Divide and conquer method for proving gaps of frustration free Hamiltonians

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Abstract. Providing system-size independent lower bounds on the spectral gap of local Hamiltonian is in general a hard problem. For the case of finite-range, frustration free Hamiltonians on a spin lattice of arbitrary dimension, we show that a property of the ground state space is sufficient to obtain such a bound. We furthermore show that such a condition is necessary and equivalent to a constant spectral gap. Thanks to this equivalence, we can prove that for gapless models in any dimension, the spectral gap on regions of diameter $n$ is at most $o\left(\frac{\log(n)^{2+\epsilon}}{n}\right)$ for any positive $\epsilon$.

Keywords: quantum phase transitions, rigorous results in statistical mechanics, spin chains, ladders and planes
### 1. Introduction

Many-body quantum systems are often described by local Hamiltonians on a lattice, in which every site interacts only with few other sites around it, and the range of the interactions is given in terms of the metric of the lattice. One of the most important properties of these Hamiltonians is the so-called spectral gap: the difference between the two lowest energy levels of the operator. The low-temperature behavior of the model (and in particular of its ground states) relies on whether the spectral gap is lower bounded by a constant which is independent on the number of particles (a situation usually referred to as gapped), or on the contrary the spectral gap tends to zero as we take the number of particle to infinity (the gapless case).

Quantum phase transitions are described by points in the phase diagram were the spectral gap vanishes [5, 27], and therefore understanding the behavior of the spectral gap is required in order to classify different phases of matter. A constant spectral gap implies exponential decay of correlations in the groundstate [15, 25], and it is conjectured (and proven in 1D) that entanglement entropy will obey an area law [13]. Moreover, the computational complexity of preparing the groundstate via an adiabatic

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3 We are using the terminology as it is frequently used in the quantum information community. In other contexts, one could only be interested in the thermodynamic limit, and the situation we have denoted as gapless does not necessarily imply that there is a continuous spectrum above the groundstate energy in such limit.

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preparation scheme [10] is given by the inverse of the spectral gap, implying that groundstates of gapped models can be prepared efficiently. It is also believed that it is possible to give synthetic descriptions of such groundstates in terms of Projected Entangled Paris States (PEPS) [28], and to prepare them with a quantum computer [29].

Because of the importance of the spectral gap, there is a large history of powerful results in mathematical physics regarding whether some systems are gapped or not, such as the Lieb–Schultz–Mattis theorem [18] and its higher dimensional generalization [14, 24], the so-called ‘martingale method’ for spin chains [23], the local gap thresholds by Knabe [17] and by Gosset and Mozgunov [12]. Cubitt, Perez-Garcia and Wolf have shown [9] that the general problem of determining, given a finite description of the local interactions, whether a 2D local Hamiltonian is gapped or not is undecidable. Nonetheless, this result does not imply that it is not possible to study the spectral gap of some specific models, and the problem can be decidable if we restrict to specific subclasses of interactions.

While these results have constituted tremendous progress, there is still a lack of practical tools for studying the gap for large classes of lattice systems, especially in dimensions greater than one. In this paper we consider frustration-free, finite range local Hamiltonian on spin lattices, and we present a technique for proving a lower bound on the spectral gap. Compared to the other methods for bounding the spectral gap that are available in the literature, the one we propose uses a recursive strategy that is more naturally targeted to spin models in dimension higher than 1, and which we hope might allow to generalize some of the results that at the moment have only been proved in 1D.

The approach we present is based on a property of the groundstate space reminiscent of the ‘martingale method’. A description of the groundstate space might not be available in all cases, but it is easily obtained for tensor network models such as PEPS [28]. We are able to prove that this condition is also necessary in gapped systems, obtaining an equivalence with the spectral gap. More specifically, we will define two versions of the martingale condition, a strong and a weak one, and we will show that the spectral gap implies the strong one. The strong martingale condition implies the weak one, hence completing the loop of equivalences. This ‘self-improving’ loop will allow us to give an upper bound on the rate at which the spectral gap vanishes in gapless systems, as any rate slower than that allows us to prove a constant spectral gap.

In order to prove the equivalence between the strong martingale condition and the spectral gap, we will use a tool known as the Detectability lemma [2, 3]. We will also show that if the Detectability lemma operator contracts the energy by a constant factor, then the system is gapped. This condition is reminiscent of the ‘converse Detectability lemma’ [4, 11], but we do not know whether these two conditions are equivalent.

Proving gaps of Hermitian operators has a long history in the setting of (thermal) stochastic evolution of classical spin systems. In this setting, there are numerous tools for bounding the spectral gap of the stochastic generator (which in turn allows to bound the mixing time of the process) both for classical [8, 19–22, 26] and for quantum commuting Hamiltonians [16].

