Gapless phases of frustration-free spin 1/2 chains

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Abstract

We consider a family of frustration free qubit chains with nearest interactions and explore conditions under which the system is gapless. In particular, for an arbitrary 2-qubit state ψ, we consider an n-qubit chain quantum system with Hamiltonian $H_n(\psi)$ defined as the sum of rank-1 projectors onto ψ applied to consecutive pairs of qubits. The main result is that the spectral gap will be upper bounded by $1/(n-1)$ if the eigenvalues of a certain 2×2 matrix has the same non-zero absolute value. On the way to the final result, we explore the ground state structure of $H_n(\psi)$ with open boundary condition as well as the one of $H_n^\circ(\psi)$ with periodic boundary condition. Moreover, since that certain 2×2 matrix plays an important role, we also list and prove its structural properties.

Contents

1 Introduction

Whether a quantum spin chain is gapped or gapless in thermodynamic limit is crucial property that we need to study. In this paper, we will provide a sufficient condition that makes the quantum spin chain with nearest neighbor interaction gapless. My exposition is based on the paper [1] by Bravyi and Gosset. Let

$\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be a normalized two-qubit state, consider an n-qubit chain with open boundary condition and the Hamiltonian defined by

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

The Hamiltonian $H_n(\psi)$ is a sum of rank-1 projections onto the state ψ, and $|\psi\rangle\langle\psi|_{i,i+1}$ is an abbreviation for the operator $\mathbb{1} \otimes \cdots \otimes |\psi\rangle\langle\psi| \otimes \cdots \otimes \mathbb{1}$ which acts nontrivially on qubit $i, i+1$. With respect to the Hamiltonian in equation (1), we say it is frustration-free if the smallest eigenvalue of the Hamiltonian is 0, in other words, the ground state energy is 0. As a result in section 3.1, we will see that this quantum spin chain is always frustration-free, and for almost all choices of ψ, the ground space has dimension $n+1$.

The spectral gap in a frustration-free model is defined to be the smallest positive eigenvalue of the Hamiltonian, in other words, it is the one separating the ground states and excited states. To study the (spectral) gap of this type of Hamiltonian, we define the following 2 by 2 matrix

$$T_\psi = \begin{pmatrix} \langle\psi|01\rangle & \langle\psi|11\rangle \\ -\langle\psi|00\rangle & -\langle\psi|10\rangle \end{pmatrix},$$

where $|0\rangle, |1\rangle$ are the standard basis of $\mathbb{C}^2$. In this paper, we will state the necessary condition of the eigenvalues of the matrix T_ψ which guarantees that the Hamiltonian $H_n(\psi)$ gapless. In particular, the following is the main theorem.

Theorem. *Let $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ be an arbitrary state. If the eigenvalues of T_ψ have the same non-zero absolute value, then the spectral gap is at most $1/(n-1)$.*

To prove this theorem we not only need to explore the ground space structure of $H_n(\psi)$ for open boundary conditions, but also need to understand the ground space structure of $H_n^\circ(\psi)$ for periodic boundary conditions. We can build an orthonormal basis for ground space of $H_n(\psi)$, but are not able to do so for the ground space of $H_n^\circ(\psi)$. But anyhow, we still can know how large the space is, namely, we will show, in section 3.2, that depending on the choice of ψ, the ground space of $H_n^\circ(\psi)$ has dimension $n+1$ or 2.

Let us begin with a brief example, let us consider the case that ψ is proportional to the singlet, i.e., the antisymmetric two-qubit state $|\epsilon\rangle := |01\rangle - |10\rangle$. The claim is that the Hamiltonian $H_n(\psi)$ coincides with the well-known ferromagnetic Heisenberg chain, whose Hamiltonian is given by

$$H^{\text{Heisen}} = -\frac{1}{4}\sum_{i=1}^{n-1} \hat{\sigma}_i \cdot \hat{\sigma}_{i+1},$$

where $\hat{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$, σ^i represents the usual Pauli matrices for $i \in \{x, y, z\}$. The ground space of the ferromagnetic Heisenberg chain is spanned by the symmetric states, and it is not hard to find out that the symmetric states are also ground states of $H_n(\epsilon)$ since the state ϵ is orthogonal to the symmetric states. The following proposition points out the details of the connection between $H_n(\epsilon)$ and H^{Heisen}.

Proposition 1. *There exists a unique state ξ up to a phase such that for $a > 0, b \in \mathbb{R}$,*

$$-(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z) = a|\xi\rangle\langle\xi| + b\mathbb{1}.$$

Proof. The LHS can be expanded as the following

$$
\begin{aligned}
-(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z) &= -\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \\
&= \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & -2 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.
\end{aligned}
$$

On the other hand, suppose $|\xi\rangle == \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$, then the RHS becomes

$$
a|\xi\rangle\langle\xi| + b\mathbb{1} = \begin{pmatrix} ax_1^2 + b & ax_1x_2 & ax_1x_3 & ax_1x_4 \\ ax_2x_1 & ax_2^2 + b & ax_2x_3 & ax_2x_4 \\ ax_3x_1 & ax_3x_2 & ax_3^2 + b & ax_3x_4 \\ ax_4x_1 & ax_4x_2 & ax_4x_3 & ax_4^2 + b \end{pmatrix}.
$$

Demanding the equality, we need

$$
\begin{cases} x_1x_4 = x_1x_3 = x_1x_2 = x_3x_4 = 0, \\ ax_2x_3 = -2, \\ ax_1^2 + b = 1. \end{cases}
$$

This implies $\begin{cases} x_1 = x_4 = 0, \\ b = -1. \end{cases}$ Therefore,

$$
\begin{cases} ax_2^2 - 1 = 1, \\ ax_2x_3 = -2, \\ ax_3^2 - 1 = 1, \end{cases}
$$

implying that $\dfrac{x_3}{x_2} = -1$. In other words, $|\xi\rangle$ is proportional to the singlet $|\epsilon\rangle$. □

Using this proposition, one can write

$$
H^{\text{Heisen}} = a \sum_{i=1}^{n-1} |\xi\rangle\langle\xi|_{i,i+1} + b\mathbb{1},
$$

for some $a > 0, b \in \mathbb{R}$. It follows that the $H_n(\epsilon)$ coincides the ferromagnetic Heisenberg chain up to a overall energy shift.

We will provide basic definitions in the next section, as well as the proof of some auxiliary results. Most of the proofs are not required to understand the final proof, but it is important to know the statements. In section 3, we will state and prove the properties of the ground space of $H_n(\psi)$ and $H_n^\circ(\psi)$, and in section 4 these properties will become building blocks of the proof of the main theorem.

2 Auxiliary results

In this section we state the basic definitions and prove some necessary propositions for later use, but the proposition themselves do not depend on the model we study.

In our quantum spin chain model, each quantum spin is associated with a complex vector space. We only consider the spin-1/2 qubit, so the complex vector space associated is two dimensional, i.e., isomorphic to $\mathbb{C}^2$. When multiple spins are prepared in the system, the natural way to describe them is through the tensor product space. The following is a brief discussion on the tensor product of vector spaces.

