Chapter 1

Ground energy of multi-particle quantum walk

1.1   Introduction

With our proof that the ground state problem for a single-particle quantum walk is QMA-complete, we would now like to examine the corresponding problem for the multi-particle quantum walk. The similarities between the two systems make us expect that very similar results will hold for the multi-particle case, but we will again need to examine the problem in a lot of detail.

In particular, the QMA-completeness for the single particle walk was relatively straightforward, in that there is really only one particle to deal with. Because of this, we understand the dynamics and can exactly analyze the system on which things interact, leading to exact solutions for the energies of the resulting Hamiltonian. With the MPQW, a full analysis is currently beyond our knowledge, and our universality construction relied on a reduction to the cases with at most two interacting particles. In order to show that finding the ground energy of a MPQW is QMA-complete using our techniques, we'd need to again reduce to the case of a small number of particles.

To make this reduction, we will show that the problem is QMA-hard when restricted to the problem where the interaction term adds (almost) no energy to the ground state, so that the ground state is contained within the span of single-particle states that don't overlap. With this restriction, we will still have correlations between many particles, but we will be able to analyze the correlations and determine the corresponding ground energy.

1.2   MPQW Hamiltonian ground-energy problem

In order to make things precise, we will fix a particular finite-range interaction, and show that with this fixed interaction, the resulting question is QMA-complete to solve. In particular let $\mathcal{U}$ be an interaction with finite support and no negative coefficients. For a particular graph G, we can then define a Hamiltonian on such a graph as [**TO DO:** *find a correct way*

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to define $\mathcal{U}$]

$$H_{f,G} = \sum_{(i,j)\in E(G)} a_i a_j + a_j a_i + \sum_{i,j \in V(G)} U_{d(i,j)}(n_i, n_j) = H_{G,\text{move}} + H_{G,\text{int}}. \qquad (1.1)$$

Note that because of the positivity restrictions placed on $\mathcal{U}$, we have that $H_{G,\text{int}}$ is positive semi-definite, and thus the ground energy of $H_{f,G}$ is at least the ground energy of $H_{G,\text{move}}$.

With this particular interaction, we can then construct the corresponding problem.

Note that these Hamiltonians actually act on an infinite dimensional Hilbert space, in that the number of particles is unbounded. In order to reduce the complexity of these problems to a reasonable amount, we restrict our attention to a particular number of particles. Once again, as each term in the Hamiltonian preserves the number of particles, we have that $H_{\mathcal{U},G}$ decomposes into blocks with a particular particle number, and we represent these blocks as $\overline{H}_{\mathcal{U},G}^N$.

Problem 1 ($\mathcal{U}$-interaction MPQW Hamiltonion)**.** Given as input a K-vertex graph G, a number of particles N, a real number c, and a precision parameter $\epsilon = 1/T$, where the positive integers N and T are given in unary, and the graph G is given as its adjacency matrix (a $K \times K$ symmetric 0-1 matrix), the $\mathcal{U}$-interaction MPQW Hamiltonian problem is to determine whether the smallest eigenvalue of $\overline{H}_{\mathcal{U},G}^N$ is at most c or is at least $c + \epsilon$, with a promise that one of these two cases hold.

1.2.1   MPQW Hamiltonian is contained in QMA

To prove that $\mathcal{U}$-interaction MPQW Hamiltonian problem is contained in QMA, we provide a verification algorithm satisfying the requirements of Definition **??**. In the Definition this algorithm is specified by a circuit involving only one measurement of the output qubit at the end of the computation. The procedure we describe below, which contains intermediate measurements in the computational basis, can be converted into a verification circuit of the desired form by standard techniques.

We are given an instance specified by G, N, c, and ϵ. We are also given an input state $|\phi\rangle$ of n_{input} qubits, where $n_{\text{input}} = \lceil \log_2 D_N \rceil$ and D_N is the dimension of $\mathcal{Z}_N(G)$ as given in equation (**??**). Note, using the inequality $\binom{a}{b} \le a^b$ in equation (**??**), that $n_{\text{input}} = \mathcal{O}(K \log(N + K))$, where $K = |V|$ is the number of vertices in the graph G. We embed $\mathcal{Z}_N(G)$ into the space of n_{input} qubits straightforwardly as the subspace spanned by the first D_N standard basis vectors (with lexicographic ordering, say). The first step of the verification procedure is to measure the projector onto this space $\mathcal{Z}_N(G)$. If the measurement outcome is 1 then the resulting state $|\phi'\rangle$ is in $\mathcal{Z}_N(G)$ and we continue; otherwise we reject.

In the second step of the verification procedure, the goal is to measure $\bar{H}_G^N$ in the state $|\phi'\rangle$. The Hamiltonian $\bar{H}_G^N$ is sparse and efficiently row-computable, with norm

$$\left\| \bar{H}_G^N \right\| \le \left\| H_G^N \right\| \le N \left\| A(G) \right\| + \left\| \sum_{k \in V} \hat{n}_k (\hat{n}_k - 1) \right\| \le NK + N^2.$$

We use phase estimation (see for example [**?**]) to estimate the energy of $|\phi'\rangle$, using sparse Hamiltonian simulation [**?**] to approximate evolution according to $\bar{H}_G^N$. We choose the pa-

rameters of the phase estimation so that, with probability at least $\frac{2}{3}$, it produces an approx-imation E of the energy with error at most $\frac{\epsilon}{4}$. This can be done in time poly($N, K, \frac{1}{\epsilon}$). If $E \leq c + \frac{\epsilon}{2}$ then we accept; otherwise we reject.

We now show that this verification procedure satisfies the completeness and soundness requirements of Definition **??**. For a yes instance, an eigenvector of $\bar{H}_G^N$ with eigenvalue $e \leq c$ is accepted by this procedure as long as the energy E computed in the phase estimation step has the desired precision. To see this, note that we measure $|E - e| \leq \frac{\epsilon}{4}$, and hence $E \leq c + \frac{\epsilon}{4}$, with probability at least $\frac{2}{3}$. For a no instance, write $|\phi'\rangle \in \mathcal{Z}_N(G)$ for a state obtained after passing the first step. The value E computed by the subsequent phase estimation step satisfies $E \geq c + \frac{3\epsilon}{4}$ with probability at least $\frac{2}{3}$, in which case the state is rejected. From this we see that the probability of accepting a no instance is at most $\frac{1}{3}$.

1.2.2   Reduction to frustration-free case

While showing that this problem is contained in QMAis relatively easy, the reduction to

1.3   Constructing the underlying graph for QMA-hardness

At this point, we will want to explicitly construct the graph for which our QMA-hardness result will hold. As such, we will at this point restrict our attention to a particular interaction, $\mathcal{U}$. While the basic idea behind these graphs will not change, the exact graph will depend on both the smallest distance that the interactions occur, as well as the largest distance. We will want to construct a foundational graph that does not have a two-particle ground state, and also we will want to ensure that our connections between these building blocks will not have multiple particles interacting except on specially chosen building blocks.

As such, let us assume that the minimum distance that the interaction $\mathcal{U}$ has non-zero interactions is $d_{\min}$, while the maximum distance is $d_{\max}$. Our graph will only depend on these two quantities.

1.3.1   Gate graphs

In this subsection we define a class of graphs (*gate graphs*) and a diagrammatic notation for them (*gate diagrams*) that will allow us to construct the overall graph. We will also discuss the MPQW Hamiltonian acting on these graphs, with a particular emphasis on the low-energy states.

Every gate graph is constructed using a specific, finite-sized graph g_0 as a building block. This graph is shown in Figure **??** (for graphs with $d_{\min} <= 3$ and discussed in Section **??**. In Section **??** we define gate graphs and gate diagrams. A gate graph is obtained by adding edges and self-loops (in a prescribed way) to a collection of disjoint copies of g_0.

[**TO DO:** *Rewrite this intro*]

In Section **??** we discuss the ground states of the Bose-Hubbard model on gate graphs. For any gate graph G, the smallest eigenvalue $\mu(G)$ of the adjacency matrix $A(G)$ satisfies $\mu(G) \geq -1 - 3\sqrt{2}$. It is convenient to define the constant

$$e_1 = -1 - 3\sqrt{2}. \tag{1.2}$$

When $\mu(G) = e_1$ we say G is an e_1-gate graph. We focus on the frustration-free states of e_1-gate graphs (recall from Definition **??** that $|\phi\rangle \in \mathcal{Z}_N(G)$ is frustration free iff $H(G,N)|\phi\rangle = 0$). We show that all such states live in a convenient subspace (called $\mathcal{I}(G,N)$) of the N-particle Hilbert space. This subspace has the property that no two (or more) particles ever occupy vertices of the same copy of g_0. The restriction to this subspace makes it easier to analyze the ground space.

In Section **??** we consider a class of subspaces that, like $\mathcal{I}(G,N)$, are defined by a set of constraints on the locations of N particles in an e_1-gate graph G. We state an "Occupancy Constraints Lemma" (proven in Appendix **??**) that relates a subspace of this form to the ground space of the Bose-Hubbard model on a graph derived from G.

1.3.1.1 The graph g_0

The graph g_0 shown in Figure **??** is constructed using the method of Chapter **??**, with the single qubit circuit with

The graph g_0 shown in Figure **??** is closely related to a single-qubit circuit $\mathcal{C}_0$ with eight gates U_j for $j \in [8]$, where

$$U_1 = U_2 = U_7 = U_8 = H \qquad U_3 = U_5 = HT \qquad U_4 = U_6 = (HT)^\dagger$$

with

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}.$$

In this section we map this circuit to the graph g_0. The mapping we use can be generalized to map an arbitrary quantum circuit with any number of qubits to a graph, but for simplicity we focus here on g_0. In Appendix **??** we discuss the more general mapping and use it to prove that computing (in a certain precise sense specified in the Appendix) the smallest eigenvalue of a sparse, efficiently row-computable symmetric 0-1 matrix is QMA-complete.

Starting with the circuit $\mathcal{C}_0$, we apply the Feynman-Kitaev circuit-to-Hamiltonian mapping [**?**, **?**] (up to a constant term and overall multiplicative factor) to get the Hamiltonian

$$-\sqrt{2} \sum_{t=1}^{8} \left(U_t^\dagger \otimes |t\rangle\langle t+1| + U_t \otimes |t+1\rangle\langle t| \right). \tag{1.3}$$

This Hamiltonian acts on the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^8$, where the second register (the "clock register") has periodic boundary conditions (i.e., we let $|8+1\rangle = |1\rangle$). The ground space of (1.3) is spanned by so-called history states

$$|\phi_z\rangle = \frac{1}{\sqrt{8}} \big(|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle) + H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle) \big), \quad z \in \{0,1\},$$

that encode the history of the computation where the circuit $\mathcal{C}_0$ is applied to $|z\rangle$. One can easily check that $|\phi_z\rangle$ is an eigenstate of the Hamiltonian with eigenvalue $-2\sqrt{2}$.

Now we modify (1.3) to give a symmetric 0-1 matrix. The trick we use is a variant of one used in references [**?**, **?**] for similar purposes.

The nonzero standard basis matrix elements of (1.3) are integer powers of $\omega = e^{i\frac{\pi}{4}}$. Note that ω is an eigenvalue of the 8×8 shift operator

$$S = \sum_{j=0}^{7} |j + 1 \text{ mod } 8\rangle\langle j|$$

with eigenvector

$$|\omega\rangle = \frac{1}{\sqrt{8}} \sum_{j=0}^{7} \omega^{-j}|j\rangle.$$

For each operator $-\sqrt{2}H, -\sqrt{2}HT$, or $-\sqrt{2}(HT)^{\dagger}$ appearing in equation (1.3), define another operator acting on $\mathbb{C}^2 \otimes \mathbb{C}^8$ by replacing nonzero matrix elements with powers of the operator S, namely $\omega^k \mapsto S^k$. Write $B(U)$ for the operator obtained by making this replacement in U, e.g.,

$$-\sqrt{2}HT = \begin{pmatrix} \omega^4 & \omega^5 \\ \omega^4 & \omega \end{pmatrix} \mapsto B(HT) = \begin{pmatrix} S^4 & S^5 \\ S^4 & S \end{pmatrix}.$$

We adjoin an 8-level ancilla and we make this replacement in equation (1.3). This gives

$$H_{\text{prop}} = \sum_{t=1}^{8} \left(B(U_t)^{\dagger}_{13} \otimes |t\rangle\langle t + 1|_2 + B(U_t)_{13} \otimes |t + 1\rangle\langle t|_2 \right), \tag{1.4}$$

a symmetric 0-1 matrix acting on $\mathbb{C}^2 \otimes \mathbb{C}^8 \otimes \mathbb{C}^8$, where the second register is the clock register and the third register is the ancilla register on which the S operators act (the subscripts indicate which registers are acted upon). It is an insignificant coincidence that the clock and ancilla registers have the same dimension.

Note that H_{prop} commutes with S (acting on the 8-level ancilla) and therefore is block diagonal with eight sectors. In the sector where S has eigenvalue ω, it is identical to the Hamiltonian we started with, equation (1.3). There is also a sector (where S has eigenvalue ω^*) where the Hamiltonian is the entrywise complex conjugate of the one we started with. We add a term to H_{prop} that assigns an energy penalty to states in any of the other six sectors, ensuring that none of these states lie in the ground space of the resulting operator.

Now we can define the graph g_0. Each vertex in g_0 corresponds to a standard basis vector in the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^8 \otimes \mathbb{C}^8$. We label the vertices (z, t, j) with $z \in \{0, 1\}$ describing the state of the computational qubit, $t \in [8]$ giving the state of the clock, and $j \in \{0, \ldots, 7\}$ describing the state of the ancilla. The adjacency matrix is

$$A(g_0) = H_{\text{prop}} + H_{\text{penalty}}$$

where the penalty term

$$H_{\text{penalty}} = \mathbb{I} \otimes \mathbb{I} \otimes \left(S^3 + S^4 + S^5 \right)$$

acts nontrivially on the third register. The graph g_0 is shown in Figure ??.

Now consider the ground space of $A(g_0)$. Note that H_{prop} and H_{penalty} commute, so they can be simultaneously diagonalized. Furthermore, H_{penalty} has smallest eigenvalue $-1 - \sqrt{2}$

(with eigenspace spanned by $|\omega\rangle$ and $|\omega^*\rangle$) and first excited energy -1. The norm of H_{prop} satisfies $\|H_{\text{prop}}\| \leq 4$, which follows from the fact that H_{prop} has four ones in each row and column (with the remaining entries all zero).

The smallest eigenvalue of $A(g_0)$ lives in the sector where H_{penalty} has eigenvalue $-1-\sqrt{2}$ and is equal to

$$-2\sqrt{2} + (-1 - \sqrt{2}) = -1 - 3\sqrt{2} = -5.24\ldots. \tag{1.5}$$

This is the constant e_1 from equation (1.2). To see this, note that in any other sector H_{penalty} has eigenvalue at least -1 and every eigenvalue of $A(g_0)$ is at least -5 (using the fact that $H_{\text{prop}} \geq -4$). An orthonormal basis for the ground space of $A(g_0)$ is furnished by the states

$$|\psi_{z,0}\rangle = \frac{1}{\sqrt{8}}\big(|z\rangle(|1\rangle + |3\rangle + |5\rangle + |7\rangle) + H|z\rangle(|2\rangle + |8\rangle) + HT|z\rangle(|4\rangle + |6\rangle)\big)|\omega\rangle \tag{1.6}$$

$$|\psi_{z,1}\rangle = |\psi_{z,0}\rangle^* \tag{1.7}$$

where $z \in \{0, 1\}$.

Note that the amplitudes of $|\psi_{z,0}\rangle$ in the above basis contain the result of computing either the identity, Hadamard, or HT gate acting on the "input" state $|z\rangle$.

1.3.1.2 Gate graphs

We use three different schematic representations of the graph g_0 (defined in Section **??**), as depicted in Figure **??**. We call these Figures *diagram elements*; they are also the simplest examples of *gate diagrams*, which we define shortly.

The black and grey circles in a diagram element are called "nodes." Each node has a label (z, t). The only difference between the three diagram elements is the labeling of their nodes. In particular, the nodes in the diagram element $U \in \{\mathbb{I}, H, HT\}$ correspond to values of $t \in [8]$ where the first register in equation (1.6) is either $|z\rangle$ or $U|z\rangle$. For example, the nodes for the H diagram element have labels with $t \in \{1, 3\}$ (where $|\psi_{z,0}\rangle$ contains the "input" $|z\rangle$) or $t = \{2, 8\}$ (where $|\psi_{z,0}\rangle$ contains the "output" $H|z\rangle$). We draw the input nodes in black and the output nodes in grey.

The rules for constructing gate diagrams are simple. A gate diagram consists of some number $R \in \{1, 2, \ldots\}$ of diagram elements, with self-loops attached to a subset $\mathcal{S}$ of the nodes and edges connecting a set $\mathcal{E}$ of pairs of nodes. A node may have a single edge or a single self-loop attached to it, but never more than one edge or self-loop and never both an edge and a self-loop. Each node in a gate diagram has a label (q, z, t) where $q \in [R]$ indicates the diagram element it belongs to. An example is shown in Figure **??**. Sometimes it is convenient to draw the input nodes on the right-hand side of a diagram element; e.g., in Figure **??** the node closest to the top left corner is labeled $(q, z, t) = (3, 0, 2)$.

To every gate diagram we associate a *gate graph* G with vertex set

$$\{(q, z, t, j)\colon q \in [R],\ z \in \{0, 1\},\ t \in [8],\ j \in \{0, \ldots, 7\}\}$$

and adjacency matrix

$$A(G) = \mathbb{I}_q \otimes A(g_0) + h_{\mathcal{S}} + h_{\mathcal{E}} \tag{1.8}$$

$$h_{\mathcal{S}} = \sum_{\mathcal{S}} |q, z, t\rangle\langle q, z, t| \otimes \mathbb{I}_j \tag{1.9}$$

$$h_{\mathcal{E}} = \sum_{\mathcal{E}} \left(|q, z, t\rangle + |q', z', t'\rangle\right)\left(\langle q, z, t| + \langle q', z', t'|\right) \otimes \mathbb{I}_j. \tag{1.10}$$

The sums in equations (1.9) and (1.10) run over the set of nodes with self-loops $(q, z, t) \in \mathcal{S}$ and the set of pairs of nodes connected by edges $\{(q, z, t), (q', z', t')\} \in \mathcal{E}$, respectively. We write $\mathbb{I}_q$ and $\mathbb{I}_j$ for the identity operator on the registers with variables q and j, respectively. We see from the above expression that each self-loop in the gate diagram corresponds to 8 self-loops in the graph G, and an edge in the gate diagram corresponds to 8 edges and 16 self-loops in G.

Since a node in a gate graph never has more than one edge or self-loop attached to it, equations (1.9) and (1.10) are sums of orthogonal Hermitian operators. Therefore

$$\|h_{\mathcal{S}}\| = \max_{\mathcal{S}} \||q, z, t\rangle\langle q, z, t| \otimes \mathbb{I}_j\| = 1 \quad \text{if } \mathcal{S} \neq \emptyset \tag{1.11}$$

$$\|h_{\mathcal{E}}\| = \max_{\mathcal{E}} \|(|q, z, t\rangle + |q', z', t'\rangle)(\langle q, z, t| + \langle q', z', t'|) \otimes \mathbb{I}_j\| = 2 \quad \text{if } \mathcal{E} \neq \emptyset \tag{1.12}$$

for any gate graph. (Of course, this also shows that $\|h_{\mathcal{S}'}\| = 1$ and $\|h_{\mathcal{E}'}\| = 2$ for any nonempty subsets $\mathcal{S}' \subseteq \mathcal{S}$ and $\mathcal{E}' \subseteq \mathcal{E}$.)

[**TO DO:** *Change this to the updated types with every vertex having a self-loop*]

1.3.1.3 Frustration-free states for a given interaction range

Consider the adjacency matrix $A(G)$ of a gate graph G, and note (from equation (1.8) that its smallest eigenvalue $\mu(G)$ satisfies

$$\mu(G) \geq e_1$$

since $h_{\mathcal{S}}$ and $h_{\mathcal{E}}$ are positive semidefinite and $A(g_0)$ has smallest eigenvalue e_1. In the special case where $\mu(G) = e_1$, we say G is an e_1-gate graph.

Definition 1. An e_1-gate graph is a gate graph G such that the smallest eigenvalue of its adjacency matrix is $e_1 = -1 - 3\sqrt{2}$.

When G is an e_1-gate graph, a single-particle ground state $|\Gamma\rangle$ of $A(G)$ satisfies

$$(\mathbb{I} \otimes A(g_0))\,|\Gamma\rangle = e_1|\Gamma\rangle \tag{1.13}$$

$$h_{\mathcal{S}}|\Gamma\rangle = 0 \tag{1.14}$$

$$h_{\mathcal{E}}|\Gamma\rangle = 0. \tag{1.15}$$

Indeed, to show that a given gate graph G is an e_1-gate graph, it suffices to find a state $|\Gamma\rangle$ satisfying these conditions. Note that equation (1.13) implies that $|\Gamma\rangle$ can be written as a superposition of the states

$$|\psi_{z,a}^q\rangle = |q\rangle|\psi_{z,a}\rangle, \quad z, a \in \{0, 1\},\ q \in [R]$$

where $|\psi_{z,a}\rangle$ is given by equations (1.6) and (1.7). The coefficients in the superposition are then constrained by equations (1.14) and (1.15).

Example 1. As an example, we show the gate graph in Figure **??** is an e_1-gate graph. As noted above, equation (1.13) lets us restrict our attention to the space spanned by the eight states $|\psi_{z,a}^q\rangle$ with $z, a \in \{0, 1\}$ and $q \in \{1, 2\}$. In this basis, the operators $h_{\mathcal{S}}$ and $h_{\mathcal{E}}$ only have nonzero matrix elements between states with the same value of $a \in \{0, 1\}$. We therefore solve for the e_1 energy ground states with $a = 0$ and those with $a = 1$ separately. Consider a ground state of the form

$$\left(\tau_1|\psi_{0,a}^1\rangle + \nu_1|\psi_{1,a}^1\rangle\right) + \left(\tau_2|\psi_{0,a}^2\rangle + \nu_2|\psi_{1,a}^2\rangle\right)$$

and note that in this case (1.14) implies $\tau_1 = 0$. Equation (1.15) gives

$$\begin{pmatrix}\tau_2 \\ \nu_2\end{pmatrix} = \begin{cases} HT\begin{pmatrix}-\tau_1 \\ -\nu_1\end{pmatrix} & a = 0 \\ (HT)^*\begin{pmatrix}-\tau_1 \\ -\nu_1\end{pmatrix} & a = 1. \end{cases}$$

We find two orthogonal e_1-energy states, which are (up to normalization)

$$|\psi_{1,0}^1\rangle - \frac{e^{i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi_{0,0}^2\rangle - |\psi_{1,0}^2\rangle\right) \tag{1.16}$$

$$|\psi_{1,1}^1\rangle - \frac{e^{-i\frac{\pi}{4}}}{\sqrt{2}}\left(|\psi_{0,1}^2\rangle - |\psi_{1,1}^2\rangle\right). \tag{1.17}$$

We interpret each of these states as encoding a qubit that is transformed at each set of input/output nodes in the gate diagram in Figure **??**. The encoded qubit begins on the input nodes of the first diagram element in the state

$$\begin{pmatrix}\tau_1 \\ \nu_1\end{pmatrix} = \begin{pmatrix}0 \\ 1\end{pmatrix}$$

because the self-loop penalizes the basis vectors $|\psi_{0,a}^1\rangle$. On the output nodes of diagram element 1, the encoded qubit is in the state where either HT (if $a = 0$) or its complex conjugate (if $a = 1$) has been applied. The edges in the gate diagram ensure that the encoded qubit on the input nodes of diagram element 2 is minus the state on the output nodes of diagram element 1.