In the classical setting, the theorems establish an intimate link between the mixing time of a stochastic semigroup (the Glauber dynamics) and the correlation properties
in the thermal state at a specified temperature: for sufficiently regular lattices and boundary conditions, correlations between two observables are exponentially decaying (as a function of the distance between their supports) if and only if the Glauber dynamics at the same temperature mixes rapidly (in a time $O(\log(N))$, where $N$ is the volume of the system). All of the proofs of the classical results in some way or another rely on showing that exponential decay of correlations implies a log-Sobolev inequality of the semi-group, and in the other direction, that the log-Sobolev inequality implies a spectral gap inequality, which in turn implies exponential decay of correlation. We will take inspiration from a weaker form of the classical theorem that shows the equivalence between spectral gap of the semigroup and exponential decay of correlation.

The paper is organized as follows. In section 2, we will describe the main assumption on the groundstate space that implies the spectral gap, and then we will state the main results. In section 3 we will recall some useful tools, namely the detectability lemma and its converse. In section 4, we will finally prove the main theorem, together with the local gap threshold.

2. Main results

2.1. Setup and notation

Let us start by fixing the notation and recalling some common terminology in quantum spin systems. We will consider a $D$-dimensional lattice $\Gamma$ (the standard example being $\Gamma = \mathbb{Z}^D$, but the same results will hold for any graph which can be isometrically embedded in $\mathbb{R}^D$). At each site $x \in \Gamma$ we associate a finite-dimensional Hilbert space $\mathcal{H}_x$, and for simplicity we will assume that they all have the same dimension $d$. For every finite subset $\Lambda \subset \Gamma$, the associated Hilbert space $\mathcal{H}_\Lambda$ is given by $\otimes_{x \in \Lambda} \mathcal{H}_x$, and the corresponding algebra of observables is $\mathcal{A}_\Lambda = \mathcal{B}(\mathcal{H}_\Lambda)$. If $\Lambda \subset \Lambda'$ we will identify $\mathcal{A}_\Lambda$ as the subalgebra $\mathcal{A}_\Lambda \otimes 1_{\Lambda' \setminus \Lambda} \subset \mathcal{A}_{\Lambda'}$. If $P$ is an orthogonal projector, we will denote by $P_{\perp}$ the complementary projection $1 - P$.

A local Hamiltonian is a map associating each finite $\Lambda \subset \Gamma$ to a Hermitian operator $H_\Lambda$, given by

$$H_\Lambda = \sum_{X \subset \Lambda} h(X),$$

where $h(X) \in \mathcal{A}_X$ is Hermitian. We will denote the orthogonal projector on the groundstate space of $H_\Lambda$ (i.e. the eigenprojector corresponding to the smallest eigenvalue of $H_\Lambda$) as $P_\Lambda$. We will make the following assumptions on the interactions $h(X)$:

**(Finite range)** there exist a positive $r$ such that $h(X)$ is zero whenever the diameter of $X$ is larger than $r$. The quantity $r$ will be denoted the range of $h$;

**(Frustration freeness)** for every $X$, $h(X)P_\Lambda = E_0(X)P_\Lambda$, where $E_0(X)$ is the lowest eigenvalue of $h(X)$.

Note that frustration freeness implies that $P_\Lambda P_{\Lambda'} = P_{\Lambda'}$ whenever $\Lambda \subset \Lambda'$. By applying a global energy shift, we can replace $h(X)$ with $h(X) - E_0(X)$, and we will assume that $E_0(X) = 0$ for every $X$, so that $H_\Lambda \geq 0$. 

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Definition 1 (Spectral gap). For every $\Lambda$, we will denote by $\lambda_\Lambda$ the difference between the two lowest distinct eigenvalues of $H_\Lambda$ (which, since we have assumed that 0 is the lowest eigenvalue, is the same as the smallest non-zero eigenvalue of $H_\Lambda$). This quantity will be called the spectral gap of $H_\Lambda$, and it can be expressed as follows:

$$\lambda_\Lambda = \inf \frac{\langle \varphi | H_\Lambda | \varphi \rangle}{\langle \varphi | P_\Lambda | \varphi \rangle}.$$  \hfill (1)

We will interpret this as a ratio of two quadratic functionals on $H_\Lambda$:

$$\text{Var}_\Lambda(\varphi) = \langle \varphi | \varphi \rangle - \langle \varphi | P_\Lambda | \varphi \rangle = \langle \varphi | P_\Lambda^\perp | \varphi \rangle;$$  \hfill (2)

$$\mathcal{E}_\Lambda(\varphi) = \langle \varphi | H_\Lambda | \varphi \rangle.$$  \hfill (3)

We will use the symbol $\text{Var}_\Lambda(\varphi)$ since the functional can be thought as a type of variance: it equals $\| \varphi - P_\Lambda | \varphi \|_2^2$, it is always positive and vanishes only on states in $P_\Lambda$. We can then rewrite equation (1) as the following optimization problem: $\lambda_\Lambda$ is the largest constant such that $\lambda_\Lambda \text{Var}_\Lambda(\varphi) \leq \mathcal{E}_\Lambda(\varphi)$.