Definition 1. Let V, W be two vector spaces of dimension m and n respectively. Then the *tensor product* of V and W, denoted $V \otimes W$, is an mn dimensional vector space. If $\{|v_1\rangle, \ldots, |v_m\rangle\}$ and $\{|w_1\rangle, \ldots, |w_n\rangle\}$ are bases for V and W, then $\{|v_i\rangle \otimes |w_j\rangle\}$ is a basis for $V \otimes W$. We often abbreviate them as $|vw\rangle$ for the tensor product $|v\rangle \otimes |w\rangle$. These tensor products satisfies the following basic properties

1. For scalar z in the filed and $|v\rangle \in V$, $|w\rangle \in W$,

$$z(|v\rangle \otimes |w\rangle) = (z|v\rangle) \otimes |w\rangle = |v\rangle \otimes (z|w\rangle).$$

2. For $|v_1\rangle, |v_2\rangle \in V$, $|w\rangle \in W$,

$$(|v_1\rangle + |v_2\rangle) \otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle.$$

3. For $|v\rangle \in V$, $|w_1\rangle, |w_2\rangle \in W$,

$$|v\rangle \otimes (|w_1\rangle + |w_2\rangle) = |v\rangle \otimes |w_1\rangle + |v\rangle \otimes |w_2\rangle.$$

Definition 2. Let $A : V \to V'$, $B : W \to W'$ be two linear maps between finite dimensional vector spaces. The natural way to define the tensor product of two linear maps is the following, let $|v\rangle \in V, |w\rangle \in W$ be two vectors, then

$$(A \otimes B)(|v\rangle \otimes |w\rangle) := A|v\rangle \otimes B|w\rangle,$$

and extend linearly. If one chooses bases for vector spaces V and W, a matrix representation known as *Kronecker product* is defined as

$$A \otimes B := \begin{bmatrix} A_{11}B & A_{12}B & \cdots & A_{1n}B \\ A_{21}B & A_{22}B & \cdots & A_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1}B & A_{m2}B & \cdots & A_{mn}B \end{bmatrix},$$

where A is an m by n matrix and B is a p by q matrix, and $A \otimes B$ is an mp by nq matrix.

As an example, the tensor product of vectors $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ and $\begin{bmatrix} 3 \\ 4 \end{bmatrix}$ is the vector

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 1 \times 3 \\ 1 \times 4 \\ 2 \times 3 \\ 2 \times 4 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ 6 \\ 8 \end{bmatrix}.$$

The following is a formal discussion of vector norm and operator norm in a Hilbert space.

Definition 3. An *inner product* on a complex vector space V is a map

$$\langle \cdot | \cdot \rangle : V \times V \to \mathbb{C}$$

such that for all $x, y, z \in V$ and $\lambda, \mu \in \mathbb{C}$:

1. $\langle x | \lambda y + \mu z \rangle = \lambda \langle x | y \rangle + \mu \langle x | z \rangle$ (linear in the second argument);
2. $\langle y | x \rangle = \overline{\langle x | y \rangle}$ (Hermitian symmetric);
3. $\langle x | x \rangle \geq 0$ (nonnegative);
4. $\langle x | x \rangle = 0$ if and only if $x = 0$ (positive definite).

The vector norm induced by inner product on V is defined by

$$\|x\| = \sqrt{\langle x | x \rangle}.$$

Definition 4. Let $A : V \to V'$ be a linear map between two normed vector spaces. A is *bounded* if there is a constant $M \geq 0$ such that

$$\|Ax\| \leq M\|A\| \quad \text{for all } x \in V.$$

If A is a bounded operator, then we define the *operator norm* $\|A\|$ of A by

$$\|A\| = \inf\{M : \|Ax\| \leq M\|x\| \text{ for all } x \in V\}.$$

Equivalent expressions for $\|A\|$ are:

$$\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{x}; \quad \|A\| = \sup_{\|x\| \leq 1} \|Ax\|; \quad \|A\| = \sup_{\|x\| = 1} \|Ax\|.$$

There is an equivalent expression for the vector norm, which is stated in the following proposition. This property will be useful in the proof of Lemma 1.

Proposition 2. *Let X be an inner product space. If $x \in X$, then*

$$\|x\| = \sup_{y \in X, \|y\| = 1} |\langle y, x \rangle|.$$

Proof. Let $y \in X$ such that $\|y\| = 1$. Then by Cauchy-Schwarz, one obtains

$$|\langle y, x\rangle| \leq \|y\|\|x\| \leq \|x\|.$$

On the other hand, let $y = \frac{x}{\|x\|}$, then

$$\|x\| \geq |\langle y, x\rangle| = \frac{\langle x, x\rangle}{\|x\|} = \|x\|,$$

then we complete the proof. □

The following proposition is an important inequality that we shall use in the proof of the main theorem in section 4.2.

Proposition 3. *For a real number x, $|e^{\mathrm{i}x} - 1| \leq |x|$.*

Proof. One can write x as an integral, i.e. $x = \int_0^x 1dy$. On the other hand, we note that $e^{ix} - 1 = \int_0^x ie^{iy}dy$. So,

$$\begin{aligned} |e^{ix} - 1| &\leq \int_0^x |ie^{iy}|dy \\ &\leq \int_0^x |1|dy \\ &= |x|, \end{aligned}$$

as required. □

Since the main theorem is about the smallest eigenvalue of a linear map, we would like to give an official name to the collection of eigenvalues of a linear map.

Definition 5. Let $A : V \to V$ be a linear map between two finite dimensional vector spaces, λ is an eigenvalue of A if there exists a nonzero vector $v \in V$ such that $Av = \lambda v$. The *spectrum* of A, denoted as $\sigma(A)$, is a set of eigenvalues of A.

One nice property of spectrum of a linear map in quantum mechanics is that it is invariant under unitary transformation, and any evolution of quantum system is described by a unitary transformations[5]. The details are in the following proposition.

Proposition 4. *Let $H : V \to V$ be a linear operator on a finite dimensional complex vector space V. Then for any unitary operator U on V,*

$$\sigma(T) = \sigma(U^*TU).$$

I.e., the spectrum is invariant under conjugation.

Proof. It suffices to show that the characteristic polynomial of T and U^*TU are identical. So,

$$\begin{aligned} \det(U^*TU - x\mathbb{1}) &= \det(U^*(T - x\mathbb{1})U) \\ &= \det U^* \cdot \det(T - x\mathbb{1}) \cdot \det U \\ &= \det U^* \cdot \det U \cdot \det(T - x\mathbb{1}) \\ &= \det(T - x\mathbb{1}) \end{aligned}$$

as required. $\square$

Definition 6. Let V be an inner product space, and $A : V \to V$ be a linear map, A is a *positive operator* if

$$\langle Av, v\rangle \geq 0$$

for all $v \in V$. Moreover, if $B : V \to V$ is another linear map, we say $A \geq B$ if $A - B$ is positive.

The spectral theorem is the most useful tool in the study of operators on inner product space. We state the theorem in this paper, the proof can be found in [6].

Theorem (Complex spectral theorem)**.** *Let V be a complex vector space, $A : V \to V$ be a linear transformation. Then the following are equivalent.*

1. $A^*A = AA^*$, where A^* is the adjoint of A .
2. A has a diagonal matrix with respect to some orthonormal basis of V.
3. V has an orthonormal basis consisting of eigenvectors of A.

In particular, let $\lambda \in \sigma(A)$ be an eigenvalue, and V_λ be the invariant subspace of A (also known as the eigenspace of λ), and let P_λ be the orthogonal projection onto V_λ. Then

$$\sum_{\lambda\in\sigma(A)} P_\lambda = \mathbb{1}, \quad \sum_{\lambda\in\sigma(A)} \lambda P_\lambda = A.$$

Utilizing the spectral theorem, we prove the following two propositions with similar strategies. They play almost the same role in the proof of an important lemma.

Proposition 5. *Let $A : V \to V$ be a positive operator. If λ_1 is the smallest positive eigenvalue of A, then*

$$A^2 \geq \lambda_1 A.$$

Proof. Using spectral decomposition, we get $A = \sum_{\lambda\in\sigma(A)} \lambda P_\lambda$. So,

$$A^2 = \sum_{\lambda\in\sigma(A)} \lambda^2 P_\lambda \geq \sum_{\lambda\in\sigma(A)} \lambda_1(\lambda P_\lambda) = \lambda_1 A. \quad \square$$

Proposition 6. *Let $A : V \to V$ be a positive operator. If $\sigma(A) = \{0 \leq \lambda_1 \leq \cdots \leq \lambda_n\}$, and γ is a non-negative number such that*

$$A^2 \geq \gamma A.$$

Then $\lambda_1 \geq \gamma$.