In this example, each single-particle ground state encodes a single-qubit computation. Later we show how N-particle frustration-free states on e_1-gate graphs can encode computations on N qubits. Recall from Definition **??** that a state $|\Gamma\rangle \in \mathcal{Z}_N(G)$ is said to be frustration free iff $H(G, N)|\Gamma\rangle = 0$. Note that $H(G, N) \geq 0$, so an N-particle frustration-free state is necessarily a ground state. Putting this together with Lemma **??**, we see that the existence of an N-particle frustration-free state implies

$$\lambda_N^1(G) = \lambda_{N-1}^1(G) = \ldots = \lambda_1^1(G) = 0,$$

i.e., there are N'-particle frustration-free states for all $N' \leq N$.

We prove that the graph g_0 has no two-particle frustration-free states. By Lemma **??**, it follows that g_0 has no N-particle frustration-free states for $N \geq 2$.

Lemma 1. $\lambda_2^1(g_0) > 0$.

Proof. Suppose (for a contradiction) that $|Q\rangle \in \mathcal{Z}_2(g_0)$ is a nonzero vector in the nullspace of $H(g_0, 2)$, so

$$H_{g_0}^2|Q\rangle = \left(A(g_0) \otimes \mathbb{I} + \mathbb{I} \otimes A(g_0) + 2 \sum_{v \in g_0} |v\rangle\langle v| \otimes |v\rangle\langle v| \right) |Q\rangle = 2e_1|Q\rangle.$$

This implies

$$A(g_0) \otimes \mathbb{I}|Q\rangle = \mathbb{I} \otimes A(g_0)|Q\rangle = e_1|Q\rangle$$

since $A(g_0)$ has smallest eigenvalue e_1 and the interaction term is positive semidefinite. We can therefore write

$$|Q\rangle = \sum_{z,a,x,y \in \{0,1\}} Q_{za,xy}|\psi_{z,a}\rangle|\psi_{x,y}\rangle$$

with $Q_{za,xy} = Q_{xy,za}$ (since $|Q\rangle \in \mathcal{Z}_2(g_0)$) and

$$(|v\rangle\langle v| \otimes |v\rangle\langle v|) |Q\rangle = 0 \tag{1.18}$$

for all vertices $v = (z, t, j) \in g_0$. Using this equation with $|v\rangle = |0, 1, j\rangle$ gives

$$Q_{00,00}\langle 0, 1, j|\psi_{0,0}\rangle^2 + 2Q_{01,00}\langle 0, 1, j|\psi_{0,1}\rangle\langle 0, 1, j|\psi_{0,0}\rangle + Q_{01,01}\langle 0, 1, j|\psi_{0,1}\rangle^2$$
$$= \frac{1}{64} \left(Q_{00,00}i^{-j} + 2Q_{01,00} + Q_{01,01}i^j \right)$$
$$= 0$$

for each $j \in \{0, \dots, 7\}$. The only solution to this set of equations is $Q_{00,00} = Q_{01,00} = Q_{01,01} = 0$. The same analysis, now using $|v\rangle = |1, 1, j\rangle$, gives $Q_{10,10} = Q_{11,10} = Q_{11,11} = 0$. Finally, using equation (1.18) with $|v\rangle = |0, 2, j\rangle$ gives

$$\frac{1}{64}\langle 0|H|1\rangle\langle 0|H|0\rangle \left(2Q_{10,00}i^{-j} + 2Q_{10,01} + 2Q_{11,00} + 2Q_{11,01}i^j \right)$$
$$= \frac{1}{64} \left(Q_{10,00}i^{-j} + Q_{10,01} + Q_{11,00} + Q_{11,01}i^j \right)$$
$$= 0$$

for all $j \in \{0, \dots, 7\}$, which implies that $Q_{10,00} = Q_{11,01} = 0$ and $Q_{11,00} = -Q_{10,01}$. Thus, up to normalization,

$$|Q\rangle = |\psi_{1,0}\rangle|\psi_{0,1}\rangle + |\psi_{0,1}\rangle|\psi_{1,0}\rangle - |\psi_{11}\rangle|\psi_{00}\rangle - |\psi_{00}\rangle|\psi_{11}\rangle.$$

Now applying equation (1.18) with $|v\rangle = |0, 4, j\rangle$, we see that the quantity

$$\frac{1}{64} \left(2\langle 0|HT|1\rangle\langle 0|(HT)^*|0\rangle - 2\langle 0|(HT)^*|1\rangle\langle 0|HT|0\rangle \right) = \frac{1}{64} \left(e^{i\frac{\pi}{4}} - e^{-i\frac{\pi}{4}} \right)$$

must be zero, which is a contradiction. Hence we conclude that the nullspace of $H(g_0, 2)$ is empty. $\qquad\square$

We now characterize the space of N-particle frustration-free states on an e_1-gate graph G. Define the subspace $\mathcal{I}(G, N) \subset \mathcal{Z}_N(G)$ where each particle is in a ground state of $A(g_0)$ and no two particles are located within the same diagram element:

$$\mathcal{I}(G, N) = \text{span}\{\text{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle \dots |\psi_{z_N,a_N}^{q_N}\rangle)\colon z_i, a_i \in \{0, 1\},\ q_i \in [R],\ q_i \neq q_j \text{ whenever } i \neq j\}. \tag{1.19}$$

Lemma 2. *Let G be an e_1-gate graph. A state $|\Gamma\rangle \in \mathcal{Z}_N(G)$ is frustration free if and only if*

$$(A(G) - e_1)^{(w)} |\Gamma\rangle = 0 \ \ \text{for all } w \in [N] \tag{1.20}$$

$$|\Gamma\rangle \in \mathcal{I}(G, N). \tag{1.21}$$

Proof. First suppose that equations (1.20) and (1.21) hold. From (1.21) we see that $|\Gamma\rangle$ has no support on states where two or more particles are located at the same vertex. Hence

$$\sum_{k \in V} \hat{n}_k\, (\hat{n}_k - 1) |\Gamma\rangle = 0. \tag{1.22}$$

Putting together equations (1.20) and (1.22), we get

$$H(G, N)|\Gamma\rangle = \left(H_G^N - Ne_1\right) |\Gamma\rangle = 0,$$

so $|\Gamma\rangle$ is frustration free.

To complete the proof, we show that if $|\Gamma\rangle$ is frustration free, then conditions (1.20) and (1.21) hold. By definition, a frustration-free state $|\Gamma\rangle$ satisfies

$$H(G, N)|\Gamma\rangle = \left(\sum_{w=1}^{N} (A(G) - e_1)^{(w)} + \sum_{k \in V} \hat{n}_k\, (\hat{n}_k - 1)\right) |\Gamma\rangle = 0. \tag{1.23}$$

Since both terms in the large parentheses are positive semidefinite, they must both annihilate $|\Gamma\rangle$ (similarly, each term in the first summation must be zero). Hence equation (1.20) holds. Let G_{rem} be the graph obtained from G by removing all of the edges and self-loops in the gate diagram of G. In other words,

$$A(G_{\text{rem}}) = \sum_{q=1}^{R} |q\rangle\langle q| \otimes A(g_0) = \mathbb{I} \otimes A(g_0).$$

Noting that

$$H(G, N) \geq H(G_{\text{rem}}, N) \geq 0,$$

we see that equation (1.23) also implies

$$H(G_{\text{rem}}, N)|\Gamma\rangle = 0. \tag{1.24}$$

Since each of the R components of G_{rem} is an identical copy of g_0, the eigenvalues and eigenvectors of $H(G_{\text{rem}}, N)$ are characterized by Lemma **??** (along with knowledge of the eigenvalues and eigenvectors of g_0). By Lemma 1 and Lemma **??**, no component has a two- (or more) particle frustration-free state. Combining these two facts, we see that in an N-particle frustration-free state, every component of G_{rem} must contain either 0 or 1 particles, and the nullspace of $H(G_{\text{rem}}, N)$ is the space $\mathcal{I}(G, N)$. From equation (1.24) we get $|\Gamma\rangle \in \mathcal{I}(G, N)$. $\qquad\square$

Note that if $\mathcal{I}(G, N)$ is empty then Lemma 2 says that G has no N-particle frustration-free states. For example, this holds for any e_1-gate graph G whose gate diagram has $R < N$ diagram elements.

A useful consequence of Lemma 2 is the fact that every k-particle reduced density matrix of an N-particle frustration-free state $|\Gamma\rangle$ on an e_1-gate graph G (with $k \leq N$) has all of its support on k-particle frustration-free states. To see this, note that for any partition of the N registers into subsets A (of size k) and B (of size $N - k$), we have

$$\mathcal{I}(G, N) \subseteq \mathcal{I}(G, k)_A \otimes \mathcal{Z}_{N-k}(G)_B.$$

Thus, if condition (1.21) holds, then all k-particle reduced density matrices of $|\Gamma\rangle$ are contained in $\mathcal{I}(G, k)$. Furthermore, (1.20) is a statement about the single-particle reduced density matrices, so it also holds for each k-particle reduced density matrix. From this we see that each reduced density matrix of $|\Gamma\rangle$ is frustration free.

1.3.2 Gadgets

In Example 1 we saw how a single-particle ground state can encode a single-qubit computation. In this Section we see how a two-particle frustration-free state on a suitably designed e_1-gate graph can encode a two-qubit computation. We design specific e_1-gate graphs (called *gadgets*) that we use in Section ?? to prove that Bose-Hubbard Hamiltonian is QMA-hard. For each gate graph we discuss, we show that the smallest eigenvalue of its adjacency matrix is e_1 and we solve for all of the frustration-free states.

We first design a gate graph where, in any two-particle frustration-free state, the locations of the particles are synchronized. This "move-together" gadget is presented in Section ??. In Section ??, we design gadgets for two-qubit gates using four move-together gadgets, one for each two-qubit computational basis state. Finally, in Section ?? we describe a small modification of a two-qubit gate gadget called the "boundary gadget."

The circuit-to-gate graph mapping described in Section ?? uses a two-qubit gate gadget for each gate in the circuit, together with boundary gadgets in parts of the graph corresponding to the beginning and end of the computation.

The gate diagram for the *move-together gadget* is shown in Figure ??. Using equation (1.8), we write the adjacency matrix of the corresponding gate graph G_W as

$$A(G_W) = \sum_{q=1}^{6} |q\rangle\langle q| \otimes A(g_0) + h_\mathcal{E} \tag{1.25}$$

where $h_\mathcal{E}$ is given by (1.10) and $\mathcal{E}$ is the set of edges in the gate diagram (in this case $h_\mathcal{S} = 0$ as there are no self-loops).

We begin by solving for the single-particle ground states, i.e., the eigenvectors of (1.25) with eigenvalue $e_1 = -1 - 3\sqrt{2}$. As in Example 1, we can solve for the states with $a = 0$ and $a = 1$ separately, since

$$\langle \psi^j_{x,1} | h_\mathcal{E} | \psi^i_{z,0} \rangle = 0$$

for all $i, j \in \{1, \ldots, 6\}$ and $x, z \in \{0, 1\}$. We write a single-particle ground state as

$$\sum_{i=1}^{6} \left(\tau_i | \psi^i_{0,a} \rangle + \nu_i | \psi^i_{1,a} \rangle \right)$$

and solve for the coefficients τ_i and ν_i using equation (1.15) (in this case equation (1.14) is automatically satisfied since $h_{\mathcal{S}} = 0$). Enforcing (1.15) gives eight equations, one for each edge in the gate diagram:

$$\tau_3 = -\tau_1 \qquad\qquad \frac{1}{\sqrt{2}}(\tau_1 + \nu_1) = -\tau_6$$

$$\tau_4 = -\nu_1 \qquad\qquad \frac{1}{\sqrt{2}}(\tau_1 - \nu_1) = -\tau_5$$

$$\nu_3 = -\tau_2 \qquad\qquad \frac{1}{\sqrt{2}}(\tau_2 + \nu_2) = -\nu_5$$

$$\nu_4 = -\nu_2 \qquad\qquad \frac{1}{\sqrt{2}}(\tau_2 - \nu_2) = -\nu_6.$$

There are four linearly independent solutions to this set of equations, given by

Solution 1: $\quad \tau_1 = 1 \quad \tau_3 = -1 \quad \tau_5 = -\dfrac{1}{\sqrt{2}} \quad \tau_6 = -\dfrac{1}{\sqrt{2}} \quad$ all other coefficients 0

Solution 2: $\quad \nu_1 = 1 \quad \tau_4 = -1 \quad \tau_5 = \dfrac{1}{\sqrt{2}} \quad \tau_6 = -\dfrac{1}{\sqrt{2}} \quad$ all other coefficients 0

Solution 3: $\quad \nu_2 = 1 \quad \nu_4 = -1 \quad \nu_5 = -\dfrac{1}{\sqrt{2}} \quad \nu_6 = \dfrac{1}{\sqrt{2}} \quad$ all other coefficients 0

Solution 4: $\quad \tau_2 = 1 \quad \nu_3 = -1 \quad \nu_5 = -\dfrac{1}{\sqrt{2}} \quad \nu_6 = -\dfrac{1}{\sqrt{2}} \quad$ all other coefficients 0.

For each of these solutions, and for each $a \in \{0, 1\}$, we find a single-particle state with energy e_1. This result is summarized in the following Lemma.

Lemma 3. G_W *is an e_1-gate graph. A basis for the eigenspace of $A(G_W)$ with eigenvalue e_1 is*

$$|\chi_{1,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{1.26}$$

$$|\chi_{2,a}\rangle = \frac{1}{\sqrt{3}}|\psi^1_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{0,a}\rangle + \frac{1}{\sqrt{6}}|\psi^5_{0,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{0,a}\rangle \tag{1.27}$$

$$|\chi_{3,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{1,a}\rangle - \frac{1}{\sqrt{3}}|\psi^4_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle + \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{1.28}$$

$$|\chi_{4,a}\rangle = \frac{1}{\sqrt{3}}|\psi^2_{0,a}\rangle - \frac{1}{\sqrt{3}}|\psi^3_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^5_{1,a}\rangle - \frac{1}{\sqrt{6}}|\psi^6_{1,a}\rangle \tag{1.29}$$

where $a \in \{0, 1\}$.

In Figure ?? we have used a shorthand $\alpha, \beta, \gamma, \delta$ to identify four nodes of the move-together gadget; these are the nodes with labels $(q, z, t) = (1, 0, 1), (1, 1, 1), (2, 1, 1), (2, 0, 1)$, respectively. We view α and γ as "input" nodes and β and δ as "output" nodes for this gate diagram. It is natural to associate each single-particle state $|\chi_{i,a}\rangle$ with one of these four nodes. We also associate the set of 8 vertices represented by the node with the corresponding node, e.g.,

$$S_\alpha = \{(1, 0, 1, j) : j \in \{0, \dots, 7\}\}.$$

Looking at equation (1.26) (and perhaps referring back to equation (1.6)) we see that $|\chi_{1,a}\rangle$ has support on vertices in S_α but not on vertices in S_β, S_γ, or S_δ. Looking at the picture on the right-hand side of the equality sign in Figure **??**, we think of $|\chi_{1,a}\rangle$ as localized at the node α, with no support on the other three nodes. The states $|\chi_{2,a}\rangle, |\chi_{3,a}\rangle, |\chi_{4,a}\rangle$ are similarly localized at nodes β, γ, δ. We view $|\chi_{1,a}\rangle$ and $|\chi_{3,a}\rangle$ as input states and $|\chi_{2,a}\rangle$ and $|\chi_{4,a}\rangle$ as output states.

Now we turn our attention to the two-particle frustration-free states of the move-together gadget, i.e., the states $|\Phi\rangle \in \mathcal{Z}_2(G_W)$ in the nullspace of $H(G_W, 2)$. Using Lemma 2 we can write

$$|\Phi\rangle = \sum_{a,b \in \{0,1\}, I,J \in [4]} C_{(I,a),(J,b)} |\chi_{I,a}\rangle |\chi_{J,b}\rangle \tag{1.30}$$

where the coefficients are symmetric, i.e.,

$$C_{(I,a),(J,b)} = C_{(J,b),(I,a)}, \tag{1.31}$$

and where

$$\langle \psi_{z,a}^q | \langle \psi_{x,b}^q | \Phi \rangle = 0 \tag{1.32}$$

for all $z, a, x, b \in \{0, 1\}$ and $q \in [6]$.

The move-together gadget is designed so that each solution $|\Phi\rangle$ to these equations is a superposition of a term where both particles are in input states and a term where both particles are in output states. The particles move from input nodes to output nodes together. We now solve equations (1.30)–(1.32) and prove the following.

Lemma 4. *A basis for the nullspace of $H(G_W, 2)$ is*

$$|\Phi_{a,b}\rangle = \mathrm{Sym}\left(\frac{1}{\sqrt{2}}|\chi_{1,a}\rangle|\chi_{3,b}\rangle + \frac{1}{\sqrt{2}}|\chi_{2,a}\rangle|\chi_{4,b}\rangle\right), \quad a, b \in \{0, 1\}. \tag{1.33}$$

There are no N-particle frustration-free states on G_W for $N \geq 3$, i.e.,

$$\lambda_N^1(G_W) > 0 \quad \text{for } N \geq 3.$$

Proof. The states $|\Phi_{a,b}\rangle$ manifestly satisfy equations (1.30) and (1.31), and one can directly verify that they also satisfy (1.32) (the nontrivial cases to check are $q = 5$ and $q = 6$).

To complete the proof that (1.33) is a basis for the nullspace of $H(G_W, 2)$, we verify that any state satisfying these conditions must be a linear combination of these four states. Applying equation (1.32) gives

$$\langle \psi_{0,a}^1 | \langle \psi_{0,b}^1 | \Phi \rangle = \frac{1}{3} C_{(1,a),(1,b)} = 0 \qquad \langle \psi_{1,a}^1 | \langle \psi_{1,b}^1 | \Phi \rangle = \frac{1}{3} C_{(2,a),(2,b)} = 0$$

$$\langle \psi_{1,a}^2 | \langle \psi_{1,b}^2 | \Phi \rangle = \frac{1}{3} C_{(3,a),(3,b)} = 0 \qquad \langle \psi_{0,a}^2 | \langle \psi_{0,b}^2 | \Phi \rangle = \frac{1}{3} C_{(4,a),(4,b)} = 0$$

$$\langle \psi_{0,a}^1 | \langle \psi_{1,b}^1 | \Phi \rangle = \frac{1}{3} C_{(1,a),(2,b)} = 0 \qquad \langle \psi_{0,a}^2 | \langle \psi_{1,b}^2 | \Phi \rangle = \frac{1}{3} C_{(4,a),(3,b)} = 0$$

$$\langle \psi_{0,a}^3 | \langle \psi_{1,b}^3 | \Phi \rangle = \frac{1}{3} C_{(1,a),(4,b)} = 0 \qquad \langle \psi_{0,a}^4 | \langle \psi_{1,b}^4 | \Phi \rangle = \frac{1}{3} C_{(2,a),(3,b)} = 0$$

for all $a, b \in \{0, 1\}$. Using the fact that all of these coefficients are zero, and using equation (1.31), we get

$$|\Phi\rangle = \sum_{a,b\in\{0,1\}} \left(C_{(1,a),(3,b)} \left(|\chi_{1,a}\rangle|\chi_{3,b}\rangle + |\chi_{3,b}\rangle|\chi_{1,a}\rangle \right) + C_{(2,a),(4,b)} \left(|\chi_{2,a}\rangle|\chi_{4,b}\rangle + |\chi_{4,b}\rangle|\chi_{2,a}\rangle \right) \right).$$

Finally, applying equation (1.32) again gives

$$\langle\psi_{0,a}^6|\langle\psi_{1,b}^6|\Phi\rangle = \frac{1}{6}C_{(2,a),(4,b)} - \frac{1}{6}C_{(1,a),(3,b)} = 0.$$

Hence

$$|\Phi\rangle = \sum_{a,b\in\{0,1\}} C_{(1,a),(3,b)} \left(|\chi_{1,a}\rangle|\chi_{3,b}\rangle + |\chi_{3,b}\rangle|\chi_{1,a}\rangle + |\chi_{2,a}\rangle|\chi_{4,b}\rangle + |\chi_{4,b}\rangle|\chi_{2,a}\rangle \right),$$

which is a superposition of the states $|\Phi_{a,b}\rangle$.

Finally, we prove that there are no frustration-free ground states of the Bose-Hubbard model on G_W with more than two particles. By Lemma **??**, it suffices to prove that there are no frustration-free three-particle states.

Suppose (for a contradiction) that $|\Gamma\rangle \in \mathcal{Z}_3(G_W)$ is a normalized three-particle frustration-free state. Write

$$|\Gamma\rangle = \sum D_{(i,a),(j,b),(k,c)}|\chi_{i,a}\rangle|\chi_{j,b}\rangle|\chi_{k,c}\rangle.$$

Note that each reduced density matrix of $|\Gamma\rangle$ on two of the three subsystems must have all of its support on two-particle frustration-free states (see the remark following Lemma 2), i.e., on the states $|\Phi_{a,b}\rangle$. Using this fact for the subsystem consisting of the first two particles, we see in particular that

$$(i, j) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \implies D_{(i,a),(j,b),(k,c)} = 0 \tag{1.34}$$

(since $|\Phi_{a_1,a_2}\rangle$ only has support on vectors $|\chi_{i,a}\rangle|\chi_{j,b}\rangle$ with $i, j \in \{(1, 3), (3, 1), (2, 4), (4, 2)\}$).

Using this fact for subsystems consisting of particles $2, 3$ and $1, 3$, respectively, gives

$$(j, k) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \implies D_{(i,a),(j,b),(k,c)} = 0 \tag{1.35}$$
$$(i, k) \notin \{(1, 3), (3, 1), (2, 4), (4, 2)\} \implies D_{(i,a),(j,b),(k,c)} = 0. \tag{1.36}$$

Putting together equations (1.34), (1.35), and (1.36), we see that $|\Gamma\rangle = 0$. This is a contradiction, so no three-particle frustration-free states exist. □

Next we show how this gadget can be used to build gadgets the implement two-qubit gates.

1.3.2.1 Two-qubit gate gadget

In this Section we define a gate graph for each of the two-qubit unitaries

$$\{\text{CNOT}_{12}, \text{CNOT}_{21}, \text{CNOT}_{12}(H \otimes \mathbb{I}), \text{CNOT}_{12}(HT \otimes \mathbb{I})\}.$$

Here CNOT_{12} is the standard controlled-not gate with the second qubit as a target, whereas CNOT_{21} has the first qubit as target.

We define the gate graphs by exhibiting their gate diagrams. For the three cases

$$U = \text{CNOT}_{12}(\tilde{U} \otimes \mathbb{I})$$

with $\tilde{U} \in \{\mathbb{I}, H, HT\}$, we associate U with the gate diagram shown in Figure **??**. In the Figure we also indicate a shorthand used to represent this gate diagram. As one might expect, for the case $U = \text{CNOT}_{21}$, we use the same gate diagram as for $U = \text{CNOT}_{12}$; however, we use the slightly different shorthand shown in Figure **??**.

