and connecting input vertices to output vertices satisfies

$$\mathrm{Tr}(|y\rangle\langle y|G_J \dots G_2 G_1) = \mathrm{PM}(\Gamma). \tag{3.32}$$

Notice that each gadget in Fig. 3.7 is a bipartite graph where all input vertices are on the side A and all output vertices are on side B. Hence Γ is a bipartite graph with positive edge weights. Then $\mathrm{PM}(\Gamma)$ can be approximated to ε relative error with probability at least $3/4$ by Lemma 18. □

We will need the following lemma to relate the state that the prepare with the target Gibbs state.

Lemma 20. *Fix a Hermitian operators H, Q, and constants $\beta, \varepsilon > 0$. Consider the Gibbs state*

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})} \tag{3.33}$$

and the approximation to the Gibbs state

$$\rho' = \frac{e^{-\beta H + Q}}{\mathrm{Tr}(e^{-\beta H + Q})}. \tag{3.34}$$

Suppose $\|Q\| \le \epsilon$. Then $\|\rho - \rho'\|_1 \le 2(1 - e^{-\epsilon})$.

Proof. Let $\mathcal{Z} = \mathrm{Tr}(e^{-\beta H})$ and $\mathcal{Z}' = \mathrm{Tr}(e^{-\beta H + Q})$ and

$$|\psi\rangle = \frac{1}{\sqrt{\mathcal{Z}}} \sum_{x \in \{0,1\}^n} e^{-\beta H/2}|x\rangle|x\rangle \qquad |\psi'\rangle = \frac{1}{\sqrt{\mathcal{Z}'}} \sum_{x \in \{0,1\}^n} e^{-\beta H/2 + Q/2}|x\rangle|x\rangle$$

By Uhlmann's theorem we have

$$F(\rho, \rho') \ge |\langle \psi | \psi' \rangle|^2 = \frac{1}{\mathcal{Z}\mathcal{Z}'} \left(\mathrm{Tr}(e^{-\beta H/2} e^{-\beta H/2 + Q/2})\right)^2$$

Now using the Golden-Thompson inequality we have

$$\mathrm{Tr}(e^{-\beta H/2} e^{-\beta H/2 + Q/2}) \ge \mathrm{Tr}(e^{-\beta H + Q/2}) \ge \mathcal{Z} e^{-\epsilon/2},$$

where we used $\|Q\| \le \epsilon$ and Weyl's inequality. Therefore

$$F(\rho, \rho') \ge e^{-\epsilon} \frac{\mathcal{Z}^2}{\mathcal{Z}\mathcal{Z}'} = e^{-\epsilon} \mathcal{Z}/\mathcal{Z}' \ge e^{-2\epsilon},$$

where we used $\mathcal{Z}' \le \mathcal{Z} e^{\epsilon}$ which follows from Weyl's inequality. Finally, using the relationship between fidelity and trace distance gives

$$\|\rho - \rho'\|_1 \ge 2(1 - \sqrt{F(\rho, \rho')}) \ge 2(1 - e^{-\epsilon})$$

□

We are now in place to prove Theorem 11.

Proof of Theorem 11. Let $\varepsilon > 0$ be given. By Lemma 17 there is a sequence of $J = \mathcal{O}((1+\beta^2)n^5\varepsilon^{-1})$ operators which act nontrivially as $h(t)$ such that

$$e^{-\beta H+Q} = G_J \dots G_2 G_1 \tag{3.35}$$

where $||Q|| \leq \varepsilon/8$. Consider the state

$$\rho' = \frac{e^{-\beta H+Q}}{\mathrm{Tr}(e^{-\beta H+Q})} \tag{3.36}$$

from Lemma 19 and its measured distribution

$$p'(x) = \langle x|\rho'|x\rangle. \tag{3.37}$$

Then the marginal probabilities are given by

$$\begin{aligned} p'_j(y) &= \sum_{z\in\{0,1\}^{n-j}} p'(yz) \\ &= \sum_{z\in\{0,1\}^{n-j}} \langle yz|\rho'|yz\rangle \\ &= \frac{\mathrm{Tr}(|y\rangle\langle y|G_J \dots G_2 G_1)}{\mathrm{Tr}(G_J \dots G_2 G_1)} \end{aligned} \tag{3.38}$$

By Lemma 19 η relative error approximations for each of the quantities above can be computed in $\mathsf{poly}(\beta, n, \varepsilon^{-1})$ where $\eta^{-1} = \mathsf{poly}(\varepsilon^{-1})$ and all of the estimates succeed with probability at least 3/4. By Lemma 12 these estimates can be used to produce a state $|\psi'_p\rangle$ satisfying

$$\||\psi'_p\rangle - |\psi_p\rangle\| \leq \varepsilon \tag{3.39}$$

where $|\psi_p\rangle = \sum_{x\in\{0,1\}^n} \sqrt{p'(x)}|x\rangle$. Consider the quantum sample

$$|\phi\rangle = \sum_{x\in\{0,1\}^n} \langle x|\rho|x\rangle. \tag{3.40}$$

By Lemma 20 $||\rho' - \rho||_1 \leq \varepsilon$. Because the trace distance is upper bound for the total variation distance of the measured distributions we have

$$\sum_x |\langle x|\rho'|x\rangle - \langle x|\rho|x\rangle| \leq \varepsilon. \tag{3.41}$$

However, the 1 norm is an upper bound for the 2 norm so we have

$$\||\psi_p\rangle - |\phi\rangle\| \leq \varepsilon. \tag{3.42}$$

By the triangle inequality on Eq. (3.39) and Eq. (3.42) we have

$$\||\psi'_p\rangle - |\phi\rangle\| \leq 2\varepsilon. \tag{3.43}$$

Let $\mathcal{F} = \beta^{-1} \log \mathrm{Tr}(e^{-\beta H})$ and $S(\rho) = -\mathrm{Tr}(\rho \log \rho)$ denote the free energy and the von Neumann entropy. Taking $\beta = \mathcal{O}(n\varepsilon^{-1})$ is sufficient to ensure that

$$|\mathrm{Tr}(\rho H) - F| \leq \frac{\varepsilon}{2} \tag{3.44}$$

and

$$|\lambda - F| \leq \frac{\varepsilon}{2} \tag{3.45}$$

and hence $|\mathrm{Tr}(\rho H) - \lambda| \leq \varepsilon$. Hence $\mathrm{Tr}(|\psi'_p\rangle\langle\psi'_p|H)$ is an additive error approximation of λ.

□

Note that the algorithm of Bravyi and Gosset uses a different Markov chain [JS89b] which also permits for the appearance of the stoquastic local terms $YY - XX$ and Z. Our proof requires the use of the Jerrum, Sinclair, and Vigoda chain [JSV04] because of the requirement to compute the marginals rather than just the partition function. We conjecture that some other techniques may be able to prepare all of the models considered in [BG17].

Conjecture 4. *It is possible to prepare the ground state of a Hamiltonian with nonnegative edge weights and local terms $XX + YY, YY - XX$, and Z in polynomial time on a quantum computer.*

We close this section with two corollaries extending Theorem 11 to antiferromagnetic Hamiltonians on bipartite graphs and to purifications of the Gibbs state.

Corollary 2 (Antiferromagnetic ground state for bipartite G)**.** *Consider the antiferromagnetic XY-model Hamiltonian*

$$H_A = \sum_{i,j} w_{i,j}(X_i X_j + Y_i Y_j). \tag{3.46}$$

Then an approximate ground state for H_A can be prepared with the same runtime and approximation guarantees as in Theorem 11.