Proof. Using spectral decomposition again, we get $A = \sum_{\lambda_i\in\sigma(A)} \lambda_i P_{\lambda_i}$. Then,

$$\lambda_i^2 \geq \gamma\lambda_i$$

for each i, in particular, $\lambda_1 \geq \gamma$. $\square$

The following theorem is crucial in the proof of proposition 12, the proof can be found in [2].

Theorem (Weyl's Perturbation Theorem). *Let A and B be Hermitian matrices with eigenvalues $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$ and $\lambda_1(B) \geq \cdots \geq \lambda_n(B)$, respectively. Then*

$$\max_j |\lambda_j(A) - \lambda_j(B)| \leq \|A - B\|.$$

The last auxiliary result in this section is Knabe's lemma. This lemma was originally proposed as a technique for proving that the periodic chain is gapped in the thermodynamic limit [1]. Let $\gamma(\psi, n)$ and $\gamma^\circ(\psi, n)$ denote the smallest non-zero eigenvalue of Hamiltonian $H_n(\psi)$ and $H_n^\circ(\psi)$, respectively. In the proof of main theorem we need Knabe's result to connect two different types of spectral gap, $\gamma(\psi, n)$ and $\gamma^\circ(\psi, n)$. For self-consistency, we prove this lemma here.

Lemma (Knabe's Lemma). *[4] For all $m \geq n \geq 2$,*

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

We provide an informal proof of general version of this type of result. Consider a frustration-free N-qubit chain with periodic boundary condition and the Hamiltonian H is given by

$$H = \sum_{i=1}^{N} P_{i,i+1},$$

where $P_{i,i+1}$ is a projection operator acting on two consecutive qubits. Let $n < N$, consider the subsystem which consists of n consecutive qubits that starts at the ith qubit with the Hamiltonian

$$h_{n,i} = \sum_{j=i}^{i+n-2} P_{j,j+1},$$

where $P_{j,j+1} = P_{j+N,j+N+1}$. We will try to get an inequality of the form

$$H^2 \geq \alpha \sum_{i=1}^{N} h_{n,i}^2 - \beta H \tag{2}$$

by adjusting the coefficients α and β. To achieve this, we note that there are three types of terms in H^2,

$$P_{i,i+1}^2 = P_{i,i+1}, \quad P_{i,i+1}P_{i+1,i+2} + P_{i+1,i+2}P_{i,i+1}, \quad 2P_{i,i+1}P_{j,j+1}\ (j \geq i+2).$$

Fix $m \in \{1, \ldots, N\}$, we shall count how many times the term $P_{m,m+1}P_{m+1,m+2}$ will appear in $\sum_{i=1}^{N} h_{n,i}^2$, but this is equivalent to find out how many ways of choosing n consecutive qubits out of N qubits such that it contains the sites $m, m+1, m+2$. It turns out that there are $n-2$ ways. Therefore, we choose $\alpha = 1/(n-2)$. On the other hand, each term of type 1 appears $n-1$ times in $\sum_{i=1}^{N} h_{n,i}^2$, and there is one more copy in H, so choose $\beta = 1/(n-2)$.

It remains to show that the choice of α and β also gives the inequality of type 3 terms. Fix $x, y \in \{1, \ldots, N\}$ and $y \geq x+2$, we look at the term $P_{x,x+1}P_{y,y+1}$. Regardless the choice of n, when $y = x+2$, it will give the largest possible multiplicity of $P_{x,x+1}P_{y,y+1}$, and the multiplicity is $n-3$. Since the coefficient α is greater than $n-3$, i.e., $(n-3)/(n-1) < 1$, the type 3 terms is less in the LHS. So we showed that the inequality is true with good choice of coefficients.

Since $h_{n,i}$ is Hermitian, we know that $h_{n,i}^2$ is positive by the following inspection:

$$\langle h_{n,i}^2 \psi | \psi \rangle = \langle h_{n,i} \psi | h_{n,i} \psi \rangle \geq 0$$

for any state ψ. Denote the smallest eigenvalue (the energy gap) of $h_{n,i}$ as $\gamma(n)$, directly using Proposition 5, one gets

$$h_{n,i}^2 \geq \gamma(n) h_{n,i}. \tag{3}$$

Now, using equation (3), equation (2) becomes

$$\begin{aligned} H^2 &\geq \frac{1}{n-2} \sum_{i=1}^{N} h_{n,i}^2 - \frac{1}{n-2} H \\ &\geq \gamma(n) \frac{1}{n-2} \sum_{i=1}^{N} h_{n,i} - \frac{1}{n-2} H \\ &= \gamma(n) \frac{n-1}{n-2} H - \frac{1}{n-2} H \\ &= \frac{n-1}{n-2} \left(\gamma(n) - \frac{1}{n-1} \right) H. \end{aligned}$$

Using the Proposition 6, one gets

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

it follows that Knabe's lemma is just the case that we restrict to the specific family of Hamiltonian $H_n(\psi)$.

3 Ground space structure

3.1 Open boundary conditions

We first consider the Hamiltonian $H_n(\psi)$ for open boundary condition. In this section we will build ground space explicitly for $H_n(\psi)$, and we will show that the dimension of the ground space will (almost) not depend on the choice of the state ψ.

3.1.1 Product state

Let us consider the simple case that $\psi = \psi_1 \otimes \psi_2$ is a product state first. According to the Proposition 4, the spectrum is invariant under the unitary transformation. Therefore, we are free to choose any basis to work with. In order to have a nice illustration of what are the ground states, we work in a basis such that we can write

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

where

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

In particular, choose $|1\rangle = \dfrac{|\psi_1\rangle}{\|\psi_1\|}$, and choose $|0\rangle$ that is orthogonal to $|1\rangle$ and norm 1. This guarantees that there exists coefficients $c, s \in \mathbb{C}$ such that $\psi_2 = s^*|0\rangle - c^*|1\rangle$. Let us look at an example with $n = 3$ first. In this case, the Hamiltonian is

$$H_3(\psi) = |1v^\perp\rangle\langle 1v^\perp| \otimes \mathbb{1} + \mathbb{1} \otimes |1v^\perp\rangle\langle 1v^\perp|.$$

Consider the set of states $\{|vvv\rangle, |v^\perp vv\rangle, |0v^\perp v\rangle, |00v^\perp\rangle\}$, by direct inspection, we know they are pairwise orthogonal ground states, the following is part of the calculation

$$\langle v^\perp vv|0v^\perp v\rangle = \langle v^\perp|0\rangle\langle v|v^\perp\rangle\langle v|v\rangle = 0,$$

and

$$\begin{aligned}\Big(|1v^\perp\rangle\langle 1v^\perp| \otimes \mathbb{1} + \mathbb{1} \otimes |1v^\perp\rangle\langle 1v^\perp|\Big)|0v^\perp v\rangle &= |1v^\perp\rangle\langle 1v^\perp|0v^\perp\rangle \otimes |v\rangle + |0\rangle \otimes |1v^\perp\rangle\langle 1v^\perp|v^\perp v\rangle \\ &= 0.\end{aligned}$$

In general, define $|g_i\rangle = |0^{i-1}v^\perp v^{n-i}\rangle$ for $i = 1, \ldots, n$, and $|g_0\rangle = |v\rangle^{\otimes n}$. Then $\mathcal{G} = \{|g_i\rangle\}_{i=0}^n$ is a set of ground states of $H_n(\psi)$ that are pairwise orthogonal. The following proposition shows that $\mathcal{G}$ is a basis.

Proposition 7. *Suppose $s \neq 0$. Then the states $g_0, \ldots, g_n$ form an orthonormal basis for the ground space of $H_n(\psi)$.*

Proof. Since $\mathcal{G}$ consists pairwise orthogonal ground states of $H_n(\psi)$, it suffices to show that the ground space has at most $n+1$ dimension. There exists a standard basis of Hilbert space of n qubits, in particular, define strings $x = (x_1, \ldots, x_n), y = (y_1, \ldots, y_n)$. Then the states $\{|x\rangle\},\ x \in \{0,1\}^n$ forms a basis of Hilbert space of n qubits, also known as the standard computational basis. Since $s \neq 0$, $|0\rangle$ and $|v\rangle$are linearly independent, so the states $\{|y\rangle\},\ y \in \{0, v\}^n$ also forms a basis.

