

Gapped and gapless phases of frustration-free spin- $\frac{1}{2}$ chains

Sergey Bravyi* David Gosset^{†‡}

Abstract

We consider a family of translation-invariant quantum spin chains with nearest-neighbor interactions and derive necessary and sufficient conditions for these systems to be gapped in the thermodynamic limit. More precisely, let ψ be an arbitrary two-qubit state. We consider a chain of n qubits with open boundary conditions and Hamiltonian $H_n(\psi)$ which is defined as the sum of rank-1 projectors onto ψ applied to consecutive pairs of qubits. We show that the spectral gap of $H_n(\psi)$ is upper bounded by $1/(n-1)$ if the eigenvalues of a certain 2×2 matrix simply related to ψ have equal non-zero absolute value. Otherwise, the spectral gap is lower bounded by a positive constant independent of n (depending only on ψ). A key ingredient in the proof is a new operator inequality for the ground space projector which expresses a monotonicity under the partial trace. This monotonicity property appears to be very general and might be interesting in its own right. As an extension of our main result, we obtain a complete classification of gapped and gapless phases of frustration-free translation-invariant spin-1/2 chains with nearest-neighbor interactions.

*IBM T.J. Watson Research Center, Yorktown Heights, NY

[†]Walter Burke Institute for Theoretical Physics and Institute for Quantum Information and Matter, California Institute of Technology

[‡]Department of Combinatorics & Optimization and Institute for Quantum Computing, University of Waterloo

Contents

1	Introduction	2
1.1	Sketch of the proof	5
2	Structure of the ground space	7
2.1	Open boundary conditions	7
2.2	Periodic boundary conditions	9
3	Gapless phase	10
4	Monotonicity under the partial trace	14
5	Gapped phase	20
5.1	Correlation functions	22
5.2	Region exclusion lemmas	25
5.3	Proof of the gapped phase theorem	29
5.4	Specializing to product states	30
6	Acknowledgments	31
	Appendix	33
	Qubit chains with higher rank projectors	33

1 Introduction

Many properties of quantum spin chains depend crucially on whether the Hamiltonian is gapped or gapless in the thermodynamic limit. Ground states of gapped Hamiltonians are weakly entangled, as quantified by the entanglement area law [1, 2, 3], and exhibit an exponential decay of correlation functions [4]. For such systems the ground energy and the ground state itself can be efficiently computed using algorithms based on Matrix Product States [5, 6, 7, 8]. On the other hand, ground states of gapless spin chains can exhibit drastic violations of the entanglement area law [9, 10, 11, 12], and computing the ground energy can be quantum-NP hard [13, 14]. Spin chain models studied in physics usually become gapless along quantum phase transition lines separating distinct gapped phases [15]. Deciding whether a given family of Hamiltonians is gapped or gapless in the thermodynamic limit is therefore a fundamental problem.

In this paper we provide a complete solution of this problem for a class of translation-invariant chains of qubits with nearest-neighbor interactions. Let $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be a fixed two-qubit state with $\|\psi\| = 1$. Consider a chain of n qubits with open boundary conditions and define a Hamiltonian

$$H_n(\psi) = \sum_{i=1}^{n-1} |\psi\rangle\langle\psi|_{i,i+1}. \quad (1)$$

Here each term is a rank-1 projector onto ψ applied to a consecutive pair of qubits. We shall refer to ψ as the *forbidden state* since the Hamiltonian penalizes adjacent qubits for

being in the state ψ . As we will see in Section 2, the Hamiltonian $H_n(\psi)$ is frustration-free for any choice of ψ , that is, ground states of $H_n(\psi)$ are zero eigenvectors of each individual projector $|\psi\rangle\langle\psi|_{i,i+1}$ and the ground energy of $H_n(\psi)$ is zero. Furthermore, the ground state degeneracy of $H_n(\psi)$ is equal to $n + 1$ for almost all choices of ψ .

We are interested in the spectral gap separating the ground states and the excited states of $H_n(\psi)$ or, equivalently, the smallest non-zero eigenvalue of $H_n(\psi)$. To state our results, define a 2×2 matrix

$$T_\psi = \begin{pmatrix} \langle\psi|0,1\rangle & \langle\psi|1,1\rangle \\ -\langle\psi|0,0\rangle & -\langle\psi|1,0\rangle \end{pmatrix}. \quad (2)$$

Here $|0\rangle, |1\rangle$ is the standard basis of \mathbb{C}^2 . As we will see, the matrix T_ψ is crucial for understanding the structure of the ground space of $H_n(\psi)$. In this paper we prove that the eigenvalues of T_ψ determine if $H_n(\psi)$ is gapped or gapless. Our main result is the following.

Theorem 1. *Let ψ be an arbitrary two-qubit state. Suppose the eigenvalues of T_ψ have equal non-zero absolute value. Then the spectral gap of $H_n(\psi)$ is at most $1/(n - 1)$. Otherwise the spectral gap of $H_n(\psi)$ is lower bounded by a positive constant independent of n , which depends only on the forbidden state ψ .*

We now motivate our choice of the model Eq. (1), highlight previous work on related models, and provide some intuition for why the eigenvalues of T_ψ appear in the statement of the theorem. An informal sketch of the proof is provided in Section 1.1. Below we write $\gamma(\psi, n)$ for the spectral gap of $H_n(\psi)$.

The family of Hamiltonians defined in Eq. (1) includes some well-known quantum models as special cases. For example, choosing ψ proportional to $|0,1\rangle - |1,0\rangle$ (the singlet state) one can easily check that $H_n(\psi)$ coincides with the ferromagnetic Heisenberg chain up to an overall energy shift. For this model $H_n(\psi)$ has spectral gap $\gamma(\psi, n) = 1 - \cos(\pi/n)$ which decays as n^{-2} for large n [16]. Note that in this case T_ψ is proportional to the identity matrix, so Theorem 1 gives an upper bound $\gamma(\psi, n) \leq 1/(n - 1)$. Koma and Nachtergaele studied a one-parameter deformation of the Heisenberg chain known as the ferromagnetic XXZ chain with kink boundary conditions [16]. In this example ψ is proportional to $|0,1\rangle - q|1,0\rangle$ for $q > 0$ and the spectral gap of $H_n(\psi)$ is given by

$$\gamma(\psi, n) = 1 - 2(q + q^{-1})^{-1} \cos(\pi/n)$$

for all $n \geq 2$, see [16] for details. One can check that T_ψ is a diagonal matrix with eigenvalues $\mu_1 = (1 + q^2)^{-1/2}$ and $\mu_2 = q(1 + q^2)^{-1/2}$. It follows that $|\mu_1| \neq |\mu_2|$ for any $q \neq 1$ and Theorem 1 asserts that $H_n(\psi)$ has a constant spectral gap. We note that in the two special cases considered above the Hamiltonian has a symmetry which enables an exact computation of the spectral gap. Such symmetries are not available for a general state ψ .

The exact results summarized above may suggest that the Hamiltonian $H_n(\psi)$ is gapless if ψ is a maximally entangled state and gapped otherwise. Theorem 1 demonstrates that this naive intuition is wrong. Indeed, choose ψ proportional to $\sqrt{1-p}|0,0\rangle + \sqrt{p}|1,1\rangle$ for some $0 < p < 1$. Then the matrix T_ψ has eigenvalues $\pm i\sqrt{p(1-p)}$ and Theorem 1 implies that $H_n(\psi)$ is gapless for all p as above.

As a simple application of Theorem 1, we now map out the phase diagram of $H_n(\psi)$ restricted to the subset of *real* states $\psi \in \mathbb{R}^2 \otimes \mathbb{R}^2$. Using the Schmidt decomposition any

real two-qubit state can be written as

$$|\psi_{\pm}\rangle = R(\theta_1) \otimes R(\theta_2) \left[\sqrt{1-p}|0,0\rangle \pm \sqrt{p}|1,1\rangle \right], \quad R(\theta) \equiv \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}, \quad (3)$$

for some $0 \leq p \leq 1/2$ and $\theta_i \in [0, \pi]$. Since the spectrum of $H_n(\psi_{\pm})$ is invariant under a simultaneous rotation of all qubits, the spectral gap depends only on two parameters $\theta_2 - \theta_1$ and p . One can easily check that the eigenvalues of T_{ψ_+} have equal non-zero magnitude iff

$$p > 0 \quad \text{and} \quad \sin^2(\theta_2 - \theta_1) \leq \frac{4}{2 + (p(1-p))^{-1/2}}.$$

On the other hand, the eigenvalues of T_{ψ_-} have equal non-zero magnitude iff either $p = 1/2$, or $\sin(\theta_2 - \theta_1) = 0$ and $0 < p < 1$. These conditions determine the gapless phase of the model for the special case of real states ψ . The gapped and gapless regions for ψ_+ as a function of $p, \theta_2 - \theta_1$ are shown in Fig. 1. A surprising feature is that the gapless phase occupies a finite volume in the parameter space. In contrast, most of the models studied in physics only become gapless along phase transition lines which have zero measure in the parameter space.

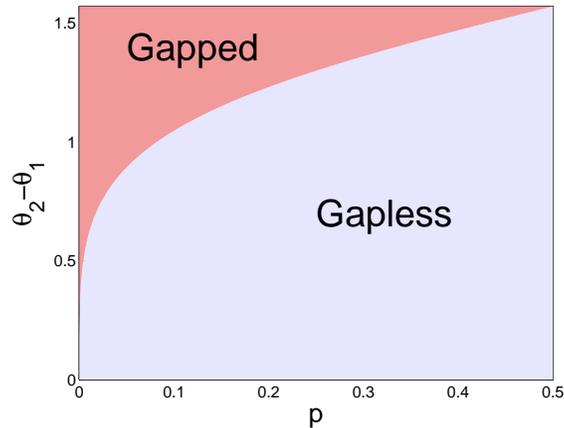


Figure 1: (Color Online) Phase diagram of the unfrustrated qubit chain $H_n(\psi)$ where ψ has real amplitudes. We use the parameterization $|\psi_{\pm}\rangle = R(\theta_1) \otimes R(\theta_2) [\sqrt{1-p}|0,0\rangle \pm \sqrt{p}|1,1\rangle]$ and we show the gapped and gapless phases for ψ_+ as a function of $\theta_2 - \theta_1 \in [0, \pi/2]$ and $p \in [0, 1/2]$. The phase diagram is symmetric under flipping the sign of $\theta_2 - \theta_1$ and under the transformation $\theta_2 - \theta_1 \rightarrow \pi - (\theta_2 - \theta_1)$. The sector corresponding to ψ_- is not shown since it has a simple description: ψ_- is in the gapless phase iff either $p = 1/2$, or $\sin(\theta_2 - \theta_1) = 0$ and $0 < p < 1$.

While it is possible to construct frustration-free translation-invariant Hamiltonians on qubits which are composed of projectors of rank 2 or 3, one can show that there are only a handful of such examples. In the Appendix we describe them and for each we determine if the system is gapped or gapless. Taken together with our main result, this gives a complete classification of gapped and gapless phases for frustration-free translation-invariant qubit

chains with nearest-neighbor interactions. Note that the restriction to Hamiltonians which are sums of projectors is without loss of generality.¹

There are several open questions related to our work. We do not know if the gapless phase of the model Eq. (1) can be connected to some known universality class of critical spin chains and whether the upper bound $1/(n-1)$ on the spectral gap in Theorem 1 is tight. It is a challenging open problem to generalize our results to qudits, i.e., to map out the phase diagram of translation-invariant frustration-free spin chains for d -dimensional spins with $d \geq 3$. A natural analogue of the Hamiltonian defined in Eq. (1) is

$$H_n(\Pi) = \sum_{j=1}^{n-1} \Pi_{j,j+1}, \quad (4)$$

where Π is a rank- r projector acting on $\mathbb{C}^d \otimes \mathbb{C}^d$. It was shown by Movassagh et al [17] that such chains are frustration-free for any Π and n whenever $r \leq d^2/4$. Their results also suggest that the Hamiltonian $H_n(\Pi)$ may be generically frustrated for $r > d^2/4$ and n sufficiently large. On the other hand, when $r > d^2/4$, the Hamiltonian is frustration-free for certain special choices of Π and n ; the famous AKLT model [18] or the model based on Motzkin paths [11] provide examples of frustration-free chains with $d = r = 3$. In general there is no efficient algorithm for testing whether $H_n(\Pi)$ is frustration-free for a given n and there are indications that this problem may be computationally hard [19]. It is therefore natural to focus on the case $r \leq d^2/4$, where the chain is guaranteed to be frustration-free. A next step could be to investigate the phase diagram of a chain of qutrits ($d = 3$) with projectors of rank $r = 1, 2$.

Finally, if one moves from frustration-free one-dimensional chains to general two-dimensional systems, the problem of distinguishing between gapped and gapless phases of translation-invariant Hamiltonians becomes undecidable [20] which leaves no hope for mapping out the full phase diagram of such systems.

1.1 Sketch of the proof

Gapless phase. In Section 3 we consider the case when eigenvalues of T_ψ have the same non-zero magnitude and prove that the spectral gap of $H_n(\psi)$ is at most $1/(n-1)$. The proof uses a result of Knabe [21] relating the spectral gap of $H_n(\psi)$ to that of the following Hamiltonian

$$H_n^\circ(\psi) = H_n(\psi) + |\psi\rangle\langle\psi|_{n,1} \quad (5)$$

which describes the chain with periodic boundary conditions. The other ingredient in the proof is a detailed understanding of the ground state degeneracy of $H_n^\circ(\psi)$. We will see that $H_n^\circ(\psi)$ is always frustration-free, but its ground state degeneracy can be smaller than that of

¹Suppose instead we consider a frustration-free qubit chain $H = \sum_{i=1}^{n-1} h_{i,i+1}$ where h has smallest eigenvalue zero (which can be arranged by adding a constant times the identity). Since H is frustration-free, it has the same null space as $H' = \sum_{i=1}^{n-1} \Pi_{i,i+1}$ where Π projects onto the range of h . Using this fact and the inequality $cH' \leq H \leq \|h\|H'$, where c is the smallest non-zero eigenvalue of h , we see that H is gapped if and only if H' is.

$H_n(\psi)$. In particular, if T_ψ^n is not proportional to the identity operator then $H_n^\circ(\psi)$ has a two-dimensional ground space whereas $H_n(\psi)$ has an $n+1$ -dimensional ground space. Otherwise, if $T_\psi^n \sim I$, then both Hamiltonians $H_n(\psi)$ and $H_n^\circ(\psi)$ have ground space degeneracy $n+1$.

We now sketch how these two ingredients can be used to prove the stated result. For ease of presentation we focus on the example considered above, where ψ_+ is of the form given in Eq. (3). Recall that the spectrum of $H_n(\psi_+)$ depends only on the two parameters $\theta_2 - \theta_1, p$. We can plot the ground state degeneracy of $H_n^\circ(\psi_+)$ as a function of these two parameters. As described in the previous paragraph, this function takes the value 2 or $n+1$ depending on whether or not $T_{\psi_+}^n$ is proportional to the identity. The black lines in Figures 2(a) and 2(b) show the curves where the ground state degeneracy is equal to $n+1$, for $n=10$ and $n=50$ respectively. Everywhere else ($0 < p \leq \frac{1}{2}$ and $\theta_2 - \theta_1 \in [0, \pi/2]$) the ground state degeneracy is 2. For reference we show the red and blue regions from Figure 1, which correspond to the gapped and gapless phases of the open boundary chain in the thermodynamic limit. As one might guess by looking at the Figure, the black curves become dense in the blue region when $n \rightarrow \infty$. If we consider a point ψ_+ in this blue region which does not sit directly on one of the black curves then the eigenvalue gap of $H_n^\circ(\psi_+)$ is equal to its third smallest eigenvalue. However as $n \rightarrow \infty$ this point ψ_+ becomes arbitrarily close to a black curve, where the Hamiltonian has ground state degeneracy $n+1$ and third smallest eigenvalue equal to zero. Using a bound on its derivative one can show that as a result the third eigenvalue of $H_n^\circ(\psi_+)$ takes arbitrarily small values as $n \rightarrow \infty$. Finally, Knabe's result implies that this can occur only if the spectral gap of $H_n(\psi_+)$ is at most $1/(n-1)$. This argument has to be modified slightly for states ψ_+ which, for some n , lie directly on one of the black curves and for general (complex) states ψ .

Gapped phase. In Sections 4,5 we prove that the spectral gap of $H_n(\psi)$ is lower bounded by a positive constant independent of n if the eigenvalues of T_ψ have distinct magnitudes or if both eigenvalues are equal to zero. Our starting point is a general method for bounding the spectral gap of frustration-free spin chains due to Nachtergaele [22], see Lemma 3 in Section 5. To apply this method one has to manipulate expressions that involve the projector onto the ground space of $H_n(\psi)$ which we denote G_n . The main technical difficulty that we had to overcome is a lack of an explicit expression for G_n which prevents us from straightforwardly applying Nachtergaele's bound. Our proof is therefore indirect and is based on establishing some features of the ground space which allow us to control G_n sufficiently well. The key technical ingredient is a new operator inequality which expresses a monotonicity of the ground space projectors under the partial trace. More precisely, we show that

$$\text{Tr}_n(G_n) \geq G_{n-1}. \quad (6)$$

where the partial trace is taken over the n -th qubit. Using the fact that the Hamiltonians $H_n(\psi)$ are frustration-free one can easily check that $\text{Tr}_n(G_n)$ and G_{n-1} have the same support, that is, Eq. (6) is equivalent to saying that all non-zero eigenvalues of $\text{Tr}_n(G_n)$ are at least one. Our proof of this monotonicity property, presented in Section 4, applies to general frustration-free chains of qubits composed of rank-1 projectors. Neither translation-invariance nor the conditions of Theorem 1 are needed for the proof of Eq. (6). We note that Eq. (6) differs from the well-known monotonicity property $G_n \leq G_{n-1} \otimes I$. The latter follows trivially from the fact that $H_n(\psi)$ is frustration-free, whereas Eq. (6) holds for more subtle reasons.