Proof. Let $Z_A = \prod_{i \in A} Z_i$ be the unitary operator where Z acts on each qubit on the A side of the vertex partition. Then

$$H_{XY} = Z_A H Z_A. \tag{3.47}$$

Hence H_{XY} has the same ground state energy as H and the state $|\tilde{\psi}\rangle$ from Theorem 11 can be used to give an approximate ground state for H_{XY} because $Z_A|\tilde{\psi}\rangle$ satisfies

$$|\langle\tilde{\psi}|Z_A H_{XY} Z_A|\tilde{\psi}\rangle - \lambda| \leq \varepsilon. \tag{3.48}$$

□

Consider the thermofield double state

$$|\mathrm{TFD}\rangle = \frac{1}{\sqrt{\mathcal{Z}(\beta)}} \sum_{x \in \{0,1\}^n} e^{-\beta H/2} |x\rangle_L |x\rangle_R \tag{3.49}$$

on the Hilbert space $\mathcal{H}_L \otimes \mathcal{H}_R$ where each tensor factor is an n-qubit system. $|\text{TFD}\rangle$ is a purification of the thermal state ρ because

$$\text{Tr}_R\left(|\text{TFD}\rangle\langle\text{TFD}|\right) = \frac{e^{-\beta H}}{\mathcal{Z}(\beta)}. \tag{3.50}$$

Corollary 3 (Thermofield double state preparation)**.** *The thermofield double state $|TFD\rangle$ can be prepared with the same runtime and approximation guarantees as in Theorem 11.*

Proof. For a bitstring $xy \in \{0,1\}^{2n}$ the measured distribution is $q(xy) = \langle xy|\text{TFD}\rangle\langle\text{TFD}|xy\rangle$. For any bitstrings l and r of length $0 \leq i, j \leq n$ respectively, the marginal probability distribution is given by

$$\begin{aligned} q_{i,j}(l,r) &= \sum_{\substack{u\in\{0,1\}^{n-i} \\ v\in\{0,1\}^{n-j}}} \langle lurv|\text{TFD}\rangle\langle\text{TFD}|lurv\rangle \\ &= \text{Tr}\left(\left(|r\rangle\langle r| \otimes |l\rangle\langle l|\right)|\text{TFD}\rangle\langle\text{TFD}|\right) \\ &= \frac{1}{\mathcal{Z}(\beta)}\text{Tr}\big(|r\rangle\langle r|e^{-\beta H/2}|l\rangle\langle l|e^{-\beta H/2}\big). \end{aligned} \tag{3.51}$$

Then by Lemma 17, for a fixed $\varepsilon > 0$, there is an efficiently computable sequence of $K = \mathsf{poly}(\beta, n, \varepsilon^{-1})$ operators which act nontrivially as $h(t)$ such that

$$e^{(-\beta H+R)/2} = G_K \ldots G_2 G_1 \tag{3.52}$$

where $||R|| \leq \varepsilon/4$. Then the marginal probabilities for the measured distribution of the thermofield double state

$$|\text{TFD}'\rangle = \frac{1}{\text{Tr}(e^{-\beta H+R})} \sum_{x\in\{0,1\}^n} e^{(-\beta H+R)/2}|x\rangle_L|x\rangle_R \tag{3.53}$$

are given by

$$\frac{\text{Tr}(|r\rangle\langle r|G_K \ldots G_2 G_1|l\rangle\langle l|G_K \ldots G_2 G_1)}{\text{Tr}(e^{-\beta H+R})}. \tag{3.54}$$

This quotient of traces which can be approximated by Lemma 19. Hence an approximation $|\text{TFD}'\rangle$ which is close to $|\text{TFD}\rangle$ in the one-norm by Lemma 20 can be prepared via Lemma 12 with high probability. □

Hence the Gibbs state and ground state of some ferromagnetic XY models can be prepared efficiently on a quantum computer. The same holds for antiferromagnetic models defined on bipartite graphs.

3.2.2 Griffiths inequality

We now show that expectation values of certain Pauli observables with respect to Gibbs states of ferromagnetic systems satisfy a nonnegativity condition known as a Griffiths inequality [Gri67]. The results are more naturally stated in terms of the X and Z operators, but these Hamiltonians are unitarily equivalent to the ferromagnetic XY Hamiltonians considered above. Let

$$K = \sum_{i,j} \left(-a_{ij} X_i X_j - b_{ij} Z_i Z_j\right)$$

where $b_{ij}, a_{ij} \geq 0$. Let $B = \mathrm{CNOT}(H \otimes I)$ be the two qubit unitary which maps from the computational to the Bell basis.

Lemma 21 ([BLU16])**.** *The $2n$-qubit Hamiltonian $K' = B^{\dagger\otimes n}\left(K \otimes I + I \otimes K\right) B^{\otimes n}$ is stoquastic.*

In the following we write $X(s) = \prod_j X_j^{s_j}$ and $Z(r) = \prod_j Z_j^{r_j}$.

Theorem 12. *Let $\rho = e^{-\beta K}/\mathcal{Z}(\beta)$ be the Gibbs state of K at inverse temperature β. Then*

$$\mathrm{Tr}(\rho Z(r) X(s)) \geq 0$$

for all $r, s \in \{0,1\}^n$.

Proof. Consider the Gibbs state of the Hamiltonian

$$K' = B^{\dagger\otimes n}\left(K \otimes I + I \otimes K\right) B^{\otimes n}$$

at inverse temperature $\beta/2$. Up to a positive normalizing constant that will not be important to us, it is

$$\rho' = B^{\dagger\otimes n}\left(e^{-\beta/2K} \otimes e^{-\beta/2K}\right) B^{\otimes n}.$$

From Lemma 21 we have

$$\langle y|\rho'|x\rangle \geq 0 \qquad x, y \in \{0,1\}^{2n}.$$

Applying this equation with $x = 0^{2n}$ and $y = rs$ for some strings $r, s \in \{0,1\}^n$ and using the fact that

$$B^{\otimes n}|rs\rangle = X(s)Z(r)|\Phi_n\rangle \qquad |\Phi_n\rangle = \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle|x\rangle,$$

we get

$$\begin{aligned} 0 \leq \langle rs|\rho'|0^{2n}\rangle &= \langle \Phi_n| Z(r)X(s)\left(e^{-\beta/2K} \otimes e^{-\beta/2K}\right)|\Phi_n\rangle && (3.55)\\ &= \frac{1}{2^n} \sum_{t,u\in\{0,1\}^n} \langle t|Z(r)X(s)e^{-\beta/2K}|u\rangle\langle t|e^{-\beta/2K}|u\rangle && (3.56)\\ &= \frac{1}{2^n}\mathrm{Tr}(Z(r)X(s)e^{-\beta K}), && (3.57) \end{aligned}$$

where we used the fact that $\langle t|e^{-\beta/2K}|u\rangle = \langle u|e^{-\beta/2K}|t\rangle$. □

Considering $U = HSH$ which satisfies $UXU^\dagger = X$, $UYU^\dagger = Z$, and $UZU^\dagger = -Y$ gives $\mathrm{Tr}(\rho_{XY} Z(r)) = -\mathrm{Tr}(\rho Y(r)) = i^{|r|}\mathrm{Tr}(\rho Z(r)X(r))$ where $\rho_{XY} = U^\dagger \rho U$.

3.3 Symmetric stoquastic Hamiltonians

In this section, we show how to compute the ground state energy and corresponding eigenvectors of a stoquastic local Hamiltonians with runtime that improves if the underlying interaction graph has a sufficiently rich automorphism group. Results are stated in terms of computing the minimum eigenvalue of a stoquastic Hamiltonian, but the statements also apply to computing the maximum eigenvalue of Hamiltonians with nonnegative matrix entries in a straightforward way.