Roughly speaking, the two-qubit gate gadgets work as follows. In Figure **??** there are four move-together gadgets, one for each two-qubit basis state $|00\rangle, |01\rangle, |10\rangle, |11\rangle$. These enforce the constraint that two particles must move through the graph together. The connections between the four diagram elements labeled $1, 2, 3, 4$ and the move-together gadgets ensure that certain frustration-free two-particle states encode two-qubit computations, while the connections between diagram elements $1, 2, 3, 4$ and $5, 6, 7, 8$ ensure that there are no additional frustration-free two-particle states (i.e., states that do not encode computations).

To describe the frustration-free states of the gate graph depicted in Figure **??**, first recall the definition of the states $|\chi_{1,a}\rangle, |\chi_{2,a}\rangle, |\chi_{3,a}\rangle, |\chi_{4,a}\rangle$ from equations (1.26)–(1.29). For each of the move-together gadgets $xy \in \{00, 01, 10, 11\}$ in Figure **??**, write

$$|\chi_{L,a}^{xy}\rangle$$

for the state $|\chi_{L,a}\rangle$ with support (only) on the gadget labeled xy. Write

$$U(a) = \begin{cases} U & \text{if } a = 0 \\ U^* & \text{if } a = 1 \end{cases}$$

and similarly for $\tilde{U}$ (we use this notation throughout the paper to indicate a unitary or its elementwise complex conjugate).

In Appendix **??** we prove the following Lemma, which shows that G_U is an e_1-gate graph and solves for its frustration-free states.

Lemma 5. *Let $U = \text{CNOT}_{12}(\tilde{U} \otimes \mathbb{I})$ where $\tilde{U} \in \{\mathbb{I}, H, HT\}$. The corresponding gate graph G_U is defined by its gate diagram shown in Figure **??**. The adjacency matrix $A(G_U)$ has ground energy e_1; a basis for the corresponding eigenspace is*

$$|\rho_{z,a}^{1,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^1\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{5+z}\rangle - \sqrt{\frac{3}{8}}\sum_{x,y=0}^{1}\tilde{U}(a)_{yz}|\chi_{1,a}^{yx}\rangle \quad |\rho_{z,a}^{2,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^2\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^{6-z}\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{2,a}^{zx}\rangle$$

$$(1.37)$$

$$|\rho_{z,a}^{3,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^3\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^7\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{3,a}^{xz}\rangle \qquad |\rho_{z,a}^{4,U}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^4\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^8\rangle - \sqrt{\frac{3}{8}}\sum_{x=0}^{1}|\chi_{4,a}^{x(z\oplus x)}\rangle$$

$$(1.38)$$

where $z, a \in \{0, 1\}$. A basis for the nullspace of $H(G_U, 2)$ is

$$\text{Sym}(|T_{z_1,a,z_2,b}^U\rangle), \quad z_1, z_2, a, b \in \{0, 1\} \tag{1.39}$$

where

$$|T^U_{z_1,a,z_2,b}\rangle = \frac{1}{\sqrt{2}}|\rho^{1,U}_{z_1,a}\rangle|\rho^{3,U}_{z_2,b}\rangle + \frac{1}{\sqrt{2}}\sum_{x_1,x_2=0}^{1} U(a)_{x_1x_2,z_1z_2}|\rho^{2,U}_{x_1,a}\rangle|\rho^{4,U}_{x_2,b}\rangle \tag{1.40}$$

for $z_1, z_2, a, b \in \{0, 1\}$. There are no N-particle frustration-free states on G_U for $N \geq 3$, i.e.,

$$\lambda^1_N(G_U) > 0 \quad \text{for } N \geq 3.$$

We view the nodes labeled $\alpha, \beta, \gamma, \delta$ in Figure **??** as "input" nodes and those labeled $\epsilon, \zeta, \eta, \theta$ as "output nodes". Each of the states $|\rho^{i,U}_{x,y}\rangle$ is associated with one of the nodes, depending on the values of $i \in \{1, 2, 3, 4\}$ and $x \in \{0, 1\}$. For example, the states $|\rho^{1,U}_{0,0}\rangle$ and $|\rho^{1,U}_{0,1}\rangle$ are associated with input node α since they both have nonzero amplitude on vertices of the gate graph that are associated with α (and zero amplitude on vertices associated with other labeled nodes).

The two-particle state $\text{Sym}(|T^U_{z_1,a,z_2,b}\rangle)$ is a superposition of a term

$$\text{Sym}\left(\frac{1}{\sqrt{2}}|\rho^{1,U}_{z_1,a}\rangle|\rho^{3,U}_{z_2,b}\rangle\right)$$

with both particles located on vertices corresponding to input nodes and a term

$$\text{Sym}\left(\frac{1}{\sqrt{2}}\sum_{x_1,x_2\in\{0,1\}} U(a)_{x_1x_2,z_1z_2}|\rho^{2,U}_{x_1,a}\rangle|\rho^{4,U}_{x_2,b}\rangle\right)$$

with both particles on vertices corresponding to output nodes. The two-qubit gate $U(a)$ is applied as the particles move from input nodes to output nodes.

1.3.2.2   Boundary gadget

The *boundary gadget* is shown in Figure **??**. This gate diagram is obtained from Figure **??** (with $\tilde{U} = \mathbb{I}$) by adding self-loops. The adjacency matrix is

$$A(G_{\text{bnd}}) = A(G_{\text{CNOT}_{12}}) + h_{\mathcal{S}}$$

where

$$h_{\mathcal{S}} = \sum_{z=0}^{1}(|1, z, 1\rangle\langle 1, z, 1| \otimes \mathbb{I}_j + |2, z, 5\rangle\langle 2, z, 5| \otimes \mathbb{I}_j + |3, z, 1\rangle\langle 3, z, 1| \otimes \mathbb{I}_j).$$

The single-particle ground states (with energy e_1) are superpositions of the states $|\rho^{i,U}_{z,a}\rangle$ from Lemma 5 that are in the nullspace of $h_{\mathcal{S}}$. Note that

$$\langle\rho^{j,U}_{x,b}|h_{\mathcal{S}}|\rho^{i,U}_{z,a}\rangle = \delta_{a,b}\delta_{x,z}\left(\delta_{i,1}\delta_{j,1} + \delta_{i,2}\delta_{j,2} + \delta_{i,3}\delta_{j,3}\right)\frac{1}{8}\cdot\frac{1}{8}$$

(one factor of $\frac{1}{8}$ comes from the normalization in equations (1.37)–(1.38) and the other factor comes from the normalization in equation (1.6)), so the only single-particle ground states are

$$|\rho^{\text{bnd}}_{z,a}\rangle = |\rho^{4,U}_{z,a}\rangle$$

with $z, a \in \{0, 1\}$. Thus there are no two- (or more) particle frustration-free states, because no superposition of the states (1.39) lies in the subspace

$$\text{span}\{\text{Sym}(|\rho_{z,a}^{4,U}\rangle |\rho_{x,b}^{4,U}\rangle) \colon z, a, x, b \in \{0, 1\}\}$$

of states with single-particle reduced density matrices in the ground space of $A(G_{\text{bnd}})$. We summarize these results as follows.

Lemma 6. *The smallest eigenvalue of $A(G_{bnd})$ is e_1, with corresponding eigenvectors*

$$|\rho_{z,a}^{bnd}\rangle = \frac{1}{\sqrt{8}}|\psi_{z,a}^4\rangle - \frac{1}{\sqrt{8}}|\psi_{z,a}^8\rangle - \sqrt{\frac{3}{8}} \sum_{x=0,1} |\chi_{4,a}^{x(z\oplus x)}\rangle. \tag{1.41}$$

There are no frustration-free states with two or more particles, i.e., $\lambda_N^1(G_{bnd}) > 0$ for $N \geq 2$.

1.3.3 Gate graph for a given circuit

For any n-qubit, M-gate verification circuit $\mathcal{C}_X$ of the form described above, we associate a gate graph G_X. The gate diagram for G_X is built using the gadgets described in Section **??**; specifically, we use M two-qubit gadgets and $2(n-1)$ boundary gadgets. Since each two-qubit gadget and each boundary gadget contains 32 diagram elements, the total number of diagram elements in G_X is $R = 32(M + 2n - 2)$.

We now present the construction of the gate diagram for G_X. We also describe some gate graphs obtained as intermediate steps that are used in our analysis in Section **??**. The reader may find this description easier to follow by looking ahead to Figure **??**, which illustrates this construction for a specific 3-qubit circuit.

1. **Draw a grid** with columns labeled $j = 0, 1, \ldots, M + 1$ and rows labeled $i = 1, \ldots, n$ (this grid is only used to help describe the diagram).

2. **Place gadgets in the grid to mimic the quantum circuit.** For each $j = 1, \ldots, M$, place a gadget for the two-qubit gate U_j between rows 1 and $s(j)$ in the jth column. Place boundary gadgets in rows $i = 2, \ldots, n$ of column 0 and in the same rows of column $M + 1$. Write G_1 for the gate graph associated with the resulting diagram.

3. **Connect the nodes within each row.** First add edges connecting the nodes in rows $i = 2, \ldots, n$; call the resulting gate graph G_2. Then add edges connecting the nodes in row 1; call the resulting gate graph G_3.

4. **Add self-loops to the boundary gadgets.** In this step we add self-loops to enforce initialization of ancillas (at the beginning) and the proper output of the circuit (at the end). For each row $k = n_{\text{in}} + 1, \ldots, n$, add a self-loop to node δ (as shown in Figure **??**) of the corresponding boundary gadget in column $r = 0$, giving the gate diagram for G_4. Finally, add a self-loop to node α of the boundary gadget (as in Figure **??**) in row 2 and column $M + 1$, giving the gate diagram for G_X.

Figure **??** illustrates the step-by-step construction of G_X using a simple 3-qubit circuit with four gates

$$\text{CNOT}_{12}\left(\text{CNOT}_{13}HT \otimes \mathbb{I}\right)\text{CNOT}_{21}\text{CNOT}_{13}.$$

In this example, two of the qubits are input qubits (so $n_{\text{in}} = 2$), while the third qubit is an ancilla initialized to $|0\rangle$. Following the convention described in Section **??**, we take qubit 2 to be the output qubit. (In this example the circuit is not meant to compute anything interesting; its only purpose is to illustrate our method of constructing a gate graph).

We made some choices in designing this circuit-to-gate graph mapping that may seem arbitrary (e.g., we chose to place boundary gadgets in each row except the first). We have tried to achieve a balance between simplicity of description and ease of analysis, but we expect that other choices could be made to work.

1.3.3.1   Notation for G_X

We now introduce some notation that allows us to easily refer to a subset $\mathcal{L}$ of the diagram elements in the gate diagram for G_X.

Recall from Section **??** that each two-qubit gate gadget and each boundary gadget is composed of 32 diagram elements. This can be seen by looking at Figure **??** and noting (from Figure **??**) that each move-together gadget comprises 6 diagram elements.

For each of the two-qubit gate gadgets in the gate diagram for G_X, we focus our attention on the four diagram elements labeled 1–4 in Figure **??**. In total there are $4M$ such diagram elements in the gate diagram for G_X: in each column $j \in \{1, \ldots, M\}$ there are two in row 1 and two in row $s(j)$. When $U_j \in \{\text{CNOT}_{1s(j)}, \text{CNOT}_{1s(j)}\left(H \otimes \mathbb{I}\right), \text{CNOT}_{1s(j)}\left(HT \otimes \mathbb{I}\right)\}$ the diagram elements labeled $1, 2$ are in row 1 and those labeled $3, 4$ are in row $s(j)$; when $U_j = \text{CNOT}_{s(j)1}$ those labeled $1, 2$ are in row $s(j)$ and those labeled $3, 4$ are in row 1. We denote these diagram elements by triples (i, j, d). Here i and j indicate (respectively) the row and column of the grid in which the diagram element is found, and d indicates whether it is the leftmost ($d = 0$) or rightmost ($d = 1$) diagram element in this row and column. We define

$$\mathcal{L}_{\text{gates}} = \{(i, j, d) : i \in \{1, s(j)\}, \ j \in [M], \ d \in \{0, 1\}\} \tag{1.42}$$

to be the set of all such diagram elements.

For example, in Figure **??** the first gate is

$$U_1 = \text{CNOT}_{13},$$

so the gadget from Figure **??** (with $\tilde{U} = 1$) appears between rows 1 and 3 in the first column. The diagram elements labeled $1, 2, 3, 4$ from Figure **??** are denoted by $(1, 1, 0), (1, 1, 1), (3, 1, 0), (3, 1, 1)$, respectively. The second gate in Figure **??** is $U_2 = \text{CNOT}_{21}$, so the gadget from Figure **??** (with $\tilde{U} = 1$) appears between rows 2 and 1; in this case the diagram elements labeled $1, 2, 3, 4$ in Figure **??** are denoted by $(2, 2, 0), (2, 2, 1), (1, 2, 0), (1, 2, 1)$, respectively.

We also define notation for the boundary gadgets in G_X. For each boundary gadget. we focus on a single diagram element, labeled 4 in Figure **??**. For the left hand-side and right-hand side boundary gadgets, respectively, we denote these diagram elements as

$$\mathcal{L}_{\text{in}} = \{(i, 0, 1) : i \in \{2, \ldots, n\}\} \tag{1.43}$$
$$\mathcal{L}_{\text{out}} = \{(i, M + 1, 0) : i \in \{2, \ldots, n\}\}. \tag{1.44}$$

Definition 2. Let $\mathcal{L}$ be the set of diagram elements

$$\mathcal{L} = \mathcal{L}_{\text{in}} \cup \mathcal{L}_{\text{gates}} \cup \mathcal{L}_{\text{out}}$$

where $\mathcal{L}_{\text{in}}$, $\mathcal{L}_{\text{gates}}$, and $\mathcal{L}_{\text{out}}$ are given by equations (1.43), (1.42), and (1.44), respectively.

Finally, it is convenient to define a function F that describes horizontal movement within the rows of the gate diagram for G_X. The function F takes as input a two-qubit gate $j \in [M]$, a qubit $i \in \{2, \ldots, n\}$, and a single bit and outputs a diagram element from the set $\mathcal{L}$. If the bit is 0 then F outputs the diagram element in row i that appears in a column $0 \le k < j$ with k maximal (i.e., the closest diagram element in row i to the left of column j):

$$F(i, j, 0) = \begin{cases} (i, k, 1) & \text{where } 1 \le k < j \text{ is the largest } k \text{ such that } s(k) = i, \text{ if it exists} \\ (i, 0, 1) & \text{otherwise.} \end{cases}$$
$$(1.45)$$

On the other hand, if the bit is 1, then F outputs the diagram element in row i that appears in a column $j < k \le M + 1$ with k minimal (i.e., the closest diagram element in row i to the right of column j).

$$F(i, j, 1) = \begin{cases} (i, k, 0) & \text{where } j < k \le M \text{ is the smallest } k \text{ such that } s(k) = j, \text{ if it exists} \\ (i, M + 1, 0) & \text{otherwise.} \end{cases}$$
$$(1.46)$$

1.3.3.2   Occupancy constraints graph

In this Section we define an occupancy constraints graph $G_X oc$. Along with G_X and the number of particles n, this determines a subspace $\mathcal{I}(G_X, G_X oc, n) \subset \mathcal{Z}_n(G_X)$ through equation (**??**). We will see in Section **??** how low-energy states of the Bose-Hubbard model that live entirely within this subspace encode computations corresponding to the quantum circuit $\mathcal{C}_X$. This fact is used in the proof of Theorem **??**, which shows that the smallest eigenvalue $\lambda_n^1(G_X, G_X oc)$ of

$$H(G_X, G_X oc, n) = H(G_X, n)\big|_{\mathcal{I}(G_X, G_X oc, n)}$$

is related to the maximum acceptance probability of the circuit.

We encode quantum data in the locations of n particles in the graph G_X as follows. Each particle encodes one qubit and is located in one row of the graph G_X. Since all two-qubit gates in $\mathcal{C}_X$ involve the first qubit, the location of the particle in the first row determines how far along the computation has proceeded. We design the occupancy constraints graph to ensure that low-energy states of $H(G_X, G_X oc, n)$ have exactly one particle in each row (since there are n particles and n rows), and so that the particles in rows $2, \ldots, n$ are not too far behind or ahead of the particle in the first row. To avoid confusion, we emphasize that not *all* states in the subspace $\mathcal{I}(G_X, G_X oc, n)$ have the desired properties—for example, there are states in this subspace with more than one particle in a given row. We see in the next Section that states with low energy for $H(G_X, n)$ that also satisfy the occupancy constraints (i.e., low-energy states of $H(G_X, G_X oc, n)$) have the desired properties.

We now define $G_X oc$, which is a simple graph with a vertex for each diagram element in G_X. Each edge in $G_X oc$ places a constraint on the locations of particles in G_X. The graph $G_X oc$ only has edges between diagram elements in the set $\mathcal{L}$ from Definition 2; we define the edge set $E(G_X oc)$ by specifying pairs of diagram elements $L_1, L_2 \in \mathcal{L}$. We also indicate (in bold) the reason for choosing the constraints, which will become clearer in Section **??**.

1. **No two particles in the same row.** For each $i \in [n]$ we add constraints between diagram elements $(i, j, c) \in \mathcal{L}$ and $(i, k, d) \in \mathcal{L}$ in row i but in different columns, i.e.,

$$\{(i, j, c), (i, k, d)\} \in E(G_X oc) \text{ whenever } j \neq k. \tag{1.47}$$

2. **Synchronization with the particle in the first row.** For each $j \in [M]$ we add constraints between row 1 and row $s(j)$:

$$\{(1, j, c), (s(j), k, d)\} \in E(G_X oc) \text{ whenever } k \neq j \text{ and } (s(j), k, d) \neq F(s(j), j, c).$$

For each $j \in [M]$ we also add constraints between row 1 and rows $i \in [n] \setminus \{1, s(j)\}$:

$$\{(1, j, c), (i, k, d)\} \in E(G_X oc) \text{ whenever } (i, k, d) \notin \{F(i, j, 0), F(i, j, 1)\}.$$

1.4   Proof of QMA-hardness for MPQW ground energy

Theorem **??** bounds the smallest eigenvalue $\lambda_n^1(G_X, G_X oc)$ of $H(G_X, G_X oc, n)$. To prove the Theorem, we investigate a sequence of Hamiltonians starting with $H(G_1, n)$ and $H(G_1, G_X oc, n)$ and then work our way up to the Hamiltonian $H(G_X, G_X oc, n)$ by adding positive semidefinite terms.

For each Hamiltonian we consider, we solve for the nullspace and the smallest nonzero eigenvalue. To go from one Hamiltonian to the next, we use the following "Nullspace Projection Lemma," which was used (implicitly) in reference [**?**]. The Lemma bounds the smallest nonzero eigenvalue $\gamma(H_A + H_B)$ of a sum of positive semidefinite Hamiltonians H_A and H_B using knowledge of the smallest nonzero eigenvalue $\gamma(H_A)$ of H_A and the smallest nonzero eigenvalue $\gamma(H_B|_S)$ of the restriction of H_B to the nullspace S of H_A.

We prove the Lemma in Section **??**. When we apply this Lemma, we are usually interested in an asymptotic limit where $c, d \ll \|H_B\|$ and the right-hand side of (**??**) is $\Omega(\frac{cd}{\|H_B\|})$.

Our proof strategy, using repeated applications of the Nullspace Projection Lemma, is analogous to that of reference [**?**], where the so-called Projection Lemma was used similarly. Our technique has the advantage of not requiring the terms we add to our Hamiltonian to have "unphysical" problem-size dependent coefficients (it also has this advantage over the method of perturbative gadgets [**?**, **?**]). This allows us to prove results about the "physically realistic" Bose-Hubbard Hamiltonian. A similar technique based on Kitaev's Geometric Lemma was used recently in reference [**?**] (however, that method is slightly more computation intensive, requiring a lower bound on $\gamma(H_B)$ as well as bounds on $\gamma(H_A)$ and $\gamma(H_B|_S)$).

1.4.1 Single-particle ground-states

We begin by discussing the graphs

$$G_1, G_2, G_3, G_4, G_X$$

(as defined in Section **??**; see Figure **??**) in more detail and deriving some properties of their adjacency matrices.

The graph G_1 has a component for each of the two-qubit gates $j \in [M]$, for each of the boundary gadgets $i = 2, \ldots, n$ in column 0, and for each of the boundary gadgets $i = 2, \ldots, n$ in column $M + 1$. In other words

$$G_1 = \underbrace{\left(\bigcup_{i=2}^{n} G_{\text{bnd}} \right)}_{\text{left boundary}} \cup \underbrace{\left(\bigcup_{j=1}^{M} G_{U_j} \right)}_{\text{two-qubit gates}} \cup \underbrace{\left(\bigcup_{i=2}^{n} G_{\text{bnd}} \right)}_{\text{right boundary}}. \tag{1.48}$$

We use our knowledge of the adjacency matrices of the components G_{bnd} and G_{U_j} to understand the ground space of $A(G_1)$. Recall (from Section **??**) that the smallest eigenvalue of $A(G_{U_j})$ is

$$e_1 = -1 - 3\sqrt{2}$$

(with degeneracy 16) which is also the smallest eigenvalue of $A(G_{\text{bnd}})$ (with degeneracy 4). For each diagram element $L \in \mathcal{L}$ and pair of bits $z, a \in \{0, 1\}$ there is an eigenstate $|\rho_{z,a}^L\rangle$ of $A(G_1)$ with this minimal eigenvalue e_1. In total we get sixteen eigenstates

$$|\rho_{z,a}^{(1,j,0)}\rangle, |\rho_{z,a}^{(1,j,1)}\rangle, |\rho_{z,a}^{(s(j),j,0)}\rangle, |\rho_{z,a}^{(s(j),j,1)}\rangle, \quad z, a \in \{0, 1\}$$

for each two-qubit gate $j \in [M]$, four eigenstates

$$|\rho_{z,a}^{(i,0,1)}\rangle, \quad z, a \in \{0, 1\}$$

for each boundary gadget $i \in \{2, \ldots, n\}$ in column 0, and four eigenstates

$$|\rho_{z,a}^{(i,M+1,0)}\rangle, \quad z, a \in \{0, 1\}$$

for each boundary gadget $i \in \{2, \ldots, n\}$ in column $M + 1$. The set

$$\left\{ |\rho_{z,a}^L\rangle \colon z, a \in \{0, 1\}, \ L \in \mathcal{L} \right\}$$

is an orthonormal basis for the ground space of $A(G_1)$.

We write the adjacency matrices of G_2, G_3, G_4, and G_X as

$$A(G_2) = A(G_1) + h_1 \qquad\qquad A(G_4) = A(G_3) + \sum_{i=n_{\text{in}}+1}^{n} h_{\text{in},i}$$

$$A(G_3) = A(G_2) + h_2 \qquad\qquad A(G_X) = A(G_4) + h_{\text{out}}.$$

From step 3 of the construction of the gate diagram in Section **??**, we see that h_1 and h_2 are both sums of terms of the form

$$(|q, z, t\rangle + |q', z, t'\rangle)(\langle q, z, t| + \langle q', z, t'|) \otimes \mathbb{I}_j,$$

where h_1 contains a term for each edge in rows $2, \ldots, n$ and h_2 contains a term for each of the $2(M-1)$ edges in the first row. The operators

$$h_{\text{in},i} = |(i,0,1),1,7\rangle\langle(i,0,1),1,7| \otimes \mathbb{I} \quad h_{\text{out}} = |(2,M+1,0),0,5\rangle\langle(2,M+1,0),0,5| \otimes \mathbb{I} \tag{1.49}$$

correspond to the self-loops added in the gate diagram in step 4 of Section **??**.