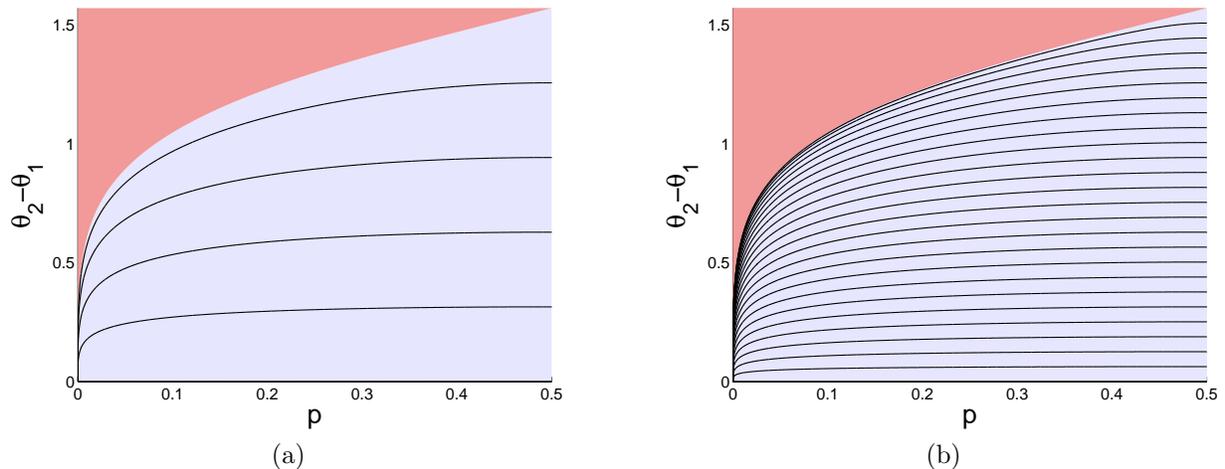


Figure 2: (Color Online) Depiction of the ground state degeneracy of $H_n^\circ(\psi_+)$ where ψ_+ is of the form given in Eq. (3). The black lines are curves in the $(\theta_2 - \theta_1, p)$ plane where $H_n^\circ(\psi)$ has ground state degeneracy equal to $n + 1$. Here we plot the curves for (a) $n = 10$ and (b) $n = 50$. For any point which does not lie on one of these curves (for $0 < p \leq \frac{1}{2}$ and $\theta_2 - \theta_1 \in [0, \pi/2]$), the ground state degeneracy of $H_n^\circ(\psi)$ is two. We also show the gapped (red) and gapless (blue) regions for the chain with open boundary conditions. As $n \rightarrow \infty$ the black curves become dense in the blue region.

We proceed by showing that a quantum state which is completely mixed over the ground space of the n -qubit chain (i.e., proportional to the projector G_n) exhibits an exponential decay of correlations for certain local observables, see Lemma 4 in Section 5.1. In Section 5.2 we use the decay of correlations and Eq. (6) to prove several “Region Exclusion” lemmas. Here we consider a partition of the chain into three or more regions and define local ground space projectors associated with each region. Loosely speaking, the Region Exclusion lemmas state that the global ground space projector associated with the entire chain can be approximated by a certain operator built from the local ground space projectors. The latter are defined on subsets of qubits where some of the chosen regions are excluded from the chain (hence the name of the lemmas). By repeatedly applying the Region Exclusion lemmas in Section 5.3 we arrive at the condition used in Nachtergaele’s bound, thus proving a constant lower bound on the gap.

2 Structure of the ground space

In this section we describe the ground spaces of $H_n(\psi)$ and $H_n^\circ(\psi)$, the Hamiltonians for the chain with open and periodic boundary conditions respectively (defined in Eqs. (1,5)).

2.1 Open boundary conditions

We first consider the Hamiltonian $H_n(\psi)$ for the chain with open boundary conditions. We begin with the simple case where $\psi = \psi_1 \otimes \psi_2$ is a product state. It is always possible to

choose the basis states $|0\rangle$ and $|1\rangle$ so that

$$|\psi\rangle = |1\rangle \otimes |v^\perp\rangle$$

where

$$|v\rangle = c|0\rangle + s|1\rangle, \quad |v^\perp\rangle = s^*|0\rangle - c^*|1\rangle, \quad \text{and} \quad |c|^2 + |s|^2 = 1.$$

For each $i = 1, \dots, n$ define an n -qubit state $|g_i\rangle = |0^{i-1}v^\perp v^{n-i}\rangle$. Also define $|g_0\rangle = |v^{\otimes n}\rangle$. For example, choosing $n = 4$ one gets

$$\begin{aligned} |g_0\rangle &= |v \ v \ v \ v \rangle, \\ |g_1\rangle &= |v^\perp \ v \ v \ v \rangle, \\ |g_2\rangle &= |0 \ v^\perp \ v \ v \rangle, \\ |g_3\rangle &= |0 \ 0 \ v^\perp \ v \rangle, \\ |g_4\rangle &= |0 \ 0 \ 0 \ v^\perp \rangle. \end{aligned}$$

Loosely speaking, the states g_i can be viewed as “domain walls” where $|0\rangle$ and $|v\rangle$ represent two different values of a magnetization. By direct inspection we see that g_0, \dots, g_n are pairwise orthogonal ground states of $H_n(\psi)$.

Proposition 1. *Suppose $s \neq 0$. Then the states g_0, \dots, g_n form an orthonormal basis for the ground space of $H_n(\psi)$.*

Proof. It suffices to show that the ground space of $H_n(\psi)$ has dimension at most $n+1$. Define $\tilde{0} \equiv 0$ and $\tilde{1} \equiv v$. Given any binary string $x = (x_1, \dots, x_n)$, define $\tilde{x} \equiv (\tilde{x}_1, \dots, \tilde{x}_n)$. Note that $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ are linearly independent since $s \neq 0$. Therefore the states $|\tilde{x}\rangle$, $x \in \{0, 1\}^n$ form a basis (non-orthonormal) for the Hilbert space of n qubits. Suppose $|g\rangle$ is a ground state of $H_n(\psi)$. Then $|g\rangle = \sum_x a_x |\tilde{x}\rangle$ for some complex coefficients a_x . A simple calculation shows that

$${}_{i,i+1}\langle\psi|g\rangle = s^2 \sum_{x: (x_i, x_{i+1})=(1,0)} a_x |\tilde{x}_1, \dots, \tilde{x}_{i-1}, \tilde{x}_{i+2}, \dots, \tilde{x}_n\rangle$$

for any $i = 1, \dots, n-1$. On the other hand, ${}_{i,i+1}\langle\psi|g\rangle = 0$ since $|g\rangle$ is a ground state of $H_n(\psi)$. This is possible only if $a_x = 0$ for all strings x that contain at least one consecutive pair $(1, 0)$. Thus $|g\rangle$ belongs to a subspace spanned by vectors $|0^i v^{n-i}\rangle$, where $i = 0, \dots, n$. This shows that the ground subspace of $H_n(\psi)$ has dimension at most $n+1$. \square

Now consider the case where ψ is entangled. In this case we can still construct the ground space of $H_n(\psi)$ although, in contrast with the product state case, we are not able to obtain an orthonormal basis. The matrix T_ψ defined in Eq. (2) plays a crucial role.

One can easily check that $\det(T_\psi) \neq 0$ whenever ψ is entangled and

$$\langle\psi|(I \otimes T_\psi) = \det(T_\psi)\langle\epsilon|, \tag{7}$$

where $|\epsilon\rangle = |0, 1\rangle - |1, 0\rangle$ is the antisymmetric state of two qubits. This shows that the ground space of $H_2(\psi) = |\psi\rangle\langle\psi|_{1,2}$ is the image of the 2-qubit symmetric subspace under the map $1 \otimes T_\psi$. A similar characterization holds for $H_n(\psi)$ with $n > 2$. In particular, define

$$T_\psi^{\text{all}} = I \otimes T_\psi \otimes T_\psi^2 \otimes \dots \otimes T_\psi^{n-1}. \tag{8}$$

The following Proposition is a special case of a result presented in [23] (and has been used previously in, e.g., [24]).

Proposition 2. *Suppose $\det(T_\psi) \neq 0$. Then the ground space of $H_n(\psi)$ is the image of the n -qubit symmetric subspace under the linear map T_ψ^{all} .*

Proof. Using Eq. (7) and the fact that $M \otimes M|\epsilon\rangle = \det(M)|\epsilon\rangle$ we get

$$(T_\psi^{\text{all}})^\dagger |\psi\rangle \langle \psi|_{j,j+1} T_\psi^{\text{all}} = |\epsilon\rangle \langle \epsilon|_{j,j+1} \otimes B_j \quad (9)$$

for each $j = 1, \dots, n-1$, where B_j is a positive operator acting on qubits in the set $[n] \setminus \{j, j+1\}$. From Eq. (9) we see that the nullspace of $(T_\psi^{\text{all}})^\dagger H_n(\psi) T_\psi^{\text{all}}$ is equal to the symmetric subspace. The result follows since T_ψ^{all} is invertible. \square

Combining Propositions 1,2 and noting that the symmetric subspace of n qubits has dimension $n+1$, we conclude that the ground space of $H_n(\psi)$ has dimension $n+1$ for almost any choice of ψ (the only exception is when $s = 0$ and ψ is a symmetric product state).

2.2 Periodic boundary conditions

We now consider the Hamiltonian $H_n^\circ(\psi)$ for the chain with periodic boundary conditions. It is well-known that $H_n^\circ(\psi)$ is frustration-free for any choice of ψ , see for instance [23, 25, 26]. However in this paper we will only need to deal with periodic boundary conditions in the case where ψ is an entangled state. Accordingly, in this section we assume that $\det(T_\psi) \neq 0$. For any such ψ we compute the dimension of the zero energy ground space of $H_n^\circ(\psi)$. We will see that it takes different values depending on the choice of ψ . This contrasts with the open boundary chain which has ground space dimension $n+1$ whenever ψ is entangled.

Here and throughout the paper we use the symbol \sim to mean proportional to.

Proposition 3. *Suppose $T_\psi^n \sim I$. Then the ground space of $H_n^\circ(\psi)$ has dimension $n+1$. Otherwise, $H_n^\circ(\psi)$ has a two-fold degenerate ground space.*

Proof. Note that $H_n^\circ(\psi)$ has the same rank as

$$T_\psi^{\text{all}\dagger} H_n^\circ(\psi) T_\psi^{\text{all}} = T_\psi^{\text{all}\dagger} H_n(\psi) T_\psi^{\text{all}} + T_\psi^{\text{all}\dagger} |\psi\rangle \langle \psi|_{n,1} T_\psi^{\text{all}}. \quad (10)$$

where T_ψ^{all} is given by Eq. (8). Both terms on the right-hand side are positive semidefinite and, by Proposition 2, the nullspace of the first term is the symmetric subspace. If $T_\psi^n \sim I$ then the second term in Eq. (10) can be written as $|\epsilon\rangle \langle \epsilon|_{n,1} \otimes B_n$ where B_n is positive and $|\epsilon\rangle = |0,1\rangle - |1,0\rangle$. Since this term annihilates every state in the symmetric subspace we see that in this case the nullspace of Eq. (10) is $(n+1)$ -dimensional.

If T_ψ^n is not proportional to the identity we show that there are exactly two states in the symmetric subspace which are annihilated by the second term in Eq. (10). We consider two cases depending on whether or not T_ψ^n is defective (has only one eigenvector).

First consider the case where T_ψ^n has two linearly independent eigenvectors $|v_1\rangle, |v_2\rangle$. Note that the last term in Eq. (10) projects qubits $n, 1$ onto a state

$$|\phi\rangle = (T_\psi^{n-1\dagger} \otimes I)|\psi\rangle \sim (T_\psi^{n\dagger} \otimes I)|\epsilon\rangle = \left(T_\psi^{n\dagger}|0\rangle\right)|1\rangle - \left(T_\psi^{n\dagger}|1\rangle\right)|0\rangle.$$

The last equality makes it clear that $|\phi\rangle$ and $|\epsilon\rangle$ are linearly independent whenever T_ψ^n is not proportional to the identity. Thus the nullspace of Eq. (10) is spanned by n -qubit symmetric

states that are orthogonal to $|\phi\rangle$ on any pair of qubits. One can easily check that the only two-qubit symmetric states orthogonal to $|\phi\rangle$ are $|v_1 \otimes v_1\rangle$ and $|v_2 \otimes v_2\rangle$. Likewise, one can check that the only n -qubit symmetric states orthogonal to $|\phi\rangle$ on any pair of qubits are linear combinations of $|v_1\rangle^{\otimes n}$ and $|v_2\rangle^{\otimes n}$. Thus Eq. (10) has a two-dimensional nullspace and therefore the same is true for $H_n^\circ(\psi)$.

Next suppose T_ψ^n is defective, i.e., has only one eigenvector. Let us work in a basis where $|0\rangle$ is this eigenvector, so

$$T_\psi^n = \begin{pmatrix} b & a \\ 0 & b \end{pmatrix}$$

for some $a, b \in \mathbb{C}$ with $a \neq 0$. Then the last term in Eq. (10) projects onto a state

$$|\phi\rangle = (T_\psi^{n-1} \otimes I)|\psi\rangle \sim (T_\psi^{n-1} \otimes I)|\epsilon\rangle = b^*|\epsilon\rangle + a^*|11\rangle.$$

Since $a \neq 0$, the states $|\phi\rangle$ and $|\epsilon\rangle$ span the same subspace as $|11\rangle$ and $|\epsilon\rangle$. Therefore the nullspace of Eq. (10) is spanned by n -qubit symmetric states that are orthogonal to $|11\rangle$ on any pair of qubits. One can easily check that the only such states are linear combinations of $|0\rangle^{\otimes n}$ and the n -qubit W-state

$$|100 \dots 0\rangle + |010 \dots 0\rangle + \dots + |00 \dots 01\rangle.$$

Thus Eq. (10) has a two-dimensional nullspace and therefore the same is true for $H_n^\circ(\psi)$. \square

3 Gapless phase

In this section we prove the first part of Theorem 1, namely,

Gapless phase theorem. *Suppose the eigenvalues of T_ψ have the same non-zero absolute value. Then $\gamma(\psi, n) \leq 1/(n-1)$ for all $n \geq 2$.*

Recall that $\gamma(\psi, n)$ denotes the smallest non-zero eigenvalue of $H_n(\psi)$. In addition we write $\gamma^\circ(\psi, n)$ for the smallest non-zero eigenvalue of the Hamiltonian $H_n^\circ(\psi)$ with periodic boundary conditions, see Eq. (5).

To prove the gapless phase theorem we use the following lemma, proven by Knabe [21], which relates the smallest non-zero eigenvalues of the chains with periodic and open boundary conditions. Knabe's result, presented in Section 2 of reference [21], applies to more general frustration-free spin chains but here we specialize to the case at hand.

Lemma 1 (Knabe [21]). *For all $m \geq n > 2$,*

$$\gamma^\circ(\psi, m) \geq \frac{n-1}{n-2} \left(\gamma(\psi, n) - \frac{1}{n-1} \right). \quad (11)$$

This lemma was originally proposed as a technique for proving that the periodic chain is gapped in the thermodynamic limit. This follows from the lemma if one can show that there exists a finite n for which the open chain has a gap strictly larger than $1/(n-1)$. Here we

apply the lemma in the opposite direction. We use the following strategy which works for some (but not all) ψ satisfying the conditions of the gapless phase theorem. First we apply the argument sketched in Section 1.1 to show that $\gamma^\circ(\psi, m)$ can take arbitrarily small values for large enough m . Then we apply Knabe's lemma to infer that $\gamma(\psi, n) \leq 1/(n-1)$ for any $n > 2$ since otherwise Eq. (11) would provide a constant lower bound on $\gamma^\circ(\psi, m)$ for all $m \geq n$, leading to a contradiction. Note also that $\gamma(\psi, 2) = 1$ since $H_2(\psi) = |\psi\rangle\langle\psi|$.

For some states ψ we are not able to use the above strategy directly; however in these cases we choose a state ϕ which can be taken arbitrarily close to ψ for which the strategy can be applied. The result for ψ then follows by continuity. In order to handle these cases (and for other portions of the proof) we will need the following straightforward bound on how much the eigenvalues of $H_n(\psi)$ (or $H_n^\circ(\psi)$) can change as ψ varies. Write

$$e_1(\psi, n) \leq e_2(\psi, n) \leq \dots \leq e_{2^n}(\psi, n) \quad \text{and} \quad e_1^\circ(\psi, n) \leq e_2^\circ(\psi, n) \leq \dots \leq e_{2^n}^\circ(\psi, n)$$

for the eigenvalues of $H_n(\psi)$ and $H_n^\circ(\psi)$ respectively.

Proposition 4. *Let ψ and ϕ satisfy $\|\psi\| = \|\phi\| = 1$. Then*

$$|e_j(\psi, n) - e_j(\phi, n)| \leq 2n \|\psi - \phi\| \quad \text{and} \quad |e_j^\circ(\psi, n) - e_j^\circ(\phi, n)| \leq 2n \|\psi - \phi\|$$

for each $j = 1, \dots, 2^n$.