In order to simplify the proofs, we will also make the following extra assumption on the interactions $h(X)$:

(Local projections) Every $h(X)$ is an orthogonal projection.

Remark 1. The assumption that every $h(X)$ is an orthogonal projection is not a fundamental restriction. Let us denote by $E_1(X)$ (resp. $E_{\max}(X)$) the second-smallest eigenvalue (resp. the largest eigenvalue) of $h(X)$, and remember that we have assumed that the lowest eigenvalue of each $h(X)$ is zero. If we then assume the two following conditions

(Local gap) $e = \inf_X E_1(X) > 0$;

(Local boundness) $E = \sup_X E_{\max}(X) < \infty$;

then we can see that for every finite $\Lambda \subset \Gamma$:

$$e \sum_{X \subset \Lambda} P_X^\perp \leq H_\Lambda \leq E \sum_{X \subset \Lambda} P_X^\perp,$$

where we have denoted by $P_X$ the projector on the groundstate of $h(X)$. Therefore $H_\Lambda$ will have a non-vanishing spectral gap if and only the spectral gap of the Hamiltonian composed of projectors $\sum_X P_X^\perp$ is not vanishing. This shows that, as far as we are interested in the behavior of the spectral gap, requiring local gap and local boundness is equivalent to requiring that the interactions $h(X)$ are projectors.

Given a local Hamiltonian $H$ which is finite range and frustration free it is easy to see that interactions can be partitioned into $g$ groups, referred to as ‘layers’, in such a way that every layer consists of non-overlapping (and therefore commuting) terms. For a fixed $\Lambda \subset \Gamma$, let us index the layers from 1 to $g$, and denote $L_i$ the orthogonal projector on the common groundstate space of the interactions belonging to group $i$. Since they are commuting, $L_i$ can also be seen as the product of the groundstate space
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projectors of each interaction term. For any given ordering of \( \{1, \ldots, g\} \), we can then define the product \( L = \prod_{i=1}^{g} L_i \) (different orders of the product will in general give rise to different operators). Any operator constructed in this fashion is called an approximate ground state projector.

2.2. Statement of the results

We will now state the main assumptions needed in the proof of the spectral gap theorem. In order to do so, we will need to introduce some notation for the overlap between groundstate spaces of different regions.

**Definition 2.** Let \( A, B \) be finite subsets of \( \Gamma \). Let \( P_{A \cup B}, P_A, \) and \( P_B \) be respectively the orthogonal projectors on the ground state space of \( H_{A \cup B}, H_A, \) and \( H_B \). Then we define

\[
\delta(A, B) = \|(P_A - P_{A \cup B})(P_B - P_{A \cup B})\|.
\]

(4)

**Remark 2.** Because of frustration freedom, we have \( P_A P_{A \cup B} = P_{A \cup B} P_A = P_{A \cup B} \) and the same holds for \( P_B \). In turn this imply that

\[
(P_A - P_{A \cup B})(P_B - P_{A \cup B}) = P_A P_B - P_{A \cup B},
\]

so that \( \delta(A, B) \) can be both seen as a measure of the overlap between \( (P_A - P_{A \cup B}) \) and \( (P_B - P_{A \cup B}) \) (the cosine of the first principal angle between the two subspaces), as well as a measure of how much \( P_{A \cup B} \) can be approximated by \( P_A P_B \).

The intuition behind definition 2 is that in a gapped system, if \( l \) is the diameter of the largest ball contained in \( A \cap B \), then \( \delta(A, B) \) should be a fast decaying function of \( l \). In this setting we will refer to the ‘size’ of the overlap of \( A \) and \( B \) as \( l \) (see figure 1(b)). One might also hope that \( \delta(A, B) \) only depends on \( l \) and not on the size of \( A \Delta B = (A \cup B) \setminus (A \cap B) \). This is captured by the following assumption:

**Condition 1.** There exists a positive function \( \delta(l) \) with exponential decay in \( l \), i.e. \( \delta(l) \leq c e^{l} \) for some \( 0 < \alpha < 1 \) and \( c > 0 \), such that for every connected \( A \) and \( B \), such that \( A \cap B \) has size \( l \), the following bound holds:

\[
\delta(A, B) \leq \delta(l).
\]

(5)
We will now present some weaker versions of condition 1. As we will show later, they will all turn out to be equivalent, but it might be hard to verify the stronger versions in some concrete examples. The first relaxation we have is to require a slower decay of the function $\delta(l)$.

Condition 2. There exists a positive function $\delta(l)$ with polynomial decay in $l$, i.e. $\delta(l) \leq cl^{-\alpha}$ for some $\alpha > 0$ and $c > 0$, such that for every connected $A$ and $B$, such that $A \cap B$ has size $l$, equation (5) holds.