Let $|\phi\rangle = \sum_y a_y|y\rangle$ be a ground state, then calculation shows

$$\Big(|\psi\rangle\langle\psi|_{i,i+1}\Big)|\phi\rangle = s^2 \sum_{y:(y_i,y_{i+1})=(v,0)} a_y|y_1, \ldots, y_{i-1}, y_{i+2}, \ldots, y_n\rangle.$$

Since $|\phi\rangle$ is a ground state, this forces the coefficients of basis states having consecutive pair $(v, 0)$ in it to be 0, in other words, $|\phi\rangle$ is in the span of states $|0^i v^{n-i}\rangle$, where $i = 0, \ldots, n$. This shows that the dimension of ground space of $H_n(\psi)$ is at most $n+1$. □

3.1.2 Entangled state

For another case that when ψ is entangled, we are not able to construct such an orthonormal basis as before, but at least we still can build the ground space of $H_n(\psi)$, and the matrix T_ψ is crucial. Let us first prove some properties of T_ψ.

Proposition 8. *If $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ is an entangled state, then* $\det T_\psi \neq 0$.

Proof. We prove the contrapositive. Suppose that $\det T_\psi = 0$, let $\psi = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$, for $a, b, c, d \in \mathbb{C}$. Then $\det T_\psi = 0$

gives that $ad - bc = 0$, in other words,

$$\frac{a}{b} = \frac{c}{d} = k,$$

for some ration $k \in \mathbb{C}$. It follows that $\psi = \begin{pmatrix} b \\ d \end{pmatrix} \otimes \begin{pmatrix} k \\ 1 \end{pmatrix}$, which is a product. □

Proposition 9. *For any $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$,*

$$\langle\psi|(\mathbb{1} \otimes T_\psi) = \det(T_\psi)\langle\epsilon|, \tag{4}$$

where $|\epsilon\rangle = |01\rangle - |10\rangle$is the antisymmetric state of two qubits.

Proof. Let $\psi = \begin{pmatrix} \psi_{00} \\ \psi_{01} \\ \psi_{10} \\ \psi_{11} \end{pmatrix}$. Paring left hand side with $|\epsilon\rangle$, we obtain

$$\langle\psi|(\mathbb{1} \otimes T_\psi)|\epsilon\rangle = \begin{pmatrix} \overline{\psi_{00}} & \overline{\psi_{01}} & \overline{\psi_{10}} & \overline{\psi_{11}} \end{pmatrix} \begin{pmatrix} \langle\psi|01\rangle & \langle\psi|11\rangle & & \\ -\langle\psi|00\rangle & -\langle\psi|10\rangle & & \\ & & \langle\psi|01\rangle & \langle\psi|11\rangle \\ & & -\langle\psi|00\rangle & -\langle\psi|10\rangle \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}.$$

Calculation gives us that $\langle\psi|(\mathbb{1} \otimes T_\psi)|\epsilon\rangle = 2\det T_\psi$. □

With equation (4) in hand, we are able to prove the fact about the ground state space of the smallest system $H_2(\psi)$.

Proposition 10. *The ground space of $H_2(\psi) = |\psi\rangle\langle\psi|$ is the image of the 2-qubit symmetric subspace under the map $\mathbb{1} \otimes T_\psi$. In other words,*

$$\ker H_2(\psi) = (\mathbb{1} \otimes T_\psi)(V_{\text{sym}}),$$

where $V_{\text{sym}} = \mathbb{C}\text{-span}(|00\rangle, |11\rangle, |01\rangle + |10\rangle)$.

Proof. Let us prove the inclusion $(\mathbb{1} \otimes T_\psi)(V_{\text{sym}}) \subseteq \ker H_2(\psi)$ first. Let $|\phi\rangle \in V_{\text{sym}}$. Using equation (4), we obtain

$$\langle\psi|(\mathbb{1} \otimes T_\psi)|\phi\rangle = \det T_\psi \langle\epsilon|\phi\rangle = 0,$$

showing that $(\mathbb{1} \otimes T_\psi)|\phi\rangle$ is a ground state. The inclusion $\ker H_2(\psi) \subseteq (\mathbb{1} \otimes T_\psi)(V_{\text{sym}})$ can be shown by using dimensionality to argue. Note that $|\psi\rangle\langle\psi|$ is rank-1 projector, then $\dim(\ker H_2) = 3$. Since $\det T_\psi \neq 0$ (note that we are assuming ψ is entangled), we know $\det(\mathbb{1} \otimes T_\psi) \neq 0$. Therefore, $\dim(\mathbb{1} \otimes T_\psi(V_{\text{sym}})) = 3$, and hence $\ker H_2(\psi) = (\mathbb{1} \otimes T_\psi)(V_{\text{sym}})$. □

The above proposition reveals the structure of the 2-qubit chain, one can generalize this local behavior to the n-qubit chain by defining

$$T_\psi^{\text{all}} = \mathbb{1} \otimes T_\psi \otimes T_\psi^2 \otimes \cdots \otimes T_\psi^{n-1},$$

where T_ψ^k is kth power of T_ψ. The motivation of such definition is when we locally look at this operator, say $k, k+1$ sites, one can rewrite the operator as $T_\psi^k \otimes T_\psi^{k+1} = (T_\psi^k \otimes T_\psi^k)(\mathbb{1} \otimes T_\psi)$. This allows us to use equation (4) to proceed the derivation. Before moving to the ground state structure of the general $H_n(\psi)$ ($n > 2$) case, we need the following property of the antisymmetric state and a fact about the determinant of tensor product of two matrices.

Proposition 11. *Let A be an operator on $\mathbb{C}^2$, then $|\epsilon\rangle$ is an eigenvector of $A \otimes A$ with eigenvalue* $\det(A)$.

Proof. This can be shown by direct calculation. Let $A = (a_{ij})$, where $i, j = 1, 2$, then

$$A \otimes A|\epsilon\rangle = \begin{pmatrix} a_{11}a_{11} & a_{11}a_{12} & a_{12}a_{11} & a_{12}a_{12} \\ a_{11}a_{21} & a_{11}a_{22} & a_{12}a_{21} & a_{12}a_{22} \\ a_{21}a_{11} & a_{21}a_{12} & a_{22}a_{11} & a_{22}a_{12} \\ a_{21}a_{21} & a_{21}a_{22} & a_{22}a_{21} & a_{22}a_{22} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = (a_{11}a_{22} - a_{12}a_{21}) \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \det A|\epsilon\rangle.$$

Another way to see that $|\epsilon\rangle$ is an eigenvector of $A \otimes A$ is using the swap operator S defined as $S(u \otimes v) := v \otimes u$. It follows that $S|\epsilon\rangle = -|\epsilon\rangle$. Noting that the commutator $[A \otimes A, S] = 0$, together with the fact that $\dim(V_{\text{antisym}}) = 1$, we know that $|\epsilon\rangle$ is an eigenvector of $A \otimes A$. □

Fact. *Let $A \in \mathrm{Mat}_n(\mathbb{C})$, $B \in \mathrm{Mat}_m(\mathbb{C})$, then* $\det(A \otimes B) = (\det A)^m (\det B)^n$.

One can see this fact by direct inspection

$$\det(A \otimes B) = \det(A \otimes \mathbb{1} \cdot \mathbb{1} \otimes B) = \det(A \otimes \mathbb{1}) \det(\mathbb{1} \otimes B) = (\det A)^m (\det B)^n.$$

Then we are able to prove the final result in this section, i.e., the dimension of ground state of $H_n(\psi)$ with ψ is an entangled state is $n + 1$.