Proof. The proof of the two inequalities is almost identical so here we prove only the first one. We use the Weyl inequality for perturbed eigenvalues (see for example Corollary III.2.6 of reference [27]) which in this case says $|e_j(\psi, n) - e_j(\phi, n)| \leq \|H_n(\psi) - H_n(\phi)\|$. To complete the proof we bound

$$\begin{aligned} \|H_n(\psi) - H_n(\phi)\| &\leq \sum_{i=1}^{n-1} \||\psi\rangle\langle\psi|_{i,i+1} - |\phi\rangle\langle\phi|_{i,i+1}\| \\ &= \frac{(n-1)}{2} \|(|\psi\rangle - |\phi\rangle) (\langle\psi| + \langle\phi|) + (|\psi\rangle + |\phi\rangle) (\langle\psi| - \langle\phi|) \| \\ &\leq (n-1) \|(|\psi\rangle - |\phi\rangle) (\langle\psi| + \langle\phi|) \| \\ &\leq 2(n-1) \||\psi\rangle - |\phi\rangle\| \end{aligned}$$

where in the last line we used the fact that $\||\psi\rangle + |\phi\rangle\| \leq 2$ (since $|\psi\rangle$ and $|\phi\rangle$ are normalized). \square

We now proceed to the proof of the gapless phase theorem.

Proof. First we claim that the eigenvalues of $H_n(\psi)$ and absolute values of the eigenvalues of T_ψ are invariant under a transformation $\psi \rightarrow (U \otimes U)\psi$ where U is an arbitrary single-qubit unitary operator. Indeed, let $\psi' = (U \otimes U)\psi$. Then Eq. (1) implies $H_n(\psi') = U^{\otimes n} H_n(\psi) (U^\dagger)^{\otimes n}$ and Eq. (7) implies $T_{\psi'} = (\det U)^{-1} \cdot U T_\psi U^\dagger$. Thus the eigenvalues of $H_n(\psi')$ and magnitudes of the eigenvalues of $T_{\psi'}$ do not depend on U . We shall use the freedom in choosing U to bring ψ into a certain canonical form as defined below.

Proposition 5. For any $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2$ there exists a single-qubit unitary U such that

$$(U \otimes U)|\psi\rangle = (\alpha + i\beta)|0, 1\rangle + (\alpha + i\gamma)|1, 0\rangle + \delta|1, 1\rangle \quad (12)$$

for some real coefficients $\alpha, \beta, \gamma, \delta$.

Since the proof is rather straightforward, we shall postpone it until the end of this section. From now on we can assume that ψ has the canonical form as in the right-hand side of Eq. (12). Substituting this canonical form into Eq. (2) one gets

$$T_\psi = \begin{pmatrix} \alpha - i\beta & \delta \\ 0 & -(\alpha - i\gamma) \end{pmatrix}. \quad (13)$$

The eigenvalues of this matrix are $\alpha - i\beta$ and $-(\alpha - i\gamma)$, with magnitudes $\sqrt{\alpha^2 + \beta^2}$ and $\sqrt{\alpha^2 + \gamma^2}$. By assumption of the theorem, the eigenvalues have the same magnitude and thus $\gamma = \pm\beta$. We consider the two cases $\gamma = \pm\beta$ separately and we show that $\gamma(\psi, n) \leq \frac{1}{n-1}$ in each case.

Case 1: $\gamma = \beta$

Fix n and let $m \geq n$ be even. Setting $\beta = \gamma$ in Eq. (13) and taking the square we see that $T_\psi^2 \sim I$. Since m is even we get $T_\psi^m \sim I$ and therefore $e_3^\circ(\psi, m) = 0$ by Proposition 3. Let $|\phi_m\rangle$ be a normalized state which satisfies

$$\|\phi_m - \psi\| \leq \frac{1}{m^2}$$

and such that the eigenvalues of T_{ϕ_m} have different magnitudes and are both non-zero. This guarantees that $T_{\phi_m}^m$ is not proportional to the identity and $\det(T_{\phi_m}) \neq 0$. Then, by Propositions 3 and 4,

$$\gamma^\circ(\phi_m, m) = e_3^\circ(\phi_m, m) = e_3^\circ(\phi_m, m) - e_3^\circ(\psi, m) \leq \frac{2}{m}.$$

Applying Lemma 1 gives

$$e_{n+2}(\phi_m, n) = \gamma(\phi_m, n) \leq \frac{1}{n-1} + \frac{n-2}{n-1} \gamma^\circ(\phi_m, m) \leq \frac{1}{n-1} + \frac{2}{m} \left(\frac{n-2}{n-1} \right)$$

for all even $m \geq n$, and using Propositions 3 and 4 again we have

$$\begin{aligned} \gamma(\psi, n) &= e_{n+2}(\phi_m, n) + (e_{n+2}(\psi, n) - e_{n+2}(\phi_m, n)) \\ &\leq e_{n+2}(\phi_m, n) + \frac{2n}{m^2} \\ &\leq \frac{1}{n-1} + \frac{2}{m} \left(\frac{n-2}{n-1} \right) + \frac{2n}{m^2}. \end{aligned}$$

The result follows since $m \geq n$ can be taken arbitrarily large.

Case 2: $\gamma = -\beta$

Let $\alpha + i\beta = re^{-i\pi(\theta + \frac{1}{2})}$ where θ and r are positive real numbers. Here $r < 1$ since ψ is normalized and $r > 0$ since the eigenvalues of T_ψ are assumed to be non-zero. We first consider the case where θ is irrational. In this case the convergents of the continued fraction expansion of θ give sequences of positive integers $\{p_j\}$ and $\{q_j\}$ with

$$\left| \frac{p_j}{q_j} - \theta \right| \leq \frac{1}{q_j^2}, \quad (14)$$

$\gcd(p_j, q_j) = 1$, and where $\{q_j\}$ diverges. Here we shall omit the first two convergents obtained by the standard continued fraction expansion, in order to guarantee that the sequence $\{q_j\}$ is strictly increasing and $q_j \geq 2$ for all j .

Define $\theta_j = \frac{p_j}{q_j}$, and let

$$|\Psi_j\rangle = re^{-i\pi(\theta_j + \frac{\pi}{2})}|0, 1\rangle + re^{i\pi(\theta_j + \frac{\pi}{2})}|1, 0\rangle + \delta|1, 1\rangle.$$

Then

$$\|\Psi_j - \psi\| = r\sqrt{2} |e^{i\pi(\theta_j - \theta)} - 1| \leq r\sqrt{2} |\pi(\theta_j - \theta)| \leq \frac{\sqrt{2}\pi}{q_j^2} \quad (15)$$

where we used the inequality $|e^{ix} - 1| \leq |x|$, Eq. (14), and the fact that $r < 1$. Note that

$$T_{\Psi_j} = \begin{pmatrix} ire^{i\pi\theta_j} & \delta \\ 0 & ire^{-i\pi\theta_j} \end{pmatrix}$$

has eigenvalues $E_1 = ire^{i\pi\theta_j}$ and $E_2 = ire^{-i\pi\theta_j}$. We have $E_1 \neq E_2$, which follows from the fact that θ_j is not an integer, since $q_j \geq 2$. Thus T_{Ψ_j} is diagonalizable. Furthermore, $E_1^{q_j} = E_2^{q_j}$, and therefore (using the fact that it is diagonalizable) $T_{\Psi_j}^{q_j} \sim I$. Hence $e_3^\circ(\Psi_j, q_j) = 0$ by Proposition 3. On the other hand $T_\psi^{q_j}$ is not proportional to the identity since θ is irrational, hence $\gamma^\circ(\psi, q_j) = e_3^\circ(\psi, q_j)$. Using these facts and Proposition 4 we have

$$\gamma^\circ(\psi, q_j) = (e_3^\circ(\psi, q_j) - e_3^\circ(\Psi_j, q_j)) \leq 2q_j \|\Psi_j - \psi\| \leq \frac{2\sqrt{2}\pi}{q_j}.$$

Now for all j such that $q_j \geq n$ we get

$$\gamma(\psi, n) \leq \frac{1}{n-1} + \frac{n-2}{n-1} \gamma^\circ(\psi, q_j) \leq \frac{1}{n-1} + \left(\frac{n-2}{n-1} \right) \frac{2\sqrt{2}\pi}{q_j}$$

and hence $\gamma(\psi, n) \leq \frac{1}{n-1}$ since the sequence $\{q_j\}$ diverges and the second term can be made arbitrarily small.

It remains to consider the case where θ is rational. In this case, for any ϵ we may choose θ' to be an irrational number satisfying $|\theta' - \theta| \leq \epsilon$. Letting

$$|\phi\rangle = re^{-i\pi(\theta' + \frac{\pi}{2})}|0, 1\rangle + re^{i\pi(\theta' + \frac{\pi}{2})}|0, 1\rangle + \delta|1, 1\rangle$$

we may now apply the above proof to get $\gamma(\phi, n) = e_{n+2}(\phi, n) \leq \frac{1}{n-1}$. Now using Proposition 4 we get

$$\begin{aligned} \gamma(\psi, n) &= e_{n+2}(\phi, n) + (e_{n+2}(\psi, n) - e_{n+2}(\phi, n)) \leq \frac{1}{n-1} + 2n \|\phi - \psi\| \\ &\leq \frac{1}{n-1} + 2nr\sqrt{2\pi}\epsilon \end{aligned}$$

where in the second line we used the same reasoning as Eq. (15). Since ϵ can be chosen arbitrarily small we get $\gamma(\psi, n) \leq \frac{1}{n-1}$. \square

Finally, let us prove Proposition 5.

Proof. Recall that a transformation $\psi \rightarrow (U \otimes U)\psi$ maps T_ψ to $(\det U)^{-1} \cdot UT_\psi U^\dagger$. Here U is an arbitrary unitary operator. We shall choose a sequence of such transformations that bring T_ψ into the canonical form defined in Eq. (13) which is equivalent to Eq. (12). First, choose U such that $|0\rangle$ is an eigenvector of T_ψ . This is always possible since any complex matrix has at least one eigenvector. Now we can assume that

$$T_\psi = \begin{bmatrix} \mu_1 & \delta \\ 0 & \mu_2 \end{bmatrix}$$

for some complex coefficients μ_1, μ_2, δ . Next choose $U = e^{-i\theta/2}I$ where the phase θ satisfies $\text{Re}(e^{i\theta}(\mu_1 + \mu_2)) = 0$. This maps T_ψ to $e^{i\theta}T_\psi$ and now we can assume that $\text{Re}(\mu_1 + \mu_2) = 0$. Finally, choosing $U = \text{diag}(e^{i\theta}, e^{-i\theta})$ one can map δ to $e^{2i\theta}\delta$ without changing μ_1, μ_2 . Thus we can make δ real. This brings T_ψ into the canonical form defined in Eq. (13). \square

4 Monotonicity under the partial trace

In this section we establish a relationship between the ground space projectors describing a chain of n and $n-1$ qubits. Our result holds in a more general setting than considered elsewhere in this paper since we do not assume translation invariance.

Let $\psi_1, \psi_2, \dots, \psi_{m-1}$ be an arbitrary sequence of normalized two-qubit states. For each $n = 2, \dots, m$ define a Hamiltonian

$$H_n(\psi_1, \psi_2, \dots, \psi_{n-1}) = \sum_{j=1}^{n-1} |\psi_j\rangle\langle\psi_j|_{j,j+1} \quad (16)$$

which describes a chain of n qubits. This Hamiltonian is frustration-free for any choice of $\psi_1, \dots, \psi_{n-1}$ (this follows directly from Proposition 6 given below). Let \mathcal{G}_n be the ground space of $H_n(\psi_1, \psi_2, \dots, \psi_{n-1})$ and G_n be the projector onto \mathcal{G}_n . We adopt the convention $H_1 = 0$ and $\mathcal{G}_1 = \mathbb{C}^2$.

First, we note that $\mathcal{G}_n \subseteq \mathcal{G}_{n-1} \otimes \mathbb{C}^2$ due to the fact that the considered Hamiltonians are frustration-free. This results in a trivial monotonicity property $G_n \leq G_{n-1} \otimes I$. Below we prove that one also has a different type of monotonicity, namely $\text{Tr}_n(G_n) \geq G_{n-1}$, where Tr_n represents the partial trace over the n -th qubit.

Lemma 2 (Monotonicity). *For each $n = 2, \dots, m$ one has*

$$\mathrm{Tr}_n(G_n) \geq G_{n-1}. \quad (17)$$

Given the simplicity and generality of Eq. (17), one may be tempted to ask whether it holds for some trivial reason unrelated to the structure of the considered Hamiltonians. We have observed numerically that Eq. (17) can be false if G_{n-1} and G_n are chosen as projectors onto random linear subspaces $\mathcal{G}_{n-1} \subseteq (\mathbb{C}^2)^{\otimes(n-1)}$ and $\mathcal{G}_n \subseteq \mathcal{G}_{n-1} \otimes \mathbb{C}^2$, even if the dimensions of \mathcal{G}_{n-1} and \mathcal{G}_n match those of the ground subspaces of $H_{n-1}(\psi_1, \dots, \psi_{n-2})$ and $H_n(\psi_1, \dots, \psi_{n-1})$. Thus any proof of the monotonicity property must exploit the special structure of the projectors G_n . In the absence of an explicit formula for G_n , one has to rely on some indirect arguments in order to derive Eq. (17). This partially explains why the proof of the lemma given below is rather cumbersome.

Proof of Lemma 2. We use induction in n . The base of the induction is $n = 2$. In this case $G_2 = I - |\psi_1\rangle\langle\psi_1|$ and thus $\mathrm{Tr}_2(G_2) = 2I - \mathrm{Tr}_2(|\psi_1\rangle\langle\psi_1|) \geq I = G_1$. Here we used the fact that the partial trace of any two-qubit state is a density matrix which has eigenvalues at most one. We now prove the induction step. For brevity denote $\psi \equiv \psi_{n-1}$ such that the last term in $H_n(\psi_1, \dots, \psi_{n-1})$ is $|\psi\rangle\langle\psi|_{n-1,n}$.

First consider the case where ψ is unentangled, that is, $\psi = \alpha \otimes \beta$ for some single-qubit states α, β . In this case the result follows trivially without using the inductive hypothesis, since $\mathcal{G}_{n-1} \otimes \beta^\perp \subseteq \mathcal{G}_n$ which implies $G_n \geq G_{n-1} \otimes |\beta^\perp\rangle\langle\beta^\perp|$ and thus $\mathrm{Tr}(G_n) \geq G_{n-1}$.

In the remainder of the proof we consider the case where ψ is entangled (i.e., not a product state). Write the Schmidt decomposition of ψ as

$$|\psi\rangle = \sqrt{p_0}|w_0\rangle|v_0\rangle + \sqrt{p_1}|w_1\rangle|v_1\rangle \quad (18)$$

where $\langle w_i|w_j\rangle = \langle v_i|v_j\rangle = \delta_{ij}$ and $p_0, p_1 > 0$ with $p_0 + p_1 = 1$.

Let $G_n^\perp = I - G_n$. Obviously, $\mathrm{Tr}_n(G_n) = 2I - \mathrm{Tr}_n(G_n^\perp)$. Furthermore, the trivial monotonicity $\mathcal{G}_n \subseteq \mathcal{G}_{n-1} \otimes \mathbb{C}^2$ implies that $\mathrm{Tr}_n(G_n)$ has all of its support on \mathcal{G}_{n-1} , that is, $\mathrm{Tr}_n(G_n) = \mathrm{Tr}_n(G_n)G_{n-1} = G_{n-1}\mathrm{Tr}_n(G_n)$. Define an operator

$$R_n \equiv G_{n-1}\mathrm{Tr}_n(G_n^\perp)G_{n-1}. \quad (19)$$

The above implies that

$$\mathrm{Tr}_n(G_n) = G_{n-1}\mathrm{Tr}_n(G_n)G_{n-1} = 2G_{n-1} - R_n \geq (2 - \|R_n\|)G_{n-1}. \quad (20)$$

Thus it suffices to prove that $\|R_n\| \leq 1$.

Choose an arbitrary orthonormal basis

$$g_1, g_2, \dots, g_r \in \mathcal{G}_{n-2}, \quad \langle g_\alpha|g_\beta\rangle = \delta_{\alpha,\beta}. \quad (21)$$

Also choose an arbitrary orthonormal basis

$$h_1, h_2, \dots, h_s \in \mathcal{G}_{n-1}, \quad \langle h_i|h_j\rangle = \delta_{i,j}. \quad (22)$$

In general the dimensions r and s of the spaces \mathcal{G}_{n-2} and \mathcal{G}_{n-1} will depend on the states $\psi_1, \dots, \psi_{n-2}$ but we will not need an explicit expression for them. We will however need to use the fact that $s > r$, which we now establish. The following proposition is a special case of the result presented in [17]; we include a proof here for completeness.

Proposition 6. *Let D_n be the dimension of \mathcal{G}_n . Then $D_n > D_{n-1}$ for all $2 \leq n \leq m$.*

Proof. Recall our convention that $\mathcal{G}_1 = \mathbb{C}^2$, so $D_1 = 2$. On the other hand $H_2(\psi_1) = |\psi_1\rangle\langle\psi_1|_{1,2}$ and $D_2 = 3$, which confirms $D_2 > D_1$. We now establish that $D_n - D_{n-1} \geq D_{n-1} - D_{n-2}$ for all $n \geq 3$. This is sufficient to complete the proof since it implies $D_n - D_{n-1} \geq D_2 - D_1 = 1$.