We prove that G_1, G_2, G_3, G_4, and G_X are e_1-gate graphs.

Lemma 7. *The smallest eigenvalues of G_1, G_2, G_3, G_4 and G_X are*

$$\mu(G_1) = \mu(G_2) = \mu(G_3) = \mu(G_4) = \mu(G_X) = e_1.$$

Proof. We showed in the above discussion that $\mu(G_1) = e_1$. The adjacency matrices of G_2, G_3, G_4, and G_X are obtained from that of G_1 by adding positive semidefinite terms (h_1, h_2, $h_{\text{in},i}$, and h_{out} are all positive semidefinite). It therefore suffices to exhibit an eigenstate $|\varrho\rangle$ of $A(G_1)$ with

$$h_1|\varrho\rangle = h_2|\varrho\rangle = h_{\text{in},i}|\varrho\rangle = h_{\text{out}}|\varrho\rangle = 0$$

(for each $i \in \{n_{\text{in}}+1, \ldots, n\}$). There are many states $|\varrho\rangle$ satisfying these conditions; one example is

$$|\varrho\rangle = |\rho_{0,0}^{(1,1,0)}\rangle$$

which is supported on vertices where h_1, h_2, $h_{\text{in},i}$, and h_{out} have no support. $\qquad\square$

1.4.1.1   Multi-particle Hamiltonian

We now outline the sequence of Hamiltonians considered in the following Sections and describe the relationships between them. As a first step, in Section **??** we exhibit a basis $\mathcal{B}_n$ for the nullspace of $H(G_1, n)$ and we prove that its smallest nonzero eigenvalue is lower bounded by a positive constant. We then discuss the restriction

$$H(G_1, G_X oc, n) = H(G_1, n)\big|_{\mathcal{I}(G_1, G_X oc, n)} \tag{1.50}$$

in Section **??**, where we prove that a subset $\mathcal{B}_{\text{legal}} \subset \mathcal{B}_n$ is a basis for the nullspace of (1.50), and that its smallest nonzero eigenvalue is also lower bounded by a positive constant.

For the remainder of the proof we use the Nullspace Projection Lemma (Lemma **??**) four times, using the decompositions

$$H(G_2, G_X oc, n) = H(G_1, G_X oc, n) + H_1\big|_{\mathcal{I}(G_2, G_X oc, n)} \tag{1.51}$$

$$H(G_3, G_X oc, n) = H(G_2, G_X oc, n) + H_2\big|_{\mathcal{I}(G_3, G_X oc, n)} \tag{1.52}$$

$$H(G_4, G_X oc, n) = H(G_3, G_X oc, n) + \sum_{i=n_{\text{in}}+1}^{n} H_{\text{in},i}\big|_{\mathcal{I}(G_4, G_X oc, n)} \tag{1.53}$$

$$H(G_X, G_X oc, n) = H(G_4, G_X oc, n) + H_{\text{out}}\big|_{\mathcal{I}(G_X, G_X oc, n)} \tag{1.54}$$

where

$$H_1 = \sum_{w=1}^{n} h_1^{(w)} \qquad H_{\text{in},i} = \sum_{w=1}^{n} h_{\text{in},i}^{(w)} \qquad H_2 = \sum_{w=1}^{n} h_2^{(w)} \qquad H_{\text{out}} = \sum_{w=1}^{n} h_{\text{out}}^{(w)}$$

are all positive semidefinite, with $h_1, h_2, h_{\mathrm{in},i}, h_{\mathrm{out}}$ as defined in Section **??**. Note that in writing equations (1.51), (1.52), (1.53), and (1.54), we have used the fact (from Lemma 7) that the adjacency matrices of the graphs we consider all have the same smallest eigenvalue e_1. Also note that

$$\mathcal{I}(G_i, G_X oc, n) = \mathcal{I}(G_X, G_X oc, n)$$

for $i \in [4]$ since the gate diagrams for each of the graphs G_1, G_2, G_3, G_4 and G_X have the same set of diagram elements.

Let S_k be the nullspace of $H(G_k, G_X oc, n)$ for $k = 1, 2, 3, 4$. Since these positive semidefinite Hamiltonians are related by adding positive semidefinite terms, their nullspaces satisfy

$$S_4 \subseteq S_3 \subseteq S_2 \subseteq S_1 \subseteq \mathcal{I}(G_X, G_X oc, n).$$

We solve for $S_1 = \mathrm{span}(\mathcal{B}_{\mathrm{legal}})$ in Section **??** and we characterize the spaces S_2, S_3, and S_4 in Section **??** in the course of applying our strategy.

For example, to use the Nullspace Projection Lemma to lower bound the smallest nonzero eigenvalue of $H(G_2, G_X oc, n)$, we consider the restriction

$$\left(H_1\big|_{\mathcal{I}(G_2, G_X oc, n)}\right)\bigg|_{S_1} = H_1\big|_{S_1}. \tag{1.55}$$

We also solve for S_2, which is equal to the nullspace of (1.55). To obtain the corresponding lower bounds on the smallest nonzero eigenvalues of $H(G_k, G_X oc, n)$ for $k = 2, 3, 4$ and $H(G_X, G_X oc, n)$, we consider restrictions

$$H_2\big|_{S_2}, \quad \sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i}\big|_{S_3}, \quad \text{and} \quad H_{\mathrm{out}}\big|_{S_4}.$$

Analyzing these restrictions involves extensive computation of matrix elements. To simplify and organize these computations, we first compute the restrictions of each of these operators to the space S_1. We present the results of this computation in Section **??**; details of the calculation can be found in Section **??**. In Section **??** we proceed with the remaining computations and apply the Nullspace Projection Lemma three times using equations (1.51), (1.52), and (1.53). Finally, in Section **??** we apply the Lemma again using equation (1.54) and we prove Theorem **??**.

1.4.2 Configurations

In this Section we use Lemma **??** to solve for the nullspace of $H(G_1, n)$, i.e., the n-particle frustration-free states on G_1. Lemma **??** describes how frustration-free states for G_1 are built out of frustration-free states for its components.

To see how this works, consider the example from Figure **??**. In this example, with $n = 3$, we construct a basis for the nullspace of $H(G_1, 3)$ by considering two types of eigenstates. First, there are frustration-free states

$$\mathrm{Sym}(|\rho_{z_1,a_1}^{L_1}\rangle|\rho_{z_2,a_2}^{L_2}\rangle|\rho_{z_3,a_3}^{L_3}\rangle) \tag{1.56}$$

where $L_k = (i_k, j_k, d_k) \in \mathcal{L}$ belong to different components of G_1. That is to say, $j_w \neq j_t$ unless $j_w = j_t \in \{0, 5\}$, in which case $i_w \neq i_t$ (in this case the particles are located either at the left or right boundary, in different rows of G_1). There are also frustration-free states where two of the three particles are located in the same two-qubit gadget $J \in [M]$ and one of the particles is located in a diagram element L_1 from a different component of the graph. These states have the form

$$\text{Sym}(|T^J_{z_1,a_1,z_2,a_2}\rangle|\rho^{L_1}_{z_3,a_3}\rangle) \tag{1.57}$$

where

$$|T^J_{z_1,a_1,z_2,a_2}\rangle = \frac{1}{\sqrt{2}}|\rho^{(1,J,0)}_{z_1,a_1}\rangle|\rho^{(s(J),J,0)}_{z_2,a_2}\rangle + \frac{1}{\sqrt{2}}\sum_{x_1,x_2 \in \{0,1\}} U_J(a_1)_{x_1 x_2, z_1 z_2}|\rho^{(1,J,1)}_{x_1,a_1}\rangle|\rho^{(s(J),J,1)}_{x_2,a_2}\rangle \tag{1.58}$$

and $L_1 = (i, j, k) \in \mathcal{L}$ satisfies $j \neq J$. Each of the states (1.56) and (1.57) is specified by 6 "data" bits $z_1, z_2, z_3, a_1, a_2, a_3 \in \{0, 1\}$ and a "configuration" indicating where the particles are located in the graph. The configuration is specified either by three diagram elements $L_1, L_2, L_3 \in \mathcal{L}$ from different components of G_1 or by a two-qubit gate $J \in [M]$ along with a diagram element $L_1 \in \mathcal{L}$ from a different component of the graph.

We now define the notion of a configuration for general n. Informally, we can think of an n-particle configuration as a way of placing n particles in the graph G_1 subject to the following restrictions. We first place each of the n particles in a component of the graph, with the restriction that no boundary gadget may contain more than one particle and no two-qubit gadget may contain more than two particles. For each particle on its own in a component (i.e., in a component with no other particles), we assign one of the diagram elements $L \in \mathcal{L}$ associated to that component. We therefore specify a configuration by a set of two-qubit gadgets $J_1, \ldots, J_Y$ that contain two particles, along with a set of diagram elements $L_k \in \mathcal{L}$ that give the locations of the remaining $n - 2Y$ particles. We choose to order the Js and the Ls so that each configuration is specified by a unique tuple $(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$. For concreteness, we use the lexicographic order on diagram elements in the set $\mathcal{L}$: $L_A = (i_A, j_A, d_A)$ and $L_B = (i_B, j_B, d_B)$ satisfy $L_A < L_B$ iff either $i_A < i_B$, or $i_A = i_B$ and $j_A < j_B$, or $(i_A, j_A) = (i_B, j_B)$ and $d_A < d_B$.

Definition 3 (Configuration). An n-particle configuration on the gate graph G_1 is a tuple

$$(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$$

with $Y \in \{0, \ldots, \lfloor \frac{n}{2} \rfloor\}$, ordered integers

$$1 \leq J_1 < J_2 < \cdots < J_Y \leq M,$$

and lexicographically ordered diagram elements

$$L_1 < L_2 < \cdots < L_{n-2Y}, \qquad L_k = (i_k, j_k, d_k) \in \mathcal{L}.$$

We further require that each L_k is from a different component of G_1, i.e.,

$$j_w = j_t \implies j_w \in \{0, M+1\} \text{ and } i_w \neq i_t,$$

and we require that $j_u \neq J_v$ for all $u \in [n - 2Y]$ and $v \in [Y]$.

In Figure **??** we give some examples of configurations (for the example from Figure **??** with $n = 3$) and we introduce a diagrammatic notation for them.

For any configuration and n-bit strings $\vec{z}$ and $\vec{a}$, there is a state in the nullspace of $H(G_1, n)$, given by

$$\text{Sym}(|T_{z_1,a_1,z_2,a_2}^{J_1}\rangle \ldots |T_{z_{2Y-1},a_{2Y-1},z_{2Y},a_{2Y}}^{J_Y}\rangle|\rho_{z_{2Y+1},a_{2Y+1}}^{L_1}\rangle \ldots |\rho_{z_n,a_n}^{L_{n-2Y}}\rangle). \tag{1.59}$$

The ordering in the definition of a configuration ensures that each distinct choice of configuration and n-bit strings $\vec{z}, \vec{a}$ gives a different state.

Definition 4. Let $\mathcal{B}_n$ be the set of all states of the form (1.59), where $(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$ is a configuration and $\vec{z}, \vec{a} \in \{0, 1\}^n$.

Lemma 8. *The set $\mathcal{B}_n$ is an orthonormal basis for the nullspace of $H(G_1, n)$. Furthermore,*

$$\gamma(H(G_1, n)) \geq \mathcal{K}_0 \tag{1.60}$$

where $\mathcal{K}_0 \in (0, 1]$ is an absolute constant.

Proof. Each component of G_1 is either a two-qubit gadget or a boundary gadget (see equation (1.48)). The single-particle states of $A(G_1)$ with energy e_1 are the states $|\rho_{z,a}^L\rangle$ for $L \in \mathcal{L}$ and $z, a \in \{0, 1\}$, as discussed in Section **??**. Each of these states has support on only one component of G_1. In addition, G_1 has a two-particle frustration-free state for each two-qubit gadget $J \in [M]$ and bits z, a, x, b, namely $\text{Sym}(|T_{z,a,x,b}^J\rangle)$. Furthermore, no component of G_1 has any three- (or more) particle frustration-free states. Using these facts and applying Lemma **??**, we see that $\mathcal{B}_n$ spans the nullspace of $H(G_1, n)$.

Lemma **??** also expresses each eigenvalue of $H(G_1, n)$ as a sum of eigenvalues for its components. We use this fact to obtain the desired lower bound on the smallest nonzero eigenvalue. Our analysis proceeds on a case-by-case basis, depending on the occupation numbers for each component of G_1 (the values $N_1, \ldots, N_k$ in Lemma **??**).

First consider any set of occupation numbers where some two-qubit gate gadget $J \in [M]$ contains 3 or more particles. By Lemma **??** and Lemma **??**, any such eigenvalue is at least $\lambda_3^1(G_{U_J})$, which is a positive constant by Lemma 5. Next consider a case where some boundary gadget contains more than one particle. The corresponding eigenvalues are similarly lower bounded by $\lambda_2^1(G_{\text{bnd}})$, which is also a positive constant by Lemma 6. Finally, consider a set of occupation numbers where each two-qubit gadget contains at most two particles and each boundary gadget contains at most one particle. The smallest eigenvalue with such a set of occupation numbers is zero. The smallest nonzero eigenvalue is either

$$\gamma(H(G_{U_J}, 1)), \gamma(H(G_{U_J}, 2)) \text{ for some } J \in [M], \text{ or } \gamma(H(G_{\text{bnd}}, 1)).$$

However, these quantities are at least some positive constant since $H(G_{U_J}, 1)$, $H(G_{U_J}, 2)$, and $H(G_{\text{bnd}}, 1)$ are nonzero constant-sized positive semidefinite matrices.

Now combining the lower bounds discussed above and using the fact that, for each $J \in [M]$, the two-qubit gate U_J is chosen from a fixed finite gate set (given in (**??**)), we see that $\gamma(H(G_1, n))$ is lower bounded by the positive constant

$$\min\{\lambda_3^1(G_U), \lambda_2^1(G_{\text{bnd}}), \gamma(H(G_U, 1)), \gamma(H(G_U, 2)), \gamma(H(G_{\text{bnd}}, 1)): U \text{ is from the gate set } (\textbf{??})\}. \tag{1.61}$$

The condition $\mathcal{K}_0 \leq 1$ can be ensured by setting $\mathcal{K}_0$ to be the minimum of 1 and (1.61). □

Note that the constant $\mathcal{K}_0$ can in principle be computed using (1.61): each quantity on the right-hand side can be evaluated by diagonalizing a specific finite-dimensional matrix.

1.4.2.1 Legal configurations

In this section we define a subset of the n-particle configurations that we call legal configurations, and we prove that the subset of the basis vectors in $\mathcal{B}_n$ that have legal configurations spans the nullspace of $H(G_1, G_X oc, n)$.

We begin by specifying the set of legal configurations. Every legal configuration

$$(J_1, \ldots, J_Y, L_1, \ldots, L_{n-2Y})$$

has $Y \in \{0, 1\}$. The legal configurations with $Y = 0$ are

$$((1, j, d_1), F(2, j, d_2), F(3, j, d_3), \ldots, F(n, j, d_n)) \tag{1.62}$$

where $j \in [M]$ and where $\vec{d} = (d_1, \ldots, d_n)$ satisfies $d_i \in \{0, 1\}$ and $d_1 = d_{s(j)}$. (Recall that the function F, defined in equations (1.45) and (1.46), describes horizontal movement of particles.) The legal configurations with $Y = 1$ are

$$(j, F(2, j, d_2), \ldots, F(s(j) - 1, j, d_{s(j)-1}), F(s(j) + 1, j, d_{s(j)+1}), \ldots, F(n, j, d_n)) \tag{1.63}$$

where $j \in \{1, \ldots, M\}$ and $d_i \in \{0, 1\}$ for $i \in [n] \setminus \{1, s(j)\}$. Although the values d_1 and $d_{s(j)}$ are not used in equation (1.63), we choose to set them to

$$d_1 = d_{s(j)} = 2$$

for any legal configuration with $Y = 1$. In this way we identify the set of legal configurations with the set of pairs $j, \vec{d}$ with $j \in [M]$ and

$$\vec{d} = (d_1, d_2, d_3, \ldots, d_n)$$

satisfying

$$d_1 = d_{s(j)} \in \{0, 1, 2\} \quad \text{and} \quad d_i \in \{0, 1\} \text{ for } i \notin \{1, s(j)\}.$$

The legal configuration is given by equation (1.62) if $d_1 = d_{s(j)} \in \{0, 1\}$ and equation (1.63) if $d_1 = d_{s(j)} = 2$.

The examples in Figures **??**, **??**, and **??** show legal configurations whereas the examples in Figures **??**, **??**, and **??** are illegal. The legal examples correspond to $j = 1$, $\vec{d} = (1, 1, 1)$; $j = 2$, $\vec{d} = (2, 2, 0)$; and $j = 1$, $\vec{d} = (1, 0, 1)$, respectively. We now explain why the other examples are illegal. Looking at (1.63), we see that the configuration $(3, (2, 0, 1))$ depicted in Figure **??** is illegal since $F(2, 3, 0) = (2, 2, 1) \neq (2, 0, 1)$ and $F(2, 3, 1) = (2, 4, 0) \neq (2, 0, 1)$. The configuration in Figure **??** is illegal since there are two particles in the same row. Looking at equation (1.62), we see that the configuration $((1, 1, 1), (2, 2, 0), (3, 5, 0))$ in Figure **??** is illegal since $(3, 5, 0) \notin \{F(3, 1, 0), F(3, 1, 1)\} = \{(3, 0, 1), (3, 3, 0)\}$.

We now identify the subset of basis vectors $\mathcal{B}_{\text{legal}} \subset \mathcal{B}_n$ that have legal configurations. We write each such basis vector as

$$|j, \vec{d}, \vec{z}, \vec{a}\rangle = \begin{cases} \text{Sym}\left(|\rho_{z_1,a_1}^{(1,j,d_1)}\rangle \displaystyle\bigotimes_{i=2}^{n} |\rho_{z_i,a_i}^{F(i,j,d_i)}\rangle\right) & d_1 = d_{s(j)} \in \{0,1\} \\[2em] \text{Sym}\left(|T_{z_1,a_1,z_{s(j)},a_{s(j)}}^{j}\rangle \displaystyle\bigotimes_{\substack{i=2 \\ i \neq s(j)}}^{n} |\rho_{z_i,a_i}^{F(i,j,d_i)}\rangle\right) & d_1 = d_{s(j)} = 2 \end{cases} \tag{1.64}$$

where $j, \vec{d}$ specifies the legal configuration and $\vec{z}, \vec{a} \in \{0,1\}^n$. (Note that the bits in $\vec{z}$ and $\vec{a}$ are ordered slightly differently than in equation (1.59); here the labeling reflects the indices of the encoded qubits).

Definition 5. Let

$$\mathcal{B}_{\text{legal}} = \left\{|j, \vec{d}, \vec{z}, \vec{a}\rangle : j \in [M], \ d_1 = d_{s(j)} \in \{0,1,2\} \text{ and } \ d_i \in \{0,1\} \text{ for } i \notin \{1, s(j)\}, \ \vec{z}, \vec{a} \in \{0,1\}^n\right\}$$

and $\mathcal{B}_{\text{illegal}} = \mathcal{B}_n \setminus \mathcal{B}_{\text{illegal}}$.

The basis $\mathcal{B}_n = \mathcal{B}_{\text{legal}} \cup \mathcal{B}_{\text{illegal}}$ is convenient when considering the restriction to the subspace $\mathcal{I}(G_1, G_X oc, n)$. Letting Π_0 be the projector onto $\mathcal{I}(G_1, G_X oc, n)$, the following Lemma (proven in Section **??**) shows that the restriction

$$\Pi_0\big|_{\text{span}(\mathcal{B}_n)} \tag{1.65}$$

is diagonal in the basis $\mathcal{B}_n$. The Lemma also bounds the diagonal entries.

Lemma 9. *Let Π_0 be the projector onto $\mathcal{I}(G_1, G_X oc, n)$. For any $|j, \vec{d}, \vec{z}, \vec{a}\rangle \in \mathcal{B}_{legal}$, we have*

$$\Pi_0|j, \vec{d}, \vec{z}, \vec{a}\rangle = |j, \vec{d}, \vec{z}, \vec{a}\rangle. \tag{1.66}$$

Furthermore, for any two distinct basis vectors $|\phi\rangle, |\psi\rangle \in \mathcal{B}_{illegal}$, we have

$$\langle\phi|\Pi_0|\phi\rangle \leq \frac{255}{256} \tag{1.67}$$

$$\langle\phi|\Pi_0|\psi\rangle = 0. \tag{1.68}$$

We use this Lemma to characterize the nullspace of $H(G_1, G_X oc, n)$ and bound its smallest nonzero eigenvalue.

Lemma 10. *The nullspace S_1 of $H(G_1, G_X oc, n)$ is spanned by the orthonormal basis $\mathcal{B}_{legal}$. Its smallest nonzero eigenvalue is*

$$\gamma(H(G_1, G_X oc, n)) \geq \frac{\mathcal{K}_0}{256} \tag{1.69}$$

where $\mathcal{K}_0 \in (0,1]$ is the absolute constant from Lemma 8.