Let $G = (V, E)$ be a graph with automorphism group $\mathcal{G}$. Fix a stoquastic 2-qubit Hamiltonian h which acts symmetrically on the two qubits and consider the Hamiltonian

$$H = \sum_{(i,j)\in E} h_{ij} \tag{3.58}$$

where h_{ij} acts as h on qubits i, j and trivially elsewhere. Then the ground energy of H can be computed efficiently if the action of $\mathcal{G}$ on $\{0,1\}^n$ has orbits satisfying conditions in the following theorem.

Theorem 13 (Maximum eigenvalue for 2-local stoquastic Hamiltonians)**.** *Consider the automorphism group $\mathcal{G}$ of G acting on $\{0,1\}^n$ by permuting the bits. If the ratios of the sizes of orbits $|\mathcal{G}\cdot x|/|\mathcal{G}\cdot y|$, canonical representatives of the quotient $\{0,1\}^n/\mathcal{G}$, and the canonical representative $\bar{x} \in \{0,1\}^n/\mathcal{G}$ of $x \in \{0,1\}^n$ can be computed in time T, then the minimum eigenvector coincides with that of a $k \times k$ matrix with entries computable in time $O(n^2T)$ where $k = |\{0,1\}^n/\mathcal{G}|$.*

This theorem can be used to compute the ground energy of Hamiltonians defined on starlike trees with nearly uniform arm lengths and also on double stars in polynomial time. For local terms $-|\phi_s\rangle\langle\phi_s| = -|00\rangle\langle 00| + s(|00\rangle\langle 11| + |11\rangle\langle 00|) + s^2|11\rangle\langle 11|$, the smallest two eigenvalues can be computed using the following techniques and assuming Conjecture 3.

For each element $\phi \in \mathcal{G}$ there is an associated unitary transformation U_ϕ which permutes the qubits according to ϕ. For any $x \in \{0,1\}^n$, an orbit state $|\mathcal{G}\cdot x\rangle$ can be defined with normalization factor related to the number of orbits or the number of stabilizers

$$|\mathcal{G}\cdot x\rangle = \frac{1}{\sqrt{|\mathcal{G}\cdot x|}} \sum_{y\in\mathcal{G}\cdot x} |y\rangle = \frac{1}{\sqrt{|\mathcal{G}||\mathcal{G}_x|}} \sum_{\phi\in\mathcal{G}} U_\phi|x\rangle. \tag{3.59}$$

The orbit states are an orthonormal basis for their span. It will be important to note that each U_ϕ commutes with H because for each local term we have

$$U_\phi^\dagger h_{ij} U_\phi = h_{\phi(i)\phi(j)} \tag{3.60}$$

and hence

$$U_\phi^\dagger H U_\phi = H \tag{3.61}$$

because ϕ is an automorphism. We can combine this with the nonnegative amplitudes to get the following lemma.

Lemma 22. *Let $|\psi\rangle$ be an eigenvector of H with eigenvalue λ and nonnegative real amplitudes in the standard basis. Then there is a state $|\mathcal{G}\cdot\psi\rangle$ which is a nonnegative linear combination of orbit states $|\mathcal{G}\cdot x\rangle$ which is an eigenvector of H with eigenvalue λ.*

Proof. By assumption, we have

$$|\psi\rangle = \sum_{x\in\{0,1\}^n} p_x|x\rangle \tag{3.62}$$

for some $p_x \geq 0$. Then consider the state

$$|\mathcal{G}\cdot\psi\rangle = \frac{1}{\sqrt{N}}\sum_{\phi\in\mathcal{G}} U_\phi|\psi\rangle \tag{3.63}$$

where $\sqrt{N}$ is a normalization factor. Note that the sum is not zero because all of the coefficients are nonnegative real numbers with at least one strictly positive. Then each term in the sum in Eq. (3.63) is an eigenstate with eigenvalue λ because H is invariant under conjugation by U_ϕ and

$$\begin{aligned} HU_\phi|\psi\rangle &= U_\phi H U_\phi^\dagger U_\phi|\psi\rangle \\ &= \lambda U_\phi|\psi\rangle. \end{aligned} \tag{3.64}$$

Hence $|\mathcal{G}\cdot\psi\rangle$ is an eigenvector of H with eigenvalue λ. Furthermore, $|\mathcal{G}\cdot\psi\rangle$ is a nonnegative linear combination of orbit states because

$$\begin{aligned} |\mathcal{G}\cdot\psi\rangle &= \frac{1}{\sqrt{N}}\sum_{\phi\in\mathcal{G}} U_\phi|\psi\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{\phi\in\mathcal{G}}\sum_{x\in\{0,1\}^n} U_\phi p_x|x\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{x\in\{0,1\}^n} p_x \sum_{\phi\in\mathcal{G}} U_\phi|x\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{x\in\{0,1\}^n} p_x|\mathcal{G}_x|\sum_{y\in\mathcal{G}\cdot x}|y\rangle \\ &= \frac{1}{\sqrt{N}}\sum_{x\in\{0,1\}^n} p_x\sqrt{|\mathcal{G}||\mathcal{G}_x|}|\mathcal{G}\cdot x\rangle \end{aligned} \tag{3.65}$$

where the last line uses the orbit-stabilizer theorem. Hence we can write

$$|\mathcal{G}\cdot\psi\rangle = \sqrt{\frac{|\mathcal{G}|}{N}}\sum_{\bar{x}\in\{0,1\}^n/\mathcal{G}}\sqrt{|\mathcal{G}_{\bar{x}}|}\left(\sum_{x\in\mathcal{G}\cdot\bar{x}} p_x\right)|\mathcal{G}\cdot\bar{x}\rangle \tag{3.66}$$

which is a nonnegative linear combination of orbit states as desired. □

To prove Theorem 13, we also need to compute the matrix elements of H in the orbit basis.

Lemma 23. *The matrix element $\langle \mathcal{G}\cdot y|H|\mathcal{G}\cdot x\rangle$ can be computed in time $O(n^2T)$ if there are algorithms to determine the ratios of the sizes of orbits $|\mathcal{G}\cdot x|/|\mathcal{G}\cdot y|$ and determine the canonical representative $\bar{x}$ of a bitstring $x\in\{0,1\}^n$ in time T.*

Proof. We compute quantities $H|\mathcal{G}\cdot x\rangle$ as

$$\begin{aligned} H|\mathcal{G}\cdot x\rangle &= \frac{1}{\sqrt{|\mathcal{G}\cdot x|}}\sum_{y\in\mathcal{G}\cdot x} H|y\rangle \\ &= \frac{1}{\sqrt{|\mathcal{G}\cdot x||\mathcal{G}_x|}}\sum_{\phi\in\mathcal{G}} HU_\phi|x\rangle \\ &= \frac{1}{\sqrt{|\mathcal{G}||\mathcal{G}_x|}}\sum_{\phi\in\mathcal{G}} U_\phi H|x\rangle \end{aligned} \tag{3.67}$$

Because H is a local Hamiltonian defined by an interaction graph, $H|x\rangle = \sum_i c_i|z_i\rangle$ is supported on $O(n^2)$ many bitstrings c_i. For each z_i compute the canonical representative $\bar{z}_i$ in time T. Next determine if they are part of the same orbit as y by computing $\bar{y}$ in time T. Finally compute the ratio $|\mathcal{G}\cdot x|/|\mathcal{G}\cdot y|$ in time T and then

$$\begin{aligned} \langle \mathcal{G}\cdot y|H|\mathcal{G}\cdot x\rangle &= \sqrt{\frac{|\mathcal{G}||\mathcal{G}_y|}{|\mathcal{G}||\mathcal{G}_x|}}\sum_{i:\bar{z}_i=\bar{y}} c_i \\ &= \sqrt{\frac{|\mathcal{G}\cdot x|}{|\mathcal{G}\cdot y|}}\sum_{i:\bar{z}_i=\bar{y}} c_i. \end{aligned} \tag{3.68}$$

Hence Eq. (3.68) gives a formula for computing $\langle \mathcal{G}\cdot y|H|\mathcal{G}\cdot x\rangle$ in time $O(n^2T)$. □

We are now in position to prove Theorem 13.