Let ϕ be a general state in \mathcal{G}_n , with $n \geq 3$. Let $\gamma_1, \dots, \gamma_{D_{n-1}}$ be an orthonormal basis for \mathcal{G}_{n-1} and let $\kappa_1, \dots, \kappa_{D_{n-2}}$ be an orthonormal basis for \mathcal{G}_{n-2} . We can write

$$|\phi\rangle = \sum_{i=1}^{D_{n-1}} f_{i,0} |\gamma_i\rangle |0\rangle + f_{i,1} |\gamma_i\rangle |1\rangle$$

for some complex coefficients $\{f_{i,z}\}$. The fact that the Hamiltonian $H_n(\psi_1, \dots, \psi_{n-1})$ is frustration-free implies

$$\mathcal{G}_n = (\mathcal{G}_{n-1} \otimes \mathbb{C}^2) \cap (\mathcal{G}_{n-2} \otimes \psi_{n-1}^\perp)$$

and thus the dimension of \mathcal{G}_n is the number of linearly independent solutions to the equations

$$\langle \kappa_j \otimes \psi_{n-1} | \phi \rangle = 0 \quad \text{for all } j = 1, \dots, D_{n-2}. \quad (23)$$

This is a set of D_{n-2} linear equations for the $2D_{n-1}$ variables $\{f_{i,z}\}$. The number of linearly independent solutions satisfies $D_n \geq 2D_{n-1} - D_{n-2}$, or equivalently $D_n - D_{n-1} \geq D_{n-1} - D_{n-2}$. \square

Define $r \times s$ matrices

$$(M_0)_{\alpha,i} = \langle g_\alpha \otimes w_0 | h_i \rangle \quad \text{and} \quad (M_1)_{\alpha,i} = \langle g_\alpha \otimes w_1 | h_i \rangle. \quad (24)$$

where w_0, w_1 are defined in Eq. (18). The trivial monotonicity $\mathcal{G}_{n-1} \subseteq \mathcal{G}_{n-2} \otimes \mathbb{C}^2$ implies

$$M_0^\dagger M_0 + M_1^\dagger M_1 = I_s. \quad (25)$$

Here and below I_q denotes the identity matrix of dimension q . Furthermore, expressing $G_{n-1} = \sum_{i=1}^s |h_i\rangle\langle h_i|$ one gets

$$\langle g_\alpha | \text{Tr}_{n-1}(G_{n-1}) | g_\beta \rangle = \langle g_\alpha \otimes w_0 | G_{n-1} | g_\beta \otimes w_0 \rangle + \langle g_\alpha \otimes w_1 | G_{n-1} | g_\beta \otimes w_1 \rangle = (M_0 M_0^\dagger + M_1 M_1^\dagger)_{\alpha,\beta}.$$

Since $\text{Tr}_{n-1}(G_{n-1}) \geq G_{n-2}$ by the induction hypothesis, we infer that

$$M_0 M_0^\dagger + M_1 M_1^\dagger \geq I_r. \quad (26)$$

The usefulness of the matrices M_0, M_1 comes from the following facts. Recall that we defined $R_n = G_{n-1} \text{Tr}_n(G_n^\perp) G_{n-1}$.

Proposition 7. *Suppose ψ is entangled. Then the matrix of the operator R_n in the chosen basis $\{h_1, \dots, h_s\}$ of \mathcal{G}_{n-1} can be written as*

$$R_n = p_0 M_0^\dagger (p_0 M_0 M_0^\dagger + p_1 M_1 M_1^\dagger)^{-1} M_0 + p_1 M_1^\dagger (p_0 M_0 M_0^\dagger + p_1 M_1 M_1^\dagger)^{-1} M_1, \quad (27)$$

where $p_0, p_1 > 0$ are defined by Eq. (18).

Proposition 8. *Let r, s be arbitrary positive integers with $s \geq r$. Let M_0, M_1 be arbitrary matrices of size $r \times s$ satisfying $M_0^\dagger M_0 + M_1^\dagger M_1 = I_s$ and $M_0 M_0^\dagger + M_1 M_1^\dagger \geq I_r$. Let $p_0, p_1 > 0$ be any real positive numbers. Then the operator R_n defined by Eq. (27) satisfies $\|R_n\| \leq 1$.*

Combining Propositions 7,8, the inequality $s > r$ proved in Proposition 6, and Eqs. (25,26) one gets $\|R_n\| \leq 1$. The lemma follows from Eq. (20). \square

In the rest of this section we prove the above propositions.

Proof of Proposition 8. Denoting $x = p_1/p_0$ one can rewrite R_n as

$$R_n = M_0^\dagger (M_0 M_0^\dagger + x M_1 M_1^\dagger)^{-1} M_0 + x M_1^\dagger (M_0 M_0^\dagger + x M_1 M_1^\dagger)^{-1} M_1. \quad (28)$$

By symmetry we can assume that $x \geq 1$. Then Eq. (26) implies

$$M_0 M_0^\dagger + x M_1 M_1^\dagger = M_0 M_0^\dagger + M_1 M_1^\dagger + (x-1) M_1 M_1^\dagger \geq I_r + (x-1) M_1 M_1^\dagger.$$

Since the function $f(y) = -1/y$ is operator monotone, we arrive at $R_n \leq S_0 + S_1$, where

$$S_0 = M_0^\dagger (I_r + (x-1) M_1 M_1^\dagger)^{-1} M_0 \quad \text{and} \quad S_1 = x M_1^\dagger (I_r + (x-1) M_1 M_1^\dagger)^{-1} M_1. \quad (29)$$

Hence it suffices to prove that $\|S_0 + S_1\| \leq 1$. From Eq. (25) one infers that $\|M_0\| \leq 1$ and $\|M_1\| \leq 1$. Since M_0 has $(s-r)$ fewer rows than columns, it must have at least this many linearly independent vectors in its nullspace. From Eq. (25) one infers that for any $\phi \in \mathbb{C}^s$ with $\|\phi\| = 1$ and $M_0 \phi = 0$ we have $\|M_1 \phi\| = 1$. Thus M_1 has at least $(s-r)$ singular values equal to 1. Likewise, M_0 has at least $(s-r)$ singular values equal to 1. Note that this implies that $(s-r) \leq r$ since $M_0 M_0^\dagger$ is an $r \times r$ matrix with at least $(s-r)$ eigenvalues equal to 1. Furthermore, conditions Eqs. (25,26) and the norm of $S_0 + S_1$ are invariant under a transformation $M_{0,1} \rightarrow W M_{0,1} V$, where W and V are arbitrary unitary matrices. We can always choose W and V to bring M_1 into a diagonal form such that the diagonal matrix elements of M_1 are non-negative and non-increasing. Thus we can assume without loss of generality that

$$M_1 = \begin{bmatrix} D & 0_{r \times (s-r)} \end{bmatrix} \quad (30)$$

where

$$D = \text{diag}(d_1, d_2, \dots, d_r), \quad 1 = d_1 = \dots = d_{(s-r)} \geq d_{(s-r+1)} \geq \dots \geq d_r \geq 0. \quad (31)$$

(If $s = r$ the above equation should read $1 \geq d_1 \geq d_2 \dots \geq d_r \geq 0$.) Here and below $0_{t \times q}$ denotes an all-zeros matrix of size $t \times q$. It follows that $M_1 M_1^\dagger = D^2$ and thus

$$S_1 = \begin{bmatrix} I_{(s-r)} & 0_{(s-r) \times r} \\ 0_{r \times (s-r)} & \tilde{S}_1 \end{bmatrix}, \quad \text{where} \quad \tilde{S}_1 = x \hat{D}^2 (I_r + (x-1) \hat{D}^2)^{-1}, \quad (32)$$

and

$$\hat{D} = \text{diag}(d_{(s-r+1)}, d_{(s-r+2)}, \dots, d_r, 0_{1 \times (s-r)}). \quad (33)$$

The above arguments also show that $\phi \in \mathbb{C}^s$ is in the nullspace of M_0 iff ϕ has support on basis vectors i with $d_i = 1$. Thus we can assume wlog that

$$M_0 = \begin{bmatrix} 0_{r \times (s-r)} & M \end{bmatrix}, \quad (34)$$

where M is some matrix of size $r \times r$. Substituting Eqs. (30,34) into Eq. (25,26) yields

$$M^\dagger M = I_r - \hat{D}^2 \quad (35)$$

and

$$MM^\dagger \geq I_r - D^2. \quad (36)$$

Using the polar decomposition of M and Eq. (35) we obtain the parameterization $M = U(I_r - \hat{D}^2)^{1/2}$, where U is unitary. Then Eq. (36) is equivalent to $U(I_r - \hat{D}^2)U^\dagger \geq I_r - D^2$, or

$$U\hat{D}^2U^\dagger \leq D^2. \quad (37)$$

Using the definition of S_0 one gets

$$S_0 = \begin{bmatrix} 0_{(s-r) \times (s-r)} & 0_{(s-r) \times r} \\ 0_{r \times (s-r)} & \tilde{S}_0 \end{bmatrix}, \quad \text{where} \quad \tilde{S}_0 = M^\dagger(I_r + (x-1)D^2)^{-1}M. \quad (38)$$

Combining Eqs. (32,38), it suffices to show that $\|\tilde{S}_0 + \tilde{S}_1\| \leq 1$. Using the chosen parameterization of M one gets

$$\tilde{S}_0 = (I_r - \hat{D}^2)^{1/2}(I_r + (x-1)U^\dagger D^2 U)^{-1}(I_r - \hat{D}^2)^{1/2}. \quad (39)$$

Now Eq. (37) implies $U^\dagger D^2 U \geq \hat{D}^2$. Since $f(y) = -1/y$ is an operator monotone function, it follows that

$$(I_r + (x-1)U^\dagger D^2 U)^{-1} \leq (I_r + (x-1)\hat{D}^2)^{-1}, \quad (40)$$

that is,

$$\tilde{S}_0 + \tilde{S}_1 \leq (I_r - \hat{D}^2)(I_r + (x-1)\hat{D}^2)^{-1} + x\hat{D}^2(I_r + (x-1)\hat{D}^2)^{-1} = I. \quad (41)$$

This proves that $\|\tilde{S}_0 + \tilde{S}_1\| \leq 1$ which implies $\|S_0 + S_1\| = 1$ and thus $\|R_n\| \leq 1$. \square

Proof of Proposition 7. We first show that

$$\mathcal{G}_n^\perp = \mathcal{A} + \mathcal{B}, \quad \text{where} \quad \mathcal{A} = \mathcal{G}_{n-2} \otimes \psi \quad \text{and} \quad \mathcal{B} = \mathcal{G}_{n-1}^\perp \otimes \mathbb{C}^2. \quad (42)$$

Note that the two tensor products in \mathcal{A} and in \mathcal{B} refer to two different partitions of the chain. We use the following two general properties of the orthogonal complement (here \mathcal{W}, \mathcal{V} are subspaces of a Hilbert space)

$$(\mathcal{W} + \mathcal{V})^\perp = \mathcal{W}^\perp \cap \mathcal{V}^\perp \quad (43)$$

$$(\mathcal{W} \otimes \mathcal{V})^\perp = \mathcal{W}^\perp \otimes \mathcal{V} + \mathcal{W} \otimes \mathcal{V}^\perp + \mathcal{W}^\perp \otimes \mathcal{V}^\perp. \quad (44)$$

We have

$$\mathcal{G}_n = (\mathcal{G}_{n-1} \otimes \mathbb{C}^2) \cap (\mathcal{G}_{n-2} \otimes \psi^\perp)$$

Applying Eqs. (43,44) gives

$$\begin{aligned} \mathcal{G}_n^\perp &= (\mathcal{G}_{n-1} \otimes \mathbb{C}^2)^\perp + (\mathcal{G}_{n-2} \otimes \psi^\perp)^\perp \\ &= \mathcal{G}_{n-1}^\perp \otimes \mathbb{C}^2 + \mathcal{G}_{n-2}^\perp \otimes \psi^\perp + \mathcal{G}_{n-2} \otimes \psi + \mathcal{G}_{n-2}^\perp \otimes \psi \\ &= \mathcal{A} + \mathcal{B} \end{aligned}$$

where to get the last line we absorbed the second and fourth terms into the first, using the fact that $(G_{n-2} \otimes \mathbb{C}^2)^\perp \subseteq G_{n-1}^\perp$.

Choose an arbitrary orthonormal basis

$$e_1, e_2, \dots, e_q \in \mathcal{G}_{n-1}^\perp, \quad q = \dim(\mathcal{G}_{n-1}^\perp) \quad (45)$$

From Eq. (42) one infers that \mathcal{G}_n^\perp is spanned by

$$(\hat{e}_1, \dots, \hat{e}_M) = (g_1 \otimes \psi, \dots, g_r \otimes \psi) \cup (e_1 \otimes v_0, \dots, e_q \otimes v_0) \cup (e_1 \otimes v_1, \dots, e_q \otimes v_1).$$

where v_0, v_1 are the Schmidt vectors of ψ as defined in Eq. (18).

We now show that the Gram matrix Γ defined by

$$\Gamma_{p,q} = \langle \hat{e}_p | \hat{e}_q \rangle$$

is invertible, which implies that $\hat{e}_1, \dots, \hat{e}_M$ are linearly independent. We note that Γ has the following simple form

$$\Gamma = \begin{bmatrix} I_r & B_0 & B_1 \\ B_0^\dagger & I_q & 0 \\ B_1^\dagger & 0 & I_q \end{bmatrix} \quad (46)$$

where

$$(B_z)_{\alpha,i} = \langle g_\alpha \otimes \psi | e_i \otimes v_z \rangle = \sqrt{p_z} \langle g_\alpha \otimes w_z | e_i \rangle \quad z = 0, 1. \quad (47)$$

Define $B = [B_0 \ B_1]$, $X = BB^\dagger$, and $Y = B^\dagger B$. Note that X and Y have the same non-zero eigenvalues. Also note that Γ is invertible if none of these eigenvalues are equal to 1, since in this case

$$\Gamma^{-1} = \begin{bmatrix} (I_r - X)^{-1} & -B(I_{2q} - Y)^{-1} \\ -B^\dagger(I_r - X)^{-1} & (I_{2q} - Y)^{-1} \end{bmatrix}. \quad (48)$$

To show that Γ is invertible it therefore suffices to show that $I_r - X$ is invertible. Using Eqs. (24,47) and the identity $I = G_{n-1} + G_{n-1}^\perp$ we get

$$\frac{1}{p_0} B_0 B_0^\dagger + M_0 M_0^\dagger = I_r \quad \text{and} \quad \frac{1}{p_1} B_1 B_1^\dagger + M_1 M_1^\dagger = I_r.$$

So

$$I_r - X = I_r - B_0 B_0^\dagger - B_1 B_1^\dagger = p_0 M_0 M_0^\dagger + p_1 M_1 M_1^\dagger. \quad (49)$$

To prove that $I_r - X$ is invertible we show that this operator is positive definite:

$$p_0 M_0 M_0^\dagger + p_1 M_1 M_1^\dagger \geq \min(p_0, p_1) (M_0 M_0^\dagger + M_1 M_1^\dagger) \geq \min(p_0, p_1) I > 0$$

where we used Eq. (26) and the fact that p_0, p_1 are both positive. This completes the proof that Γ is invertible and establishes that $\hat{e}_1, \dots, \hat{e}_M$ are linearly independent.

Since we have shown that $\hat{e}_1, \dots, \hat{e}_M$ are a basis for \mathcal{G}_n^\perp , we have

$$G_n^\perp = \sum_{p,q=1}^M (\Gamma^{-1})_{p,q} |\hat{e}_p\rangle \langle \hat{e}_q|. \quad (50)$$

Substituting Eqs. (50,48) into $R_n \equiv G_{n-1} \text{Tr}_n(G_n^\perp) G_{n-1}$ and noting that $\hat{e}_\alpha = g_\alpha \otimes \psi$ with $\alpha = 1, \dots, r$ are the only basis vectors of \mathcal{G}_n^\perp which are not orthogonal to $\mathcal{G}_{n-1} \otimes \mathbb{C}^2$, we arrive at

$$R_n = \sum_{\alpha, \beta=1}^r (I_r - X)_{\alpha, \beta}^{-1} G_{n-1} (|g_\alpha\rangle\langle g_\beta| \otimes \text{Tr}_2|\psi\rangle\langle\psi|) G_{n-1}.$$

Substituting $G_{n-1} = \sum_{i=1}^s |h_i\rangle\langle h_i|$ and $\text{Tr}_2|\psi\rangle\langle\psi| = p_0|w_0\rangle\langle w_0| + p_1|w_1\rangle\langle w_1|$ into the above equation yields

$$\langle h_i | R_n | h_j \rangle = \sum_{\alpha, \beta=1}^r (I_r - X)_{\alpha, \beta}^{-1} (p_0 \langle h_i | g_\alpha \otimes w_0 \rangle \cdot \langle g_\beta \otimes w_0 | h_j \rangle + p_1 \langle h_i | g_\alpha \otimes w_1 \rangle \cdot \langle g_\beta \otimes w_1 | h_j \rangle).$$

Replacing the last two factors by matrix elements of M_0, M_1 defined in Eq. (24) and $I_r - X$ by Eq. (49) one arrives at Eq. (27). \square

5 Gapped phase

In this section we prove the second part of Theorem 1, namely

Gapped phase theorem. *Suppose the eigenvalues of T_ψ have different magnitudes or both eigenvalues are equal to zero. Then the spectral gap of $H_n(\psi)$ is lower bounded by a positive constant independent of n .*

Let us first consider the simple case when both eigenvalues of T_ψ are equal to zero. Using the canonical form of ψ established in Proposition 5 and Eq. (13) one can check that this is possible only if $|\psi\rangle = (U \otimes U)|1, 1\rangle$ for some single-qubit unitary operator U . Thus the Hamiltonian $H_n(\psi)$ is a sum of pairwise commuting projectors and $\gamma(\psi, n) \geq 1$ for all n which proves the desired lower bound.

In the rest of this section we assume that the eigenvalues of T_ψ have distinct magnitudes. In this case the eigenvectors of T_ψ must be linearly independent. Let us first introduce some notation. Suppose $S \subseteq [n]$ is a consecutive block of qubits. We shall write G_S for the projector onto the ground space of the truncated Hamiltonian

$$\sum_{\{i, i+1\} \subseteq S} |\psi\rangle\langle\psi|_{i, i+1}$$

obtained from $H_n(\psi)$ by retaining only the terms fully contained in S . The projector G_S acts trivially on all qubits in the complement of S . Note that $G_n = G_S$ in the case where S is the entire chain.