Proof. Recall from Section **??** that

$$H(G_1, G_X oc, n) = H(G_1, n)|_{\mathcal{I}(G_1, G_X oc, n)}.$$

Its nullspace is the space of states $|\kappa\rangle$ satisfying

$$\Pi_0|\kappa\rangle = |\kappa\rangle \quad \text{and} \quad H(G_1, n)|\kappa\rangle = 0$$

(recall that Π_0 is the projector onto $\mathcal{I}(G_1, G_X oc, n)$, the states satisfying the occupancy constraints). Since $\mathcal{B}_n$ is a basis for the nullspace of $H(G_1, n)$, to solve for the nullspace of $H(G_1, G_X oc, n)$ we consider the restriction (1.65) and solve for the eigenspace with eigenvalue 1. This calculation is simple because (1.65) is diagonal in the basis $\mathcal{B}_n$, according to Lemma 9. We see immediately from the Lemma that $\mathcal{B}_{\text{legal}}$ spans the nullspace of $H(G_1, G_X oc, n)$; we now show that Lemma 9 also implies the lower bound (1.69). Note that

$$\gamma(H(G_1, G_X oc, n)) = \gamma(\Pi_0 H(G_1, n)\Pi_0).$$

Let Π_{legal} and Π_{illegal} project onto the spaces spanned by $\mathcal{B}_{\text{legal}}$ and $\mathcal{B}_{\text{illegal}}$ respectively, so $\Pi_{\text{legal}} + \Pi_{\text{illegal}}$ projects onto the nullspace of $H(G_1, n)$. The operator inequality

$$H(G_1, n) \geq \gamma(H(G_1, n)) \cdot (1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})$$

implies

$$\Pi_0 H(G_1, n)\Pi_0 \geq \gamma(H(G_1, n)) \cdot \Pi_0(1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})\Pi_0.$$

Since the operators on both sides of this inequality are positive semidefinite and have the same nullspace, their smallest nonzero eigenvalues are bounded as

$$\gamma(\Pi_0 H(G_1, n)\Pi_0) \geq \gamma(H(G_1, n)) \cdot \gamma(\Pi_0(1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})\Pi_0).$$

Hence

$$\gamma(H(G_1, G_X oc, n)) = \gamma(\Pi_0 H(G_1, n)\Pi_0) \geq \mathcal{K}_0 \cdot \gamma(\Pi_0(1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})\Pi_0) \qquad (1.70)$$

where we used Lemma 8. From equations (1.67) and (1.68) we see that

$$\Pi_0|g\rangle = |g\rangle \quad \text{and} \quad \Pi_{\text{illegal}}|f\rangle = |f\rangle \qquad \implies \qquad \langle f|g\rangle\langle g|f\rangle \leq \frac{255}{256}. \qquad (1.71)$$

The nullspace of

$$\Pi_0 \left(1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}}\right) \Pi_0 \qquad (1.72)$$

is spanned by

$$\mathcal{B}_{\text{legal}} \cup \{|\tau\rangle \colon \Pi_0|\tau\rangle = 0\}.$$

To see this, note that (1.72) commutes with Π_0, and the space of $+1$ eigenvectors of Π_0 that are annihilated by (1.72) is spanned by $\mathcal{B}_{\text{legal}}$ (by Lemma 9). Any eigenvector $|g_1\rangle$ corresponding to the smallest nonzero eigenvalue of this operator therefore satisfies $\Pi_0|g_1\rangle = |g_1\rangle$ and $\Pi_{\text{legal}}|g_1\rangle = 0$, so

$$\gamma(\Pi_0(1 - \Pi_{\text{legal}} - \Pi_{\text{illegal}})\Pi_0) = 1 - \langle g_1|\Pi_{\text{illegal}}|g_1\rangle \geq \frac{1}{256}$$

using equation (1.71). Plugging this into equation (1.70) gives the lower bound (1.69). □

We now consider

$$H_1|_{S_1}, H_2|_{S_1}, H_{\mathrm{in},i}|_{S_1}, H_{\mathrm{out}}|_{S_1} \tag{1.73}$$

where these operators are defined in Section 1.4.1.1 and

$$S_1 = \mathrm{span}(\mathcal{B}_{\mathrm{legal}})$$

is the nullspace of $H(G_1, G_X oc, n)$.

We specify the operators (1.73) by their matrix elements in an orthonormal basis for S_1. Although the basis $\mathcal{B}_{\mathrm{legal}}$ was convenient in Section **??**, here we use a different basis in which the matrix elements of H_1 and H_2 are simpler. We define

$$|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \sum_{\vec{x}\in\{0,1\}^n} \left(\langle\vec{x}|\bar{U}_{j,d_1}(a_1)|\vec{z}\rangle\right)|j, \vec{d}, \vec{x}, \vec{a}\rangle \tag{1.74}$$

where

$$\bar{U}_{j,d_1}(a_1) = \begin{cases} U_{j-1}(a_1)U_{j-2}(a_1)\ldots U_1(a_1) & \text{if } d_1 \in \{0,2\} \\ U_j(a_1)U_{j-1}(a_1)\ldots U_1(a_1) & \text{if } d_1 = 1. \end{cases} \tag{1.75}$$

In each of these states the quantum data (represented by the $\vec{x}$ register on the right-hand side) encodes the computation in which the unitary $\bar{U}_{j,d_1}(a_1)$ is applied to the initial n-qubit state $|\vec{z}\rangle$ (the notation $\mathrm{In}(\vec{z})$ indicates that $\vec{z}$ is the input). The vector $\vec{a}$ is only relevant insofar as its first bit a_1 determines whether or not each two-qubit unitary is complex conjugated; the other bits of $\vec{a}$ go along for the ride. Letting $\vec{z}, \vec{a} \in \{0,1\}^n$, $j \in [M]$, and

$$\vec{d} = (d_1, \ldots, d_n) \quad \text{with} \quad d_1 = d_{s(j)} \in \{0,1,2\} \quad \text{and} \quad d_i \in \{0,1\}, \ i \notin \{1, s(j)\},$$

we see that the states (1.74) form an orthonormal basis for S_1. In Section **??** we compute the matrix elements of the operators (1.73) in this basis, which are reproduced below.

Roughly speaking, the nonzero off-diagonal matrix elements of the operator H_1 in the basis (1.74) occur between states $|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle$ and $|j, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}\rangle$ where the legal configurations $j, \vec{d}$ and $j, \vec{c}$ are related by horizontal motion of a particle in one of the rows $i \in \{2, \ldots, n\}$.

Matrix elements of H_1

$$\langle k, \vec{c}, \mathrm{In}(\vec{x}), \vec{b}|H_1|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \delta_{k,j}\delta_{\vec{a},\vec{b}}\delta_{\vec{z},\vec{x}} \cdot \begin{cases} \frac{n-1}{64} & \vec{c} = \vec{d} \\[2mm] \frac{1}{64}\displaystyle\prod_{\substack{r=1\\r\neq i}}^{n}\delta_{d_r,c_r} & d_i \neq c_i \text{ for some } i \in [n]\setminus\{1,s(j)\} \\[4mm] \frac{1}{64\sqrt{2}}\displaystyle\prod_{\substack{r=2\\r\neq s(j)}}^{n}\delta_{d_r,c_r} & (c_1,d_1) \in \{(2,0),(0,2),(1,2),(2,1)\} \\[4mm] 0 & \text{otherwise.} \end{cases}$$

$$\tag{1.76}$$

From this expression we see that $H_1|_{S_1}$ is block diagonal in the basis (1.74), with a block for each $\vec{z}, \vec{a} \in \{0,1\}^n$ and $j \in [M]$. Moreover, the submatrix for each block is the same. In Figure **??** we illustrate some of the off-diagonal matrix elements of $H_1|_{S_1}$ for the example from Figure **??**.

Next, we present the matrix elements of H_2.

Matrix elements of H_2

$$\langle k, \vec{c}, \text{In}(\vec{x}), \vec{b}|H_2|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle = f_{\text{diag}(\vec{d},j) \cdot \delta_{j,k} \delta_{\vec{a},\vec{b}} \delta_{\vec{z},\vec{x}} \delta_{\vec{c},\vec{d}}} \tag{1.77}$$
$$+ \left(f_{\text{off-diag}}(\vec{c}, \vec{d}, j) \cdot \delta_{k,j-1} + f_{\text{off-diag}}(\vec{d}, \vec{c}, k) \cdot \delta_{k-1,j}\right)\delta_{\vec{a},\vec{b}}\delta_{\vec{z},\vec{x}}$$

where

$$f_{\text{diag}}(\vec{d}, j) = \begin{cases} 0 & d_1 = 0 \text{ and } j = 1, \text{ or } d_1 = 1 \text{ and } j = M \\ \frac{1}{128} & d_1 = 2 \text{ and } j \in \{1, M\} \\ \frac{1}{64} & \text{otherwise} \end{cases} \tag{1.78}$$

and

$$f_{\text{off-diag}}(\vec{c}, \vec{d}, j) = \left(\prod_{\substack{r=2 \\ r \notin \{s(j-1), s(j)\}}}^{n} \delta_{d_r, c_r}\right) \cdot \begin{cases} \frac{1}{64\sqrt{2}} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) \in \{(2,0,0,0),(1,1,2,1)\} \\ \frac{1}{64} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) = (1,0,0,1) \\ \frac{1}{128} & (c_1, c_{s(j)}, d_1, d_{s(j-1)}) = (2,1,2,0) \\ 0 & \text{otherwise.} \end{cases}$$
$$\tag{1.79}$$

This shows that $H_2|_{S_1}$ is block diagonal in the basis (1.74), with a block for each $\vec{z}, \vec{a} \in \{0,1\}^n$. Also note that (in contrast with H_1) H_2 connects states with different values of j. In Figure **??** we illustrate some of the off-diagonal matrix elements of $H_2|_{S_1}$, for the example from Figure **??**.

Finally, we present the matrix elements of $H_{\text{in},i}$ (for $i \in \{n_{\text{in}} + 1, \ldots, n\}$) and H_{out}:

Matrix elements of $H_{\mathbf{in},i}$

For each ancilla qubit $i \in \{n_{\text{in}} + 1, \ldots, n\}$, define $j_{\text{min},i} = \min\{j \in [M]: s(j) = i\}$ to be the index of the first gate in the circuit that involves this qubit (recall from Section **??** that we consider circuits where each ancilla qubit is involved in at least one gate). The operator $H_{\text{in},i}$ is diagonal in the basis (1.74), with entries

$$\langle j, \vec{d}, \text{In}(\vec{z}), \vec{a}|H_{\text{in},i}|j, \vec{d}, \text{In}(\vec{z}), \vec{a}\rangle = \begin{cases} \frac{1}{64} & j \leq j_{\text{min},i}, \ z_i = 1, \text{ and } d_i = 0 \\ 0 & \text{otherwise.} \end{cases} \tag{1.80}$$

Matrix elements of $H_{\mathbf{out}}$

Let $j_{\text{max}} = \max\{j \in [M]: s(j) = 2\}$ be the index of the last gate $U_{j_{\text{max}}}$ in the circuit

that acts between qubits 1 and 2 (the output qubit). Then

$$\langle k, \vec{c}, \mathrm{In}(\vec{x}), \vec{b}|H_{\mathrm{out}}|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \delta_{j,k}\delta_{\vec{c},\vec{d}}\delta_{\vec{a},\vec{b}} \begin{cases} \langle\vec{x}|U_{\mathcal{C}_X}^{\dagger}(a_1)|0\rangle\langle0|_2 U_{\mathcal{C}_X}(a_1)|\vec{z}\rangle\frac{1}{64} & j \geq j_{\max} \text{ and } d_2 = 1 \\ 0 & \text{otherwise.} \end{cases}$$

$$(1.81)$$

1.4.3 Frustration-Free states

Define the $(n-2)$-dimensional hypercubes

$$\mathcal{D}_k^j = \big\{(d_1, \ldots, d_n)\colon d_1 = d_{s(j)} = k,\, d_i \in \{0,1\} \text{ for } i \in [n] \setminus \{1, s(j)\}\big\}$$

for $j \in \{1, \ldots, M\}$ and $k \in \{0, 1, 2\}$, and the superpositions

$$|\mathrm{Cube}_k(j, \vec{z}, \vec{a})\rangle = \frac{1}{\sqrt{2^{n-2}}} \sum_{\vec{d}\in\mathcal{D}_k^j} (-1)^{\sum_{i=1}^n d_i} |j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle$$

for $k \in \{0, 1, 2\}$, $j \in [M]$, and $\vec{z}, \vec{a} \in \{0,1\}^n$. For each $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$, let

$$|C(j, \vec{z}, \vec{a})\rangle = \frac{1}{2}|\mathrm{Cube}_0(j, \vec{z}, \vec{a})\rangle + \frac{1}{2}|\mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle - \frac{1}{\sqrt{2}}|\mathrm{Cube}_2(j, \vec{z}, \vec{a})\rangle. \qquad (1.82)$$

We prove

Lemma 11. *The Hamiltonian $H(G_2, G_X oc, n)$ has nullspace S_2 spanned by the states*

$$|C(j, \vec{z}, \vec{a})\rangle$$

for $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$. Its smallest nonzero eigenvalue is

$$\gamma(H(G_2, G_X oc, n)) \geq \frac{\mathcal{K}_0}{35000n}$$

where $\mathcal{K}_0 \in (0, 1]$ is the absolute constant from Lemma 8.

Proof. Recall from the previous section that $H_1|_{S_1}$ is block diagonal in the basis (1.74), with a block for each $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$. That is to say, $\langle k, \vec{c}, \mathrm{In}(\vec{x}), \vec{b}|H_1|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle$ is zero unless $\vec{a} = \vec{b}$, $k = j$, and $\vec{z} = \vec{x}$. Equation (1.76) gives the nonzero matrix elements within a given block, which we use to compute the frustration-free ground states of $H_1|_{S_1}$.

Looking at equation (1.76), we see that the matrix for each block can be written as a sum of n commuting matrices: $\frac{n-1}{64}$ times the identity matrix (case 1 in equation (1.76)), $n-2$ terms that each flip a single bit $i \notin \{1, s(j)\}$ of $\vec{d}$ (case 2), and a term that changes the value of the "special" components $d_1 = d_{s(j)} \in \{0,1,2\}$ (case 3). Thus

$$\langle j, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}|H_1|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle = \langle j, \vec{c}, \mathrm{In}(\vec{z}), \vec{a}|\frac{1}{64}(n-1) + \frac{1}{64}\sum_{i\in[n]\setminus\{1,s(j)\}} H_{\mathrm{flip},i} + \frac{1}{64}H_{\mathrm{special},j}|j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a}\rangle$$

where

$$\langle j, \vec{c}, \text{In}(\vec{z}), \vec{a} | H_{\text{flip},i} | j, \vec{d}, \text{In}(\vec{z}), \vec{a} \rangle = \delta_{c_i, d_i \oplus 1} \prod_{r \in [n] \setminus \{i\}} \delta_{c_r, d_r}$$

and

$$\langle j, \vec{c}, \text{In}(\vec{z}), \vec{a} | H_{\text{special},j} | j, \vec{d}, \text{In}(\vec{z}), \vec{a} \rangle = \begin{cases} \frac{1}{\sqrt{2}} & (c_1, d_1) \in \{(2,0), (0,2), (1,2), (2,1)\} \\ & \text{and } d_r = c_r \text{ for } r \in [n] \setminus \{1, s(j)\} \\ 0 & \text{otherwise.} \end{cases}$$

Note that these n matrices are mutually commuting, each eigenvalue of $H_{\text{flip},i}$ is ± 1, and each eigenvalue of $H_{\text{special},j}$ is equal to one of the eigenvalues of the matrix

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix},$$

which are $\{-1, 0, 1\}$. Thus we see that the eigenvalues of $H_1|_{S_1}$ within a block for some $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$ are

$$\frac{1}{64} \left(n - 1 + \sum_{i \notin \{1, s(j)\}} y_i + w \right) \tag{1.83}$$

where $y_i \in \pm 1$ for each $i \in [n] \setminus \{1, s(j)\}$ and $w \in \{-1, 0, 1\}$. In particular, the smallest eigenvalue within the block is zero (corresponding to $y_i = w = -1$). The corresponding eigenspace is spanned by the simultaneous -1 eigenvectors of each $H_{\text{flip},i}$ for $i \in [n] \setminus \{1, s(j)\}$ and $H_{\text{special},j}$. The space of simultaneous -1 eigenvectors of $H_{\text{flip},i}$ for $i \in [n] \setminus \{1, s(j)\}$ within the block is spanned by $\{|\text{Cube}_0(j, \vec{z}, \vec{a})\rangle, |\text{Cube}_1(j, \vec{z}, \vec{a})\rangle, |\text{Cube}_2(j, \vec{z}, \vec{a})\rangle\}$. The state $|C(j, \vec{z}, \vec{a})\rangle$ is the unique superposition of these states that is a -1 eigenvector of $H_{\text{special},j}$. Hence, for each block we obtain a unique state $|C(j, \vec{z}, \vec{a})\rangle$ in the space S_2. Ranging over all blocks $j \in [M]$ and $\vec{z}, \vec{a} \in \{0,1\}^n$, we get the basis described in the Lemma.

The smallest nonzero eigenvalue within each block is $\frac{1}{64}$ (corresponding to $y_i = -1$ and $w = 0$ in equation (1.83)), so

$$\gamma(H_1|_{S_1}) = \frac{1}{64}. \tag{1.84}$$

To get the stated lower bound, we use Lemma ?? with $H(G_2, G_X oc, n) = H_A + H_B$ where

$$H_A = H(G_1, G_X oc, n) \qquad H_B = H_1|_{\mathcal{I}(G_2, G_X oc, n)}$$

(as in equation (1.51)), along with the bounds

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{256} \qquad \gamma(H_B|_{S_1}) = \gamma(H_1|_{S_1}) = \frac{1}{64} \qquad \|H_B\| \leq \|H_1\| \leq n \|h_1\| = 2n$$

from Lemma 10, equations (1.55) and (1.84), and the fact that $\|h_1\| = 2$ from (1.12). This gives

$$\gamma(H(G_2, G_X oc, n)) \geq \frac{\mathcal{K}_0}{64 \mathcal{K}_0 + 256 + 2n \cdot 64 \cdot 256} \geq \frac{\mathcal{K}_0}{35000n}$$

where we used the facts that $\mathcal{K}_0 \leq 1$ and $n \geq 1$. $\qquad \square$

For each $\vec{z}, \vec{a} \in \{0,1\}^n$ define the uniform superposition

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle = \frac{1}{\sqrt{M}} \sum_{j=1}^{M} |C\left(j, \vec{z}, \vec{a}\right)\rangle.$$

that encodes (somewhat elaborately) the history of the computation that consists of applying either $U_{\mathcal{C}_X}$ or $U_{\mathcal{C}_X}^*$ to the state $|\vec{z}\rangle$. The first bit of $\vec{a}$ determines whether the circuit $\mathcal{C}_X$ or its complex conjugate is applied.

Lemma 12. *The Hamiltonian $H(G_3, G_X oc, n)$ has nullspace S_3 spanned by the states*

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle$$

for $\vec{z}, \vec{a} \in \{0,1\}^n$. Its smallest nonzero eigenvalue is

$$\gamma(H(G_3, G_X oc, n)) \geq \frac{\mathcal{K}_0}{10^7 n^2 M^2}$$

where $\mathcal{K}_0 \in (0,1]$ is the absolute constant from Lemma 8.

Proof. Recall that

$$H(G_3, G_X oc, n) = H(G_2, G_X oc, n) + H_2|_{\mathcal{I}(G_3, G_X oc, n)}$$

with both terms on the right-hand side positive semidefinite. To solve for the nullspace of $H(G_3, G_X oc, n)$, it suffices to restrict our attention to the space

$$S_2 = \operatorname{span}\{|C(j, \vec{z}, \vec{a})\rangle \colon j \in [M], \ \vec{z}, \vec{a} \in \{0,1\}^n\} \tag{1.85}$$

of states in the nullspace of $H(G_2, G_X oc, n)$. We begin by computing the matrix elements of H_2 in the basis for S_2 given above. We use equations (1.77) and (1.82) to compute the diagonal matrix elements:

$$\langle C\left(j, \vec{z}, \vec{a}\right) |H_2|C\left(j, \vec{z}, \vec{a}\right)\rangle = \frac{1}{4}\langle \mathrm{Cube}_0(j, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_0(j, \vec{z}, \vec{a})\rangle + \frac{1}{4}\langle \mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle|H_2|\mathrm{Cube}_1(j, \vec{z}, \vec{a})\rangle$$

$$\tag{1.86}$$

$$+ \frac{1}{2}\langle \mathrm{Cube}_2(j, \vec{z}, \vec{a})|H_2|\mathrm{Cube}_2(j, \vec{z}, \vec{a})\rangle \tag{1.87}$$

$$= \begin{cases} 0 + \frac{1}{256} + \frac{1}{256} & j = 1 \\ \frac{1}{256} + \frac{1}{256} + \frac{1}{128} & j \in \{2, \ldots, M-1\} \\ \frac{1}{256} + 0 + \frac{1}{256} & j = M \end{cases} \tag{1.88}$$

$$= \begin{cases} \frac{1}{128} & j \in \{1, M\} \\ \frac{1}{64} & j \in \{2, \ldots, M-1\}. \end{cases} \tag{1.89}$$

In the second line we used equation (1.78). Looking at equation (1.77), we see that the only nonzero off-diagonal matrix elements of H_2 in this basis are of the form

$$\langle C(j-1, \vec{z}, \vec{a})|H_2|C(j, \vec{z}, \vec{a})\rangle \quad \text{or} \quad \langle C(j, \vec{z}, \vec{a})|H_2|C(j-1, \vec{z}, \vec{a})\rangle = \langle C(j-1, \vec{z}, \vec{a})|H_2|C(j, \vec{z}, \vec{a})\rangle^*$$

for $j \in \{2, \ldots, M\}$, $\vec{z}, \vec{a} \in \{0,1\}^n$. To compute these matrix elements we first use equation (1.79) to evaluate

$$\langle \mathrm{Cube}_w(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_v(j, \vec{z}, \vec{a}) \rangle$$

for $v, w \in \{0, 1, 2\}$ and $j \in \{2, \ldots, M\}$. For example, using the second case of equation (1.79), we get

$$\langle \mathrm{Cube}_1(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_0(j, \vec{z}, \vec{a}) \rangle = \frac{1}{2^{n-2}} \sum_{\vec{d} \in \mathcal{D}_0^j} \sum_{\vec{c} \in \mathcal{D}_1^{j-1}} (-1)^{\sum_{i \in [n]}(c_i + d_i)} \langle j-1, \vec{c}, \mathrm{In}(\vec{z}), \vec{a} | H_2 | j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a} \rangle$$

$$= \frac{1}{2^{n-2}} \sum_{\vec{d} \in \mathcal{D}_0^j : d_{s(j-1)} = 1} (-1) \cdot \frac{1}{64} = -\frac{1}{128}.$$

To go from the first to the second line we used the fact that, for each $\vec{d} \in \mathcal{D}_0^j$ with $d_{s(j-1)} = 1$, there is one $\vec{c} \in \mathcal{D}_1^{j-1}$ for which $\langle j-1, \vec{c}, \mathrm{In}(\vec{z}), \vec{a} | H_2 | j, \vec{d}, \mathrm{In}(\vec{z}), \vec{a} \rangle = \frac{1}{64}$ (with all other such matrix elements equal to zero). This $\vec{c}$ satisfies $c_1 = c_{s(j-1)} = 1$ and $c_{s(j)} = 0$, with all other bits equal to those of $\vec{d}$, so

$$(-1)^{\sum_{i=1}^{n}(c_i + d_i)} = (-1)^{c_1 + c_{s(j)} + c_{s(j-1)} + d_1 + d_{s(j)} + d_{s(j-1)}} = -1$$

for each nonzero term in the sum.