Proof of Theorem 13. Let H be a 2-local stoquastic Hamiltonian with local terms which act symmetrically on the two active qubits. By the Perron-Frobenius theorem, H has an eigenvector $|\psi\rangle$ with minimum eigenvalue and nonnegative real amplitudes. Hence by Lemma 22, H has a ground state which is a nonnegative linear combination of orbit states. Then the ground state

$$\lambda = \max_{|v\rangle\in\mathrm{span}\{|\mathcal{G}\cdot\bar{x}\rangle\}} \frac{\langle v|H|v\rangle}{\langle v|v\rangle} \tag{3.69}$$

is also the minimum eigenvector of the $k\times k$ matrix with entries $\langle \mathcal{G}\cdot\bar{y}|H|\mathcal{G}\cdot\bar{x}\rangle$ and rows and columns indexed by the representatives of the orbits and $k=|\{0,1\}^n/\mathcal{G}|$. By Lemma 23 each matrix element can be computed in time $O(n^2T)$. □

Notice that if $|\{0,1\}^n/\mathcal{G}|$ and T defined in Theorem 13 are bounded by a polynomial, then Theorem 13 gives a polynomial time algorithm for computing the minimum eigenvalue and corresponding eigenvector in terms of orbit states. We close this section with some example applications of Theorem 13.

Example 1 (Uniform starlike trees)**.** *Fix a constant k. For each n consider the starlike tree G with $kn+1$ vertices which has n paths of length k attached to a central vertex. Then the automorphism group $\mathcal{G}$ is isomorphic to S_n and acts on the vertices by permuting the paths. For $m < 2^k$, let m_b denote the binary representation of m which is a string of length k by possibly adding trailing zeroes. The bitstrings*

$$x_0 0_b^{n_0} 1_b^{n_1} \dots (2^k-1)_b^{n_{2^k-1}} \tag{3.70}$$

where $n_0 + n_1 + \ldots + n_{2^k-1} = n$ are a set of canonical representatives for $\{0,1\}^{kn+1}/\mathcal{G}$. Hence the number of orbits is $O(n^{2^k})$. The corresponding canonical representative of x can be computed in time $O(n)$ by reading bits $i+1$ to $i+1+k$ as a number in binary for $i = 0, \ldots, k-1$. Then the size of each orbits is the number of unique ways that the length k blocks of bits can be permuted hence the ratio of sizes of orbits is

$$\frac{|\mathcal{G} \cdot x_0 0_b^{n_0} 1_b^{n_1} \dots (2^k-1)_b^{n_{2^k-1}}|}{|\mathcal{G} \cdot y_0 0_b^{m_0} 1_b^{m_1} \dots (2^k-1)_b^{m_{2^k-1}}|} = \prod_{i=1}^{2^k-1} \frac{m_i!}{n_i!}. \tag{3.71}$$

Then by Theorem 13 the minimum eigenvalue of 2-local symmetric stoquastic Hamiltonians corresponds to that of a matrix of size $O(n^{2^k})$ in n with entries computable in polynomial time in $O(2^k n^3)$.

For a starlike tree with n legs where only $O(1)$ many have length $O(1)$ not equal to k, the above algorithm can still be used to compute the maximum eigenvalue. We now consider double stars and complete graphs.

Example 2. *(Double stars) For each n consider the graph T_n which is an edge $e^* = (x_0, y_0)$ where each endpoint also has n leaves attached to it. Then the automorphism group $\mathcal{G}$ is generated by permuting the vertices of each half individually and by exchanging the vertices appearing in each star. We consider this group acting on $\{0,1\}^{2(n+1)}$ with elements $x_0 x_1 \dots x_n y_0 y_1 \dots y_n$. Hence there are $2(n+1)n$ canonical representatives $x_0 1^k 0^{n-k} y_0 1^m 0^{n-m}$ where $k \leq m$. By computing the hamming weights $|x_1 x_2 \dots x_n|$ and $|y_1 y_2 \dots y_n|$, the canonical representative of any string $x_0 x_1 \dots x_n y_0 y_1 \dots y_n$ can be computed in time $O(n)$. Finally, the ratios of the orbits are*

$$\frac{|\mathcal{G} \cdot x_0 x y_0 y|}{|\mathcal{G} \cdot z_0 z w_0 w|} = \frac{|z|!(n-|z|)!|w|!(n-|w|)!}{|x|!(n-|x|)!|y|!(n-|y|)!} \tag{3.72}$$

Hence by Theorem 13 there is a matrix with $O(n^2)$ rows and columns with entries computable in time $O(n^3)$ with minimum eigenvalue and eigenvector corresponding to that of a stoquastic local Hamiltonian H with interaction graph T_n.

Example 3 (Complete graphs)**.** *For each n consider the complete graph K_n. The automorphism group is S_n with canonical representatives of $\{0,1\}^n/\mathcal{G}$ given by the bitstrings $0^k 1^{n-k}$. For any x, the canonical representation can be computed in time $O(n)$ and for any $x, y \in \{0,1\}^n$ we have*

$$\frac{|S_n \cdot x|}{|S_n \cdot y|} = \frac{|y|!(n-|y|)!}{|x|!(n-|x|)!} \tag{3.73}$$

where $|\cdot|$ is the Hamming weight. By Theorem 13 the minimum eigenvalue of a 2-local stoquastic Hamiltonian defined on K_n is equal to that of an $(n+1)\times(n+1)$ matrix with entries computable in time $O(n^3)$.

When H preserves Hamming weight, then the symmetry-reduced Hamiltonian is diagonal in the orbit basis and the maximum eigenvector and corresponding eigenvector can be computed by solving the optimization

$$\max_{\bar{x}\in\mathcal{G}/\{0,1\}^n} \langle \mathcal{G}\cdot\bar{x}|H|\mathcal{G}\cdot\bar{x}\rangle \tag{3.74}$$

which can often be computed by hand.

Finally, the number of orbits $|\{0,1\}^n/\mathcal{G}|$ can be computed using Burnside's lemma.

Lemma 24. *(Burnside) Let $\mathcal{G}$ be a finite group acting on a finite set X. Let $X^g = \{x\in X : g\cdot x = x\}$ be the set of points fixed by g. Then*

$$|X/\mathcal{G}| = \frac{1}{|\mathcal{G}|}\sum_{g\in\mathcal{G}} |X^g|. \tag{3.75}$$

Note that Theorem 13 can be generalized to qudits with dimension d, hypergraphs with uniform edge size c, and directed graphs by acting on the set $[d]^n$, considering strictly c-local Hamiltonians, and adjusting the symmetry condition on the local terms accordingly.

3.4 Ising Hamiltonians

The Lee-Yang theorem [LY52] guarantees that the Gibbs state of the classical Ising model is in $LY(1)$ at any temperature. We show that a certain polynomial derived from powers of a deformed Ising model satisfies a similar zero-free condition.

For a graph $G=(V,E)$, consider the deformed Ising Hamiltonian

$$H(t) = \sum_{(i,j)\in E} (|00\rangle\langle 00| + t|11\rangle\langle 11|)_{ij}. \tag{3.76}$$

The following theorem shows that a suitably normalized $\mathrm{Tr}(H(t)^k)$ converges to $1+t^k$.