Our starting point is a general lower bound on the gap of 1D frustration-free Hamiltonians due to Nachtergaele [22]. Specializing Theorem 3 of Ref. [22] to our case one gets the following lemma.

Lemma 3 (Nachtergaele [22]). *Suppose there exists an integer $r \geq 1$ and a real number $\epsilon < (r+1)^{-1/2}$ such that for all large enough n and for the partition $[n] = ABC$ with $|B| = r$ and $|C| = 1$ one has $\|G_{ABC} - G_{AB}G_{BC}\| \leq \epsilon$. Then*

$$\gamma(\psi, n) \geq \frac{\gamma(\psi, r+1)}{r+1} (1 - \epsilon(r+1)^{1/2})^2 \quad (51)$$

for all large enough n .

Note that the right-hand side of Eq. (51) is a positive constant independent of n . Thus Lemma 3 reduces the problem of lower bounding the spectral gap of $H_n(\psi)$ to that of upper bounding the quantity $\|G_{ABC} - G_{AB}G_{BC}\|$. Our main technical result is an upper bound on this quantity that decays exponentially with the size of B .

Theorem 2. *Let μ_1, μ_2 be the eigenvalues of T_ψ such that $|\mu_1| < |\mu_2|$. Define $\lambda = \mu_2/\mu_1$. Let c be the inner product between the normalized eigenvectors of T_ψ . Consider any partition $[n] = ABC$ such that $|B| = r$. Then*

$$\|G_{ABC} - G_{AB}G_{BC}\| \leq O(r^{1/2}|\lambda|^{-r/8}) + O(|c|^{r/8}), \quad (52)$$

where the constant coefficients in $O(\cdot)$ depend only on the forbidden state ψ . If $\mu_1 = 0$ then (52) holds with a formal replacement $\lambda = \infty$ which sets the first term to zero.

Note that $|c| < 1$ since the eigenvectors of T_ψ are linearly independent. Furthermore, since $|\lambda| > 1$, the right-hand side of Eq. (52) is an exponentially decaying function of r . Therefore we can choose a constant r depending only on the forbidden state ψ such that

$$\|G_{ABC} - G_{AB}G_{BC}\| \leq \epsilon \equiv \frac{1}{2(r+1)^{1/2}}$$

for all $n > r$. Substituting this into Lemma 3 one gets

$$\gamma(\psi, n) \geq \frac{\gamma(\psi, r+1)}{4(r+1)}$$

for all large enough n which proves the gapped phase theorem.

In the rest of this section we prove Theorem 2. We shall first consider the case where ψ is an entangled state ($\mu_1 \neq 0$). The main technical difficulty we had to overcome is a lack of explicit formulas for the projectors G_{ABC}, G_{AB} , and G_{BC} . At a high level, our approach is to develop a set of identities relating the global ground space projector such as G_{ABC} and the local ones such as G_A or G_{AB} . These identities hold with a small error controlled by the size of the regions. Our proof of the theorem uses three identities of this type which are stated as ‘‘Region Exclusion’’ lemmas in Section 5.2. We use the Region Exclusion lemmas to decompose the operator $G_{ABC} - G_{AB}G_{BC}$ in Eq. (52) into a sum of several terms and to show that the norm of each term is exponentially small in r , see Section 5.3. The proof of the Region Exclusion lemmas combines two ingredients: monotonicity of the ground space projectors under the partial trace (established in Section 4) and the fact that certain correlation functions in the ground space decay exponentially (established in Section 5.1).

In Section 5.4 we consider the case where ψ is a product state ($\mu_1 = 0$). In this case the orthonormal basis for the ground space constructed in Section 2.1 gives an explicit formula for the ground space projector. We use this formula to establish the Region Exclusion lemmas (for the $\mu_1 = 0$ case) in a more direct way. The corresponding special case of the theorem then follows from the Region Exclusion identities.

Before proceeding, let us establish some notation and conventions. Recall that a local unitary transformation $\psi \rightarrow (U \otimes U)\psi$ preserves eigenvalues of $H_n(\psi)$ and maps T_ψ to

$(\det U)^{-1} \cdot UT_\psi U^\dagger$, see Section 3. We shall choose the unitary U to fix one of the eigenvectors of T_ψ . Specifically, in the rest of this section we shall assume that

$$T_\psi|0\rangle = \mu_1|0\rangle \quad \text{and} \quad T_\psi|v\rangle = \mu_2|v\rangle \quad (53)$$

for some state

$$|v\rangle = c|0\rangle + s|1\rangle, \quad \text{where } |c|^2 + s^2 = 1 \text{ and } s > 0.$$

Note that c is the inner product between the eigenvectors of T_ψ , as defined in the statement of Theorem 2. It will also be convenient to define a state

$$|v^\perp\rangle = s|0\rangle - c^*|1\rangle.$$

Given a set of qubits S and a single-qubit state $|\theta\rangle$ we shall write $|\theta\rangle_S$ for the product state $|\theta\rangle^{\otimes |S|}$. We shall write $|\theta\rangle\langle\theta|_S$ for the projector onto this state and $|\theta\rangle\langle\theta|_S^\perp = I_S - |\theta\rangle\langle\theta|_S$.

5.1 Correlation functions

In this section we show that certain ground space correlation functions decay exponentially. Specifically, define

$$\tau(i, j, n) = \text{Tr}(G_n|1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_j), \quad (54)$$

and

$$\tau(n) = \text{Tr}(G_n|v^\perp\rangle\langle v^\perp|_n) \quad (55)$$

where $1 \leq i < j \leq n$. For notational convenience we have suppressed the dependence of these functions on the forbidden state ψ . Our main result in this section is as follows.

Lemma 4. *The sequence $\{\tau(n)\}_{n \geq 2}$ is monotonically increasing and has a finite limit $\tau(\infty)$ such that*

$$0 \leq \tau(\infty) - \tau(n) \leq O(n|\lambda|^{-2n}) \quad \text{for all } n \geq 2. \quad (56)$$

Furthermore,

$$\tau(i, j, n) \leq O((j-i) \cdot |\lambda|^{-2(j-i)}) \quad \text{for all } 1 \leq i < j \leq n. \quad (57)$$

Here the constant coefficients in $O(\cdot)$ depend only on the forbidden state ψ .

Proof. Let us define yet another correlation function

$$\sigma(i, j, n) = \max_{\phi \in \mathcal{G}_n} \langle \phi | (|1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_j) | \phi \rangle, \quad (58)$$

where the maximum is over normalized ground states, that is, $\|\phi\| = 1$.

Proposition 9.

$$\sigma(i, j, n) \leq |\lambda|^{-2(j-i)} \frac{s^2}{1 - |c|} \quad (59)$$

for $1 \leq i < j \leq n$.

Proof. Define

$$|\psi^r\rangle = |v^\perp 1\rangle - (\lambda^*)^r |1v^\perp\rangle$$

Using Eq. (53) we see that $\langle 1|T_\psi = \mu_2\langle 1|$ and $\langle v^\perp|T_\psi = \mu_1\langle v^\perp|$. Therefore

$$\langle \psi^r|(I \otimes T_\psi^r) \sim \mu_2^r \langle v^\perp 1| - (\lambda\mu_1)^r \langle 1v^\perp| \sim \langle v^\perp 1| - \langle 1v^\perp| \sim \langle \epsilon|, \quad (60)$$

where $|\epsilon\rangle = |0, 1\rangle - |1, 0\rangle$ (recall that \sim means proportional to). Comparing Eq. (7) and Eq. (60) one infers that ψ^1 is the forbidden state, that is, $\psi \sim \psi^1$.

Let $\phi \in \mathcal{G}_n$ be a normalized state (i.e., $\|\phi\| = 1$) for which the maximum in Eq. (58) is achieved, so

$$\sigma(i, j, n) = \langle \phi| (|1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_j) |\phi\rangle.$$

Since $\phi \in \mathcal{G}_n$, by Proposition 2 it can be written $|\phi\rangle = I \otimes T_\psi \otimes T_\psi^2 \dots \otimes T_\psi^{n-1} |\chi\rangle$ where $|\chi\rangle$ belongs to the symmetric subspace. Using this fact and Eq. (60) we see that

$${}_{i,j}\langle \psi^{j-i}|\phi\rangle = 0 \quad (61)$$

for all integers $1 \leq i < j \leq n$. Writing

$$|\phi\rangle = |0\rangle_i |\phi_0^i\rangle_{[n]\setminus i} + |v\rangle_i |\phi_1^i\rangle_{[n]\setminus i}$$

and substituting this into Eq. (61) one gets

$$s \left({}_j\langle 1|\phi_0^i\rangle - \lambda^{j-i} {}_j\langle v^\perp|\phi_1^i\rangle \right) = 0$$

which implies

$$\langle \phi_1^i| (|v^\perp\rangle\langle v^\perp|_j) |\phi_1^i\rangle = \frac{1}{|\lambda|^{2(j-i)}} \langle \phi_0^i| (|1\rangle\langle 1|_j) |\phi_0^i\rangle. \quad (62)$$

Using the fact that $|\phi\rangle$ is normalized we have

$$1 = \langle \phi|\phi\rangle = \langle \phi_0^i|\phi_0^i\rangle + \langle \phi_1^i|\phi_1^i\rangle + 2\text{Re}(c\langle \phi_0^i|\phi_1^i\rangle). \quad (63)$$

We upper bound the magnitude of the third term using the Cauchy-Schwarz and the arithmetic/geometric mean inequality:

$$|c\langle \phi_0^i|\phi_1^i\rangle| \leq |c| \sqrt{\langle \phi_0^i|\phi_0^i\rangle \langle \phi_1^i|\phi_1^i\rangle} \leq \frac{|c|}{2} (\langle \phi_0^i|\phi_0^i\rangle + \langle \phi_1^i|\phi_1^i\rangle).$$

Substituting this into Eq. (63) yields

$$1 \geq (1 - |c|) (\langle \phi_0^i|\phi_0^i\rangle + \langle \phi_1^i|\phi_1^i\rangle) \geq (1 - |c|) \langle \phi_0^i|\phi_0^i\rangle$$

and hence $\langle \phi_0^i|\phi_0^i\rangle \leq \frac{1}{1-|c|}$. Using this fact and Eq. (62) we obtain

$$\langle \phi_1^i| (|v^\perp\rangle\langle v^\perp|_j) |\phi_1^i\rangle \leq \frac{|\lambda|^{-2(j-i)}}{1 - |c|}$$

and thus

$$\sigma(i, j, n) = \langle \phi| (|1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_j) |\phi\rangle = s^2 \langle \phi_1^i| (|v^\perp\rangle\langle v^\perp|_j) |\phi_1^i\rangle \leq |\lambda|^{-2(j-i)} \frac{s^2}{1 - |c|}.$$

□

Now we are ready to prove Eq. (56). First, applying the Monotonicity Lemma (Lemma 2) to the left-right flipped chain yields $\text{Tr}_1(G_n) \geq G_{n-1}$. Therefore

$$\tau(n) = \text{Tr}(\text{Tr}_1(G_n)|v^\perp\rangle\langle v^\perp|_{n-1}) \geq \text{Tr}(G_{n-1}|v^\perp\rangle\langle v^\perp|_{n-1}) = \tau(n-1),$$

that is, $\tau(n)$ is monotonically increasing.

Inserting the identity decomposition $I = |0\rangle\langle 0| + |1\rangle\langle 1|$ on the first qubit in Eq. (55) one gets

$$\tau(n) = \text{Tr}(G_n|1\rangle\langle 1|_1 \otimes |v^\perp\rangle\langle v^\perp|_n) + \text{Tr}(G_n|0\rangle\langle 0|_1 \otimes |v^\perp\rangle\langle v^\perp|_n). \quad (64)$$

The first term in Eq. (64) is upper bounded by $(n+1)\sigma(1, n, n)$ since we can decompose $G_n = \sum_{a=0}^n |g_a\rangle\langle g_a|$ using some orthonormal basis $\{g_a\}$ of \mathcal{G}_n and use the fact that

$$\langle g_a|(|1\rangle\langle 1|_1 \otimes |v^\perp\rangle\langle v^\perp|_n)|g_a\rangle \leq \sigma(1, n, n)$$

for each individual state g_a . The second term in Eq. (64) is upper bounded by $\tau(n-1)$, which follows from $G_n \leq I \otimes G_{n-1}$. Thus

$$\tau(n) \leq (n+1)\sigma(1, n, n) + \tau(n-1).$$

Proposition 9 implies $\sigma(1, n, n) = O(|\lambda|^{-2n})$, that is,

$$0 \leq \tau(n) - \tau(n-1) \leq O(n|\lambda|^{-2n}).$$

This shows that $\tau(n)$ has a finite limit $\tau(\infty)$ at $n \rightarrow \infty$. Summing up the series produces the desired bound Eq. (56).

The proof of Eq. (57) follows a similar strategy. First consider the case $i = 1, j = n$. The same argument used above shows that

$$\tau(1, n, n) \leq (n+1)\sigma(1, n, n) = O(n|\lambda|^{-2n}). \quad (65)$$

Next suppose $i \geq 2$ and $j = n$. Inserting the identity decomposition $I = |0\rangle\langle 0| + |1\rangle\langle 1|$ on the first qubit, using the fact that $G_n \leq I \otimes G_{n-1}$, and noting that $|1\rangle\langle 1|_i \leq I$, one gets

$$\begin{aligned} \tau(i, n, n) &\leq \tau(i-1, n-1, n-1) + \text{Tr}(G_n|1\rangle\langle 1|_1 \otimes |1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_n) \\ &\leq \tau(i-1, n-1, n-1) + \tau(1, n, n). \end{aligned} \quad (66)$$

This shows that

$$\tau(i, n, n) \leq \sum_{k=n-i+1}^n \tau(1, k, k). \quad (67)$$

Substituting Eq. (65) into this bound and summing up the series, we get

$$\tau(i, n, n) \leq O((n-i)|\lambda|^{-2(n-i)}) \quad \text{for all } i = 1, \dots, n-1. \quad (68)$$

(Here we included the case $i = 1$ which was handled in Eq. (65)).

Finally, consider the case $j \leq n-1$. Inserting the identity decomposition $I = |v\rangle\langle v| + |v^\perp\rangle\langle v^\perp|$ on the n -th qubit, using the fact that $G_n \leq G_{n-1} \otimes I$, and noting that $|v^\perp\rangle\langle v^\perp|_j \leq I$, one gets

$$\tau(i, j, n) \leq \tau(i, j, n-1) + \text{Tr}(G_n|1\rangle\langle 1|_i \otimes |v^\perp\rangle\langle v^\perp|_j \otimes |v^\perp\rangle\langle v^\perp|_n) \leq \tau(i, j, n-1) + \tau(i, n, n).$$

This shows that

$$\tau(i, j, n) \leq \sum_{m=j}^n \tau(i, m, m). \quad (69)$$

Combining this with Eq. (67) leads to the desired bound Eq. (57). \square

5.2 Region exclusion lemmas

To perform manipulations with ground space projectors that involve several regions we now prove three region exclusion lemmas. These lemmas allow one to exclude one of the regions from certain operators built from ground space projectors.

The first region exclusion lemma states that $G_{ABC}|v\rangle\langle v|_{BC} \approx G_{AB} \otimes I_C|v\rangle\langle v|_{BC}$.

Region Exclusion Lemma 5. *Let $[n] = ABC$ with $|B| = j$. Then*

$$\|(G_{ABC} - G_{AB} \otimes I_C)|v\rangle\langle v|_{BC}\|^2 \leq O(|c|^j) + O(j|\lambda|^{-j})$$

Here the constant coefficients in $O(\cdot)$ depend only on the forbidden state ψ .