We perform a similar calculation using cases 1, 3, and 4 in equation (1.79) to obtain

$$\langle \mathrm{Cube}_w(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_v(j, \vec{z}, \vec{a}) \rangle = \begin{cases} -\frac{1}{128} & (w, v) = (1, 0) \\ \frac{1}{128\sqrt{2}} & (w, v) \in \{(2,0), (1,2)\} \\ -\frac{1}{256} & (w, v) = (2, 2) \\ 0 & \text{otherwise.} \end{cases}$$

Hence

$$\langle C(j-1, \vec{z}, \vec{a}) | H_2 | C(j, \vec{z}, \vec{a}) \rangle$$

$$= \frac{1}{4} \langle \mathrm{Cube}_1(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_0(j, \vec{z}, \vec{a}) \rangle - \frac{1}{2\sqrt{2}} \langle \mathrm{Cube}_2(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_0(j, \vec{z}, \vec{a}) \rangle$$

$$+ \frac{1}{2} \langle \mathrm{Cube}_2(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_2(j, \vec{z}, \vec{a}) \rangle - \frac{1}{2\sqrt{2}} \langle \mathrm{Cube}_1(j-1, \vec{z}, \vec{a}) | H_2 | \mathrm{Cube}_2(j, \vec{z}, \vec{a}) \rangle$$

$$= -\frac{1}{128}.$$

Combining this with equation (1.89), we see that $H_2|_{S_2}$ is block diagonal in the basis (1.85), with a block for each pair of n-bit strings $\vec{z}, \vec{a} \in \{0,1\}^n$. Each of the 2^{2n} blocks is equal to the $M \times M$ matrix

$$\frac{1}{128} \begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \ddots & \vdots \\ 0 & 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

This matrix is just $\frac{1}{128}$ times the Laplacian of a path of length M, whose spectrum is well known. In particular, it has a unique eigenvector with eigenvalue zero (the all-ones vector) and its eigenvalue gap is $2(1 - \cos(\frac{\pi}{M})) \geq \frac{4}{M^2}$. Thus for each of the 2^{2n} blocks there is an eigenvector of $H_2|_{S_2}$ with eigenvalue 0, equal to the uniform superposition $|\mathcal{H}(\vec{z}, \vec{a})\rangle$ over the M states in the block. Furthermore, the smallest nonzero eigenvalue within each block is at least $\frac{1}{32M^2}$. Hence

$$\gamma(H_2|_{S_2}) \geq \frac{1}{32M^2}. \tag{1.90}$$

To get the stated lower bound on $\gamma(H(G_3, G_X oc, n))$, we apply Lemma **??** with

$$H_A = H(G_2, G_X oc, n) \qquad H_B = H_2|_{\mathcal{I}(G_3, G_X oc, n)}$$

and

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{35000n} \qquad \gamma(H_B|_{S_2}) = \gamma(H_2|_{S_2}) \geq \frac{1}{32M^2} \qquad \|H_B\| \leq \|H_2\| \leq n\|h_2\| = 2n \tag{1.91}$$

from Lemma 11, equation (1.90), and the fact that $\|h_2\| = 2$ from (1.12). This gives

$$\gamma(H(G_3, G_X oc, n)) \geq \frac{\mathcal{K}_0}{32M^2 \mathcal{K}_0 + 35000n + 2n(35000n)(32M^2)}$$
$$\geq \frac{\mathcal{K}_0}{M^2 n^2 (32 + 35000 + 70000 \cdot 32)} \geq \frac{\mathcal{K}_0}{10^7 M^2 n^2}. \qquad \square$$

Lemma 13. *The nullspace S_4 of $H(G_4, G_X oc, n)$ is spanned by the states*

$$|\mathcal{H}(\vec{z}, \vec{a})\rangle \quad where \quad \vec{z} = z_1 z_2 \ldots z_{n_{in}} \underbrace{00 \ldots 0}_{n - n_{in}} \tag{1.92}$$

for $\vec{a} \in \{0,1\}^n$ and $z_1, \ldots, z_{n_{in}} \in \{0,1\}$. Its smallest nonzero eigenvalue satisfies

$$\gamma(H(G_4, G_X oc, n)) \geq \frac{\mathcal{K}_0}{10^{10} M^3 n^3}$$

where $\mathcal{K}_0 \in (0, 1]$ is the absolute constant from Lemma 8.

Proof. Using equation (1.80), we find

$$\langle C(k, \vec{x}, \vec{b})|H_{in,i}|C(j, \vec{z}, \vec{a})\rangle = \delta_{k,j}\delta_{\vec{x},\vec{z}}\delta_{\vec{a},\vec{b}}\left(\frac{1}{4}\langle \text{Cube}_0(j, \vec{z}, \vec{a})|H_{in,i}|\text{Cube}_0(j, \vec{z}, \vec{a})\rangle\right.$$
$$+ \frac{1}{4}\langle \text{Cube}_1(j, \vec{z}, \vec{a})|H_{in,i}|\text{Cube}_1(j, \vec{z}, \vec{a})\rangle$$
$$\left.+ \frac{1}{2}\langle \text{Cube}_2(j, \vec{z}, \vec{a})|H_{in,i}|\text{Cube}_2(j, \vec{z}, \vec{a})\rangle\right)$$
$$= \delta_{k,j}\delta_{\vec{x},\vec{z}}\delta_{\vec{a},\vec{b}}\left(\frac{1}{64}\delta_{z_i,1}\right)\begin{cases} \frac{1}{4} \cdot \frac{1}{2} + \frac{1}{4} \cdot \frac{1}{2} + \frac{1}{2} \cdot \frac{1}{2} & j < j_{min,i} \\ \frac{1}{4} + 0 + 0 & j = j_{min,i} \\ 0 + 0 + 0 & j > j_{min,i} \end{cases}$$

for each $i \in \{n_{\mathrm{in}} + 1, \ldots, n\}$. Hence

$$\langle \mathcal{H}(\vec{x}, \vec{b})| \sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i} |\mathcal{H}(\vec{z}, \vec{a})\rangle = \frac{1}{M} \delta_{\vec{x}, \vec{z}} \delta_{\vec{a}, \vec{b}} \sum_{i=n_{\mathrm{in}}+1}^{n} \frac{1}{64} \left(\frac{j_{\mathrm{min},i} - 1}{2} + \frac{1}{4} \right) \delta_{z_i, 1}.$$

Therefore

$$\sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i} \big|_{S_3}$$

is diagonal in the basis $\{|\mathcal{H}(\vec{z}, \vec{a})\rangle : \vec{z}, \vec{a} \in \{0, 1\}^n\}$. The zero eigenvectors are given by equation (1.92), and the smallest nonzero eigenvalue is

$$\gamma \left(\sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i} \big|_{S_3} \right) \geq \frac{1}{256M}. \tag{1.93}$$

since $j_{\mathrm{min},i} \geq 1$. To get the stated lower bound we now apply Lemma **??** with

$$H_A = H(G_3, G_X oc, n) \qquad H_B = \sum_{i=n_{\mathrm{in}}+1}^{n} H_{\mathrm{in},i} \big|_{\mathcal{I}(G_4, G_X oc, n)}$$

and

$$\gamma(H_A) \geq \frac{\mathcal{K}_0}{10^7 M^2 n^2} \qquad \gamma(H_B|_{S_3}) \geq \frac{1}{256M} \qquad \|H_B\| \leq n \left\| \sum_{i=n_{\mathrm{in}}+1}^{n} h_{\mathrm{in},i} \right\| = n$$

where we used Lemma 12, equation (1.93), and the fact that $\left\| \sum_{i=n_{\mathrm{in}}+1}^{n} h_{\mathrm{in},i} \right\| = 1$ (from equation (1.11)). This gives

$$\gamma \left(H(G_4, G_X oc, n) \right) \geq \frac{\mathcal{K}_0}{256 M \mathcal{K}_0 + 10^7 n^2 M^2 + n(256M)(10^7 n^2 M^2)}$$

$$\geq \frac{\mathcal{K}_0}{(M^3 n^3)(256 + 10^7 + 256 \cdot 10^7)} \geq \frac{\mathcal{K}_0}{10^{10} M^3 n^3}. \qquad \square$$

1.4.4   The occupancy constraints lemma

1.4.4.1   Definitions and notation

In this Section we establish notation and we describe how the gate graph $G^\square$ is constructed from G and G^{occ}. We also define two related gate graphs $G^\triangle$ and $G^\Diamond$ that we use in our analysis.

Let us first fix notation for the gate graph G and the occupancy constraints graph G^{occ}. Write the adjacency matrix of G as (see equation (1.8))

$$A(G) = \sum_{q=1}^{R} |q\rangle\langle q| \otimes A(g_0) + h_{\mathcal{E}^G} + h_{\mathcal{S}^G}$$

where $h_{\mathcal{E}^G}$ and $h_{\mathcal{S}^G}$ are determined (through equations (1.10) and (1.9)) by the sets $\mathcal{E}^G$ and $\mathcal{S}^G$ of edges and self-loops in the gate diagram for G, and where g_0 is the 128-vertex graph from Figure **??**. Recall that the occupancy constraints graph G^{occ} is a simple graph with vertices labeled $q \in [R]$, one for each diagram element in G. We write $E(G^{\mathrm{occ}}) \subseteq \binom{[R]}{2} = \{\{x, y\} : x, y \in [R], x \neq y\}$ for the edge set of G^{occ}.

Definition of $G^{\square}$

To ensure that the ground space has the appropriate form, the construction of $G^{\square}$ is slightly different depending on whether R is even or odd. The following description handles both cases.

1. Replace each diagram element $q \in [R]$ in the gate diagram for G as shown in Figure **??**, with diagram elements labeled $q_{\text{in}}, q_{\text{out}}$ and $d(q, s)$ where $q, s \in [R]$ and $q \neq s$ if R is even. Each node (q, z, t) in the gate diagram for G is mapped to a new node $\text{new}(q, z, t)$ as shown by the black and grey arrows, i.e.,

$$\text{new}(q, z, t) = \begin{cases} (q_{\text{in}}, z, t) & \text{if } (q, z, t) \text{ is an input node} \\ (q_{\text{out}}, z, t) & \text{if } (q, z, t) \text{ is an output node.} \end{cases} \tag{1.94}$$

   Edges and self-loops in the gate diagram for G are replaced by edges and self-loops between the corresponding nodes in the modified diagram.

2. For each edge $\{q_1, q_2\} \in E(G^{\text{occ}})$ in the occupancy constraints graph we add four diagram elements of the type shown in Figure **??** (i.e., diagram elements corresponding to the identity). We refer to these diagram elements by labels $e_{ij}(q_1, q_2)$ with $i, j \in \{0, 1\}$. For these diagram elements the labeling function is symmetric, i.e., $e_{ij}(q_1, q_2) = e_{ji}(q_2, q_1)$ whenever $\{q_1, q_2\} \in E(G^{\text{occ}})$.

3. For each non-edge $\{q_1, q_2\} \notin E(G^{\text{occ}})$ with $q_1, q_2 \in [R]$ and $q_1 \neq q_2$ we add 8 diagram elements of the type shown in Figure **??**. We refer to these diagram elements as $e_{ij}(q_1, q_2)$ and $e_{ij}(q_2, q_1)$ with $i, j \in \{0, 1\}$; when $\{q_1, q_2\} \notin E(G^{\text{occ}})$ the labeling function is not symmetric, i.e., $e_{ij}(q_1, q_2) \neq e_{ji}(q_2, q_1)$. If R is odd we also add $4R$ diagram elements labeled $e_{ij}(q, q)$ with $i, j \in \{0, 1\}$ and $q \in [R]$.

4. Finally, we add edges and self-loops to the gate diagram as shown in Figure **??**. This gives the gate diagram for $G^{\square}$.

The set of diagram elements in the gate graph for $G^{\square}$ is indexed by

$$L^{\square} = Q_{\text{in}} \cup D \cup E_{\text{edges}} \cup E_{\text{non-edges}} \cup Q_{\text{out}} \tag{1.95}$$

where

$$Q_{\text{in}} = \{q_{\text{in}} : q \in [R]\} \tag{1.96}$$
$$D = \{d(q, s) : q, s \in [R] \text{ and } q \neq s \text{ if } R \text{ is even}\} \tag{1.97}$$
$$E_{\text{edges}} = \{e_{ij}(q, s) : i, j \in \{0, 1\}, \{q, s\} \in E(G^{\text{occ}}) \text{ and } q < s\}$$
$$E_{\text{non-edges}} = \{e_{ij}(q, s) : i, j \in \{0, 1\}, \{q, s\} \notin E(G^{\text{occ}}) \text{ and } q \neq s \text{ if } R \text{ is even}\}$$
$$Q_{\text{out}} = \{q_{\text{out}} : q \in [R]\}. \tag{1.98}$$

The total number of diagram elements in $G^\square$ is

$$
\begin{aligned}
|L^\square| &= |Q_{\text{in}}| + |D| + |E_{\text{edges}}| + |E_{\text{non-edges}}| + |Q_{\text{out}}| \\
&= \begin{cases} R + R^2 + 4|E(G^{\text{occ}})| + 4\left(R^2 - 2|E(G^{\text{occ}})|\right) + R & R \text{ odd} \\ R + R\left(R-1\right) + 4|E(G^{\text{occ}})| + 4\left(R(R-1) - 2|E(G^{\text{occ}})|\right) + R & R \text{ even} \end{cases} \\
&= \begin{cases} 5R^2 + 2R - 4|E(G^{\text{occ}})| & R \text{ odd} \\ 5R^2 - 3R - 4|E(G^{\text{occ}})| & R \text{ even.} \end{cases}
\end{aligned}
$$

In both cases this is upper bounded by $7R^2$ as claimed in the statement of the Lemma. Write

$$
A(G^\square) = \sum_{l \in L^\square} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^\square} + h_{\mathcal{E}^\square} \tag{1.99}
$$

where $\mathcal{S}^\square$ and $\mathcal{E}^\square$ are the sets of self-loops and edges in the gate diagram for $G^\square$.

We now focus on the input nodes of diagram elements in Q_{in} and the output nodes of the diagram elements in Q_{out}. These are the nodes indicated by the black and grey arrows in Figure ??. Write $\mathcal{E}^0 \subset \mathcal{E}^\square$ and $\mathcal{S}^0 \subset \mathcal{S}^\square$ for the sets of edges and self-loops that are incident on these nodes in the gate diagram for $G^\square$. Note that the sets $\mathcal{E}^0$ and $\mathcal{S}^0$ are in one-to-one correspondence with (respectively) the sets $\mathcal{E}^G$ and $\mathcal{S}^G$ of edges and self-loops in the gate diagram for G. The other edges and self-loops in $G^\square$ do not depend on the sets of edges and self-loops in G. Writing

$$
\mathcal{S}^\triangle = \mathcal{S}^\square \setminus S^0 \qquad \mathcal{E}^\triangle = \mathcal{E}^\square \setminus \mathcal{E}^0,
$$

we have

$$
h_{\mathcal{S}^\square} = h_{\mathcal{S}^0} + h_{\mathcal{S}^\triangle} \qquad h_{\mathcal{E}^\square} = h_{\mathcal{E}^0} + h_{\mathcal{E}^\triangle}. \tag{1.100}
$$

Definition of $G^\triangle$

The gate diagram for $G^\triangle$ is obtained from that of $G^\square$ by removing all edges and self-loops attached to the input nodes of the diagram elements in Q_{in} and the output nodes of the diagram elements in Q_{out}. Its adjacency matrix is

$$
A(G^\triangle) = \sum_{l \in L^\square} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^\triangle} + h_{\mathcal{E}^\triangle}. \tag{1.101}
$$

Note that $G^\triangle = G^\square$ whenever the gate diagram for G contains no edges or self-loops.

Definition of $G^\diamond$

We also define a gate graph $G^\diamond$ with gate diagram obtained from that of $G^\triangle$ by removing all edges (but leaving the self-loops). Note that $G^\diamond$ has a component for each diagram element $l \in L^\square$. The components corresponding to diagram elements without a self-loop (those with $l \in L^\square \setminus E_{\text{non-edges}}$) have adjacency matrix $A(g_0)$; those with a self-loop ($l \in E_{\text{non-edges}}$) have

adjacency matrix $A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}$, so

$$A(G^\diamond) = \sum_{l \in L^\square} |l\rangle\langle l| \otimes A(g_0) + h_{\mathcal{S}^\triangle} \qquad (1.102)$$

$$= \sum_{l \in L^\square \backslash E_{\text{non-edges}}} |l\rangle\langle l| \otimes A(g_0) + \sum_{l \in E_{\text{non-edges}}} |l\rangle\langle l| \otimes (A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}). \quad (1.103)$$

Example

We provide an example of this construction in Figure **??** (which shows a gate graph and an occupancy constraints graph) and Figure **??** (which describes the derived gate graphs $G^\square$, $G^\triangle$, and $G^\diamond$).

1.4.5   The gate graph $G^\diamond$

We now solve for the e_1-energy ground states of the adjacency matrix $A(G^\diamond)$. Write g_1 for the graph with adjacency matrix

$$A(g_1) = A(g_0) + |1,1\rangle\langle 1,1| \otimes \mathbb{I}$$

(i.e., g_0 with 8 self-loops added), so (recalling equation (1.103)) each component of $G^\diamond$ is either g_0 or g_1. Recall from Section **??** that $A(g_0)$ has four orthonormal e_1-energy ground states $|\psi_{z,a}\rangle$ with $z, a \in \{0,1\}$. It is also not hard to verify that the e_1-energy ground space of $A(g_1)$ is spanned by two of these states $|\psi_{0,a}\rangle$ for $a \in \{0,1\}$. Now letting $|\psi^l_{z,a}\rangle = |l\rangle|\psi_{z,a}\rangle$, we choose a basis $\mathcal{W}$ for the e_1-energy ground space of $A(G^\diamond)$ where each basis vector is supported on one of the components:

$$\mathcal{W} = \{|\psi^l_{z,a}\rangle \,:\, z, a \in \{0,1\}, \, l \in L^\square \backslash E_{\text{non-edges}}\} \cup \{|\psi^l_{0,a}\rangle \,:\, a \in \{0,1\}, \, l \in E_{\text{non-edges}}\}. \quad (1.104)$$

The eigenvalue gap of $A(G^\diamond)$ is equal to that of either $A(g_0)$ or $A(g_1)$. Since g_0 and g_1 are specific 128-vertex graphs we can calculate their eigenvalue gaps using a computer; we get $\gamma(A(g_0) - e_1) = 0.7785\ldots$ and $\gamma(A(g_1) - e_1) = 0.0832\ldots$. Hence

$$\gamma(A(G^\diamond) - e_1) \geq 0.0832\ldots > \frac{1}{13}. \qquad (1.105)$$

The ground space of $A(G^\diamond)$ has dimension

$$|\mathcal{W}| = 4|L^\square| - 2|E_{\text{non-edges}}| = \begin{cases} 4\left(5R^2 + 2R - 4|E(G^{\text{occ}})|\right) - 2\left(4R^2 - 8|E(G^{\text{occ}})|\right) & R \text{ odd} \\ 4\left(5R^2 - 3R - 4|E(G^{\text{occ}})|\right) - 2\left(4R(R-1) - 8|E(G^{\text{occ}})|\right) & R \text{ even} \end{cases}$$

$$= \begin{cases} 12R^2 + 8R & R \text{ odd} \\ 12R^2 - 4R & R \text{ even}. \end{cases} \qquad (1.106)$$

We now consider the N-particle Hamiltonian $H(G^\diamond, N)$ and characterize its nullspace.

Lemma 14. *The nullspace of $H(G^\diamond, N)$ is*

$$\mathcal{I}_\diamond = \operatorname{span}\{\operatorname{Sym}(|\psi^{q_1}_{z_1,a_1}\rangle|\psi^{q_2}_{z_2,a_2}\rangle \ldots |\psi^{q_N}_{z_N,a_N}\rangle) : |\psi^{q_i}_{z_i,a_i}\rangle \in \mathcal{W} \text{ and } q_i \neq q_j \text{ for all distinct } i, j \in [N]\}$$

where $\mathcal{W}$ is given in equation (1.104). The smallest nonzero eigenvalue satisfies $\gamma(H(G^\diamond, N)) > \frac{1}{300}$.

Proof. For the first part of the proof we use the fact that the basis vectors $|\psi^l_{z,a}\rangle \in \mathcal{W}$ span the e_1-eigenspace of the component $G^\diamond_l$ of $G^\diamond$ corresponding to the diagram element $l \in L^\square$, i.e., the nullspace of $H(G^\diamond_l, 1)$. Furthermore, no component of $G^\diamond$ supports a two-particle frustration-free state, i.e., $\lambda^1_2(g_0) > 0$ and $\lambda^1_2(g_1) > 0$ (by Lemma 1). Now applying Lemma **??** we see that $\mathcal{I}_\diamond$ is the nullspace of $H(G^\diamond, N)$. We also see that the smallest nonzero eigenvalue $\gamma(H(G^\diamond, N))$ is either $\lambda^1_2(g_0)$, $\lambda^1_2(g_1)$, $\gamma(H(g_0, 1))$, or $\gamma(H(g_1, 1))$. These constants can be calculated numerically using a computer; they are $\lambda^1_2(g_0) = 0.0035\ldots$, $\lambda^1_2(g_1) = 0.0185\ldots$, $\gamma(H(g_0, 1)) = 0.7785\ldots$, and $\gamma(H(g_1, 1)) = 0.0832\ldots$. Hence

$$\gamma(H(G^\diamond, N)) \geq \min\{\lambda^1_2(g_0), \lambda^1_2(g_1), \gamma(H(g_0, 1)), \gamma(H(g_1, 1))\} > \frac{1}{300}. \qquad \square$$

1.4.6 The adjacency matrix of the gate graph $G^\triangle$

We begin by solving for the e_1-energy ground space of the adjacency matrix $A(G^\triangle)$. From equations (1.101) and (1.102) we have

$$A(G^\triangle) = A(G^\diamond) + h_{\mathcal{E}^\triangle}. \tag{1.107}$$

Recall the e_1-energy ground space of $A(G^\diamond)$ is spanned by $\mathcal{W}$ from equation (1.104). Since $h_{\mathcal{E}^\triangle} \geq 0$ it follows that $A(G^\triangle) \geq e_1$. To solve for the e_1-energy groundpsace of $A(G^\triangle)$ we construct superpositions of vectors from $\mathcal{W}$ that are in the nullspace of $h_{\mathcal{E}^\triangle}$. To this end we consider the restriction

$$h_{\mathcal{E}^\triangle}\big|_{\operatorname{span}(\mathcal{W})}. \tag{1.108}$$

We now show that it is block diagonal in the basis $\mathcal{W}$ and we compute its matrix elements.

First recall from equation (1.10) that

$$h_{\mathcal{E}^\triangle} = \sum_{\{(l,z,t),(l',z',t')\} \in \mathcal{E}^\triangle} (|l, z, t\rangle + |l', z', t'\rangle)(\langle l, z, t| + \langle l', z', t'|) \otimes \mathbb{I}. \tag{1.109}$$

The edges $\{(l, z, t), (l', z', t')\} \in \mathcal{E}^\triangle$ can be read off from Figure **??** and Figure **??**, respectively (referring back to Figure **??** for our convention regarding the labeling of nodes on a diagram element). The edges from Figure **??** are

$$\{(q_{\text{in}}, z, t), (d(q, 1), z, t')\}, \{(d(q, 2), z, t), (d(q, 3), z, t')\}, \ldots, \{(d(q, R), z, t), (q_{\text{out}}, z, t')\} \tag{1.110}$$

with $q \in [R]$ and $(z, t, t') = (0, 7, 3)$ or $(1, 5, 1)$, and where $d(q, q)$ does not appear if R is even (i.e., $d(q, q-1)$ is followed by $d(q, q+1)$). The edges from Figure **??** are

$$\{(d(q, s), 0, 1), (e_{00}(q, s), \alpha(q, s), 1)\}, \{(d(q, s), 1, 3), (e_{10}(q, s), \alpha(q, s), 1)\}, \tag{1.111}$$
$$\{(d(q, s), 0, 5), (e_{01}(q, s), \alpha(q, s), 1)\}, \{(d(q, s), 1, 7), (e_{11}(q, s), \alpha(q, s), 1)\}$$

with $q, s \in [R]$ and $q \neq s$ if R is even, and where

$$\alpha(q,s) = \begin{cases} 1 & q > s \text{ and } \{q,s\} \in E(G^{\mathrm{occ}}) \\ 0 & \text{otherwise.} \end{cases}$$

The set $\mathcal{E}^{\triangle}$ consists of all edges (1.110) and (1.111).