Theorem 1. *Suppose* $\det(T_\psi) \neq 0$, *then the ground state of $H_n(\psi)$ is the image of the n-qubit symmetric subspace under the linear map T_ψ^{all}.*

Proof. In this proof we write T to denote $T_\psi$for simplicity. We want to show that $\ker H_n(\psi) = T^{\text{all}}(V_{\text{sym}})$, where V_{sym} is the symmetric subspace of n-qubit. The key input here is equation (4). Consider the expression

$$(T^{\text{all}})^* |\psi\rangle\langle\psi|_{j,j+1} (T^{\text{all}}) \tag{5}$$

for some j. To simplify this, we only need to take a close look at sites j and $j + 1$, since $|\psi\rangle\langle\psi|_{j,j+1} = \mathbb{1} \otimes \cdots \otimes |\psi\rangle\langle\psi| \otimes \cdots \otimes \mathbb{1}$, and other sites are simply positive operators in the form of $T^{k*}T^k$, for some k. Using equation (4) and Proposition 11, we get

$$\begin{aligned} (T^j \otimes T^{j+1})^* |\psi\rangle\langle\psi| (T^j \otimes T^{j+1}) &= (T^j \otimes T^j)^* (\mathbb{1} \otimes T)^* |\psi\rangle\langle\psi| (\mathbb{1} \otimes T)(T^j \otimes T^j) \\ &= |\det T_\psi|^2 \cdot (T^j \otimes T^j)^* |\epsilon\rangle\langle\epsilon| (T^j \otimes T^j) \\ &= (|\det T_\psi|^2 |\det T^j|) \cdot |\epsilon\rangle\langle\epsilon|. \end{aligned}$$

Therefore, one can rewrite equation (5) as

$$(T^{\text{all}})^* |\psi\rangle\langle\psi|_{j,j+1} (T^{\text{all}}) = |\epsilon\rangle\langle\epsilon|_{j,j+1} \otimes B_j, \tag{6}$$

for some positive operator B_j that only act on all n qubits except j and $j + 1$. Using equation (6) one can write

$$
\begin{aligned}
(T^{\text{all}})^* H_n(\psi)(T^{\text{all}}) &= \sum_{j=1}^{n-1} (T^{\text{all}})^* |\psi\rangle\langle\psi|_{j,j+1} (T^{\text{all}}) \\
&= \sum_{j=1}^{n-1} |\epsilon\rangle\langle\epsilon|_{j,j+1} \otimes B_j,
\end{aligned}
$$

from there we immediately see that $\ker\left((T^{\text{all}})^* H_n(\psi)(T^{\text{all}})\right) = V_{\text{sym}}$.

Using the above fact, we know that $\det(T^{\text{all}}) \neq 0$. Now, it suffices to show that

$$
\ker H_n = T^{\text{all}}\left[\ker\left((T^{\text{all}})^* H_n(\psi)(T^{\text{all}})\right)\right].
$$

Let $|\phi\rangle$ be a state in the right hand side, let $|\sigma\rangle \in \ker\left((T^{\text{all}})^* H_n(\psi)(T^{\text{all}})\right)$ such that $T^{\text{all}}|\sigma\rangle = |\phi\rangle$. Then

$$
0 = (T^{\text{all}})^* H_n(\psi)(T^{\text{all}})|\sigma\rangle = (T^{\text{all}})^* H_n(\psi)|\phi\rangle.
$$

Since $T^{\text{all}*}$ is invertible, we deduce that $|\phi\rangle \in \ker H_n$, namely, $T^{\text{all}}\left[\ker\left((T^{\text{all}})^* H_n(\psi)(T^{\text{all}})\right)\right] \subseteq \ker H_n$. Still, since T^{all} is full-rank, the dimension in both sides are equal, and we complete our proof. □

Combining Proposition 7 and Theorem 1, together with the fact that the symmetric subspace of n-qubit chain is $n+1$ dimensional, we conclude that for almost all choices of ψ (except when $\psi = |1\rangle \otimes |v^{\perp}\rangle$ is a product, $|v\rangle = c|0\rangle + s|1\rangle$, and $s = 0$), the ground space of $H_n(\psi)$ is $n+1$ dimensional.

3.2 Periodic boundary conditions

Consider the Hamiltonian $H_n^{\circ}(\psi)$ for the chain with periodic boundary condition. Here we only consider the case that ψ is entangled, and according to Proposition 8, $\det(T_\psi) \neq 0$. Compare with the open boundary condition $H_n(\psi)$, we will see that the ground space of $H_n^{\circ}(\psi)$ is not always $n+1$ dimensional. Depending on the choice of the state ψ, it might have smaller ground state.

The symbol $\sim$ is shorthand for proportional to.

Theorem 2. *Suppose $T_\psi^n \sim \mathbb{1}$. 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. As what we did in the proof of Theorem 1, we note that $H_n^{\circ}(\psi)$ has the same rank as

$$
(T_\psi^{\text{all}})^* H_n^{o} T_\psi^{\text{all}} = (T_\psi^{\text{all}})^* H_n T_\psi^{\text{all}} + (T_\psi^{\text{all}})^* |\psi\rangle\langle\psi|_{n,1} T_\psi^{\text{all}}. \tag{7}
$$

By Theorem 1, the kernel of the first term in the RHS is the symmetric subspace V_{sym}.

If $T_\psi^n \sim \mathbb{1}$, using equation (4) and Proposition 11, we observe that

$$
\begin{aligned}
(T_\psi^{n-1} \otimes \mathbb{1})^* |\psi\rangle\langle\psi|_{n,1} (T_\psi^{n-1} \otimes \mathbb{1}) &= (T_\psi^{n-1} \otimes T_\psi^{n-1})^* (\mathbb{1} \otimes T_\psi)^* |\psi\rangle\langle\psi|_{n,1} (\mathbb{1} \otimes T_\psi)(T_\psi^{n-1} \otimes T_\psi^{n-1}) \\
&= |\epsilon\rangle\langle\epsilon| \otimes B_n,
\end{aligned}
$$

for some positive operator B_n. It follows that the kernel of equation (7) is still the symmetric subspace with dimension $n+1$.

Now, suppose T_ψ^n is not proportional to the identity. To write down the specific basis of the ground space, we need to know whether the matrix T_ψ^n has two linearly independent eigenvectors or not. So suppose first that v_1, v_2 are two linearly independent eigenvectors, and note that the the second term in RHS of equation (7) projects qubits $n, 1$ onto a state $|\phi\rangle = (T_\psi^{n-1} \otimes \mathbb{1})^* |\psi\rangle$. In particular, using equation (4) and Proposition 11, one finds

$$
\begin{aligned}
|\phi\rangle = (T_\psi^{n-1} \otimes \mathbb{1})^* |\psi\rangle &= (T_\psi^{n} \otimes \mathbb{1})^* (T_\psi^{-1} \otimes T_\psi^{-1})^* (\mathbb{1} \otimes T_\psi)^* |\psi\rangle \\
&\sim (T_\psi^{n} \otimes \mathbb{1})^* (|0,1\rangle - |1,0\rangle) \\
&= (T_\psi^{n*}|0\rangle) \otimes |1\rangle - (T_\psi^{n*}|1\rangle) \otimes |0\rangle.
\end{aligned}
$$

Clearly, $|\phi\rangle$ and $|\epsilon\rangle$ are linear independent. Since the kernel of sum of positive operators are just the intersection of the kernel of each positive operator in the sum, the ground states of LHS in equation (7) are the symmetric states that are orthogonal to $|\phi\rangle$ on any pair of qubits. We claim that the only two-qubit states that are orthogonal to $|\phi\rangle$ are $|v_1 \otimes v_1\rangle$ and $|v_2 \otimes v_2\rangle$. Indeed, for $i \in \{1, 2\}$,

$$
\begin{aligned}
\langle v_i \otimes v_i | \phi\rangle &\sim \langle v_i \otimes v_i | T_\psi^{n*} \otimes \mathbb{1} | 01\rangle - \langle v_i \otimes v_i | T_\psi^{n*} \otimes \mathbb{1} | 10\rangle \\
&= \langle T_\psi^{n} v_i \otimes v_i | 01\rangle - \langle T_\psi^{n} v_i \otimes v_i | 10\rangle \\
&= \overline{\lambda_i^n} \langle v_i \otimes v_i | \epsilon\rangle = 0,
\end{aligned}
$$

where λ_i is the eigenvalue associate to the eigenvector v_i of the matrix T_ψ. Therefore, $(|v_i\rangle^{\otimes n})_{i=1}^2$ forms a basis kernel of the RHS in equation (7), it follows that $\dim(\ker H_n^\circ(\psi)) = 2$ since they have the same rank.