Proof. Define $P \equiv G_{ABC}$ and $Q \equiv G_{AB} \otimes I_C$. Using the fact that $PQ = QP = P$ one can write the quantity we wish to bound as

$$\|(P - Q)|v\rangle\langle v|_{BC}\|^2 \leq \text{Tr}_A \langle v_{BC} | (P - Q)^2 | v_{BC} \rangle = \text{Tr}(Q|v\rangle\langle v|_{BC}) - \text{Tr}(P|v\rangle\langle v|_{BC}). \quad (70)$$

Define

$$\theta(n, r) = \text{Tr}(G_n \cdot I_{n-r} \otimes |v\rangle\langle v|^{\otimes r}). \quad (71)$$

One can rewrite Eq. (70) as

$$\|(P - Q)|v\rangle\langle v|_{BC}\|^2 \leq \theta(i + j, j) - \theta(i + j + k, j + k), \quad (72)$$

where $i = |A|$, $j = |B|$, and $k = |C|$. Representing $|v\rangle\langle v| = I - |v^\perp\rangle\langle v^\perp|$ on the last qubit in Eq. (71) and using the monotonicity property $\text{Tr}_n(G_n) \geq G_{n-1}$ from Lemma 2 one gets

$$\theta(n, r) \geq \theta(n - 1, r - 1) - \xi(n, r - 1), \quad (73)$$

where

$$\xi(n, r) \equiv \text{Tr}(G_n \cdot I_{n-r-1} \otimes |v\rangle\langle v|^{\otimes r} \otimes |v^\perp\rangle\langle v^\perp|). \quad (74)$$

From Eq. (73) we get

$$\theta(i + j, j) \leq \theta(i + j + k, j + k) + \sum_{r=j}^{j+k-1} \xi(i + r + 1, r)$$

and plugging into Eq. (72) gives

$$\|(P - Q)|v\rangle\langle v|_{BC}\|^2 \leq \sum_{r=j}^{j+k-1} \xi(i + r + 1, r). \quad (75)$$

To complete the proof we now show that $\xi(n, r)$ has an upper bound which is exponentially small in r and does not depend on n . Partition the chain as $[n] = A'B'B''C'$, where $|C'| = 1$, $|B'| = \lfloor r/2 \rfloor$, $|B''| = \lceil r/2 \rceil$, and $|A'| = n - 1 - r$. Using the fact that $|v\rangle\langle v|_{B''} \leq I$ we get

$$\xi(n, r) \leq \langle v_{B'} | L_{B'} | v_{B'} \rangle, \quad \text{where} \quad L_{B'} \equiv \text{Tr}_{A'B''C'}(G_n |v^\perp\rangle\langle v^\perp|_{C'}). \quad (76)$$

Using the second part of Lemma 4 we have

$$\text{Tr}(L_{B'} |1\rangle\langle 1|_m) = \tau(m, n, n) = O((n - m)|\lambda|^{-2(n-m)}) \quad \text{for any } m \in B'. \quad (77)$$

Note that $n - m \geq r/2$ for any $m \in B'$. Let $|0\rangle\langle 0|_{B'}^\perp = I - |0\rangle\langle 0|_{B'}$. It follows that

$$\text{Tr}(L_{B'} |0\rangle\langle 0|_{B'}^\perp) \leq \sum_{m \in B'} \text{Tr}(L_{B'} |1\rangle\langle 1|_m) \leq O(1) \sum_{m=n-r}^{n-r/2} (n - m) |\lambda|^{-2|n-m|} = O(r|\lambda|^{-r}). \quad (78)$$

Thus $L_{B'}$ has almost all its weight on the basis vector $|0_{B'}\rangle$ and an exponentially small weight $O(r|\lambda|^{-r})$ on the space orthogonal to $|0_{B'}\rangle$. Furthermore, the first part of Lemma 4 implies that $\text{Tr}(L_{B'}) = \tau(n) = \tau(\infty) - O(n|\lambda|^{-2n})$. Combining this fact and Eq. (78) results in

$$L_{B'} = \tau(\infty) |0\rangle\langle 0|_{B'} + E \quad \text{where} \quad \|E\| \leq O(r|\lambda|^{-r}). \quad (79)$$

Therefore

$$\xi(n, r) \leq \langle v_{B'} | L_{B'} | v_{B'} \rangle = \tau(\infty) |\langle 0|v\rangle|^{2|B'|} + O(r|\lambda|^{-r}) \leq \tau(\infty) |c|^{(r-2)} + O(r|\lambda|^{-r}). \quad (80)$$

Finally, substituting this into Eq. (75) gives

$$\|(P - Q) |v\rangle\langle v|_{BC}\|^2 \leq \sum_{r=j}^{j+k-1} \xi(i+r+1, r) \leq \sum_{r=j}^{\infty} \xi(i+r+1, r) \leq O(|c|^j) + O(j|\lambda|^{-j}). \quad (81)$$

□

The second region exclusion lemma concerns the operator $G_{ABCD} |v\rangle\langle v|_C^\perp$ (recall that $|v\rangle\langle v|_C^\perp = I - |v\rangle\langle v|_C$).

Region Exclusion Lemma 6. *Consider any partition $[n] = ABCD$ with $|B| = j$. Then*

$$\|(G_{ABCD} - |0\rangle\langle 0|_A \otimes G_{BCD}) |v\rangle\langle v|_C^\perp\|^2 \leq O(j|\lambda|^{-2j}).$$

Here the constant coefficient in $O(\cdot)$ depends only on the forbidden state ψ .

Proof. For brevity denote $P \equiv G_{ABCD}$ and $Q \equiv |0\rangle\langle 0|_A \otimes G_{BCD}$. Then

$$\|(P - Q) |v\rangle\langle v|_C^\perp\|^2 \leq \text{Tr}((P - Q)^2 |v\rangle\langle v|_C^\perp).$$

Taking into account that $G_{ABCD} G_{BCD} = G_{ABCD}$ gives

$$\|(P - Q) |v\rangle\langle v|_C^\perp\|^2 \leq \text{Tr}(P |v\rangle\langle v|_C^\perp) + \text{Tr}(Q |v\rangle\langle v|_C^\perp) - 2\text{Tr}(P |0\rangle\langle 0|_A \otimes |v\rangle\langle v|_C^\perp).$$

Substituting $|0\rangle\langle 0|_A = I - |0\rangle\langle 0|_A^\perp$ in the last term results in

$$\|(P - Q)|v\rangle\langle v|_C^\perp\|^2 \leq \text{Tr}(Q|v\rangle\langle v|_C^\perp) - \text{Tr}(P|v\rangle\langle v|_C^\perp) + 2\text{Tr}(P|0\rangle\langle 0|_A^\perp \otimes |v\rangle\langle v|_C^\perp).$$

Applying the Monotonicity Lemma (Lemma 2) one gets $\text{Tr}_A(G_{ABCD}) \geq G_{BCD}$. This shows that

$$\text{Tr}(Q|v\rangle\langle v|_C^\perp) - \text{Tr}(P|v\rangle\langle v|_C^\perp) = \text{Tr}(G_{BCD}|v\rangle\langle v|_C^\perp) - \text{Tr}(G_{ABCD}|v\rangle\langle v|_C^\perp) \leq 0$$

and therefore

$$\|(P - Q)|v\rangle\langle v|_C^\perp\|^2 \leq 2\text{Tr}(P|0\rangle\langle 0|_A^\perp \otimes |v\rangle\langle v|_C^\perp) \leq 2 \sum_{m \in A} \sum_{m' \in C} \text{Tr}(G_{ABCD}|1\rangle\langle 1|_m \otimes |v^\perp\rangle\langle v^\perp|_{m'}).$$

One can recognize the last term as the correlation function $\tau(m, m', n)$ defined in Section 5.1. Using the second part of Lemma 4 one gets

$$\|(P - Q)|v\rangle\langle v|_C^\perp\|^2 \leq \sum_{m \in A} \sum_{m' \in C} O\left((m' - m)|\lambda|^{-2(m' - m)}\right) \leq O(1) \cdot \sum_{r=j}^{\infty} r(r-j)|\lambda|^{-2r} = O(j|\lambda|^{-2j}).$$

Here we denoted $r = m' - m$ so that $r \geq |B| = j$. We also used the fact that the number of pairs (m, m') with $m \in A$ and $m' \in C$ such that $m' - m = r$ is at most $r - |B| = r - j$. \square

The third and final region exclusion lemma involves operators built from the ground space projectors as follows. Given any bipartition $[n] = AB$, where A and B are consecutive blocks of qubits, define

$$G_{A>B} \equiv G_A \otimes |v\rangle\langle v|_B - G_{AB} \quad \text{and} \quad G_{A<B} \equiv |0\rangle\langle 0|_A \otimes G_B - G_{AB}.$$

Region Exclusion Lemma 7. *Consider any partition $[n] = ABC$ with $|B| = j$. Then*

$$\|G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C}\| \leq O(j^{1/2}|\lambda|^{-j/4}) + O(|c|^{j/4}). \quad (82)$$

and

$$\|G_{A<BC} - G_{A<B} \otimes |v\rangle\langle v|_C\| \leq O(j^{1/2}|\lambda|^{-j/4}) + O(|c|^{j/4}). \quad (83)$$

Here the constant coefficients in $O(\cdot)$ depend only on the forbidden state ψ .

Proof. We first show that the bound Eq. (83) follows from Eq. (82) and thus it suffices to prove the latter. To see this, consider horizontally flipping the chain so that the vertices previously labeled $1, 2, \dots, n$ are now $n, n-1, \dots, 1$. The new forbidden state is $\psi' = \text{SWAP}\psi$ where SWAP is the unitary transformation which interchanges the two qubits. The new matrix $T_{\psi'}$ is proportional to T_ψ^{-1} . From this we see that $|0'\rangle = |v\rangle$ and $|v'\rangle = |0\rangle$, and that $\lambda' = \lambda$. Using these facts we can see that Eq. (83) is just Eq. (82) applied to the left-right flipped chain.

It remains to prove Eq. (82). Let ϕ be any normalized state of ABC such that

$$\|G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C}\| = \|(G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C})\phi\|. \quad (84)$$

Partition the region B as $B = B'B''$, where $|B'| = \lfloor j/2 \rfloor$ and $|B''| = \lceil j/2 \rceil$. Define states

$$\phi^- = |v\rangle\langle v|_C^\perp \cdot \phi, \quad \phi^{-+} = |v\rangle\langle v|_{B''}^\perp \otimes |v\rangle\langle v|_C \cdot \phi, \quad \phi^{++} = |v\rangle\langle v|_{B''} \otimes |v\rangle\langle v|_C \cdot \phi.$$

One can easily check that the above states are pairwise orthogonal,

$$\phi = \phi^- + \phi^{-+} + \phi^{++} \quad \text{and} \quad 1 = \|\phi\|^2 = \|\phi^-\|^2 + \|\phi^{-+}\|^2 + \|\phi^{++}\|^2.$$

We shall bound the contributions to the right-hand side of Eq. (84) coming from ϕ^- , ϕ^{-+} , and ϕ^{++} separately.

Let us start with ϕ^- . Using the definitions of $G_{AB>C}$ and $G_{B>C}$ one gets

$$G_{AB>C} \cdot \phi^- = -G_{ABC} \cdot \phi^- \quad \text{and} \quad |0\rangle\langle 0|_A \otimes G_{B>C} \cdot \phi^- = -|0\rangle\langle 0|_A \otimes G_{BC} \cdot \phi^-.$$

Since $\phi^- = |v\rangle\langle v|_C^\perp \cdot \phi^-$ and $\|\phi^-\| \leq 1$, this results in

$$\|(G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C})\phi^-\| \leq \|(G_{ABC} - |0\rangle\langle 0|_A \otimes G_{BC})|v\rangle\langle v|_C^\perp\| \leq O(j^{1/2}|\lambda|^{-j}). \quad (85)$$

Here the last inequality follows from Lemma 6, where we set $D = \emptyset$.

Next let us consider ϕ^{-+} . Using the definitions of $G_{AB>C}$ and $G_{B>C}$ one gets

$$G_{AB>C} \cdot \phi^{-+} = (G_{AB} - G_{ABC}) \cdot \phi^{-+} \quad \text{and} \quad |0\rangle\langle 0|_A \otimes G_{B>C} \cdot \phi^{-+} = |0\rangle\langle 0|_A \otimes (G_B - G_{BC}) \cdot \phi^{-+}.$$

It follows that

$$\begin{aligned} \|(G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C})\phi^{-+}\| &\leq \|(G_{AB'B''} - |0\rangle\langle 0|_A \otimes G_{B'B''})|v\rangle\langle v|_{B''}^\perp\| \\ &\quad + \|(G_{AB'B''C} - |0\rangle\langle 0|_A \otimes G_{B'B''C})|v\rangle\langle v|_{B''}^\perp\| \end{aligned} \quad (86)$$

We can bound both terms in the right-hand side of the above equations using Lemma 6. One should choose the four regions in the statement of Lemma 6 as $(A, B, C, D) = (A, B', B'', \emptyset)$ for the first term and $(A, B, C, D) = (A, B', B'', C)$ for the second term. This results in

$$\|(G_{AB>C} - |0\rangle\langle 0|_A \otimes G_{B>C})\phi^{-+}\| \leq O(j^{1/2}|\lambda|^{-j/2}) + O(j^{1/2}|\lambda|^{-j/2}) = O(j^{1/2}|\lambda|^{-j/2}). \quad (87)$$

Finally, let us consider ϕ^{++} . We have

$$G_{AB>C} \cdot \phi^{++} = (G_{AB} - G_{ABC}) \cdot \phi^{++} \quad \text{and} \quad |0\rangle\langle 0|_A \otimes G_{B>C} \cdot \phi^{++} = |0\rangle\langle 0|_A \otimes (G_B - G_{BC}) \cdot \phi^{++}.$$

It follows that

$$\|G_{AB>C} \cdot \phi^{++}\| \leq \|(G_{(AB')B''C} - G_{(AB')B''})|v\rangle\langle v|_{B''C}\| \leq O(j^{1/2}|\lambda|^{-j/4}) + O(|c|^{j/4}). \quad (88)$$

Here we applied Lemma 5 choosing the regions in the statement of the lemma as $(A, B, C) = (AB', B'', C)$. Likewise,

$$\begin{aligned} \||0\rangle\langle 0|_A \otimes G_{B>C} \cdot \phi^{++}\| &\leq \|(G_{BC} - G_B) \cdot \phi^{++}\| \leq \|(G_{B'B''C} - G_{B'B''})|v\rangle\langle v|_{B''C}\| \\ &\leq O(j^{1/2}|\lambda|^{-j/4}) + O(|c|^{j/4}). \end{aligned} \quad (89)$$

Here we applied Lemma 5 choosing the regions in the statement of the lemma as $(A, B, C) = (B', B'', C)$. Substituting Eqs. (85,87,89) into Eq. (84) and using the triangle inequality one arrives at the desired bound Eq. (82). \square

5.3 Proof of the gapped phase theorem

Let us now prove Theorem 2 for the case where ψ is entangled, that is, $\mu_1 \neq 0$. In Section 5.4 we will see how to modify this proof to handle the product state case $\mu_1 = 0$.

Partition region B as $B = B'B''$, where $|B'| = \lfloor r/2 \rfloor$, $|B''| = \lceil r/2 \rceil$. First we note that

$$G_{AB}G_{BC} - G_{ABC} = (G_{AB} - G_{ABC})G_{BC} \quad (90)$$

and

$$G_{AB} - G_{ABC} = G_{AB} \otimes |v\rangle\langle v|_C + G_{AB} \otimes |v\rangle\langle v|_C^\perp - G_{ABC} = G_{AB>C} + G_{AB} \otimes |v\rangle\langle v|_C^\perp.$$

Here we used the notation from Lemma 7. Applying Lemma 7 to exclude region A from $G_{AB>C}$ one gets

$$G_{AB} - G_{ABC} = |0\rangle\langle 0|_A \otimes G_{B>C} + G_{AB} \otimes |v\rangle\langle v|_C^\perp + \epsilon_r \quad (91)$$

where ϵ_r denotes some operator such that

$$\|\epsilon_r\| \leq O(r^{1/2}|\lambda|^{-r/4}) + O(|c|^{r/4}).$$

Substituting the identity

$$G_{B>C} = G_B \otimes |v\rangle\langle v|_C - G_{BC} = (G_B - G_{BC}) - G_B \otimes |v\rangle\langle v|_C^\perp$$

one gets

$$\begin{aligned} G_{AB} - G_{ABC} &= |0\rangle\langle 0|_A \otimes (G_B - G_{BC}) + (G_{AB} - |0\rangle\langle 0|_A \otimes G_B) \otimes |v\rangle\langle v|_C^\perp + \epsilon_r \\ &= |0\rangle\langle 0|_A \otimes (G_B - G_{BC}) - G_{A<B'} \otimes |v\rangle\langle v|_C^\perp + \epsilon_r. \end{aligned} \quad (92)$$

Applying Lemma 7 to exclude region B'' from $G_{A<B'}$ one gets

$$G_{AB} - G_{ABC} = |0\rangle\langle 0|_A \otimes (G_B - G_{BC}) - G_{A<B'} \otimes |v\rangle\langle v|_{B''} \otimes |v\rangle\langle v|_C^\perp + \epsilon_{r/2} + \epsilon_r. \quad (93)$$

Using $(G_B - G_{BC})G_{BC} = 0$, $\|G_{A<B'}\| \leq 2$, and $G_{BC} = G_{B''C}G_{BC}$, one arrives at

$$\|(G_{AB} - G_{ABC})G_{BC}\| \leq 2\|(|v\rangle\langle v|_{B''} \otimes |v\rangle\langle v|_C^\perp)G_{B''C}\| + \|\epsilon_{r/2}\| + \|\epsilon_r\|. \quad (94)$$

Finally, partition $B'' = B''_1 B''_2$ with $|B''_1| = \lfloor |B''| \rfloor$ and $|B''_2| = \lceil |B''| \rceil$ (so that each part has size $\approx r/4$). Denote

$$\delta_{r/4} = |v\rangle\langle v|_C^\perp (G_{B''C} - |0\rangle\langle 0|_{B''_1} \otimes G_{B''_2C}).$$

Applying Lemma 6 where the four regions are chosen as $(A, B, C, D) = (B''_1, B''_2, C, \emptyset)$ one concludes that

$$\|\delta_{r/4}\| \leq O(r^{1/2}|\lambda|^{-r/4}). \quad (95)$$

Replacing $G_{B''C}$ in Eq. (94) by $|0\rangle\langle 0|_{B''_1} \otimes G_{B''_2C}$ and using Eq. (95) results in

$$\begin{aligned} \|(G_{AB} - G_{ABC})G_{BC}\| &\leq 2\| |v\rangle\langle v|_{B''} \cdot |0\rangle\langle 0|_{B''_1} \| + 2\|\delta_{r/4}\| + \|\epsilon_{r/2}\| + \|\epsilon_r\| \\ &\leq 2|\langle v|0\rangle|^{|B''_1|} + O(r^{1/2}|\lambda|^{-r/8}) + O(|c|^{r/8}) \\ &\leq O(r^{1/2}|\lambda|^{-r/8}) + O(|c|^{r/8}). \end{aligned} \quad (96)$$

This completes the proof of Theorem 2 for the case when ψ is an entangled state.

5.4 Specializing to product states

Finally consider the case $\mu_1 = 0$. This implies that $\det(T_\psi) = 0$, that is, ψ is a product state. Using the notation from Section 2.1 write

$$|\psi\rangle = |1v^\perp\rangle, \quad |v\rangle = c|0\rangle + s|1\rangle, \quad |v^\perp\rangle = s|0\rangle - c^*|1\rangle,$$

where $|c|^2 + s^2 = 1$. Here $s \neq 0$ which follows from the fact that $\mu_2 \neq 0$. It is also easily checked that $|0\rangle$ and $|v\rangle$ are eigenvectors of T_ψ corresponding to eigenvalues $\mu_1 = 0, \mu_2 = -s$ respectively.