Clearly, condition 1 implies condition 2. As formulated, conditions 1 and 2 and B require equation (5) to be satisfied homogenously for all regions $A$ and $B$ of arbitrary size. However, in order to prove a bulk spectral gap, such a strong homogeneity assumption can be relaxed. We can allow for the size of $A \cap B$, of $A$ and of $B$ to be taken into account; intuitively, we would like to have less stringent requirement if $A \cap B$ is very small compared to $A$ and $B$. In particular, we will define classes $F_k$ of sets, which have the property that they can be decomposed as overlapping unions of sets in $F_{k-1}$, with a sufficiently large overlap. Then we will only require equation (5) to hold for this specific decomposition, and moreover we will allow the bound $\delta(l)$ to depend on $k$.

The construction of the sets $F_k$ we present is a generalization of the one originally proposed by Cesi [8] and used in the context of open quantum systems by one of the authors [16].

Definition 3. For each $k \in \mathbb{N}$, let $l_k = (3/2)^{k/D}$ and denote
$$R(k) = [0, l_{k+1}] \times \cdots \times [0, l_{k+D}] \subset \mathbb{R}^D.$$ Let $F_k$ be the collection of $\Lambda \subset \Gamma$ which are contained in $R(k)$ up to translations and permutation of the coordinates.

We now show that sets in $F_k$ can be decomposed 'nicely' in terms of sets in $F_{k-1}$, as shown in Figure 2.

Proposition 1. For each $\Lambda \in F_k \setminus F_{k-1}$ and each positive integer $s \leq \frac{1}{8}l_k$, there exist $s$ distinct pairs of non-empty sets $(A_i, B_i)_{i=1}^s$ such that
(i) $\Lambda = A_i \cup B_i$ and $A_i, B_i \in F_{k-1}$, $\forall i = 1, \ldots, s$;
(ii) $\text{dist}(\Lambda \setminus A_i, \Lambda \setminus B_i) \geq \frac{l_k}{8s} - 2$.

Figure 2. Depiction of the decomposition of the region $\Lambda = A_i \cup B_i$, with $i = 1, \ldots, s$, where the intersections of sets $A_i \cap B_i$ are all non-overlapping.
(iii) \( A_i \cap B_i \cap A_j \cap B_j = \emptyset \quad \forall i \neq j. \)

We will call a set of \( s \) distinct pairs \((A_i, B_i)\) of non-empty sets satisfying the above properties an \( s \)-decomposition of \( \Lambda \).

The proof of this proposition—a minor variation over the one presented by Cesi [8]—is contained in appendix. With this definition of \( F_k \) at hand, we can now present the weakest version of condition 1.

**Condition 3.** There exists an increasing sequence of positive integers \( s_k \), with \( \sum k s_k < \infty \), such that
\[
\sum_{k=1}^{\infty} \delta_k := \sum_{k=1}^{\infty} \sup_{A \in F_k \setminus F_{k-1}} \sup \delta(A, B) < \infty,
\]
where the second supremum is taken over all \( s_k \)-decompositions \( \Lambda = A_i \cup B_i \) given by proposition 1.

It is not immediately clear from the definition that condition 3 is implied by condition 2, so we show this in the next proposition.

**Proposition 2.** Condition 2 implies condition 3 with any \( s_k \) such that \( \sum k s_k / l_k < \infty \).

**Proof.** Let \( \delta(l) \) be as in condition 1. Since for every \( \Lambda_k \in F_k \setminus F_{k-1} \) and for every \( s_k \)-decomposition \( \Lambda_k = A_i \cup B_i \) of \( \Lambda_k \), the overlap \( A_i \cap B_i \) has size at least \( l_k / 8 s_k - 2 \), then
\[
\delta_k \leq \delta \left( \frac{l_k}{8 s_k} - 2 \right).
\]
Since \( \delta(l) \) decays as \( l^{-\alpha} \) for some positive \( \alpha \), \( \delta_k \) is summable if \( \sum s_k / l_k \) is summable. \( \square \)

**Remark 3.** If we consider condition 3 with \( s_k \) growing faster than \( l_k / 3 \), then the previous proposition does not apply—note that in any case \( s_k \) has to be smaller than \( l_k / 5 \) for the construction of proposition 1 to be possible. In practice we do not need to consider such situations. In Cesi [8], \( s_k \) was chosen to be of order \( l_k^{1/3} \). As we will see later, we will be interested in choosing \( s_k \) with slower rates than that (while still having \( \sum 1 / s_k \) finite), so the condition \( s_k = \mathcal{O} \left( \frac{l_k}{k} \right) \) will not be restrictive for our purposes. So from now on, we will only consider condition 3 in the case where \( s_k = \mathcal{O} \left( \frac{l_k}{k} \right) \).