Now suppose that the the matrix T_ψ^n only has one eigenvector. For simplicity, let us work in a basis with $|0\rangle$ is the eigenvector, so

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

for some $a, b \in \mathbb{C}$, and $a \neq 0$. In this case, the last term in RHS of equation (7) projects qubits $n, 1$ onto a state

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

where the proportionality comes from the same idea above case. Since $a \neq 0$, the space spanned by $|\epsilon\rangle, |\phi\rangle$ are the same as the space spanned by $|\epsilon\rangle, |11\rangle$. Then it is not hard to finds that the ground states of LHS in equation (7) are the symmetric states that are orthogonal to $|11\rangle$ on any pair of qubits. Therefore, the only states satisfy the conditions are linear combination of $|0\rangle^{\otimes n}$ and the n-qubit state

$$
|100\ldots0\rangle + |010\ldots0\rangle + \cdots + |00\ldots01\rangle,
$$

and we obtain $\dim(\ker H_n^\circ(\psi)) = 2$ as required. □

4 Gapless phase

In this section we are going to prove the following theorem.

Theorem 3. *Suppose the eigenvalues of T_ψ has the same non-zero absolute value, then $\gamma(\psi, n) \leq 1/(n-1)$ for all $n \geq 2$.*

4.1 Auxiliary propositions

Since there is a lot to prepare to prove the theorem, we first state and prove these technical results.

In particular, we are about to study the smallest non-zero eigenvalue of $H_n(\psi)$ as well as $H_n^\circ(\psi)$. Recall that $\gamma(\psi, n)$ and $\gamma^\circ(\psi, n)$ denote the smallest non-zero eigenvalue of Hamiltonian $H_n(\psi)$ and $H_n^\circ(\psi)$, respectively. It will turn out that we are able to bound $\gamma^\circ(\psi, m)$, for some $m \geq n$. In order to connect two different eigenvalues, the following lemma is indispensable.

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

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

The proof of the lemma is stated in section 2. As we said, we will show that $\gamma^\circ(\psi, m)$ can take arbitrarily small values for large m, and use the lemma backwards to infer $\gamma(\psi, n) \leq \dfrac{1}{n-1}$. In particular, according to the lemma we know,

$$\gamma(\psi, n) \leq \frac{1}{n-1} + \frac{n-2}{n-1}(\gamma^\circ(\psi, m)),$$

as m approaches to infinity, we obtain the desired result. However, for some state ψ we can not use this strategy directly. In these cases we perturb ψ to an arbitrarily close state ϕ such that ϕ is a state that we can apply the strategy. To measure and bound how close these two states are, we need the following Proposition. Recall that $H_n(\psi)$ is an self-adjoint operator in vector space $\mathbb{C}^{2^n}$,so it has 2^n eigenvalues. Denote them as $e_i(\psi, n)$ for the ith largest eigenvalue, i.e.,

$$e_1(\psi, n) \leq e_2(\psi, n) \leq \cdots \leq e_{2^n}(\psi, n).$$

Similarly, write

$$e_1^o(\psi, n) \leq e_2^o(\psi, n) \leq \cdots \leq e_{2^n}^o(\psi, n)$$

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

Lemma 1. *Let $u, v \in \mathscr{H}$, then $\||u\rangle\langle v|\| = \|u\|\|v\|$.*

Proof. Using the definition of operator norm and Proposition2, we obtain

$$\begin{aligned}
\||u\rangle\langle v|\| &= \sup_{x\in\mathscr{H}, \|x\|=1} \||u\rangle\langle v|x\| \\
&= \sup_{x,y\in\mathscr{H}, \|x\|=\|y\|=1} \|\langle y|u\rangle\langle v|x\rangle\| \\
&= \sup_{y\in\mathscr{H}, \|y\|=1} \|\langle y|u\rangle\| \cdot \sup_{x\in\mathscr{H}, \|x\|=1} \|\langle v|x\rangle\| \\
&= \|u\|\|v\|.
\end{aligned}$$

□

Proposition 12. *Let ψ, ϕ be two normalized states, then*

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

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

Proof. The proof of two inequalities are identical so we only prove the first one. Let's begin with using Theorem 2 (Weyl's Perturbation Theorem), we obtain, in this case,

$$|e_j(\psi, n) - e_j(\phi, n)| \le \|H_n(\psi) - H_n(\phi)\|.$$

To complete the proof, we first note that for a positive operator A, we have $\|A \otimes \mathbb{1}\| = \|A\|$. To see this fact, we recall that the operator norm is the largest singular value, and the eigenvalues are just singular values for a positive operator. It then follows that $\||\psi\rangle\langle\psi|_{i,i+1} - |\phi\rangle\langle\phi|_{i,i+1}\| = \||\psi\rangle\langle\psi| - |\phi\rangle\langle\phi|\|$. To proceed, we bound

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

where in the last line we used Lemma 1 and the fact that $|\psi\rangle, |\phi\rangle$are normalized. □

We observe that the state ψ under a transformation of the form $U \otimes U$, where U is unitary, will leave eigenvalues of $H_n(\psi)$ and absolute values of the eigenvalues of T_ψ invariant. To see this, let $\psi' = (U \otimes U)\psi$, then

$$\begin{aligned}
H_n(\psi') = \sum_{i=1}^{n-1} |\psi'\rangle\langle\psi'|_{i,i+1} &= \sum_{i=1}^{n-1} (U \otimes U)|\psi\rangle\langle\psi|_{i,i+1}(U \otimes U)^* \\
&= \sum_{i=1}^{n-1} (U)^{\otimes n}|\psi\rangle\langle\psi|_{i,i+1}(U^*)^{\otimes n} \\
&= (U)^{\otimes n} H_n(\psi)(U^*)^{\otimes n}.
\end{aligned}$$

Using proposition 4 we showed the first part of the observation. For the second part, we will show that

$$T_{\psi'} = (\det U)^{-1} U T_\psi U^*.$$

Using equation (4), one obtains

$$\langle\psi'|(\mathbb{1} \otimes T_{\psi'}) = \det T_{\psi'} \langle\epsilon|. \tag{8}$$

Consider $\langle\psi|(U \otimes U)^*(U \otimes U)(\mathbb{1} \otimes T_\psi)(U \otimes U)^*$ and using equation (4) again, we have

$$\langle\psi'|(\mathbb{1} \otimes U T_\psi U^*) = \det T_\psi \langle\epsilon|(U \otimes U)^*,$$

and using Proposition 11,

$$\langle\psi'|(\mathbb{1} \otimes U T_\psi U^*) = \det T_\psi (\det U)^{-1} \langle\epsilon|. \tag{9}$$

If one can show that

$$\det T_{\psi'} = (\det U^*)^2(\det T_\psi), \tag{10}$$

then rewrite equation (8) and equation (9) and combine them we get

$$(\det T_\psi)^{-1}(\det U)\langle\psi'|(\mathbb{1}\otimes UT_\psi U^*) = (\det U)^2(\det T_\psi)^{-1}\langle\psi'|(\mathbb{1}\otimes T_{\psi'}),$$

note that we assume that ψ is entangled and hence $\det T_\psi \neq 0$. Equivalently,

$$T_{\psi'} = (\det U)^{-1}UT_\psi U^*.$$

The following proposition will prove that equation (10) is true.