We now show that the region exclusion identities presented in Lemmas 5,6,7 (for the case of entangled ψ) become exact equalities. Indeed, as was shown in Section 2.1, the ground space of $H_n(\psi)$ has an orthonormal basis g_0, \dots, g_n , where $|g_0\rangle = |v^{\otimes n}\rangle$ and $|g_i\rangle = |0^{i-1}v^\perp v^{n-i}\rangle$ for $i \geq 1$. Thus

$$G_n = \sum_{i=0}^n |g_i\rangle\langle g_i|, \quad (97)$$

We start with Lemma 6. Let $[n] = ABCD$ be an arbitrary partition such that B and C are non-empty. We have to prove that

$$(G_{ABCD} - |0\rangle\langle 0|_A \otimes G_{BCD}) \cdot |v\rangle\langle v|_C^\perp = 0. \quad (98)$$

Note that $|v\rangle\langle v|_j \cdot |g_i\rangle = |g_i\rangle$ for all $i < j \leq n$. This implies

$$|g_i\rangle\langle g_i| \cdot |v\rangle\langle v|_C^\perp = |g_i\rangle\langle g_i| \cdot |v\rangle\langle v|_C \cdot |v\rangle\langle v|_C^\perp = 0 \quad \text{for all } i \in AB.$$

Substituting Eq. (97) for G_{ABCD} and using the above identity yields

$$G_{ABCD} \cdot |v\rangle\langle v|_C^\perp = \sum_{i \in CD} |g_i\rangle\langle g_i| \cdot |v\rangle\langle v|_C^\perp = |0\rangle\langle 0|_A \otimes G_{BCD} \cdot |v\rangle\langle v|_C^\perp$$

since $|g_i\rangle = |0\rangle_A \otimes |g_{i-|A|}\rangle_{BCD}$ for all $i \in CD$. This is equivalent to Eq. (98).

Next consider Lemma 5. Let $[n] = ABC$ be any partition such that B is non-empty. We have to prove that

$$(G_{ABC} - G_{AB} \otimes I_C) \cdot |v\rangle\langle v|_{BC} = 0. \quad (99)$$

Note that for any $i \in A$ one has

$$|g_i\rangle\langle g_i| = |g_i\rangle\langle g_i|_A \otimes |v\rangle\langle v|_{BC} \quad \text{and} \quad |g_i\rangle\langle g_i|_{AB} = |g_i\rangle\langle g_i|_A \otimes |v\rangle\langle v|_B.$$

On the other hand, $|g_i\rangle\langle g_i| \cdot |v\rangle\langle v|_{BC} = 0$ for any $i \in BC$. Therefore

$$G_{ABC} \cdot |v\rangle\langle v|_{BC} = \sum_{i \in AU\{0\}} |g_i\rangle\langle g_i| \cdot |v\rangle\langle v|_{BC} = \sum_{i \in AU\{0\}} |g_i\rangle\langle g_i|_A \otimes |v\rangle\langle v|_{BC}$$

Likewise, $|g_i\rangle\langle g_i|_{AB} \cdot |v\rangle\langle v|_{BC} = 0$ for any $i \in B$. Therefore

$$(G_{AB} \otimes I_C) \cdot |v\rangle\langle v|_{BC} = \sum_{i \in AU\{0\}} |g_i\rangle\langle g_i|_{AB} \cdot |v\rangle\langle v|_{BC} = \sum_{i \in AU\{0\}} |g_i\rangle\langle g_i|_A \otimes |v\rangle\langle v|_{BC}.$$

Comparing the last two identities one arrives at Eq. (99).

Finally, note that the proof of Lemma 7 only uses Lemmas 5,6, and the fact that Eq. (83) is equivalent to Eq. (82) applied to the left-right flipped chain. In the proof of Lemma 7 we use the fact that T_ψ is invertible to establish this latter fact. In the case at hand T_ψ is not invertible but since $|\psi\rangle = |1v^\perp\rangle$ we immediately see that Eq. (83) is just the left-right flipped version of Eq. (82). So both inequalities in Lemma 7 become exact equalities.

The proof of Theorem 2 from Section 5.3 uses the Region Exclusion lemmas to establish the result. Since we have shown that each of these lemmas holds (with exact equality) for product states ψ , we see that the proof of Theorem 2 also applies in this case if one formally sets $\lambda = \infty$ in all error terms.

6 Acknowledgments

DG thanks Edward Farhi, Jeffrey Goldstone, and Sam Gutmann for many discussions about this problem when he was a graduate student. DG was supported in part by NSERC and by ARO. IQC is supported in part by the Government of Canada and the Province of Ontario. SB would like to thank Ramis Movassagh for helpful discussions. SB acknowledges NSF Grant CCF-1110941.

References

- [1] M. B. Hastings. An area law for one-dimensional quantum systems. *J. of Stat. Mech.: Theory and Experiment*, 08:P08024, 2007.
- [2] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani. An area law and sub-exponential algorithm for 1D systems. *arXiv preprint arXiv:1301.1162*, 2013.
- [3] F. Brandão and M. Horodecki. An area law for entanglement from exponential decay of correlations. *Nature Physics*, 9(11):721–726, 2013.
- [4] M. B. Hastings and T. Koma. Spectral gap and exponential decay of correlations. *Comm. Math. Phys.*, 265(3):781–804, 2006.
- [5] G. Vidal. Efficient classical simulation of slightly entangled quantum computations. *Phys. Rev. Lett.*, 91(14):147902, 2003.
- [6] D. Perez-Garcia, F. Verstraete, M. Wolf, and J. I. Cirac. Matrix Product State representations. *Quant. Inf. Comp.*, 7:401, 2007.
- [7] Z. Landau, U. Vazirani, and T. Vidick. A polynomial-time algorithm for the ground state of 1D gapped local hamiltonians. *arXiv preprint arXiv:1307.5143*, 2013.
- [8] C. T. Chubb and S. T. Flammia. Computing the degenerate ground space of gapped spin chains in polynomial time. *arXiv:1502.06967*, 2015.
- [9] D. Gottesman and M.B. Hastings. Entanglement vs. gap for one-dimensional spin systems. *New J. Phys.*, 12:025002, 2009.

- [10] S. Irani. Ground state entanglement in one dimensional translationally invariant quantum systems. *J. Math. Phys.*, 51:022101, 2010.
- [11] S. Bravyi, L. Caha, R. Movassagh, D. Nagaj, and P. Shor. Criticality without frustration for quantum spin-1 chains. *Phys. Rev. Lett.*, 109(20):207202, 2012.
- [12] R. Movassagh and P. Shor. Power law violation of the area law in quantum spin chains. *arXiv:1408.1657*, 2014.
- [13] D. Aharonov, D. Gottesman, S. Irani, and J. Kempe. The power of quantum systems on a line. *Comm. Math. Phys.*, 287(1):41–65, 2009.
- [14] S. Hallgren, D. Nagaj, and S. Narayanaswami. The local hamiltonian problem on a line with eight states is QMA-complete. *Quantum Inf. & Comp.*, 13(9-10):721–750, 2013.
- [15] Subir Sachdev. *Quantum Phase Transitions*. Cambridge University Press, 2011.
- [16] T. Koma and B. Nachtergaele. The spectral gap of the ferromagnetic XXZ-chain. *Lett. in Math. Physics*, 40(1):1–16, 1997.
- [17] R. Movassagh, E. Farhi, J. Goldstone, D. Nagaj, T. J. Osborne, and P. W. Shor. Unfrustrated qudit chains and their ground states. *Phys. Rev. A*, 82:012318, 2010.
- [18] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki. Rigorous results on valence-bond ground states in antiferromagnets. *Phys. Rev. Lett.*, 59:799–802, 1987.
- [19] D. Gottesman and S. Irani. The quantum and classical complexity of translationally invariant tiling and Hamiltonian problems. In *FOCS'09. 50th Annual IEEE Symposium on*, pages 95–104. IEEE, 2009.
- [20] T. Cubitt, D. Garcia-Perez, and M. Wolf. Undecidability of the Spectral Gap. *arXiv:1502.04573*.
- [21] S. Knabe. Energy gaps and elementary excitations for certain VBS-quantum antiferromagnets. *J. Stat. Phys.*, 52(3-4):627–638, 1988.
- [22] B. Nachtergaele. The spectral gap for some spin chains with discrete symmetry breaking. *Comm. Math. Phys.*, 175(3):565–606, 1996.
- [23] S. Bravyi. Efficient algorithm for a quantum analogue of 2-SAT. *arXiv:quant-ph/0602108*. Published in *Contemporary Mathematics*, Vol. 536, p. 33, 2011.
- [24] N. de Beaudrap, T.J. Osborne, and J. Eisert. Ground states of unfrustrated spin hamiltonians satisfy an area law. *New Journal of Physics*, 12:095007, 2010.
- [25] C. R. Laumann, R. Moessner, A. Scardicchio, and S. Sondhi. Phase transitions and random quantum satisfiability. *Quant. Inf. and Comp.*, 10(1):0001–0015, 2010.
- [26] S. Bravyi, C. Moore, and A. Russell. Bounds on the quantum satisfiability threshold. In *Proc. 1st Symposium on Innovation in Computer Science (ICS 2010)*, page 482, 2010.

[27] Rajendra Bhatia. *Matrix Analysis*. Graduate Texts in Mathematics. Springer New York, 1997.

Appendix

Qubit chains with higher rank projectors

In the main body of the paper we considered qubit chains where Π is rank-1 and $H_n(\Pi)$, defined in Eq. (4), is guaranteed to be frustration-free. Here we consider qubit chains where Π is rank-2 or rank-3 and we determine which projectors Π correspond to frustration-free chains. For each frustration-free chain we determine if the system is gapped or gapless. We say that $H_n(\Pi)$ is gapped if its spectral gap, denoted $\gamma(\Pi, n)$, is lower bounded by a positive constant independent of n (otherwise it is gapless). We shall write \mathcal{G}_n for the null space of $H_n(\Pi)$ and G_n for the projector onto this space.

The case where Π is rank-3 is trivial, so we consider it first. In this case there is a unique two-qubit state $|\chi\rangle$ in the null space of Π . If $H_n(\Pi)$ is frustration-free then there exists an n -qubit state ψ with reduced state on each pair of consecutive qubits $i, i+1$ supported entirely on χ . It follows that the rank-3 chain is frustration-free if and only if $\chi = \theta \otimes \theta$ for some single-qubit state θ . Thus $\Pi = I - |\theta\rangle\langle\theta|^{\otimes 2}$ and $H_n(\Pi)$ is a sum of pairwise commuting projectors. This shows that $H_n(\Pi)$ has unique ground state $|\theta\rangle^{\otimes n}$, and its eigenvalue gap is equal to 1, for all $n \geq 2$.

The rank-2 case is slightly more interesting. There is a trivial case where Π is a 1-local projector, i.e., $\Pi = P \otimes I$ or $\Pi = I \otimes P$; in that case $\gamma(\Pi, n) = 1$ for all $n \geq 2$. The following theorem handles all other cases.

Theorem 3. *Suppose Π is a two-qubit, rank-2 projector which cannot be written as $I \otimes P$ or $P \otimes I$ for some projector P . Then the dimension of the null space of $H_n(\Pi)$ satisfies $\dim(\mathcal{G}_n) = \dim(\mathcal{G}_4) \in \{0, 1, 2\}$ for all $n \geq 4$. Moreover, exactly one of the following holds:*

1. $\mathcal{G}_4 = \text{span}\{|\alpha\alpha\alpha\alpha\rangle\}$ for some single-qubit state α .
2. $\mathcal{G}_4 = \text{span}\{|\alpha\alpha\alpha\alpha\rangle, |\beta\beta\beta\beta\rangle\}$ for some linearly independent single-qubit states α, β .
3. $\mathcal{G}_4 = \text{span}\{|\alpha\beta\alpha\beta\rangle, |\beta\alpha\beta\alpha\rangle\}$ for some linearly independent single-qubit states α, β .
4. $\mathcal{G}_4 = \text{span}\{|\alpha\alpha\alpha\alpha\rangle, |\alpha^\perp\alpha\alpha\alpha\rangle + f|\alpha\alpha^\perp\alpha\alpha\rangle + f^2|\alpha\alpha\alpha^\perp\alpha\rangle + f^3|\alpha\alpha\alpha\alpha^\perp\rangle\}$ for some orthonormal single-qubit states α, α^\perp and non-zero $f \in \mathbb{C}$.
5. \mathcal{G}_4 is empty.

In cases 1, 2, 3, and 4, the Hamiltonian $H_n(\Pi)$ is frustration-free for all $n \geq 2$, whereas in case 5 it is frustrated for $n \geq 4$. $H_n(\Pi)$ is gapped in cases 1, 2, and 3, and it is gapped in case 4 if $|f| \neq 1$. If $|f| = 1$ in case 4 then the Hamiltonian is gapless, with spectral gap upper bounded as $\gamma(\Pi, n) \leq 2(1 - \cos(\pi/n))$.

To establish lower bounds on spectral gaps we shall use Nachtergaele's criterion [22]. Recall that Lemma 3 states this criterion for the case where Π is rank-1. More generally

if $H_n(\Pi)$ is frustration-free for $n \geq 2$ then the same bound holds for its spectral gap (with $\gamma(\psi, n)$ and $\gamma(\psi, r+1)$ replaced by $\gamma(\Pi, n)$ and $\gamma(\Pi, r+1)$ in the statement of the Lemma). For our purposes it will be sufficient to use the following weaker version of the bound.

Lemma 5. *Suppose $H_n(\Pi)$ is frustration-free for $n \geq 2$. Let $[n] = ABC$ with $|C| = 1$, $|B| = r$, and $|A| = n - r - 1$. Suppose there exist constants $0 \leq \delta < 1$ and $K > 0$ such that for all sufficiently large n we have $\|G_{ABC} - G_{AB}G_{BC}\| \leq K\delta^r$. Then $H_n(\Pi)$ is gapped.*

Proof. We can always choose r so that $K\delta^r \leq \frac{1}{2\sqrt{r+1}}$. Plugging this choice into Nachtergaele's bound with $\epsilon = \frac{1}{2\sqrt{r+1}}$ we obtain $\gamma(\Pi, n) \geq \gamma(\Pi, r+1)(4r+4)^{-1}$. \square

Proof of Theorem 3. We first establish that the range of Π is spanned by two linearly independent states ϕ, ψ which are both entangled. It is easy to check that the only two dimensional subspaces of $\mathbb{C}^2 \otimes \mathbb{C}^2$ which contain only product states are of the form $\chi \otimes \mathbb{C}^2$ or $\mathbb{C}^2 \otimes \chi$ for some single qubit state χ . By the hypothesis of the theorem Π cannot be written as $I \otimes P$ or $P \otimes I$, which implies $\text{range}(\Pi)$ does not have this form; thus it contains at least one entangled state ϕ . Let $\nu \in \text{range}(\Pi)$ be linearly independent from ϕ . It is easy to see that we can always choose $\psi = \phi + z\nu$ for some nonzero $z \in \mathbb{C}$ so that ψ is entangled.

So $\text{range}(\Pi) = \text{span}\{\phi, \psi\}$ where ψ, ϕ are both entangled (equivalently, T_ϕ and T_ψ are both invertible). Furthermore, an n -qubit state χ is in the null space of $H_n(\Pi)$ if and only if it is in the null space of $|\psi\rangle\langle\psi|_{i,i+1}$ and $|\phi\rangle\langle\phi|_{i,i+1}$ for all $i = 1, \dots, n-1$.

To complete the proof we now suppose that \mathcal{G}_4 is nonempty and we consider two cases depending on whether or not $T_\phi^{-1}T_\psi$ has two linearly independent eigenvectors. The theorem follows directly from the following propositions which handle the two cases.

Proposition 10. *Suppose Π is a two-qubit projector such that $\text{range}(\Pi) = \text{span}\{\phi, \psi\}$ where ψ, ϕ are both entangled. Suppose that $T_\phi^{-1}T_\psi$ has linearly independent eigenvectors $\{\alpha, \beta\}$ and that \mathcal{G}_4 is nonempty. Then one of the cases 1, 2, or 3 from Theorem 3 occurs. Moreover, $H_n(\Pi)$ is frustration-free for all $n \geq 2$ and it is gapped. Its ground space dimension satisfies $\dim(\mathcal{G}_n) = \dim(\mathcal{G}_4)$ for all $n \geq 4$.*

Proposition 11. *Suppose Π is a two-qubit projector such that $\text{range}(\Pi) = \text{span}\{\phi, \psi\}$ where ψ, ϕ are both entangled. Suppose that $T_\phi^{-1}T_\psi$ has only one linearly independent eigenvector $\{\alpha\}$ and that \mathcal{G}_4 is nonempty. Then case 4 from Theorem 3 occurs. Moreover, $H_n(\Pi)$ is frustration-free and has ground space dimension equal to 2 for all $n \geq 2$. It is gapped if and only if $|f| \neq 1$; if $|f| = 1$ then $\gamma(\Pi, n) \leq 2(1 - \cos(\pi/n))$.*

\square

In the remainder of this section we prove Propositions 10 and 11.

Proof of Proposition 10 We first establish that \mathcal{G}_2 is spanned by $1 \otimes T_\psi|\alpha\rangle|\alpha\rangle$ and $1 \otimes T_\psi|\beta\rangle|\beta\rangle$. These states are linearly independent (since α, β are). Since \mathcal{G}_2 is 2-dimensional it suffices to establish that it contains both of these states. Clearly each is orthogonal to $|\psi\rangle\langle\psi|$ since $|\psi\rangle \sim \langle\epsilon|I \otimes T_\psi^{-1}$ (recall $|\epsilon\rangle = |0, 1\rangle - |1, 0\rangle$). To check that they are orthogonal to $|\phi\rangle\langle\phi|$ use the fact that $\langle\phi| \sim \langle\epsilon|I \otimes T_\phi^{-1}$ and that α, β are eigenvectors of $T_\phi^{-1}T_\psi$.