Theorem 14. *Fix a connected graph G with n vertices and m edges. For any $k\in\mathbb{N}$ consider the polynomial*

$$f_k(t) = \frac{1}{m^k}\mathrm{Tr}(H(t)^k) = c_{k,0} + c_{k,1}t + \ldots + c_{k,k}t^k. \tag{3.77}$$

Fix $\varepsilon>0$. Then there exists $K=\Omega(n^3\log(\varepsilon^{-1}))$ such that for $k\geq K$ we have

$$\begin{aligned} |c_{k,j}-1| &< \varepsilon, \text{ for } j=0,k \\ |c_{k,j}| &< \varepsilon \text{ for } 0<j<k. \end{aligned} \tag{3.78}$$

Proof. For any k-tuple of edges $(e_1, e_2, \ldots, e_k)$ let $\mathcal{C}(e_1, e_2, \ldots, e_k)$ denote the set of multisets C which partition $e_1, e_2, \ldots, e_k$ and induce connected subgraphs of G. Let each multiset have weight $|C|$ equal to the number of edges in C. Then $\mathrm{Tr}(H(t)^k)$ can be expanded as

$$\begin{aligned}\mathrm{Tr}(H(t)^k) &= \sum_{(e_1,e_2,\ldots,e_k)\in E^k} \mathrm{Tr}\big(\Pi_{j=1}^k |00\rangle\langle 00|_{e_j} + t|11\rangle\langle 11|_{e_j}\big) \\ &= \sum_{(e_1,e_2,\ldots,e_k)\in E^k} \mathrm{Tr}(\Pi_{C\in\mathcal{C}(e_1,e_2\ldots,e_k)} |0_C\rangle\langle 0_C| + t^{|C|}|1_C\rangle\langle 1_C|)\end{aligned} \tag{3.79}$$

Let $D \subseteq E^k$ denote the set of tuples for which $\mathcal{C}(e_1, e_2, \ldots, e_k)$ has multiple components. Since G is connected, any tuple of edges $e_1, e_2, \ldots, e_k$ which has multiple components avoids at least one edge in G. For each edge e^*, there are $(m-1)^k$ tuples in E^k which avoid e^*. Hence the number of edge sequences which have more than one component is bounded above by $m(m-1)^k$. Then the fraction of such sequences among all m^k tuples

$$\delta := \frac{|D|}{|E^k|} = \frac{|D|}{m^k} \leq m\left(\frac{m-1}{m}\right)^k \tag{3.80}$$

goes to zero exponentially with k. Then we can analyze the above polynomial in terms of tuples in and not in D

$$\mathrm{Tr}(H(t)^k) = \sum_{(e_1,e_2\ldots,e_k)\notin D} (t^k+1) + \sum_{(e_1,e_2,\ldots,e_k\in D)} \mathrm{Tr}\left(\prod_{C\in C(e_1,e_2,\ldots,e_k)} |0_C\rangle\langle 0_C| + t^{|C|}|1_C\rangle\langle 1_C|\right). \tag{3.81}$$

Each trace term is a sum of at most 2^n terms with coefficient 1. Hence the coefficients of $f_k(t) = m^{-k}\mathrm{Tr}(H(t)^k)$ satisfy

$$\begin{aligned} 1-\delta \leq c_{k,j} &\leq 1 && \text{for } j = 0, k \\ 0 \leq c_{k,j} &\leq 2^n\delta && \text{for } 0 < j < k.\end{aligned}$$

Taking $K = \Omega(n^3 \log(\varepsilon^{-1}))$ suffices to show that

$$\begin{aligned} |c_{k,j} - 1| < \varepsilon, \text{ for } j = 0, k \\ |c_{k,j}| < \varepsilon \text{ for } 0 < j < k.\end{aligned} \tag{3.82}$$

□

It can also be shown that for large m the roots of $\mathrm{Tr}(H(t)^k)$ are on the unit circle. In order to prove this, we introduce the notion of self-inversive polynomials.

Definition 2. *A polynomial $f(x) = c_0 + c_1 x + \ldots c_n x^n$ of degree n with complex coefficients is self-inversive if*

$$c_n = e^{i\theta} c_{n-k}^*, \text{ for all } k \in [n] \text{ and fixed } \theta \in \mathbb{R}. \tag{3.83}$$

Self-inversive polynomials with sufficiently large leading coefficient satisfy the following zero-free theorem.

Theorem 15 (Self-inversive zero-free condition [LL04])**.** *If the degree n polynomial $f(x) = c_0 + c_1 x + \ldots + c_n x^n$ is self-inversive and satisfies*

$$|c_n| \geq \frac{1}{2} \sum_{j=0}^{n-1} |c_j|, \tag{3.84}$$

then all roots of $f(x)$ are on the unit circle.

We can now show that for all sufficiently large exponents k, that $\mathrm{Tr}(H(t)^k)$ has roots on the unit circle.

Theorem 16. *Let G be a connected graph with n vertices. Then there exists a $K = \Omega(n^3)$ such that if $k \geq K$, then $f_k(t) = m^{-k}\mathrm{Tr}(H(t)^k) = c_{k,0} + c_{k,1}x + \ldots + c_{k,k}t^k$ has all zeros on the unit circle.*

Proof. Fix a connected graph G with n vertices. Each local term satisfies

$$|00\rangle\langle 00| + t|11\rangle\langle 11| = tX \otimes X(|00\rangle\langle 00| + t^{-1}|11\rangle\langle 11|)X \otimes X. \tag{3.85}$$

Hence by conjugating each factor $H(t)$ by $X^{\otimes n}$ we have $t^k \mathrm{Tr}(H(t^{-1})^k) = \mathrm{Tr}(H(t)^k)$. Hence $f_k(t)$ is self-inversive. Because $f(x)$ has only non-negative coefficients we have

$$\sum_{j=0}^{n} |c_{k,j}| = \sum_{j=0}^{n} c_{k,j} = f_k(1). \tag{3.86}$$

Let $D \subseteq E^k$ be the set of tuples with more than one connected component and define

$$\delta := \frac{|D|}{m^k} \tag{3.87}$$

Then we can bound $f_k(1)$ by using the expansion into components as above

$$\begin{aligned} f_k(1) &= \frac{1}{m^k}\mathrm{Tr}(H(1)^k) \\ &= \frac{1}{m^k} \sum_{(e_1,e_2,\ldots,e_k)\in E^k} \mathrm{Tr}(h_{e_1}(1)h_{e_2}(1)\ldots h_{e_k}(1)) \\ &= \frac{1}{m^k} \sum_{(e_1,e_2,\ldots,e_k)\in D} (1^k + 1) + \frac{1}{m^k} \sum_{(e_1,e_2\ldots,e_k)\notin D} \mathrm{Tr}(h_{e_1}(1)h_{e_2}(1)\ldots h_{e_k}(1)) \\ &\leq (1-\delta)\cdot 2 + \delta \cdot 2^n. \end{aligned} \tag{3.88}$$

Next we can bound $c_{k,k}$ from below. Since each sequence not in D contributes a term t^k/m^k to the sum, we have the following lower bound on $c_{k,k}$

$$c_{k,k} \geq 1 - \frac{|D|}{m^k} = 1 - \delta. \tag{3.89}$$

Because δ is bounded above by $m((m-1)/m)^k$, taking $K = \Omega(n^3)$ is large enough that so that $\delta < 1/(1+2^n)$ and we have

$$\begin{aligned} f_k(1) &\leq 2(1-\delta) + 2^n\delta \\ &< 3(1-\delta) \leq 3c_{k,k}. \end{aligned} \tag{3.90}$$

Because $f_k(1) = c_{k,0} + c_{k,1} + \ldots c_{k,k}$, Eq. (3.90) is the sufficient condition from Theorem 15. Hence for sufficiently large k, $\mathrm{Tr}(H(t)^k)$ has roots on the unit circle. □

Based on numerical evidence, we conjecure that the conclusion of Theorem 16 holds for all values of k.