Lemma 2. *Let $U \in \mathrm{U}(2)$ be a 2 by 2 unitary matrix, $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$be a 2-qubit state. Let ψ' be the state under the unitary transformation, i.e. $|\psi'\rangle = (U \otimes U)|\psi\rangle$. Then $\det T_{\psi'} = (\det U^*)^2(\det T_\psi)$.*

Proof. The proof is just tedious calculation. With out loss of generality, we assume that ψ is entangled, otherwise, since the $U \otimes U$ brings product states to product states, the equation we want to prove is $0 = 0$. We know there exist a parametrization of 2 by 2 unitary group, i.e., one can write $U = \begin{pmatrix} a & b \\ -e^{i\phi}\overline{b} & e^{i\phi}\overline{a} \end{pmatrix}$, where $a, b \in \mathbb{C}, \phi \in \mathbb{R}$. Let $|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} \in \mathbb{C}^2 \otimes \mathbb{C}^2$. Then

$$|\psi'\rangle = \begin{pmatrix} a^2 & ab & ab & b^2 \\ -e^{i\phi}a\overline{b} & e^{i\phi}|a|^2 & -e^{i\phi}|b|^2 & e^{i\phi}\overline{a}b \\ -e^{i\phi}a\overline{b} & -e^{i\phi}|b|^2 & e^{i\phi}|a|^2 & e^{i\phi}\overline{a}b \\ e^{2i\phi}\overline{b^2} & -e^{2i\phi}\overline{ab} & -e^{2i\phi}\overline{ab} & e^{2i\phi}\overline{a^2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} a^2\alpha + ab(\beta+\gamma) + b^2\delta \\ e^{i\phi}(-a\overline{b}\alpha + |a|^2\beta - |b|^2\gamma + \overline{a}b\delta) \\ e^{i\phi}(-a\overline{b}\alpha - |b|^2\beta + |a|^2\gamma + \overline{a}b\delta) \\ e^{2i\phi}(\overline{b^2}\alpha - a\overline{b}(\beta+\gamma) + \overline{a^2}\delta) \end{pmatrix},$$

so the matrix

$$T_{\psi'} = \begin{pmatrix} e^{-i\phi}\overline{(-a\overline{b}\alpha - |b|^2\beta + |a|^2\gamma + \overline{a}b\delta)} & e^{-2i\phi}\overline{(\overline{b^2}\alpha - a\overline{b}(\beta+\gamma) + \overline{a^2}\delta)} \\ \overline{-a^2\alpha - ab(\beta+\gamma) - b^2\delta} & e^{-i\phi}\overline{(a\overline{b}\alpha + |b|^2\beta - |a|^2\gamma - \overline{a}b\delta)} \end{pmatrix}.$$

Then

$$\overline{\det T_{\psi'}} = e^{2i\phi}\Big[(-a\overline{b}\alpha - |b|^2\beta + |a|^2\gamma + \overline{a}b\delta)(a\overline{b}\alpha + |b|^2\beta - |a|^2\gamma - \overline{a}b\delta) \\ + (a^2\alpha + ab(\beta+\gamma) + b^2\delta)(\overline{b^2}\alpha - a\overline{b}(\beta+\gamma) + \overline{a^2}\delta)\Big].$$

To compute this, there are 32 terms in the expansion. We treat $\alpha, \beta, \gamma, \delta$ as "basis", and a, b, c, d as "coefficients". We compute coefficients of each basis element as the following:

$$
\begin{aligned}
\alpha^2 :& - a^2\overline{b^2} + a^2\overline{b^2} = 0,\\
\beta^2 :& |a|^2|b|^2 - |a|^2|b|^2 = 0,\\
\gamma^2 :& |a|^2|b|^2 - |a|^2|b|^2 = 0,\\
\delta^2 :& - \overline{a^2}b^2 + \overline{a^2}b^2 = 0,\\
\alpha\beta :& - ab\overline{b^2} + a^2\overline{ab} - a^2\overline{ab} + ab\overline{b^2} = 0,\\
\alpha\gamma :& - a^2\overline{ab} + ab\overline{b^2} + a^2\overline{ab} - ab\overline{b^2} = 0,\\
\alpha\delta :& 2|a|^2|b|^2 + |a|^4 + |b|^4 = (|a|^2 + |b|^2)^2 = 1,\\
\beta\gamma :& - |a|^4 - |b|^4 - 2|a|^2|b|^2 = -(|a|^2 + |b|^2)^2 = -1,\\
\beta\delta :& - \overline{a^2}ab + \overline{ab}b^2 + ab\overline{a^2} - \overline{ab}b^2 = 0,\\
\gamma\delta :& \overline{ab}b^2 - \overline{a^2}ba + ab\overline{a^2} - \overline{ab}b^2 = 0.
\end{aligned}
$$

Therefore, $\det T_{\psi'} = e^{-2i\phi}\overline{(\alpha\delta - \beta\gamma)}$. On the other hand,

$$(\det U^*)^2 \det T_\psi = e^{-2i\phi}\overline{(\alpha\delta - \beta\gamma)},$$

as required. □

Proposition 13. *For any $\psi \in \mathbb{C}^2 \otimes \mathbb{C}^2$ there exists a single-qubit unitary U such that*

$$U \otimes U|\psi\rangle = (\alpha + \mathrm{i}\beta)|01\rangle + (\alpha + \mathrm{i}\gamma)|10\rangle + \delta|11\rangle$$

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

Proof. Let $|\psi'\rangle = U \otimes U|\psi\rangle$. Recall the previous observation that the transformation $|\psi\rangle \to U \otimes U|\psi\rangle$ induces the transformation $T_\psi \to (\det U)^{-1} U T_\psi U^*$. So, to show that one can bring $|\psi\rangle$ to that canonical form, it is equivalent to show that one can bring T_ψ to

$$T_{\psi'} = \begin{pmatrix} \alpha - \mathrm{i}\beta & \delta \\ 0 & -\alpha + \mathrm{i}\gamma \end{pmatrix}.$$

We will perform a consecutive unitary transformation on ψ to bring it to the canonical form.

First, we want T_ψ to be an upper triangular matrix. Since every complex matrix is guaranteed an eigenvalue, one can change the basis so that $|0\rangle$ is an eigenvector of T_ψ. Then we can assume

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

Second, we are able to change the phase of $(\mu_1 + \mu_2)$ so that its real part is 0, or equivalently, let $U = e^{-\mathrm{i}\theta/2}\mathbb{1}$, where $\theta \in \mathbb{R}$ such that $\mathrm{Re}(e^{\mathrm{i}\theta}(\mu_1 + \mu_2)) = 0$. It remains to modify δ to be real. Noting that the unitary matrix $\begin{pmatrix} e^{\mathrm{i}\phi} & \\ & e^{-\mathrm{i}\phi} \end{pmatrix}$ can modify δ without changing μ_1, μ_2. Thus, we can assume δ is real. □

4.2 The proof of the main theorem

Let $|\psi\rangle$ be the canonical form defined in Proposition 13, and consider the matrix

$$T_\psi = \begin{pmatrix} \alpha - \mathrm{i}\beta & \delta \\ 0 & -\alpha + \mathrm{i}\gamma \end{pmatrix}.$$

Assumption of the theorem demands $|\alpha - \mathrm{i}\beta| = |\alpha - \mathrm{i}\gamma|$, equivalently, $\gamma = \pm\beta$. We divide the proof into two parts.

Proof of the case $\gamma = \beta$. When $\gamma = \beta$, we get

$$T_\psi = \begin{pmatrix} z & \delta \\ 0 & -z \end{pmatrix}$$

where $z = \alpha - \mathrm{i}\beta$. So $T_\psi^2 \sim \mathbb{1}$. Now we fix $n \geq 2$, it is clear that for every even $m \geq n$, T_ψ^m is also proportional to $\mathbb{1}$. Using Theorem 2 we find out that the dimension of the ground space of $H_m^\circ(\psi)$ is $m+1$ which is greater than 3, so $e_3^\circ(\psi, m) = 0$.