We claim that (1.108) is block diagonal with a block $\mathcal{W}_{(z,a,q)} \subseteq \mathcal{W}$ of size

$$\left| \mathcal{W}_{(z,a,q)} \right| = \begin{cases} 3R + 2 & R \text{ odd} \\ 3R - 1 & R \text{ even} \end{cases}$$

for each for each triple (z,a,q) with $z, a \in \{0,1\}$ and $q \in [R]$. Using equation (1.106) we confirm that $|\mathcal{W}| = 4R \left| \mathcal{W}_{(z,a,q)} \right|$, so this accounts for all basis vectors in $\mathcal{W}$. The subset of basis vectors for a given block is

$$\mathcal{W}_{(z,a,q)} = \left\{ |\psi_{z,a}^{q_{\mathrm{in}}}\rangle, |\psi_{z,a}^{q_{\mathrm{out}}}\rangle \right\} \cup \left\{ |\psi_{z,a}^{d(q,s)}\rangle : s \in [R], \ s \neq q \text{ if } R \text{ even} \right\}$$

$$\cup \left\{ |\psi_{\alpha(q,s),a}^{e_{zx}(q,s)}\rangle : x \in \{0,1\}, \ s \in [R], \ s \neq q \text{ if } R \text{ even} \right\}. \tag{1.112}$$

Using equation (1.109) and the description of $\mathcal{E}^{\triangle}$ from (1.110) and (1.111), one can check by direct inspection that (1.108) only has nonzero matrix elements between basis vectors in $\mathcal{W}$ from the same block. We also compute the matrix elements between vectors from the same block. For example, if R is odd or if R is even and $q \neq 1$, there are edges $\{(q_{\mathrm{in}}, 0, 7), (d(q,1), 0, 3)\}, \{(q_{\mathrm{in}}, 1, 5), (d(q,1), 1, 1)\} \in \mathcal{E}^{\triangle}$. Using the fact that $|\psi_{z,a}^{l}\rangle = |l\rangle |\psi_{z,a}\rangle$ where $|\psi_{z,a}\rangle$ is given by (1.6) and (1.7), we compute the relevant matrix elements:

$$\langle \psi_{z,a}^{q_{\mathrm{in}}} | h_{\mathcal{E}^{\triangle}} | \psi_{z,a}^{d(q,1)} \rangle$$

$$= \langle \psi_{z,a}^{q_{\mathrm{in}}} | \left(\sum_{(z',t,t') \in \{(0,7,3),(1,5,1)\}} (|q_{\mathrm{in}}, z', t\rangle + |d(q,1), z', t'\rangle)(\langle q_{\mathrm{in}}, z', t| + \langle d(q,1), z', t'|) \otimes \mathbb{I} \right) | \psi_{z,a}^{d(q,1)} \rangle$$

$$= \sum_{(z',t,t') \in \{(0,7,3),(1,5,1)\}} \langle \psi_{z,a} | (|z', t\rangle \langle z', t'| \otimes \mathbb{I}) | \psi_{z,a} \rangle = \frac{1}{8}.$$

Continuing in this manner, we compute the principal submatrix of (1.108) corresponding to the set $\mathcal{W}_{(z,a,q)}$. This matrix is shown in Figure **??**. In the Figure each vertex is associated with a state in the block and the weight on a given edge is the matrix element between the two states associated with vertices joined by that edge. The diagonal matrix elements are described by the weights on the self-loops. The matrix described by Figure **??** is the same for each block.

For each triple (z,a,q) with $z, a \in \{0,1\}$ and $q \in [R]$, define

$$|\phi_{z,a}^{q}\rangle = \begin{cases} \frac{1}{\sqrt{3R+2}} \left(|\psi_{z,a}^{q_{\mathrm{in}}}\rangle + \sum_{j \in [R]} (-1)^j \left(|\psi_{z,a}^{d(q,j)}\rangle - |\psi_{\alpha(q,j),a}^{e_{z0}(q,j)}\rangle - |\psi_{\alpha(q,j),a}^{e_{z1}(q,j)}\rangle \right) + |\psi_{z,a}^{q_{\mathrm{out}}}\rangle \right) & R \text{ odd} \\ \frac{1}{\sqrt{3R-1}} \left(|\psi_{z,a}^{q_{\mathrm{in}}}\rangle + \left(\sum_{j<q} - \sum_{j>q} \right) (-1)^j \left(|\psi_{z,a}^{d(q,j)}\rangle - |\psi_{\alpha(q,j),a}^{e_{z0}(q,j)}\rangle - |\psi_{\alpha(q,j),a}^{e_{z1}(q,j)}\rangle \right) + |\psi_{z,a}^{q_{\mathrm{out}}}\rangle \right) & R \text{ even.} \end{cases}$$
$$\tag{1.113}$$

Next we show that these states span the ground space of $A(G^{\triangle})$. The choice to omit $d(q,q)$ for R even ensures that $|\psi_{z,a}^{q_{\mathrm{in}}}\rangle$ and $|\psi_{z,a}^{q_{\mathrm{out}}}\rangle$ have the same sign in these ground states.

Lemma 15. *An orthonormal basis for the e_1-energy ground space of $A(G^\triangle)$ is given by the states*

$$\left\{|\phi_{z,a}^q\rangle :\ z, a \in \{0,1\},\ q \in [R]\right\}$$

defined by equation (1.113). The eigenvalue gap is bounded as

$$\gamma(A(G^\triangle) - e_1) > \frac{1}{(30R)^2}. \tag{1.114}$$

Proof. The e_1-energy ground space of $A(G^\triangle)$ is equal to the nullspace of (1.108). Since this operator is block diagonal in the basis $\mathcal{W}$, we can solve for the eigenvectors in the nullspace of each block. Thus, to prove the first part of the Lemma, we analyze the $|\mathcal{W}_{(z,a,q)}| \times |\mathcal{W}_{(z,a,q)}|$ matrix described by Figure **??** and show that (1.113) is the unique vector in its nullspace. We first rewrite it in a slightly different basis obtained by multiplying some of the basis vectors by a phase of -1. Specifically, we use the basis

$$\left\{|\psi_{z,a}^{q_{\rm in}}\rangle, -|\psi_{z,a}^{d(q,1)}\rangle, |\psi_{\alpha(q,1),a}^{e_{z0}(q,1)}\rangle, |\psi_{\alpha(q,1),a}^{e_{z1}(q,1)}\rangle, |\psi_{z,a}^{d(q,2)}\rangle, -|\psi_{\alpha(q,2),a}^{e_{z0}(q,2)}\rangle, -|\psi_{\alpha(q,2),a}^{e_{z1}(q,2)}\rangle, \ldots, |\psi_{z,a}^{q_{\rm out}}\rangle\right\}$$

where the state associated with each vertex on one side of a bipartition of the graph is multiplied by -1; these are the phases appearing in equation (1.113). Changing to this basis replaces the weight $\frac{1}{8}$ on each edge in Figure **??** by $-\frac{1}{8}$ and does not change the weights on the self-loops. The resulting matrix is $\frac{1}{8}L_0$, where L_0 is the Laplacian matrix of the graph shown in Figure **??**. Now we use the fact that the Laplacian of any connected graph has smallest eigenvalue zero, with a unique eigenvector equal to the all-ones vector. Hence for each block we get an eigenvector in the nullspace of (1.108)) given by (1.113). Ranging over all $z, a \in \{0,1\}$ and $q \in [R]$ gives the claimed basis for the e_1-energy ground space of $A(G^\triangle)$.

To prove the lower bound, we use the Nullspace Projection Lemma (Lemma **??**) with

$$H_A = A(G^\diamond) - e_1 \qquad H_B = h_{\mathcal{E}^\triangle}$$

and where $S = \mathrm{span}(\mathcal{W})$ is the nullspace of H_A as shown in Section 1.4.5. Since it is block diagonal in the basis $\mathcal{W}$, the smallest nonzero eigenvalue of (1.108) is equal to the smallest nonzero eigenvalue of one of its blocks. The matrix for each block is $\frac{1}{8}L_0$. Thus we can lower bound the smallest nonzero eigenvalue of $H_B|_S$ using standard bounds on the smallest nonzero eigenvalue of the Laplacian L of a graph G. In particular, Theorem 4.2 of reference [**?**] shows that

$$\gamma(L) \geq \frac{4}{|V(G)|\,\mathrm{diam}(G)} \geq \frac{4}{|V(G)|^2}$$

(where $\mathrm{diam}(G)$ is the diameter of G). Since the size of the graph in Figure **??** is either $3R - 1$ or $3R + 2$, we have

$$\gamma(H_B|_S) = \frac{1}{8}\gamma(L_0) \geq \frac{1}{8}\frac{4}{(3R+2)^2} \geq \frac{1}{32R^2}$$

since $R \geq 2$. Using this bound and the fact that $\gamma(H_A) > \frac{1}{13}$ (from equation (1.105)) and $\|H_B\| = 2$ (from equation (1.12)) and plugging into Lemma **??** gives

$$\gamma(A(G^\triangle) - e_1) \geq \frac{\frac{1}{13}\cdot\frac{1}{32R^2}}{\frac{1}{13} + \frac{1}{32R^2} + 2} \geq \frac{1}{(32+13+832)R^2} > \frac{1}{(30R)^2}. \qquad \square$$

1.4.7 The Hamiltonian $H(G^\triangle, N)$

We now consider the N-particle Hamiltonian $H(G^\triangle, N)$ and solve for its nullspace. We use the following fact about the subsets $\mathcal{W}_{(z,a,q)} \subset \mathcal{W}$ defined in equation (1.112).

Definition 6. We say $\mathcal{W}_{(z_1,a_1,q_1)}$ and $\mathcal{W}_{(z_2,a_2,q_2)}$ *overlap on a diagram element* if there exists $l \in L^\square$ such that $|\psi^l_{x_1,b_1}\rangle \in \mathcal{W}_{(z_1,a_1,q_1)}$ and $|\psi^l_{x_2,b_2}\rangle \in \mathcal{W}_{(z_2,a_2,q_2)}$ for some $x_1, x_2, b_1, b_2 \in \{0,1\}$.

Fact 1 (Key property of $\mathcal{W}_{(z,a,q)}$). *Sets $\mathcal{W}_{(z_1,a_1,q_1)}$ and $\mathcal{W}_{(z_2,a_2,q_2)}$ overlap on a diagram element if and only if $q_1 = q_2$ or $\{q_1, q_2\} \in E(G^{occ})$.*

This fact can be confirmed by direct inspection of the sets $\mathcal{W}_{(z,a,q)}$. If $q_1 = q_2 = q$ the diagram element l on which they overlap can be chosen to be $l = q_{\text{in}}$; if $q_1 \neq q_2$ and $\{q_1, q_2\} \in E(G^{occ})$ then $l = e_{z_1 z_2}(q_1, q_2) = e_{z_2 z_1}(q_2, q_1)$. Conversely, if $\{q_1, q_2\} \notin E(G^{occ})$ with $q_1 \neq q_2$, then there is no overlap.

We show that the nullspace $\mathcal{I}_\triangle$ of $H(G^\triangle, N)$ is

$$\mathcal{I}_\triangle = \text{span}\{\text{Sym}(|\phi^{q_1}_{z_1,a_1}\rangle|\phi^{q_2}_{z_2,a_2}\rangle \ldots |\phi^{q_N}_{z_N,a_N}\rangle) : z_i, a_i \in \{0,1\}, q_i \in [R], q_i \neq q_j, \text{ and } \{q_i, q_j\} \notin E(G^{occ})\}. \tag{1.115}$$

Note that $\mathcal{I}_\triangle \subset \mathcal{Z}_N(G^\triangle)$ is very similar to $\mathcal{I}(G, G^{occ}, N) \subset \mathcal{Z}_N(G)$ (from equation (??)) but with each single-particle state $|\psi^q_{z,a}\rangle \in \mathcal{Z}_N(G)$ replaced by $|\phi^q_{z,a}\rangle \in \mathcal{Z}_N(G^\triangle)$.

Lemma 16. *The nullspace of $H(G^\triangle, N)$ is $\mathcal{I}_\triangle$ as defined in equation (1.115). Its smallest nonzero eigenvalue is*

$$\gamma(H(G^\triangle, N)) > \frac{1}{(17R)^7}. \tag{1.116}$$

In addition to Fact 1, we use the following simple fact in the proof of the Lemma.

Fact 2. *Let $|p\rangle = c|\alpha_0\rangle + \sqrt{1-c^2}|\alpha_1\rangle$ with $\langle \alpha_i|\alpha_j\rangle = \delta_{ij}$ and $c \in [0,1]$. Then*

$$|p\rangle\langle p| = c^2|\alpha_0\rangle\langle \alpha_0| + M$$

where $\|M\| \leq 1 - \frac{3}{4}c^4$.

To prove this Fact, one can calculate $\|M\| = \frac{1}{2}(1-c^2) + \frac{1}{2}\sqrt{1+2c^2-3c^4}$ and use the inequality $\sqrt{1+x} \leq 1 + \frac{x}{2}$ for $x \geq -1$.

Proof of Lemma 16. Using equation (1.107) and the fact that the smallest eigenvalues of $A(G^\diamond)$ and $A(G^\triangle)$ are the same (equal to e_1, from Section 1.4.5 and Lemma 15), we have

$$H(G^\triangle, N) = H(G^\diamond, N) + \sum_{w=1}^{N} h_{\mathcal{E}^\triangle}^{(w)}\bigg|_{\mathcal{Z}_N(G^\triangle)}. \tag{1.117}$$

Recall from Lemma 14 that the nullspace of $H(G^\diamond, N)$ is $\mathcal{I}_\diamond$. We consider

$$\sum_{w=1}^{N} h_{\mathcal{E}^\triangle}^{(w)}\bigg|_{\mathcal{I}_\diamond}. \tag{1.118}$$

We show that its nullspace is equal to $\mathcal{I}_\triangle$ (establishing the first part of the Lemma), and we lower bound its smallest nonzero eigenvalue. Specifically, we prove

$$\gamma\left(\sum_{w=1}^{N} h_{\mathcal{E}^\triangle}^{(w)}\bigg|_{\mathcal{I}_\diamond}\right) > \frac{1}{(9R)^6}. \tag{1.119}$$

Now we prove equation (1.116) using this bound. We apply the Nullspace Projection Lemma (Lemma ??) with H_A and H_B given by the first and second terms in equation (1.117); in this case the nullspace of H_A is $S = \mathcal{I}_\diamond$ (from Lemma 14). Now applying Lemma ?? and using the bounds $\gamma(H_A) > \frac{1}{300}$ (from Lemma 14), $\|H_B\| \leq N\|h_{\mathcal{E}^\triangle}\| = 2N \leq 2R$ (from equation (1.12) and the fact that $N \leq R$), and the bound (1.119) on $\gamma(H_B|_S)$, we find

$$\gamma(H(G^\triangle, N)) \geq \frac{\frac{1}{300(9R)^6}}{\frac{1}{300} + \frac{1}{(9R)^6} + 2R} \geq \left(\frac{1}{9^6 + 300 + 600 \cdot 9^6}\right)\frac{1}{R^7} > \frac{1}{(17R)^7}.$$

To complete the proof we must establish that the nullspace of (1.118) is $\mathcal{I}_\triangle$ and prove the lower bound (1.119). To analyze (1.118) we use the fact (established in Section 1.4.6) that (1.108) is block diagonal with a block $\mathcal{W}_{(z,a,q)} \subset \mathcal{W}$ for each triple (z,a,q) with $z,a \in \{0,1\}$ and $q \in [R]$. The operator (1.118) inherits a block structure from this fact. For any basis vector

$$\mathrm{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle|\psi_{z_2,a_2}^{q_2}\rangle\ldots|\psi_{z_N,a_N}^{q_N}\rangle) \in \mathcal{I}_\diamond, \tag{1.120}$$

we define a set of occupation numbers

$$\mathcal{N} = \left\{N_{(x,b,r)}\colon x,b \in \{0,1\},\, r \in [R]\right\}$$

where

$$N_{(x,b,r)} = |\{j\colon |\psi_{z_j,a_j}^{q_j}\rangle \in \mathcal{W}_{(x,b,r)}\}|.$$

Now observe that (1.118) conserves the set of occupation numbers and is therefore block diagonal with a block for each possible set $\mathcal{N}$.

For a given block corresponding to a set of occupation numbers $\mathcal{N}$, we write $\mathcal{I}_\diamond(\mathcal{N}) \subset \mathcal{I}_\diamond$ for the subspace spanned by basis vectors (1.120) in the block. We classify the blocks into three categories depending on $\mathcal{N}$.

Classification of the blocks of (1.118) according to $\mathcal{N}$

Consider the following two conditions on a set $\mathcal{N} = \{N_{(x,b,r)}\colon x,b \in \{0,1\},\, r \in [R]\}$ of occupation numbers:

(a) $N_{(x,b,r)} \in \{0,1\}$ for all $x,b \in \{0,1\}$ and $r \in [R]$. If this holds, write (y_i, c_i, s_i) for the nonzero occupation numbers (with some arbitrary ordering), i.e., $N_{(y_i,c_i,s_i)} = 1$ for $i \in [N]$.

(b) The sets $\mathcal{W}_{(y_i,c_i,s_i)}$ and $\mathcal{W}_{(y_j,c_j,s_j)}$ do not overlap on a diagram element for all distinct $i,j \in [N]$.

We say a block is of type 1 if $\mathcal{N}$ satisfies (a) and (b). We say it is of type 2 if $\mathcal{N}$ does

not satisfy (a). We say it is of type 3 if $\mathcal{N}$ satisfies (a) but does not satisfy (b).

Note that every block is either of type 1, 2, or 3. We consider each type separately. Specifically, we show that each block of type 1 contains one state in the nullspace of (1.118) and, ranging over all blocks of this type, we obtain a basis for $\mathcal{I}_{\triangle}$. We also show that the smallest nonzero eigenvalue within a block of type 1 is at least $\frac{1}{32R^2}$. Finally, we show that blocks of type 2 and 3 do not contain any states in the nullspace of (1.118) and that the smallest eigenvalue within any block of type 2 or 3 is greater than $\frac{1}{(9R)^6}$. Hence, the nullspace of (1.118) is $\mathcal{I}_{\triangle}$ and its smallest nonzero eigenvalue is lower bounded as in equation (1.119).

Type 1

Note (from Definition 6) that (b) implies $q \neq r$ whenever

$$|\psi_{x,b}^q\rangle \in \mathcal{W}_{(y_i,c_i,s_i)} \text{ and } |\psi_{z,a}^r\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}$$

for distinct $i, j \in [N]$. Hence

$$\mathcal{I}_{\diamond}(\mathcal{N}) = \text{span}\{\text{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle|\psi_{z_2,a_2}^{q_2}\rangle \ldots |\psi_{z_N,a_N}^{q_N}\rangle): q_i \neq q_j \text{ and } |\psi_{z_j,a_j}^{q_j}\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}\}$$
$$= \text{span}\{\text{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle|\psi_{z_2,a_2}^{q_2}\rangle \ldots |\psi_{z_N,a_N}^{q_N}\rangle): |\psi_{z_j,a_j}^{q_j}\rangle \in \mathcal{W}_{(y_j,c_j,s_j)}\}.$$

From this we see that

$$\dim(\mathcal{I}_{\diamond}(\mathcal{N})) = \prod_{j=1}^{N} |\mathcal{W}_{(y_j,c_j,s_j)}| = \begin{cases} (3R+2)^N & R \text{ odd} \\ (3R-1)^N & R \text{ even.} \end{cases}$$

We now solve for all the eigenstates of (1.118) within the block.

It is convenient to write an orthonormal basis of eigenvectors of the $|\mathcal{W}_{(z,a,q)}| \times |\mathcal{W}_{(z,a,q)}|$ matrix described by Figure **??** as

$$|\phi_{z,a}^q(u)\rangle, \quad u \in [|\mathcal{W}_{(z,a,q)}|] \tag{1.121}$$

and their ordered eigenvalues as

$$\theta_1 \leq \theta_2 \leq \ldots \leq \theta_{|\mathcal{W}_{(z,a,q)}|}.$$

From the proof of Lemma 15, the eigenvector with smallest eigenvalue $\theta_1 = 0$ is $|\phi_{z,a}^q\rangle = |\phi_{z,a}^q(1)\rangle$ and $\theta_2 \geq \frac{1}{32R^2}$. For any $u_1, u_2, \ldots, u_N \in [|\mathcal{W}_{(z,a,q)}|]$, the state

$$\text{Sym}(|\phi_{y_1,c_1}^{s_1}(u_1)\rangle|\phi_{y_2,c_2}^{s_2}(u_2)\rangle \ldots |\phi_{y_N,c_N}^{s_N}(u_N)\rangle)$$

is an eigenvector of (1.118) with eigenvalue $\sum_{j=1}^{N} \theta_j$. Furthermore, states corresponding to different choices of $u_1, \ldots, u_N$ are orthogonal, and ranging over all $\dim(\mathcal{I}_{\diamond}(\mathcal{N}))$ choices we get every eigenvector in the block. The smallest eigenvalue within the block is $N\theta_1 = 0$ and there is a unique vector in the nullspace, given by

$$\text{Sym}(|\phi_{y_1,c_1}^{s_1}\rangle|\phi_{y_2,c_2}^{s_2}\rangle \ldots |\phi_{y_N,c_N}^{s_N}\rangle) \tag{1.122}$$

(recall $|\phi_{z,a}^q\rangle = |\phi_{z,a}^q(1)\rangle$). The smallest nonzero eigenvalue of (1.118) within the block is $(N-1)\theta_1 + \theta_2 = \theta_2 \geq \frac{1}{32R^2}$.

Finally, we show that the collection of states (1.122) obtained from all blocks of type 1 spans the space $\mathcal{I}_\triangle$. Each block of type 1 corresponds to a set of occupation numbers

$$N_{(y_1,c_1,s_1)} = N_{(y_2,c_2,s_2)} = \cdots = N_{(y_N,c_N,s_N)} = 1 \quad \text{(with all other occupation numbers zero)}$$

and gives a unique vector (1.122) in the nullspace of $H(G^\triangle, N)$. The sets $\mathcal{W}_{(y_i,c_i,s_i)}$ and $\mathcal{W}_{(y_j,c_j,s_j)}$ do not overlap on a diagram element for all distinct $i, j \in [N]$. Using Fact 1 we see this is equivalent to $s_i \neq s_j$ and $\{s_i, s_j\} \notin E(G^{\mathrm{occ}})$ for distinct $i, j \in [N]$. Hence the set of states (1.122) obtained from of all blocks of type 1 is

$$\left\{ \mathrm{Sym}(|\phi_{y_1,c_1}^{s_1}\rangle|\phi_{y_2,c_2}^{s_2}\rangle \ldots |\phi_{y_N,c_N}^{s_N}\rangle) \colon y_i, c_i \in \{0,1\}, \ s_i \in [R], \ s_i \neq s_j, \ \{s_i, s_j\} \notin E(G^{\mathrm{occ}}) \right\}$$

which spans $\mathcal{I}_\triangle$.