The main result of the paper is to show that condition 3 is sufficient to prove a spectral gap. In turn, this will imply condition 1, which as we have already seen in remark 3 implies condition 3, showing that all three conditions are equivalent.

**Theorem 3.** Let \( H \) be a finite range, frustration free, local Hamiltonian, and let \( F_k \) be as in proposition 1. Then the following are equivalent

(i) \( \inf_{k} \inf_{\Lambda \in F_k} \lambda_{\Lambda} \geq \lambda > 0 \) (or in other words, \( H \) is gapped);

(ii) \( H \) satisfies condition 1 with \( \delta(l) = \frac{1}{(1+\lambda/l^2)^{1/2}} \) for some constant \( g \);

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(iii) $H$ satisfies condition 2;

(iv) $H$ satisfied condition 3 with $s_k$ such that $\sum_k \frac{s_k}{l_k} < \infty$.

By proving the equivalence of these conditions, we are also able to show that in any gapless model, the spectral gap cannot close too slowly, since a slow enough (but still infinitesimal) gap will imply condition 3 and therefore a constant gap. The threshold is expressed in the following corollary.

**Corollary 4.** If $H$ is gapless, then for any $\Lambda \subset \Gamma$ of diameter $n$ it holds that

$$\lambda_\Lambda = o\left(\frac{\log(n)^{2+\epsilon}}{n}\right),$$

for every $\epsilon > 0$.

We also provide an independent condition for lower bounding the spectral gap. Consider again the construction of the detectability lemma, where $L = L_1 \cdots L_g$ is an approximate ground state projector.

**Theorem 5.** If there exist a constant $0 < \gamma < 1$ such

$$\mathcal{E}(L\varphi) \leq \gamma\mathcal{E}(\varphi),$$

then the spectral gap of $H$ is bounded below by $\lambda \geq \frac{1-\gamma}{4}$.  

While similar in spirit to the Converse Detectability lemma (see section 3), we do not know if these are equivalent, nor whether the hypothesis of theorem 5 is necessary.

**Remark 4 (Comparison with the ‘martingale method’).** Nachtergaele [23] presented a general method for proving the spectral gap for a class of spin-lattice models, which has become known as the martingale method. Given an increasing and absorbing sequence $\Lambda_n \to \Gamma$, and a fixed parameter $l$, it requires three conditions ($C1$–$C3$) to be satisfied uniformly along the sequence to prove a lower bound to the spectral gap. Let us briefly recall what these conditions would be if we applied them to the setting we are considering, and compare them to condition 3. The first condition, denoted ($C1$) in the original paper, is automatically satisfied by finite range interactions, which is also the case we are considering here. If we denote $A_n = \Lambda_n$ and $B_n = \Lambda_{n+1} \setminus \Lambda_{n-1}$ (where now $l$ is a parameter partially controlling the size of $A_n \cap B_n = \Lambda_n \setminus \Lambda_{n-1}$), then condition ($C2$) requires that $H_{A_n \cap B_n}$ has a spectral gap of $\gamma_l$ independently of $n$ (for every $n$ large enough). We do not need to require such assumption, since we are using a recursive proof. Condition ($C3$) can be restated, using our notation, as requiring that

$$\delta(A_n, B_n) \leq \epsilon_l < \frac{1}{\sqrt{n+1}}$$

for all $n$ large enough.

Clearly, the big difference with condition 3 is that the requirement on $\delta$ is not of asymptotic decay, but only to be bounded by a specific constant. Upon careful inspection, we see this is only a fair comparison in 1D. In higher dimensions, condition ($C2$) could be as hard to verify as the original problem of lower bounding the spectral gap, since the size of $A_n \cap B_n$ will grow with $n$. Condition ($C3$) is also clearly implied by condition 1. Therefore, one could compare the method we propose with the martingale method.
as a strengthening of condition (C3) in exchange of a weakening of condition (C2), a trade-off which we hope makes it more applicable in dimensions \( D > 1 \).

### 2.3. Example 1: translation invariant 1D spin chains

To clarify the differences between conditions 1–3, let us consider the case of 1D spin chains. We will consider a translational invariant model to further simplify the situation. Then we can take, without loss of generality, \( A = [0, n] \) and \( B = [n - d, n - d + m] \), with \( n, m, d \) being positive integers such that \( \min(m, n) > d \). The intersection \( A \cap B = [n - d, n] \) has length \( d + 1 \), so that condition 1 is equivalent to the fact that the function

\[
\delta(d) = \sup_{d < n, m} \delta([0, n], [n - d, n - d + m])
\]

has exponential decay in \( d \). Condition 2 would relax this to a polynomial decay, but both require a bound that is uniform in \( n \) and in \( m \).