Conjecture 5. *All roots of* $\mathrm{Tr}(H_{CF}(t)^k)$ *are on the unit circle for all graphs and all* $k \in \mathbb{N}$. *Here* H_{CF} *has local terms* $(1+t)(ZI+IZ) + (1-t)(II+ZZ)$ *as above.*

Numerical study 4. *We computed the roots of* $\mathrm{Tr}(H_{CF}(t)^k)$ *for various graphs* G *and exponents* k. *For graphs with* 4 *vertices, the conjecture is true when* $k \leq 64$. *For graphs with* 5 *vertices, the conjecture is true when* $k \leq 66$. *For graphs with* 6 *vertices, the conjecture is true when* $k \leq 23$ *and* $k = 30, 35, 40$. *For all graphs with* 7 *vertices, the conjecture is true for* $k \leq 10$ *and* $k = 15$. *For graphs with* 8 *vertices, the conjecture is true for* $k \leq 18$.

Finally, we investigate a similar conjecture for a quantum Hamiltonian. Recall the deformed EPR Hamiltonian from Section 3.1

$$H_s = \sum_{e \in E} (|00\rangle + s|11\rangle)(\langle 00| + s\langle 11|)_e. \tag{3.91}$$

One might hope based on the fact that the Lee-Yang theorem [LY52] can be generalized to quantum Hamiltonians as in the Suzuki-Fisher theorem [SF71] that Theorem 16 can be generalized to include some Suzuki-Fisher Hamiltonians. Based on small examples, one may be tempted to conjecture that an analogue of Theorem 16 holds for $H_E(s)$.

Conjecture 6. *All roots of* $\mathrm{Tr}(H_E(s)^k)$ *are on the unit circle for all graphs and all* k.

However, this conjecture can be falsified by explicit counterexample as below.

Numerical study 5. *We numerically computed the roots of* $\mathrm{Tr}(H_E(s)^k)$ *for various* k. *For all graphs with* $n \leq 5$ *and* $k \leq 20$, *all graphs with* 6 *vertices and* $k \leq 10$, *and all graphs with* 7 *vertices and* $k \leq 8$ *Conjecture 6 is true. For* 10^5 *random graphs with* $n \in [4, 10]$ *and* $k \leq 15$ *Conjecture 6 is true. However, for the graph with adjacency matrix*

$$\begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix} \tag{3.92}$$

and $k = 26$, $\mathrm{Tr}(H_E(s)^k)$ *has zeros off of the unit circle. The roots of this degree* 52 *polynomial were computed to* 1000 *decimal digits of accuracy. Hence Conjecture 6 is false.*

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Appendices

Appendix A

Markov chain Monte Carlo

The Markov chain Monte Carlo method is a paradigm for designing sampling algorithms by simulating random walks. We introduce notation for Markov chains and state the fundamental theorems used to bound the runtime of such algorithms. A general reference for Markov chains and their mixing times is [LPW09].

In this appendix only, Ω will always denote a finite set of states and $\mathbf{x} : \Omega \to \mathbb{R}_{\geq 0}$ a probability distribution. We view such distributions as vectors $\mathbf{x} \in \mathbb{R}^\Omega$ with components x_i for $i \in \Omega$. Linear operators P on such distributions have matrix elements P_{ij} in the standard basis $\{e_i\}_{i \in \Omega}$.

Definition 3 (Right stochastic matrix)**.** *An $n \times n$ nonnegative matrix P is a right stochastic matrix if each row sums to* 1*.*

This definition ensures that multiplication of a probability vector by a right stochastic matrix on the right yields another probability vector.

Definition 4 (Markov chain)**.** *Let Ω be a finite set and P a right stochastic matrix. The Markov chain defined by Ω and P with initial distribution $0 < \mathbf{x} \in \mathbb{R}^\Omega$ is the sequence of probability vectors $\{\mathbf{x}(t)\}_{t=0}^\infty$ defined by*

$$\mathbf{x}(t) = \mathbf{x}P^t. \tag{A.1}$$

We will also write $\mathcal{M} = (\Omega, P)$ to mean the Markov chain with state space Ω and transition matrix P where $\mathbf{x}$ will be provided as an initial condition.

Definition 5 (Ergodicity)**.** *A Markov chain $\mathcal{M} = (\Omega, P)$ is ergodic if there is a probability vector $\pi > 0$ such that for any distribution $\mathbf{x} > 0$,*

$$\lim_{s \to \infty} \mathbf{x}P^s = \pi. \tag{A.2}$$

The distribution π is known as the stationary distribution of the Markov chain. Let $\mathcal{M} = (\Omega, P)$ be a Markov chain. It is known that the following conditions imply ergodicity.

1. (Irreducible) for any $i, j \in \Omega$ there is some s such that $P_{ij}^s \neq 0$, and
2. (Lazy) for any $i \in \Omega$, $P_{ii} \geq 1/2$.
3. (Reversible) there is a distribution $\pi > 0$ such that for any $i, j \in \Omega$ the detailed balance condition
$$P_{ij}\pi_i = P_{ji}\pi_j \tag{A.3}$$
is satisfied.

All Markov chains we consider will be irreducible, lazy, and reversible. From the classical theory of Markov chains, these conditions imply that P has nonnegative eigenvalues, that there is a unique eigenvector with with maximum eigenvalue 1, and that if a distribution satisfies the detailed balance condition that it must be the stationary distribution. The Perron-Frobenius theorem is the main tool for reasoning about the spectrum of a nonnegative matrix.

Definition 6 (Directed graph of a matrix)**.** *Every $n \times n$ square matrix A has underlying directed graph X with vertex set $[n]$ and an arc from i to j if $A_{ij} \neq 0$.*

Theorem 17 (Perron-Frobenius [GR01])**.** *Suppose that A is a real nonnegative $n \times n$ matrix whose underlying directed graph is strongly connected. Then the eigenvalue of A with largest magnitude is simple and the corresponding eigenvector can be taken to have all entries strictly positive.*

We are interested in how many steps of simulation are required to sample from a distribution which approximates the stationary distribution of the Markov chain.

Definition 7 (Total variation distance)**.** *The total variation distance between two distributions $\mathbf{p}, \mathbf{q} : \Omega \to \mathbb{R}_{\geq 0}$ is defined as*
$$||\mathbf{p} - \mathbf{q}||_{\mathrm{TV}} = \frac{1}{2}\sum_{i \in \Omega} |p_i - q_i| \tag{A.4}$$

Definition 8 (Mixing time)**.** *Let $\varepsilon > 0$ be a real parameter. The mixing time is the shortest time for which simulation approaches the stationary distribution from the standard basis vector $\mathbf{e}_i$ for $i \in \Omega$*
$$t_i(\varepsilon) = \min\{t \in \mathbb{N} : \|\mathbf{e}_i P^t - \pi\|_{\mathrm{TV}} \leq \varepsilon\} \tag{A.5}$$

The two main methods for proving an upper bound on the mixing time of a Markov chain are to estimate the conductance or to estimate the multicommodity flow. These methods are intimately related to the spectral gap of the transition matrix. Suppose that the transition matrix P has eigenvalues λ_i for $1 \leq i \leq |\Omega|$ with $1 = \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{|\Omega|}$. Then the spectral gap is defined as $1 - \lambda_2$.