Recall that Theorem 1 asserts that the ground space of $H_n(\psi)$ is $n+1$ dimensional, so $\gamma(\psi, n) = e_{n+2}(\psi, n)$. We will bound $e_{n+2}(\phi_m, n)$, for a slightly perturbed state ϕ_m, in order to bound $\gamma(\psi, n)$ via

$$\gamma(\psi, n) = e_{n+2}(\phi_m, n) + \Big(e_{n+2}(\psi, n) - e_{n+2}(\phi_m, n)\Big). \tag{11}$$

For each m, let ϕ_m be a perturbed and normalized state that

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

and such that eigenvalues of T_{ϕ_m} have different nonzero magnitude. Therefore, $T_{\phi_m}^m$ is not proportional to $\mathbb{1}$ and $\det T_{\phi_m} \neq 0$. Then by Theorem 2 and Proposition 12,

$$\gamma^\circ(\phi_m, m) = e_3^\circ(\phi_m, m) = e_3^\circ(\phi_m, m) - e_3^\circ(\psi, m) \leq \frac{2}{m}. \tag{12}$$

The next step is to transform this bound to a bound of $\gamma(\phi_m, n)$ using Knabe's lemma, we get

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

Finally, using Proposition 12, equation (11) becomes

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

as desired. □

In the first part of the proof, we observed that given a matrix T_ψ so that T_ψ^n is proportional to $\mathbb{1}$ for some n, we constructed a perturbed matrix T_{ϕ_m} so that $T_{\phi_m}^m$ is not proportional to $\mathbb{1}$. This is because one can use the "subtract 0" trick to bound the smallest eigenvalue of $H_m^\circ(\phi_m)$ as we did in equation (12). In the another part of the proof, we will see that when $\gamma = -\beta$, T_ψ^m is not proportional to $\mathbb{1}$ for any m. In this case we will perturb ψ so that we can get a matrix that is proportional to $\mathbb{1}$ when we raise it to some power, and using the same trick to bound the smallest eigenvalue of $H_m^\circ(\psi)$.

Before we proceed to another case, we would like to state a fact about irrational numbers.

Fact. *[2]Every irrational number α can be uniquely expressed by an infinite simple continued fraction, and if $\frac{p_k}{q_k}$ is the kth convergent, then there exists an inequality*

$$|\alpha - \frac{p_k}{q_k}| < \frac{1}{q_k^2}.$$

Proof of the case $\beta = -\gamma$. In this case we get

$$T_\psi = \begin{pmatrix} \alpha - \mathrm{i}\beta & \delta \\ 0 & -\alpha - \mathrm{i}\beta \end{pmatrix}.$$

We will perturb ψ so that we get a matrix that is proportional to $\mathbb{1}$ if we raise it to some power. To do this, we put $\alpha + \mathrm{i}\beta$ in polar form since we do not want affect the magnitude. So, write $\alpha + \mathrm{i}\beta = re^{-\mathrm{i}\pi(\theta+\frac{1}{2})}$, where r, θ are positive real numbers, and $r < 1$ since ψ is normalized, $r > 0$ since eigenvalues of T_ψ are nonzero. Now we obtain

$$\psi = re^{-\mathrm{i}\pi(\theta+\frac{1}{2})}|01\rangle + re^{\mathrm{i}\pi(\theta+\frac{1}{2})}|10\rangle + \delta|11\rangle.$$

We shall perturb θ to meet our purpose.

We first consider θ is irrational. By the fact we stated above, there exists two sequences of positive integers $\{p_j\}, \{q_j\}$ with

$$|\frac{p_j}{q_j} - \theta| \le \frac{1}{q_j^2},$$

where $\gcd(p_j, q_j) = 1$, and $\{q_j\}$ diverges. We shall omit the first two convergent as we want q_j to be the number of qubits later on. So $q_j \ge 2$ for every j.

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

$$|\Psi_j\rangle = re^{-\mathrm{i}\pi(\theta_j+\frac{1}{2})}|01\rangle + re^{\mathrm{i}\pi(\theta_j+\frac{1}{2})}|10\rangle + \delta|11\rangle$$

be the perturbed state. The bound of the difference is

$$\begin{aligned} \|\Psi_j - \psi\| &= r\|(e^{-\mathrm{i}\pi(\theta_j+\frac{1}{2})} - e^{-\mathrm{i}\pi(\theta+\frac{1}{2})})|01\rangle + (e^{\mathrm{i}\pi(\theta_j+\frac{1}{2})} - e^{\mathrm{i}\pi(\theta+\frac{1}{2})})|10\rangle\| \\ &\le r\|e^{-\mathrm{i}\pi\theta_j} - e^{-\mathrm{i}\pi\theta}\| + r\|e^{\mathrm{i}\pi\theta_j} - e^{\mathrm{i}\pi\theta}\| \\ &= r\|e^{\mathrm{i}\pi(\theta-\theta_j)} - 1\| + r\|1 - e^{\mathrm{i}\pi(\theta-\theta_j)}\| \\ &\le 2r|\pi(\theta_j - \theta)| \\ &\le \frac{2\pi}{q_{j^2}} \end{aligned} \tag{13}$$

where we used Proposition 3 , $r \leq 1$, and $|\theta_j - \theta| \leq \frac{1}{q_j^2}$.

Now let us look at the perturbed matrix

$$T_{\Psi_j} = \begin{pmatrix} \mathrm{i} r e^{\mathrm{i}\pi\theta_j} & \delta \\ 0 & \mathrm{i} r e^{-\mathrm{i}\pi\theta_j} \end{pmatrix}.$$

The eigenvalues are not equal since θ_j is not an integer, so T_{Ψ_j} is diagonalizable. Recall that $\theta_j = \frac{p_j}{q_j}$, by simple calculation and use the fact that the matrix is diagonalizable, we found that $T_{\Psi_j}^{q_j}$ is proportional to $\mathbb{1}$. On the other hand, since θ is not rational, $T_{\psi}^{q_j}$ is not proportional to the identity. Hence by Theorem 2, $e_3^{\circ}(\Psi_j, q_j) = 0$ and $\gamma^{\circ}(\psi, q_j) = e_3^{\circ}(\psi_j, q_j)$. Then Proposition 12 reads

$$\gamma^{\circ}(\psi, q_j) = \Big(\gamma^{\circ}(\psi, q_j) - e_3^{\circ}(\Psi_j, q_j)\Big) \leq 2q_j\|\Psi_j - \psi\| \leq \frac{4\pi}{q_j}.$$

Using Knabe's lemma stated in the end of the section 2, for $q_j \geq n$, we get

$$\begin{aligned} \gamma(\psi, n) &\leq \frac{1}{n-1} + \frac{n-2}{n-1}\gamma^{\circ}(\psi, q_j) \\ &\leq \frac{1}{n-1} + (\frac{n-2}{n-1})\frac{4\pi}{q_j} \\ &\xrightarrow{j\to\infty} \frac{1}{n-1}, \end{aligned}$$

since $\{q_j\}$ diverges.

It remains to show the case that θ is rational. The idea here is that we perturb θ to a irrational θ' and apply what we just showed. In particular, for any $\varepsilon > 0$, let θ' be irrational such that $|\theta' - \theta| \leq \varepsilon$, and let

$$|\phi\rangle = re^{-\mathrm{i}\pi(\theta' + \frac{1}{2})}|01\rangle + re^{\mathrm{i}\pi(\theta' + \frac{1}{2})}|10\rangle + \delta|11\rangle.$$

The above proof implies $\gamma(\phi, n) = e_{n+2}(\phi, n) \leq \frac{1}{n-1}$. Then using the same idea in equation (13) and Proposition 12, we get

$$\begin{aligned} \gamma(\psi, n) &= e_{n+2}(\phi, n) + \Big(e_{n+2}(\psi, n) - e_{n+2}(\phi, n)\Big) \\ &\leq \frac{1}{n-1} + 2n\|\psi - \phi\| \\ &\leq \frac{1}{n-1} + 2n(2r\pi\varepsilon) \\ &\xrightarrow{\varepsilon\to 0} \frac{1}{n-1}, \end{aligned}$$

as desired. □

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