We can now consider the larger interval in each \( F_k \), namely \( \Lambda_k = [0, (3/2)^k + 1] \). Denoting \( l_k = (3/2)^k \), we can write \( \Lambda_k \) and its \( s \)-decompositions as

\[
\Lambda_k = [0, 1] \cdot l_{k+1}, \\
A^i_k = \left[ 0, \frac{1}{2} + \frac{i}{6} \right] \cdot l_{k+1}, \\
B^i_k = \left[ \frac{1}{2} + \frac{i}{6} - \frac{1}{12s}, 1 \right] \cdot l_{k+1},
\]

for \( i = 1, \ldots, s \). The overlap \( A^i_k \cap B^i_k \) has size \( \frac{l_k}{12s} \) for every \( i \). If we fix for concreteness \( s_k = l_k^{1/3} \), as in [8], then we can define

\[
n_{i,k} = \left[ \frac{1}{2} l_k + \frac{i}{6} \right], \quad m_{i,k} = \left[ \frac{1}{2} l_k - \frac{2i - 1}{12} l_k^{2/3} \right], \quad d_k = \left[ \frac{l_k^{2/3}}{12} \right],
\]

so that

\[
A^i_k = [0, n_{i,k}], \quad B^i_k = [n_{i,k} + d_k, n_{i,k} + d_k + m_{i,k}].
\]

Note that \( n_{i,k} \) and \( m_{i,k} \) are always smaller than \( 24\sqrt{3} d_k^{3/2} \). So we then see that in order to show that the model satisfies condition 3, it would be sufficient for example to verify that

\[
\delta(d) = \sup_{d < n, m \leq 24\sqrt{3} d^{3/2}} \delta([0, n], [n - d, n - d + m])
\]

is decaying polynomially fast in \( d \). Compared to equation (8), \( n \) and \( m \) are restricted given a specific \( d \), i.e. we only have to consider the case where they are at most a constant times \( d^{3/2} \). It should be clear now that this restriction on the \( n \) and \( m \) depends on the choice of the scaling of \( s_k \). Choosing faster rates of growth for \( s_k \) leads to more restrictive conditions (and thus in principle easier to verify): the downside is that this will be reflected in the numerical bound for the spectral gap, which will become worse (although finite).
2.4. Example 2: PVBS models

One notable model in dimension larger than 1 for which the original martingale method has been successfully applied is the Product Vacua and Boundary State (PVBS) model \([6, 7]\), a translation invariant, finite range, frustration free spin lattice Hamiltonian, with parameters \(D\) positive real numbers \((\lambda_1, \ldots, \lambda_D)\). We refer to the original paper for the precise definition of the model. The spectral gap of the PVBS Hamiltonian is amenable to be analyzed using the ‘1D version’ of the martingale method, applied recursively in each of the dimensions, and it has been shown that in the infinite plane the Hamiltonian is gapped if and only if not all \(\lambda_j\) are equal to 1. In this section we show that our result recovers the same finite-size limit analysis as in the original paper: for simplicity we will only do the analysis in the case of rectangular regions, with the caveat that in that case the finite-size gap closes if only one of the \(\lambda_j\) is equal to 1 (even if the GNS Hamiltonian is still gapped).

In \([7, \text{lemma } 3.3]\) it has been shown that in the case of two connected regions \(A\) and \(B\) such that \(A \cap B\) is also connected,

\[
\delta(A, B)^2 = \frac{C(A \setminus B)C(B \setminus A)}{C(A)C(B)},
\]

where \(C(X) = \sum_{x \in X} \prod_{j=1}^D \lambda_j^{2x_j}\) is the normalization constant of the model. If we now consider \(\Lambda \in \mathcal{F}_k\) to be a rectangular region (so that every \(A_i\) and \(B_i\) appearing in the geometrical construction of proposition 1 will also be rectangles), then the normalization constant \(C(\Lambda)\) will be a product of different constants in each dimension independently. Assuming without loss of generality that the dimension being cut by proposition 1 is the \(D\)th, we see that if \(\lambda_D = 1\) then

\[
\delta(A_i, B_i) = \left(\frac{|A_i \setminus B_i|}{|A_i|} \frac{|B_i \setminus A_i|}{|B_i|}\right)^{1/2} = \mathcal{O}\left(1 - \frac{1}{8s_k}\right),
\]

which is not infinitesimal.