Theorem 18 (Spectral bound [Sin92])**.** *For any $i \in \Omega$, the mixing time is bounded above as*
$$t_i(\varepsilon) \leq (1 - \lambda_2)^{-1}(\ln(\pi_i^{-1}) + \ln(\varepsilon^{-1})) \tag{A.6}$$
and bounded below as
$$\max_{x \in \Omega} t_x(\varepsilon) \geq \lambda_2(1 - \lambda_2)^{-1} \ln((2\varepsilon)^{-1})/2. \tag{A.7}$$

In general, it is difficult to give a tight estimate of the spectral gap directly. Instead, it is customary to estimate a structural property of the graph known as the conductance. Because of the detailed balance equation Eq. (A.3), we can define weights $w_{ij} = P_{ij}\pi_i = P_{ji}\pi_j$. Then the conductance Φ is

$$\Phi = \min_{S \subseteq \Omega} \frac{W(S, \overline{S})}{\pi(S)\pi(\overline{S})} \tag{A.8}$$

where $\pi(S) = \sum_{i \in S} \pi_i$ and $W(S, \overline{S}) = \sum_{i \in S, j \notin S} w_{ij}$.

Theorem 19 (Conductance bound [Sin88, JS88, JS89a, JSV04])**.** *For an irreducible, lazy, reversible Markov chain with state space Ω and transition matrix P*

$$t_x(\varepsilon) \leq \frac{2}{\Phi^2}(\ln(\pi_x^{-1}) + \ln(\varepsilon^{-1})). \tag{A.9}$$

One strategy for giving a lower bound on the conductance is to define a set of canoncial simple paths $\Gamma = \{\Gamma_{xy}\}_{x,y \in \Omega}$ from which the associated congestion

$$\rho(\Gamma) = \max_{(i,j) \in E} w_{ij} \sum_{(x,y) \in \Gamma_{ij}} \pi_x \pi_y \tag{A.10}$$

can be calculated. Then the following bound can be used in conjunction with Theorem 19.

Theorem 20 (Canonical paths bound [JS88, Sin92])**.** *An irreducible, lazy, reversible Markov chain with canonical paths Γ satisfies*

$$\Phi \geq \frac{1}{2\rho(\Gamma)}. \tag{A.11}$$

We present two Markov chains which are known to be rapidly mixing. The first is due to Jerrum and Sinclair [JS89b] and has an important place in the history of rapidly mixing Markov chains and designing approximation algorithms for the permanent. The second chain is due to Anari, Gharan, and Rezaei [AOGR16], and derives a bound on the spectral gap by using a zero-free region.

We begin with the task of sampling from perfect and near-perfect matchings almost uniformly. Given a graph $G = (V, E)$ with $2n$ vertices, denote the set of matchings of size $i \in [n]$ as M_i. Consider the Markov chain $\mathcal{M}_{\text{pm}}(G)$ with state space $\Omega_{\text{pm}} = M_n(G) \cup M_{n-1}(G)$ and transitions as follows. In any state, $M \in \Omega_{\text{pm}}$ stay in state M with probability $1/2$, otherwise select an edge $e = (u, v) \in E$ uniformly at random and

(i) if $M \in M_n(G)$ and $e \in M$, transition to the state $M - e$,

(ii) if $M \in M_{n-1}(G)$ and u, v are both unmatched, transition to the state $M + e$,

(iii) if $M \in M_{n-1}(G)$ and exactly one of u, v is matched in edge $f \in M$, then transition to the state $M + e - f$,

(iv) otherwise, do nothing.

As a consequence of irreducibility, laziness, and reversibility, it can be shown that the stationary distribution of $\mathcal{M}_{\text{pm}}$ is uniform on Ω_{pm}. Jerrum and Sinclair use the canonical paths method to show that whenever $M_n(G) \neq \emptyset$ the conductance is bounded below as

$$\Phi \geq \frac{1}{16|E|} \left(\frac{|M_n(G)|}{|M_{n-1}(G)|} \right)^2. \tag{A.12}$$

From which a bound on the runtime of sampling can be derived.

Theorem 21 (Sampling large matchings [JS89b])**.** *Let $G = (V, E)$ be a graph with $|V| = 2n$ and $M_n(G) \neq \emptyset$. Then if there is a polynomial q such that the bound*

$$\left| \frac{M_{n-1}(G)}{M_n(G)} \right| \leq q(n) \tag{A.13}$$

holds, then the associated Markov chain $\mathcal{M}_{pm}$ mixes rapidly and (almost) uniform samples form $\Omega_{pm} = M_n(G) \cup M_{n-1}(G)$ can be computed in runtime $\mathsf{poly}(n)$.

For bipartite graphs, it can be shown that augmenting $\mathcal{M}_{\text{pm}}$ with a metropolis acceptance rule results in a rapidly mixing Markov chain for sampling (almost) uniform perfect matchings on any bipartite graphs [JSV04].

The second Markov chain we consider samples from strongly-Rayleigh distributions which have homogeneous support. Let $\mu : \{0,1\}^n \to \mathbb{R}_{\geq 0}$ be a probability distribution supported only on bitstrings of weight k. Consider the Markov chain $\mathcal{M}_{\text{sr}}$ with state space $\Omega_{\text{sr}} = \text{supp}\{\mu\}$ and transitions as follows. For any state $x \in \Omega_{\text{sr}}$ stay in state x with probability $1/2$, otherwise select a random indices $i \in \{k : x_k = 1\}$ and $j \in \{k : x_k = 0\}$ and let y be the bitstring with entries

$$y_k = \begin{cases} x_k & \text{if } k \notin \{i, j\} \\ x_k \oplus 1 & \text{if } k \in \{i, j\}, \end{cases} \tag{A.14}$$

(i) if $y \in \Omega_{\text{sr}}$, then transition to y with probability $(1/2)\min\{1, \mu(y)/\mu(x)\}$,

(ii) otherwise, do nothing.

Theorem 22 (Sampling from strong-Rayleigh distributions [AOGR16])**.** *If μ is a k-homogeneous Strong-Rayleigh distribution, then the Markov chain $\mathcal{M}_{sr}$ computes (almost) samples from μ in time* $\mathsf{poly}(n)$.

The proof of rapid mixing extends previous results on balanced matroids [FM92] and decomposable Markov chains [JSTV04].

Appendix B

Numerical methods

We review techniques from the numerical experiments in this thesis by presenting Python libraries and examples. Python is a powerful language for development due to its flexible syntax, extensive library support, and interactive development environments. However, the tradeoff for this convenience is that Python programs can have poor runtime performance. For this reason, expensive computational steps are handed over to Fortran and C libraries through standard Python interoperation facilities. For performance intensive tasks, we mostly use software appearing in the netlib family of packages. The GNU scientific library [GDT+21] is an alternative to netlib if native C++ support is preferred. Other useful Python packages for numerics in quantum computing that were used in this project are mpnum for tensor networks [ZMP] and CVXPY for optimization [DB16].

B.1 Linear algebra

NumPy [HMv+20] is a C-based array programming library for Python. In addition to array creation and manipulation, NumPy includes standard linear algebra functionality such as solving systems of linear equations and matrix decompositions.

```
1 import numpy as np
2
3 # define the Pauli X matrix
4 x = np.array([[0,1],[1,0]])
5
6 # compute the eigenvalues and eigenvectors
7 np.linalg.eig(x)
```

Listing B.1: NumPy example

SciPy [VGO+20] extends NumPy with functionality that is useful for scientific computing. SciPy provides an interface to the Fortran library ARPACK [LSY98] which implements the Arnoldi method for computing eigenvalues and eigenvectors of large sparse matrices. In the Arnoldi method, the matrix A need only be specified through a subroutine which calculates $v \mapsto Av$ for any vector v in the domain. This feature can save on both runtime and memory by allowing users to provide matrices in a sparse formats or even as a subroutines.

```
import scipy

# define the Pauli X matrix in sparse format
x = scipy.sparse.coo_matrix(([1.0,1.0],([0,1],[1,0])),shape=(2,2))

# compute the maximum eigenvalue and eigenvector
scipy.sparse.linalg.eigsh(x,k=1)
```

Listing B.2: Sparse diagonalization

ARPACK allows users to specify their desired performance characteristics through optional parameters by providing the error tolerance, the number of eigenvalues required, whether eigenvectors should be saved for output, and the size of the auxiliary subspace used in the solution. Purported eigenvectors can be validated through matrix multiplication.