Now consider $n = 3$. Since \mathcal{G}_4 is nonempty, there exists a state $|\chi\rangle \in \mathcal{G}_3$, which by Proposition 2 can be written as $|\chi\rangle = 1 \otimes T_\psi \otimes T_\psi^2|s\rangle$ for some state $|s\rangle$ in the 3-qubit

symmetric subspace. Since the chain is frustration free, the first two qubits of χ have all of their support in \mathcal{G}_2 . This implies $|\chi\rangle = a|\alpha\rangle^{\otimes 3} + b|\beta\rangle^{\otimes 3}$ where a, b are not both zero. By symmetry we assume without loss of generality that $a \neq 0$. Next, imposing orthogonality to $|\phi\rangle\langle\phi|_{2,3}$ gives

$$a|\alpha\rangle (\langle\epsilon|T_\psi \otimes T_\phi^{-1}T_\psi^2|\alpha, \alpha\rangle) + b|\beta\rangle (\langle\epsilon|T_\psi \otimes T_\phi^{-1}T_\psi^2|\beta, \beta\rangle) = 0.$$

Since α, β are linearly independent, both terms must be zero. Using the fact that any two-qubit state orthogonal to ϵ is symmetric, and that $a \neq 0$, we get:

- $T_\psi|\alpha\rangle$ is an eigenvector of $T_\phi^{-1}T_\psi$, and
- If $b \neq 0$ then $T_\psi|\beta\rangle$ is an eigenvector of $T_\phi^{-1}T_\psi$.

Now recall that α, β are linearly independent eigenvectors of $T_\phi^{-1}T_\psi$. Note that $T_\phi^{-1}T_\psi$ is not proportional to the identity (since this would imply that ϕ is proportional to ψ) and therefore α, β are the only eigenvectors of $T_\phi^{-1}T_\psi$. Hence $T_\psi|\alpha\rangle$ is proportional to one of the states α, β , and if $b \neq 0$ then the same holds for $T_\psi|\beta\rangle$. However, since T_ψ is invertible, it cannot be the case that $T_\psi|\alpha\rangle \sim T_\psi|\beta\rangle$. Putting this together we see there are 4 subcases to consider (below we show that the first three correspond to cases 1., 2., 3., from the statement of the theorem and that the fourth does not occur):

Case (i): $T_\psi|\alpha\rangle \sim |\alpha\rangle$ and $T_\psi|\beta\rangle = c|\alpha\rangle + d|\beta\rangle$ where c, d are both non-zero.

In this case $T_\psi|\beta\rangle$ is not an eigenvector of $T_\phi^{-1}T_\psi$, which implies (by the facts established above) that $b = 0$ and thus $|\chi\rangle \sim |\alpha\rangle^{\otimes 3}$ is the only state in \mathcal{G}_3 . Likewise, $|\alpha\rangle^{\otimes n}$ is the only state in \mathcal{G}_n for $n \geq 3$ (since it is the unique n -qubit state such that any three consecutive qubits $i, i+1, i+2$ have all of their support on \mathcal{G}_3 .) This establishes that we are in case 1 from Theorem 3. Note that for any partition $[n] = ABC$ with $|B| \geq 1$ we have $G_{ABC} = |\alpha\rangle\langle\alpha|^{\otimes n} = G_{AB}G_{BC}$ and so the conditions of Lemma 5 are satisfied (with $\delta = 0$) and $H_n(\Pi)$ is gapped.

Case (ii): $T_\psi|\alpha\rangle \sim |\alpha\rangle$ and $T_\psi|\beta\rangle \sim |\beta\rangle$

In this case (by the facts established above) \mathcal{G}_2 is spanned by $|\alpha\rangle|\alpha\rangle$ and $|\beta\rangle|\beta\rangle$. This implies that \mathcal{G}_n is spanned by $|\alpha\rangle^{\otimes n}$ and $|\beta\rangle^{\otimes n}$ for all $n \geq 2$, so we are in case 2 of Theorem 3. One can easily construct an orthonormal basis and confirm that $\|G_n - |\alpha\rangle\langle\alpha|^{\otimes n} - |\beta\rangle\langle\beta|^{\otimes n}\| = O(|\langle\alpha|\beta\rangle|^n)$. Using this expression three times and the triangle inequality we get $\|G_{AB}G_{BC} - G_{ABC}\| \leq K|\langle\alpha|\beta\rangle|^{|B|}$ where K is a constant, for any partition $[n] = ABC$. Hence the conditions of Lemma 5 are satisfied (with $\delta = |\langle\alpha|\beta\rangle|$) and $H_n(\Pi)$ is gapped.

Case (iii): $T_\psi|\alpha\rangle \sim |\beta\rangle$ and $T_\psi|\beta\rangle \sim |\alpha\rangle$

In this case $\mathcal{G}_2 = \text{span}\{|\alpha\rangle|\beta\rangle, |\beta\rangle|\alpha\rangle\}$, which implies that for all $n \geq 2$, \mathcal{G}_n is spanned by product states $|\nu_1\rangle = |\alpha\rangle|\beta\rangle|\alpha\rangle \dots |\beta\rangle$ and $|\nu_2\rangle = |\beta\rangle|\alpha\rangle|\beta\rangle \dots |\alpha\rangle$ (the last tensor product factors are instead $|\alpha\rangle, |\beta\rangle$ respectively if n is odd). This shows that we are in case 3 of Theorem 3. Now constructing an orthonormal basis we see that $\|G_n - |\nu_1\rangle\langle\nu_1| - |\nu_2\rangle\langle\nu_2|\| = O(|\langle\alpha|\beta\rangle|^n)$. Letting $[n] = ABC$ and using this expression we get $\|G_{AB}G_{BC} - G_{ABC}\| \leq K|\langle\alpha|\beta\rangle|^{|B|}$ for some constant K . Hence the conditions of Lemma 5 are satisfied (with $\delta = |\langle\alpha|\beta\rangle|$) and $H_n(\Pi)$ is gapped.

Case (iv): $T_\psi|\alpha\rangle \sim |\beta\rangle$ and $T_\psi|\beta\rangle = c|\alpha\rangle + d|\beta\rangle$ where c, d are both non-zero.

In this final case $b = 0$ and the only state in \mathcal{G}_3 is $|\chi\rangle = 1 \otimes T_\psi \otimes T_\psi^2 |\alpha\rangle |\alpha\rangle |\alpha\rangle \sim |\alpha\rangle |\beta\rangle T_\psi |\beta\rangle$. Any non-zero state $\kappa \in \mathcal{G}_4$ must have its first three and last three qubits in the state χ . This implies in particular that κ is a product state. Furthermore, the second qubit of κ must be in the state β (look at the first three qubits) and also in the state α (look at the last three qubits), which is impossible. Therefore \mathcal{G}_4 is empty, which is a contradiction. So case (iv) does not occur. \square

Proof of Proposition 11 Define an orthonormal basis $\{|\hat{0}\rangle = |\alpha\rangle, |\hat{1}\rangle = |\alpha^\perp\rangle\}$. Since $|\hat{0}\rangle$ is the only eigenvector of $T_\phi^{-1}T_\psi$, in this basis we have

$$T_\phi^{-1}T_\psi = \begin{pmatrix} c & d \\ 0 & c \end{pmatrix} \quad (100)$$

for some $c, d \in \mathbb{C}$ with $c \neq 0$ (since $\det(T_\phi^{-1}T_\psi) \neq 0$).

First consider $n = 2$. We claim that $1 \otimes T_\psi |\hat{0}\rangle |\hat{0}\rangle$ and $1 \otimes T_\psi (|\hat{0}\rangle |\hat{1}\rangle + |\hat{1}\rangle |\hat{0}\rangle)$ span \mathcal{G}_2 . To see this note that these states are linearly independent and orthogonal to $|\psi\rangle \langle \psi|$. To show that they are also orthogonal to $|\phi\rangle \langle \phi|$, use the fact that $\langle \phi| \sim \langle \epsilon| 1 \otimes T_\phi^{-1}$ and Eq. (100).

We now show that our assumption that \mathcal{G}_4 (and therefore also \mathcal{G}_3) is nonempty implies $1 \otimes T_\psi \otimes T_\psi^2 |\hat{0}, \hat{0}, \hat{0}\rangle$ is in \mathcal{G}_3 . To reach a contradiction, assume $1 \otimes T_\psi \otimes T_\psi^2 |\hat{0}, \hat{0}, \hat{0}\rangle \notin \mathcal{G}_3$. By Proposition 2 any state $\omega \in \mathcal{G}_3$ satisfies $|\omega\rangle = I \otimes T_\psi \otimes T_\psi^2 |s\rangle$ for some $|s\rangle$ in the three-qubit symmetric subspace. The first two qubits of $|s\rangle$ must be supported entirely in \mathcal{G}_2 . Using the form of \mathcal{G}_2 derived above, we see that this implies $|s\rangle$ is a superposition of the symmetric Hamming weight zero and one states (with respect to the $\hat{0}, \hat{1}$ basis). Since $1 \otimes T_\psi \otimes T_\psi^2 |\hat{0}, \hat{0}, \hat{0}\rangle \notin \mathcal{G}_3$ (and since \mathcal{G}_3 is nonempty), we have shown that \mathcal{G}_3 is one-dimensional and contains a single state ω of the form

$$|\omega\rangle = 1 \otimes T_\psi \otimes T_\psi^2 (a|\hat{0}, \hat{0}, \hat{0}\rangle + b|\hat{1}, \hat{0}, \hat{0}\rangle + b|\hat{0}, \hat{1}, \hat{0}\rangle + b|\hat{0}, \hat{0}, \hat{1}\rangle)$$

where $b \neq 0$. By assumption there exists a state in \mathcal{G}_4 , which must have its last three and first three qubits each supported on \mathcal{G}_3 , i.e., it must be of the form $|\theta_1\rangle |\omega\rangle = |\omega\rangle |\theta_2\rangle$ for some single-qubit states θ_1, θ_2 . However this is impossible since ω is not a product state whenever $b \neq 0$. Having reached a contradiction we conclude $1 \otimes T_\psi \otimes T_\psi^2 |\hat{0}, \hat{0}, \hat{0}\rangle$ is in \mathcal{G}_3 .

Now

$${}_{2,3}\langle \phi| 1 \otimes T_\psi \otimes T_\psi^2 |\hat{0}, \hat{0}, \hat{0}\rangle \sim |\hat{0}\rangle (\langle \epsilon| T_\psi \otimes T_\phi^{-1} T_\psi^2 |\hat{0}, \hat{0}\rangle) = 0$$

implies that $T_\psi |\hat{0}\rangle$ is an eigenvector of $T_\phi^{-1}T_\psi$. By assumption this operator has only one eigenvector $|\hat{0}\rangle$, so $T_\psi |\hat{0}\rangle \sim |\hat{0}\rangle$. Thus $|\hat{0}\rangle$ is an eigenvector of both T_ψ and T_ϕ . Therefore, in the $\hat{0}, \hat{1}$ basis we have

$$T_\psi = \begin{pmatrix} x & y \\ 0 & z \end{pmatrix} \quad T_\phi = \begin{pmatrix} q & r \\ 0 & s \end{pmatrix} \quad T_\phi^{-1}T_\psi \sim \begin{pmatrix} sx & sy - rz \\ 0 & qz \end{pmatrix}$$

for some $x, y, z, q, r, s \in \mathbb{C}$. Comparing with Eq. (100) we see that $sx = qz \neq 0$. Now

$$|\psi\rangle = x^* |\hat{0}, \hat{1}\rangle - z^* |\hat{1}, \hat{0}\rangle + y^* |\hat{1}, \hat{1}\rangle \quad (101)$$

and

$$|\phi\rangle = q^* |\hat{0}, \hat{1}\rangle - s^* |\hat{1}, \hat{0}\rangle + r^* |\hat{1}, \hat{1}\rangle = (q^*/x^*) (x^* |\hat{0}, \hat{1}\rangle - z^* |\hat{1}, \hat{0}\rangle) + r^* |\hat{1}, \hat{1}\rangle. \quad (102)$$

Comparing Eqs. (101),(102) we see that $\text{range}(\Pi) = \text{span}\{|\phi\rangle, |\psi\rangle\} = \text{span}\{|\hat{1}, \hat{1}\rangle, |\nu\rangle\}$ where

$$|\nu\rangle = \frac{1}{\sqrt{1+|f|^2}} (|\hat{0}, \hat{1}\rangle - f|\hat{1}, \hat{0}\rangle) \quad (103)$$

and $f = z^*/x^*$ (note that x, z are both nonzero since $sx = qz \neq 0$). Moreover these states are orthonormal so $\Pi = |\hat{1}, \hat{1}\rangle\langle\hat{1}, \hat{1}| + |\nu\rangle\langle\nu|$.

By Proposition 2, a basis for the zero energy ground space of $\sum_i |\nu\rangle\langle\nu|_{i,i+1}$ is given by

$$T_\nu^{\text{all}} \sum_{z \in \{0,1\}^{\otimes n}, |z|=j} |\hat{z}\rangle, \quad j = 0 \dots n$$

where $T_\nu \sim \text{diag}(1, f)$ and $T_\nu^{\text{all}} = 1 \otimes T_\nu \otimes T_\nu^2 \otimes \dots \otimes T_\nu^{n-1}$. It is then easy to see that the only states in this space orthogonal to $\sum_i |\hat{1}, \hat{1}\rangle\langle\hat{1}, \hat{1}|_{i,i+1}$ are the basis vectors corresponding to $j = 0, 1$ and linear combinations thereof. These two states span \mathcal{G}_n for all $n \geq 2$; this shows that we are in case 4 of Theorem 3.

We now show that the system is gapped if $|f| \neq 1$. Without loss of generality we may assume $|f| < 1$; note that if $|f| > 1$ we may relabel the qubits $1, 2, 3, \dots, n$ as $n, n-1, \dots, 1$ (flipping the chain left to right) which sends $f \rightarrow f^{-1}$. Define $G_n^k = |0\rangle\langle 0|^{\otimes n} + |\chi^{k,n}\rangle\langle\chi^{k,n}|$ where

$$|\chi^{k,n}\rangle = \sqrt{1-|f|^2} \left(\sum_{i=1}^k f^{i-1} |\hat{0}^{\otimes i-1} \hat{1} \hat{0}^{\otimes n-i}\rangle \right) \quad 1 \leq k \leq n. \quad (104)$$

Noting that the ground space projector is $G_n = |0\rangle\langle 0|^{\otimes n} + \|\chi^{n,n}\|^{-2} |\chi^{n,n}\rangle\langle\chi^{n,n}|$ and that

$$\| |\chi^{n,n}\rangle\langle\chi^{n,n}| - |\chi^{k,n}\rangle\langle\chi^{k,n}| \| \leq 2 \| |\chi^{n,n}\rangle - |\chi^{k,n}\rangle \| \leq 2\sqrt{1-|f|^2} \left(\sum_{i=k+1}^{\infty} |f|^{2(i-1)} \right)^{1/2} = 2|f|^k,$$

we obtain

$$\|G_n^k - G_n\| \leq 1 - \|\chi^{n,n}\|^2 + \| |\chi^{n,n}\rangle\langle\chi^{n,n}| - |\chi^{k,n}\rangle\langle\chi^{k,n}| \| \leq |f|^{2n} + 2|f|^k \leq 3|f|^k.$$

Now let a partition $[n] = ABC$ be given with $|A| > |B|$ and $|C| = 1$. Using the above bound three times, the triangle inequality, and the facts that $\|G_n^k\| \leq 1$ and $|f|^{|A|} < |f|^{|B|}$, we obtain

$$\|G_{AB}G_{BC} - G_{ABC}\| \leq \|G_{AB}^{|A|}G_{BC}^{|B|} - G_{ABC}^{|A|}\| + 9|f|^{|B|}. \quad (105)$$

Using explicit expressions for $G_{AB}^{|A|}, G_{BC}^{|B|}$, and $G_{ABC}^{|A|}$ we see that $G_{AB}^{|A|}G_{BC}^{|B|} = G_{ABC}^{|A|}$ and the first term above is zero. This shows that the conditions of Lemma 5 are satisfied with $\delta = |f|$, and $H_n(\Pi)$ is gapped.

Finally, we establish that $H_n(\Pi)$ is gapless if $|f| = 1$. Using Eq. (103) we see that $H_n(\Pi)$ commutes with the total Hamming weight operator $\sum_{i=1}^n |\hat{1}\rangle\langle\hat{1}|_i$ and is therefore block diagonal with a block for each Hamming weight $0, \dots, n$. The spectral gap $\gamma(\Pi, n)$ is upper bounded by the smallest nonzero eigenvalue within any given block. The matrix of the block

with Hamming weight 1, in the orthonormal basis $\{|e_i\rangle = f^{i-1}|\hat{0}^{i-1} \hat{1} \hat{0}^{n-i}\rangle : i = 1, \dots, n\}$, is given by

$$\langle e_i | H_n(\Pi) | e_j \rangle = \begin{cases} 1, & \text{if } i = j = 1 \text{ or } i = j = n \\ 2, & \text{if } 2 \leq i = j \leq n - 1, \\ -1, & \text{if } |i - j| = 1 \\ 0, & \text{otherwise.} \end{cases}$$

This is the Laplacian matrix of the path graph of length n , and its spectrum is known. In particular, its smallest nonzero eigenvalue is $2(1 - \cos(\pi/n))$, which upper bounds $\gamma(\Pi, n)$ if $|f| = 1$. \square