On the other hand, if \(\lambda_D \neq 1\), then

\[
\delta(A_i, B_i) = \left(\frac{\sum_{x=0}^{l_A-1} \lambda_D^{2x} \sum_{x=1}^{l_B} \lambda_D^{2x}}{\sum_{x=0}^{l_A} \lambda_D^{2x} \sum_{x=0}^{l_B} \lambda_D^{2x}}\right)^{1/2},
\]

have denoted by \(l_A\) (resp. \(l_B, l\)) the length of \(A\) (resp. \(B, A \cap B\)) along dimension \(D\). Therefore

\[
\delta(A_i, B_i) \leq \begin{cases} 
\lambda_D^{l+1}[(1 - \lambda_D^{-2(l_A+1)})(1 - \lambda_D^{-2(l_B+1)})]^{-1/2} & \text{if } \lambda_D < 1, \\
\lambda_D^{l+1}[(1 - \lambda_D^{-2(l_A+1)})(1 - \lambda_D^{-2(l_B+1)})]^{-1/2} & \text{if } \lambda_D > 1.
\end{cases}
\]

If all \(\lambda_j\) are distinct from one, then the PVBS model satisfies condition 1 with

\[
\delta(l) = \frac{\lambda_l}{1 - \lambda_l^2}, \quad \lambda_* = \max\min(\lambda_i, \lambda_i^{-1}),
\]

and therefore it is gapped by theorem 15. If at least one of them is equal to 1 then \(\delta(l)\) will be lower bounded away from zero, and therefore the gap will close. Note that one
could get a better estimate on the spectral gap by following the proof of theorem 15, and using a different $\delta(l)$ in each of the dimensions, instead that just taking the worst case as we did here.

3. Detectability lemma and spectral gap

3.1. The detectability lemma and its converse

The Detectability lemma \cite{2–4} originated in the context of the quantum PCP conjecture \cite{1}. It has since then become a useful tool in many-body problems. A converse result is known as the Converse Detectability lemma \cite{4, 11}, and will also be used later. At the same time as we recall them, we will reformulate them in terms of inequalities between some quadratic functionals.

In analogy to equation (2), given $L = \prod_{i=1}^{g} L_i$ we define the following quadratic functional on $\mathcal{H}_\Lambda$

$$DL(\varphi) = \langle \varphi | \varphi \rangle - \langle \varphi | L^* L | \varphi \rangle.$$ (11)

Before stating the Detectability lemma and its converse, let us make some preliminary observations regarding $L$ and $DL(\varphi)$.

Remark 5. For any $L$ given above, denote $P$ the projector on the groundstate space of $H$. Then

1. $LP = PL = P$, and in particular $[L, P] = 0$;
2. $\|L\| \leq 1$;

Proof. (1) follows from the definition of $L$ and frustration freedom. Since $L$ is a product of projectors its norm is bounded by 1, so also (2) is trivial.

Proposition 6. For every $\varphi \in \mathcal{H}_\Lambda$ it holds that

$$DL(\varphi) \leq \text{Var}(\varphi) \leq \frac{1}{1 - \|LP^\perp\|^2} DL(\varphi),$$ (12)

and $1/(1 - \|LP^\perp\|^2)$ is the smaller constant that makes the upper bound hold true.

Proof. Let us start by observing that

$$\text{Var}(L\varphi) = \langle \varphi | L^* P^\perp L | \varphi \rangle = \langle \varphi | L^* L | \varphi \rangle - \langle \varphi | P | \varphi \rangle = \text{Var} \varphi - DL(\varphi).$$

On the one hand, since $\text{Var}$ is a positive quadratic functional, we have that $\text{Var}(L\varphi) \geq 0$ and therefore $\text{Var}(\varphi) \geq DL(\varphi)$. On the other hand we have the following bound

$$\text{Var}(\varphi) - DL(\varphi) = \langle \varphi | L^* P^\perp L | \varphi \rangle = \langle \varphi | P^\perp L^* LP^\perp | \varphi \rangle \leq \|LP^\perp\|^2 \langle \varphi | P^\perp | \varphi \rangle;$$

from which the upper bound in equation (12) follows by rearranging the terms. Optimality follows by choosing a $\varphi$ such that $\|LP^\perp \varphi\| = \|LP^\perp\| \|P^\perp \varphi\|$. 

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As can be seen from equation (12), if \( \|L_P\|^2 \) is smaller than 1, then \( DL \) is up to constants equivalent to \( \text{Var} \). The Detectability lemma and its converse then relate \( DL \) to \( \mathcal{E} \), thus allowing to connect \( \|L_P\|^2 \) to the spectral gap, via equation (1).

**Lemma 7 (Detectability lemma).** With the notation above, it holds that

\[
\mathcal{E}(L\varphi) \leq g^2 DL(\varphi). \tag{13}
\]

The proof of this statement can be found in [4, lemma 2]. A simple corollary follows:

**Corollary 8.** If \( \lambda \) is the spectral gap of \( H \), then

\[
\|L_P\|^2 \leq \frac{1}{1 + \lambda/g^2}. \tag{14}
\]

In particular, for finite systems \( \|L_P\| < 1 \).