B.2 Polynomial roots

The roots of univariate polynomials can be computed with the mpmath library [mdt23]. Polynomials are specified as lists of coefficients. Whether the first element of the list is the leading coefficient or the constant term depends on the version of mpmath.

```
from mpmath import mp

# define the polynomial x^2 + 1
my_poly = [1,0,1]

# compute the roots
roots = mp.polyroots(my_poly)

# validate one of the roots by evaluating the polynomial
mp.polyval(my_poly,roots[0])
```

Listing B.3: Solving a univariate polynomial with mpmath.

B.3 Graphs

B.3.1 Generating graphs with geng

It can be useful to verify conjectures on graphs exhaustively with numerics. The geng executable from Nauty and Traces [MP13] can be used to efficiently output all graphs with edge, vertex, and connectivity constraints specified by the user.

```
> ./geng -c 10 9:9 > tree10.txt
```

Listing B.4: Generating all trees with 10 vertices using geng.

B.3.2 Graph manipulations with NetworkX

NetworkX [HSS08] can be used to manipulate graphs including changing their, format, structure, and checking for isomorphism.

```
import networkx as nx

# read graphs in
graphs = nx.read_graph6("filepath/file.txt")

# check for isomorphism
nx.is_isomorphic(graphs[0],graphs[1])
nx.is_isomorphic(graphs[0],graphs[0])

# convert to numpy array
nx.to_numpy_array(graphs[0])
```

Listing B.5: Reading converting and checking for graphs for isomorphism.

B.4 Performance

B.4.1 High precision computing with mpmath

When higher numerical precision is required, the simplest solution is to increase the number of decimal places used in the calculations at the cost of performance. The mpmath library [mdt23] provides support for arbitrary precision real and complex floating point numbers.

```
from mpmath import mp

# set precision
mp.dps = 100
mp.prec = 400

# compare the difference in precision!
1/10 + 2/10
mp.mpf(1)/10 + mp.mpf(2)/10
```

Listing B.6: High precision arithmetic with mpmath.

B.4.2 High performance computing with Numba

Code which makes heavy use of NumPy can be compiled to LLVM using the Numba just-in-time compiler [LPS15]. In some cases this can offer a dramatic increase in performance.

```
import numpy as np
from numba import njit

# some long vector
```

```
v = np.arange(100000)

# decorate a function with @njit
@njit
def sum_of_squares(x):
  acc = 0
  for i in range(x.shape[0]):
    acc = acc + x[i]**2
  return acc

# evaluating the function for the first time cause numba to compile the
    function
sum_of_squares(v)
```

Listing B.7: Using the Numba JIT compiler.

B.4.3 Parallel computation

Program runtime can be reduced by using multiple cores. When there is no shared memory or state, it is easy to take advantage of multiple cores. The Python standard library provides a parallel map in the multiprocessing library.

```
from multiprocessing import Pool

# function to compute on many independent inputs
def inc(x):
  return x + 1

# parallel execution of inc
with Pool(12) as p:
  p.map(inc,range(10000))
```

Listing B.8: Applying a function to many arguments in parallel with multiprocessing.

B.4.4 Remote access CPUs

The faculty of mathematics at the University of Waterloo provides students with high performance, many-core computers for running computationally intensive tasks. Graduate students in the faculty of mathematics can access these machines remotely using ssh.

```
> ssh (watiam)@cpu(number).math.private.uwaterloo.ca
```

Listing B.9: Accessing the school computers. Here (watiam) should be replaced with a valid WatIAM identification and (number) is the number of the cpu listed at https://howbusy.math.uwaterloo.ca.

Long jobs should be run using `nohup nice (executable) & top -u (watiam)` in order to prevent the server from lagging and to ensure that the computation has started properly. Processes taking an unexpected amount of resources can be terminated with the `pkill` command.

B.5 Data

B.5.1 Storing data

Output data from computations can be serialized and stored in files. The Python standard library includes facilities for storing data in the widely compatible JSON format or in the compact and idiomatic pickle format.

```
import pickle
import json

data = [0,1,2,3,4,5]

# store the data using pickle
f = open("file.pkl","ab")
pickle.dump(data,f)
f.close()

# read the pickle data
f = open("file.pkl","rb")
pickle.load(f)
f.close()

# store the data using json
f = open("file.json","w")
json.dump(data,f)
f.close()

# read the json data
f = open("file.json","r")
json.load(f)
f.close()
```

Listing B.10: Writing and reading data to files.

B.5.2 Plotting data with matplotlib

Data can be plotted in Python using matplotlib [Hun07].

```
import matplotlib.pyplot as plt

def plot():
    # scatter some points
    scatter_x = list(range(-3,4))
    scatter_y = [-2,-1,0,1,0,-1,-2]
    plt.scatter(scatter_x,scatter_y,color='r',label="mountain",marker="x")

    # plot a parabola
    parabola_x = list(map(lambda x:x/100,range(-300,301)))
    parabola_y = list(map(lambda x:x**2-3,parabola_x))
    plt.plot(parabola_x,parabola_y,label="parabola")
```

```
13
14      # plot a shape
15      circle = plt.Circle((0,0),1,color="g",alpha=0.5,label="circle")
16      fig = plt.gcf()
17      ax = fig.gca()
18      ax.add_patch(circle)
19      ax.set_box_aspect(1)
20
21      # plot parameters
22      plt.legend(loc="upper right")
23      plt.xlim(-3,3)
24      plt.ylim(-3,3)
25      plt.xlabel("x axis")
26      plt.ylabel("y axis")
27      plt.title("Example plot")
28
29      # save and close plot
30      plt.savefig("example.png")
31      plt.close()
32      return
```

Listing B.11: Plotting data with matplotlib.

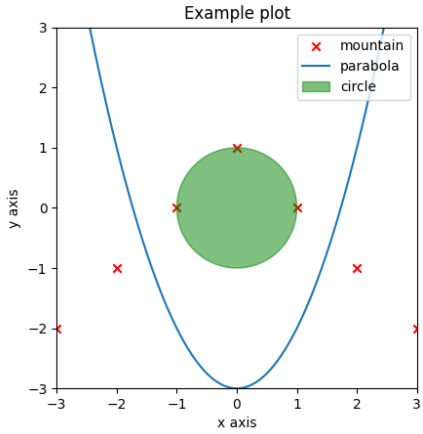


Figure B.1: Plot produced by the code in Listing B.11 featuring points, lines, and shapes.

B.6 Symbolic calculation

Sagemath [The22] amalgamates and extends NumPy, SciPy, matplotlib, and other mathematical tools in order to deliver a consistent interface for programmers. Syntactically, Sagemath is a dialect of Python which uses ^ instead of ** for exponentiation. Complex symbolic variables can be used to simplify programs. There are many algebraic features for symbolic expressions included in Sagemath. Symbolic calculations are often inefficient, but they are easy to write and reason about. A symbolic calculation can often be used to benchmark the accuracy of a faster program which is harder to understand.

```
# define a symbolic variable
z = PolynomialRing(ComplexField(),'z').gen()

# factor a symbolic polynomial
my_poly = z^2+2*z+1
my_poly.factor()
```

Listing B.12: Defining and using a symbolic variable in Sagemath.