Type 2

If $\mathcal{N}$ is of type 2 then there exist $x, b \in \{0,1\}$ and $r \in [R]$ such that $N_{(x,b,r)} \geq 2$. We show there are no eigenvectors in the nullspace of (1.118) within a block of this type and we lower bound the smallest eigenvalue within the block. Specifically, we show

$$\min_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \sum_{w=1}^N h_{\mathcal{E}^\triangle}^{(w)} |\kappa\rangle > \frac{1}{(9R)^6}. \tag{1.123}$$

First note that all $|\kappa\rangle \in \mathcal{I}_\diamond$ satisfy $(A(G^\diamond) - e_1)^{(w)}|\kappa\rangle = 0$ for each $w \in [N]$, which can be seen using the definition of $\mathcal{I}_\diamond$ and the fact that $\mathcal{W}$ spans the nullspace of $A(G^\diamond) - e_1$. Using this fact and equation (1.107), we get

$$\min_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \sum_{w=1}^N h_{\mathcal{E}^\triangle}^{(w)} |\kappa\rangle = \min_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \sum_{w=1}^N \left(A(G^\triangle) - e_1 \right)^{(w)} |\kappa\rangle. \tag{1.124}$$

Now we use the operator inequality

$$\sum_{w=1}^N \left(A(G^\triangle) - e_1 \right)^{(w)} \geq \gamma \left(\sum_{w=1}^N \left(A(G^\triangle) - e_1 \right)^{(w)} \right) \cdot \left(1 - \Pi^\triangle \right)$$

$$= \gamma(A(G^\triangle) - e_1) \cdot \left(1 - \Pi^\triangle \right) > \frac{1}{(30R)^2} \left(1 - \Pi^\triangle \right), \tag{1.125}$$

where $\Pi^\triangle$ is the projector onto the nullspace of $\sum_{w=1}^N \left(A(G^\triangle) - e_1 \right)^{(w)}$, and where in the last step we used Lemma 15. Plugging equation (1.125) into equation (1.124) gives

$$\min_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \sum_{w=1}^N h_{\mathcal{E}^\triangle}^{(w)} |\kappa\rangle > \frac{1}{(30R)^2} \left(1 - \max_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \Pi^\triangle |\kappa\rangle \right). \tag{1.126}$$

In the following we show that $\langle \kappa | \Pi^\triangle |\kappa\rangle = \langle \kappa | \Pi_{\mathcal{N}}^\triangle |\kappa\rangle$ for all $|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})$, where $\Pi_{\mathcal{N}}^\triangle$ is a Hermitian operator with

$$1 - \|\Pi_{\mathcal{N}}^\triangle\| \geq \frac{3}{4} \left(\frac{1}{4R} \right)^4 = \frac{3}{1024R^4}. \tag{1.127}$$

Plugging this into (1.126) gives

$$\min_{|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})} \langle \kappa | \sum_{w=1}^{N} h_{\mathcal{E}^\triangle}^{(w)} | \kappa \rangle > \frac{3}{(30R)^2 \cdot 1024R^4} > \frac{1}{(9R)^6}.$$

To complete the proof, we exhibit the operator $\Pi_\mathcal{N}^\triangle$ and show that its norm is bounded as (1.127). Using Lemma 15 we can write $\Pi^\triangle$ explicitly as

$$\Pi^\triangle = \sum_{(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})} \tag{1.128}$$

where

$$\mathcal{P}_{(\vec{z},\vec{a},\vec{q})} = |\phi_{z_1,a_1}^{q_1}\rangle\langle\phi_{z_1,a_1}^{q_1}| \otimes |\phi_{z_2,a_2}^{q_2}\rangle\langle\phi_{z_2,a_2}^{q_2}| \otimes \cdots \otimes |\phi_{z_N,a_N}^{q_N}\rangle\langle\phi_{z_N,a_N}^{q_N}|$$
$$\mathcal{Q} = \{(z_1,\ldots z_N, a_1,\ldots,a_N, q_1,\ldots,q_N) : z_i, a_i \in \{0,1\} \text{ and } q_i \in [R]\}.$$

For each $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}$ we also define a space

$$S_{(\vec{z},\vec{a},\vec{q})} = \text{span}(\mathcal{W}_{(z_1,a_1,q_1)}) \otimes \text{span}(\mathcal{W}_{(z_2,a_2,q_2)}) \otimes \cdots \otimes \text{span}(\mathcal{W}_{(z_N,a_N,q_N)}).$$

Note that $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ has all of its support in $S_{(\vec{z},\vec{a},\vec{q})}$, and that

$$S_{(\vec{z},\vec{a},\vec{q})} \perp S_{(\vec{z}',\vec{a}',\vec{q}')} \text{ for distinct } (\vec{z},\vec{a},\vec{q}), (\vec{z}',\vec{a}',\vec{q}') \in \mathcal{Q}. \tag{1.129}$$

Therefore $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}\mathcal{P}_{(\vec{z}',\vec{a}',\vec{q}')} = 0$ for distinct $(\vec{z},\vec{a},\vec{q}), (\vec{z}',\vec{a}',\vec{q}') \in \mathcal{Q}$. (Below we use similar reasoning to obtain a less obvious result.) Note that $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ is orthogonal to $\mathcal{I}_\diamond(\mathcal{N})$ unless

$$|\{j : (z_j, a_j, q_j) = (w, u, v)\}| = N_{(w,u,v)} \text{ for all } w, u \in \{0,1\}, v \in [R]. \tag{1.130}$$

We restrict our attention to the projectors that are not orthogonal to $\mathcal{I}_\diamond(\mathcal{N})$. Letting $\mathcal{Q}(\mathcal{N}) \subset \mathcal{Q}$ be the set of $(\vec{z},\vec{a},\vec{q})$ satisfying equation (1.130), we have

$$\langle\kappa| \sum_{(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})} |\kappa\rangle = \langle\kappa| \sum_{(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})} |\kappa\rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N}). \tag{1.131}$$

Since $N_{(x,b,r)} \geq 2$, note that in each term $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ with $(\vec{z},\vec{a},\vec{q}) \in \mathcal{Q}(\mathcal{N})$, the operator

$$|\phi_{x,b}^r\rangle\langle\phi_{x,b}^r| \otimes |\phi_{x,b}^r\rangle\langle\phi_{x,b}^r|$$

appears between two of the N registers (tensored with rank-1 projectors on the other $N-2$ registers). Using equation (1.113) we may expand $|\phi_{x,b}^r\rangle$ as a sum of states from $\mathcal{W}_{(x,b,r)}$. This gives

$$|\phi_{x,b}^r\rangle|\phi_{x,b}^r\rangle = c_0|\psi_{x,b}^{r_{\text{in}}}\rangle|\psi_{x,b}^{r_{\text{in}}}\rangle + \left(1 - c_0^2\right)^{\frac{1}{2}} |\Phi_{x,b}^r\rangle$$

where c_0 is either $\frac{1}{3R+2}$ (if R is odd) or $\frac{1}{3R-1}$ (if R is even), and where $|\psi_{x,b}^{r_{\text{in}}}\rangle|\psi_{x,b}^{r_{\text{in}}}\rangle$ is orthogonal to $|\Phi_{x,b}^r\rangle$. Note that each of the states $|\phi_{x,b}^r\rangle|\phi_{x,b}^r\rangle$, $|\psi_{x,b}^{r_{\text{in}}}\rangle|\psi_{x,b}^{r_{\text{in}}}\rangle$, and $|\Phi_{x,b}^r\rangle$ lie in the space

$$\text{span}(\mathcal{W}_{(x,b,r)}) \otimes \text{span}(\mathcal{W}_{(x,b,r)}). \tag{1.132}$$

Now applying Fact 2 gives

$$|\phi_{x,b}^r\rangle\langle\phi_{x,b}^r| \otimes |\phi_{x,b}^r\rangle\langle\phi_{x,b}^r| = c_0^2|\psi_{x,b}^{r_{\text{in}}}\rangle\langle\psi_{x,b}^{r_{\text{in}}}| \otimes |\psi_{x,b}^{r_{\text{in}}}\rangle\langle\psi_{x,b}^{r_{\text{in}}}| + M_{x,b}^r \qquad (1.133)$$

where $M_{x,b}^r$ is a Hermitian operator with all of its support on the space (1.132) and

$$\left\|M_{x,b}^r\right\| \leq 1 - \frac{3}{4}c_0^4 \leq 1 - \frac{3}{4}\left(\frac{1}{3R+2}\right)^4 \leq 1 - \frac{3}{4}\frac{1}{(4R)^4} \qquad (1.134)$$

since $R \geq 2$. For each $(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}(\mathcal{N})$ we define $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M$ to be the operator obtained from $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}$ by replacing

$$|\phi_{x,b}^r\rangle\langle\phi_{x,b}^r| \otimes |\phi_{x,b}^r\rangle\langle\phi_{x,b}^r| \mapsto M_{x,b}^r$$

on two of the registers (if $N_{(x,b,r)} > 2$ there is more than one way to do this; we fix one choice for each $(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}(\mathcal{N})$). Note that $\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M$ has all of its support in the space $S_{(\vec{z},\vec{a},\vec{q})}$. Using (1.129) gives

$$\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M \mathcal{P}_{(\vec{z}',\vec{a}',\vec{q}')}^M = 0 \text{ for distinct } (\vec{z}, \vec{a}, \vec{q}), (\vec{z}', \vec{a}', \vec{q}') \in \mathcal{Q}(\mathcal{N}).$$

Using equation (1.133) and the fact that

$$\langle\kappa|\left(|\psi_{x,b}^{r_{\text{in}}}\rangle\langle\psi_{x,b}^{r_{\text{in}}}|^{(w_1)}\right)\left(|\psi_{x,b}^{r_{\text{in}}}\rangle\langle\psi_{x,b}^{r_{\text{in}}}|^{(w_2)}\right)|\kappa\rangle = 0 \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N}) \text{ and distinct } w_1, w_2 \in [N]$$

(which can be seen from the definition of $\mathcal{I}_\diamond$), we have

$$\langle\kappa|\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}|\kappa\rangle = \langle\kappa|\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M|\kappa\rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N}).$$

Hence, letting

$$\Pi_{\mathcal{N}}^\triangle = \sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M, \qquad (1.135)$$

we have $\langle\kappa|\Pi^\triangle|\kappa\rangle = \langle\kappa|\Pi_{\mathcal{N}}^\triangle|\kappa\rangle$ for all $|\kappa\rangle \in \mathcal{I}_\diamond(\mathcal{N})$. To obtain the desired bound (1.127) on the norm of $\Pi_{\mathcal{N}}^\triangle$, we use the fact that the norm of a sum of pairwise orthogonal Hermitian operators is upper bounded by the maximum norm of an operator in the sum, so

$$\left\|\Pi_{\mathcal{N}}^\triangle\right\| = \left\|\sum_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M\right\| = \max_{(\vec{z},\vec{a},\vec{q})\in\mathcal{Q}(\mathcal{N})} \left\|\mathcal{P}_{(\vec{z},\vec{a},\vec{q})}^M\right\| = \left\|M_{x,b}^r\right\| \leq 1 - \frac{3}{4}\frac{1}{(4R)^4}. \qquad (1.136)$$

Type 3

If $\mathcal{N}$ is of type 3 then $N_{(x,b,r)} \in \{0,1\}$ for all $x, b \in \{0,1\}$ and $r \in [R]$, and

$$N_{(y,c,s)} = N_{(t,d,u)} = 1$$

for some $(y, c, s) \neq (t, d, u)$ with either $u = s$ or $\{u, s\} \in E(G^{\text{occ}})$ (using property (b) and Fact 1). We show there are no eigenvectors in the nullspace of (1.118) within a block of this type and we lower bound the smallest eigenvalue within the block. We establish the same bound (1.123) as for blocks of Type 2.

The proof is very similar to that given above for blocks of Type 2. In fact, the first part of proof is identical, from equation (1.124) up to and including equation (1.131). That is to say, as in the previous case we have

$$\langle \kappa | \sum_{(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}} \mathcal{P}_{(\vec{z}, \vec{a}, \vec{q})} | \kappa \rangle = \langle \kappa | \sum_{(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}(\mathcal{N})} \mathcal{P}_{(\vec{z}, \vec{a}, \vec{q})} | \kappa \rangle \quad \text{for all } |\kappa\rangle \in \mathcal{I}_{\Diamond}(\mathcal{N}). \tag{1.137}$$

In this case, since $N_{(y,c,s)} = N_{(t,d,u)} = 1$, in each term $\mathcal{P}_{(\vec{z}, \vec{a}, \vec{q})}$ with $(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}(\mathcal{N})$, the operator

$$|\phi_{y,c}^s\rangle\langle\phi_{y,c}^s| \otimes |\phi_{t,d}^u\rangle\langle\phi_{t,d}^u|$$

appears between two of the N registers (tensored with rank 1 projectors on the other $N - 2$ registers). Using equation (1.113) we may expand $|\phi_{y,c}^s\rangle$ and $|\phi_{t,d}^u\rangle$ as superpositions (with amplitudes $\pm\frac{1}{\sqrt{3R+2}}$ if R is odd or $\pm\frac{1}{\sqrt{3R-1}}$ if R is even) of the basis states from $\mathcal{W}_{(y,c,s)}$ and $\mathcal{W}_{(t,d,u)}$ respectively. Since $\mathcal{W}_{(y,c,s)}$ and $\mathcal{W}_{(t,d,u)}$ overlap on some diagram element, there exists $l \in L^{\square}$ such that $|\psi_{x_1,b_1}^l\rangle \in \mathcal{W}_{(y,c,s)}$ and $|\psi_{x_2,b_2}^l\rangle \in \mathcal{W}_{(t,d,u)}$ for some $x_1, x_2, b_1, b_2 \in \{0, 1\}$. Hence

$$|\phi_{y,c}^s\rangle|\phi_{t,d}^u\rangle = c_0 \left(\pm |\psi_{x_1,b_1}^l\rangle|\psi_{x_2,b_2}^l\rangle \right) + \left(1 - c_0^2\right)^{\frac{1}{2}} |\Phi_{y,c,t,d}^{s,u}\rangle$$

where c_0 is either $\frac{1}{3R+2}$ (if R is odd) or $\frac{1}{3R-1}$ (if R is even). Now applying Fact 2 we get

$$|\phi_{y,c}^s\rangle\langle\phi_{y,c}^s| \otimes |\phi_{t,d}^u\rangle\langle\phi_{t,d}^u| = c_0^2 |\psi_{x_1,b_1}^l\rangle\langle\psi_{x_1,b_1}^l| \otimes |\psi_{x_2,b_2}^l\rangle\langle\psi_{x_2,b_2}^l| + M_{y,c,t,d}^{s,u} \tag{1.138}$$

where $\|M_{y,c,t,d}^{s,u}\| \le 1 - \frac{3}{4}\left(\frac{1}{4R}\right)^4$. For each $(\vec{z}, \vec{a}, \vec{q}) \in \mathcal{Q}(\mathcal{N})$ we define $\mathcal{P}_{(\vec{z}, \vec{a}, \vec{q})}^M$ to be the operator obtained from $\mathcal{P}_{(\vec{z}, \vec{a}, \vec{q})}$ by replacing

$$|\phi_{y,c}^s\rangle\langle\phi_{y,c}^s| \otimes |\phi_{t,d}^u\rangle\langle\phi_{t,d}^u| \mapsto M_{y,c,t,d}^{s,u}$$

on two of the registers and we let $\Pi_{\mathcal{N}}^{\triangle}$ be given by (1.135). Then, as in the previous case, $\langle \kappa | \Pi^{\triangle} | \kappa \rangle = \langle \kappa | \Pi_{\mathcal{N}}^{\triangle} | \kappa \rangle$ for all $|\kappa\rangle \in \mathcal{I}_{\Diamond}(\mathcal{N})$ and using the same reasoning as before, we get the bound (1.127) on $\|\Pi_{\mathcal{N}}^{\triangle}\|$. Using these two facts we get the same bound on the smallest eigenvalue within a block of type 3 as the bound we obtained for blocks of type 2:

$$\min_{|\kappa\rangle \in \mathcal{I}_{\Diamond}(\mathcal{N})} \langle \kappa | \sum_{w=1}^{N} h_{\mathcal{E}^{\triangle}}^{(w)} | \kappa \rangle > \frac{1}{(30R)^2} \left(1 - \|\Pi_{\mathcal{N}}^{\triangle}\|\right) > \frac{1}{(9R)^6}. \qquad \square$$

1.4.8 The gate graph $G^{\square}$

We now consider the gate graph $G^{\square}$ and prove Lemma **??**. We first show that $G^{\square}$ is an e_1-gate graph. From equations (1.99), (1.100), and (1.101) we have

$$A(G^{\square}) = A(G^{\triangle}) + h_{\mathcal{E}^0} + h_{\mathcal{S}^0}. \tag{1.139}$$

Lemma 15 characterizes the e_1-energy ground space of $G^{\triangle}$ and gives an orthonormal basis $\{|\phi_{z,a}^q\rangle : z, a \in \{0, 1\}, q \in [R]\}$ for it. To solve for the e_1-energy ground space of $A(G^{\square})$, we solve for superpositions of the states $\{|\phi_{z,a}^q\rangle\}$ in the nullspace of $h_{\mathcal{E}^0} + h_{\mathcal{S}^0}$.

and using equation (1.144), we see that $\langle\Gamma'|h_{\mathcal{E}^0} + h_{\mathcal{S}^0}|\Gamma'\rangle = 0$ and therefore $\langle\Gamma'|A(G^\square)|\Gamma'\rangle = e_1$. Hence $G^\square$ is an e_1-gate graph. Moreover, the linear mapping from $\mathcal{Z}_1(G)$ to $\mathcal{Z}_1(G^\square)$ defined by

$$|\psi_{z,a}^q\rangle \mapsto |\phi_{z,a}^q\rangle \tag{1.145}$$

maps each e_1-energy eigenstate of $A(G)$ to an e_1-energy eigenstate of $A(G^\square)$.

Now consider the N-particle Hamiltonian $H(G^\square, N)$. Using equation (1.139) and the fact that both $A(G^\square)$ and $A(G^\triangle)$ have smallest eigenvalue e_1, we have

$$H(G^\square, N) = H(G^\triangle, N) + \sum_{w=1}^{N} (h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)}\bigg|_{\mathcal{Z}_N(G^\square)}.$$

Recall from Lemma 15 that the nullspace of the first term is $\mathcal{I}_\triangle$. The N-fold tensor product of the mapping (1.145) acts on basis vectors of $\mathcal{I}(G, G^{\mathrm{occ}}, N)$ as

$$\mathrm{Sym}(|\psi_{z_1,a_1}^{q_1}\rangle|\psi_{z_2,a_2}^{q_2}\rangle\ldots|\psi_{z_N,a_N}^{q_N}\rangle) \mapsto \mathrm{Sym}(|\phi_{z_1,a_1}^{q_1}\rangle|\phi_{z_2,a_2}^{q_2}\rangle\ldots|\phi_{z_N,a_N}^{q_N}\rangle), \tag{1.146}$$

where $z_i, a_i \in \{0,1\}$, $q_i \neq q_j$, and $\{q_i, q_j\} \notin E(G^{\mathrm{occ}})$. Clearly this defines an invertible linear map between the two spaces $\mathcal{I}(G, G^{\mathrm{occ}}, N)$ and $\mathcal{I}_\triangle$. Let $|\Theta\rangle \in \mathcal{I}(G, G^{\mathrm{occ}}, N)$ and write $|\Theta'\rangle \in \mathcal{I}_\triangle$ for its image under the map (1.146). Then

$$\langle\Theta'|H(G^\square, N)|\Theta'\rangle = \langle\Theta'|\sum_{w=1}^{N}(h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)}|\Theta'\rangle = \langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle\cdot\begin{cases} \frac{1}{3R+2} & R \text{ odd} \\ \frac{1}{3R-1} & R \text{ even} \end{cases} \tag{1.147}$$

where in the first equality we used the fact that $|\Theta'\rangle$ is in the nullspace $\mathcal{I}_\triangle$ of $H(G^\triangle, N)$ and in the second equality we used equation (1.144) and the fact that $\langle\phi_{z,a}^q|\phi_{x,b}^r\rangle = \langle\psi_{z,a}^q|\psi_{x,b}^r\rangle$. We now complete the proof of Lemma ?? using equation (1.147).

Case 1: $\lambda_N(G, G^{\mathbf{occ}}) \leq a$

In this case there exists a state $|\Theta\rangle \in \mathcal{I}(G, G^{\mathrm{occ}}, N)$ satisfying

$$\langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle \leq a.$$

From equation (1.147) we see that the state $|\Theta'\rangle \in \mathcal{I}_\triangle$ satisfies $\langle\Theta'|H(G^\square, N)|\Theta'\rangle \leq \frac{a}{3R-1} \leq \frac{a}{R}$.

Case 2: $\lambda_N(G, G^{\mathbf{occ}}) \geq b$

In this case

$$\lambda_N(G, G^{\mathrm{occ}}) = \min_{|\Theta\rangle\in\mathcal{I}(G,G^{\mathrm{occ}},N)}\langle\Theta|H(G, G^{\mathrm{occ}}, N)|\Theta\rangle = \min_{|\Theta\rangle\in\mathcal{I}(G,G^{\mathrm{occ}},N)}\langle\Theta|\sum_{w=1}^{N}(h_{\mathcal{E}^G} + h_{\mathcal{S}^G})^{(w)}|\Theta\rangle \geq b.$$

Now applying equation (1.147) gives

$$\min_{|\Theta'\rangle \in \mathcal{I}_\triangle} \langle \Theta'| H(G^\square, N)|\Theta'\rangle = \min_{|\Theta'\rangle \in \mathcal{I}_\triangle} \langle \Theta'| \sum_{w=1}^{N} (h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)} |\Theta'\rangle \geq \frac{1}{3R+2} b. \qquad (1.148)$$

This establishes that the nullspace of $H(G^\square, N)$ is empty, i.e., $\lambda_N^1(G^\square) > 0$, so $\lambda_N^1(G^\square) = \gamma(H(G^\square, N))$. We lower bound $\lambda_N^1(G^\square)$ using the Nullspace Projection Lemma (Lemma **??**) with

$$H_A = H(G^\triangle, N) \qquad H_B = \sum_{w=1}^{N} (h_{\mathcal{E}^0} + h_{\mathcal{S}^0})^{(w)} \bigg|_{\mathcal{Z}_N(G^\square)}$$

and where the nullspace of H_A is $S = \mathcal{I}_\triangle$. We apply Lemma **??** and use the bounds $\gamma(H_A) > \frac{1}{(17R)^7}$ (from Lemma 16), $\gamma(H_B|_S) \geq \frac{b}{3R+2}$ (from equation (1.148)), and $\|H_B\| \leq N \|h_{\mathcal{E}^0} + h_{\mathcal{S}^0}\| \leq 3N \leq 3R$ (using equations (1.12) and (1.11) and the fact that $N \leq R$) to find

$$\lambda_N^1(G^\square) = \gamma(H(G^\square, N))$$

$$\geq \frac{b}{(3R+2)(17R)^7(\frac{1}{(17R)^7} + \frac{b}{3R+2} + 3R)}$$

$$\geq \frac{b}{R^9} \cdot \frac{1}{3 + 2 + b \cdot (17)^7 + 3 \cdot (3+2)(17)^7}$$

$$> \frac{b}{(13R)^9}$$

where in the denominator we used the fact that $b \leq 1$.

1.4.9 Completeness and Soundness

1.5 Open questions