**Proof.** If \( \lambda \) is the spectral gap of \( H \), then \( \lambda \text{Var}(\varphi) \leq \mathcal{E}(\varphi) \). In particular, \( \lambda \text{Var}(L\varphi) \leq \mathcal{E}(L\varphi) \leq g^2 DL(\varphi) \). But in proposition 6 we have seen that \( \text{Var}(L\varphi) = \text{Var}(\varphi) - DL(\varphi) \), and therefore \( \text{Var}(\varphi) \leq (1 + \frac{g^2}{\lambda}) DL(\varphi) \). The result follows from optimality of the constant in equation (12). \( \square \)

**Lemma 9 (Converse DL).** With the same notation as above,

\[
DL(\varphi) \leq 4\mathcal{E}(\varphi). \tag{15}
\]

The proof of this statement can be found in [11, corollary 1]. Again, from this functional formulation we can derive the usual statement of the Converse Detectability lemma

**Corollary 10.** If \( \lambda \) is the spectral gap of \( H \), then

\[
\lambda \geq 1 - \frac{\|L_P\|^2}{4}. \tag{16}
\]

**Proof.** It follows from proposition 6. \( \square \)

We are now ready to prove theorem 5.

**Proof.** From corollary 8, we have that \( \|L_P\| < 1 \), and then proposition 6 implies that \( \lim_{n \to \infty} L^n = P \). Therefore

\[
\lim_{m \to \infty} \sum_{n=0}^{m} DL(L^n \varphi) = \lim_{m \to \infty} \sum_{n=0}^{m} \langle \varphi | (L^n)^* L^n | \varphi \rangle - \langle \varphi | (L^{n+1})^* L^{n+1} | \varphi \rangle \tag{17}
\]

\[
= \lim_{m \to \infty} \langle \varphi | \varphi \rangle - \langle \varphi | (L^{m+1})^* L^{m+1} | \varphi \rangle \tag{18}
\]

\[
= \langle \varphi | \varphi \rangle - \langle \varphi | P | \varphi \rangle = \text{Var}(\varphi). \tag{19}
\]

By applying lemma 9 to each term in the summation, we obtain that:
3.2. Spectral gap implies condition 1

Let us start by proving the following converse relationship between spectral gap and \( \delta(A, B) \).

**Theorem 11.** Let \( A, B \subset \Gamma \) be finite, and let \( l = \text{dist}((A \cup B) \setminus A, (A \cup B) \setminus B) \). If \( H_\Lambda \) for \( \Lambda = A \cup B \) is a finite range Hamiltonian with spectral gap \( \lambda_\Lambda \), then

\[
\delta(A, B) \leq \frac{1}{(1 + \lambda_\Lambda / g^2)^{l/2}},
\]

where \( g \) is a constant depending only on \( \Gamma \) and on the range of \( H \).

In order to prove this result, we will make use of the Detectability lemma. With the same notation as in lemma 7, it implies that \( \|L^qP^+_\Lambda\| \leq \frac{1}{1 + \lambda_\Lambda / g^2} \). By taking \( q \)-powers of \( L \) and iterating the previous bound \( q \) times we obtain

\[
\|L^qP^+_\Lambda\| \leq \frac{1}{(1 + \lambda_\Lambda / g^2)^{q/2}} = \varepsilon^q_\Lambda,
\]

since \( L^qP^+_\Lambda \subset P^+_\Lambda \), where we have denoted \( \varepsilon_\Lambda = (1 + \lambda_\Lambda / g^2)^{-1/2} < 1 \). Therefore, if \( H_\Lambda \) is gapped, \( L^q \) will be an exponentially good approximation of \( P_\Lambda \), with \( q \) chosen independently of \( \Lambda \). We now want to show that \( L^q \) can be split as a product of two terms \( L^q = M_A M_B \) in such a way that both \( M_A \) and \( M_B \) are good approximations to \( P_A \) and \( P_B \), using a strategy presented in [16].

**Lemma 12.** With the notation defined above, if \( q \leq l \), then there exist two operators \( M_A \) and \( M_B \), respectively acting on \( A \) and on \( B \), such that \( L^q = M_A M_B \) and the following holds:

\[
\|P_A - M_A\| \leq \varepsilon_\Lambda, \quad \|(P_A - M_A)M_B\| \leq \varepsilon^q_\Lambda;
\]

and the same holds with \( A \) and \( B \) interchanged.

**Proof.** Let us start by defining \( M_A \) and \( M_B \) as follows: we will group the projectors appearing in \( L^q \) in two disjoint groups, such that \( M_A \) will be the product (in the same order as they appear in \( L^q \)) of the projectors of one group, \( M_B \) the product of the rest, and \( L^q = M_A M_B \). In order to do so, we will consider the layers \( L_1, \ldots, L_g \) sequentially (following the order in which are multiplied in \( L \)), and then we will start again from \( L_1 \) up to \( L_g \), until we have considered \( \lfloor gq/2 \rfloor \) different layers. Each layer will be split into two parts, where terms of one of them will end up appearing in \( M_A \) and terms in the other will appear in \( M_B \). In the first layer, we will only include in \( M_A \) terms which intersect \( (A \cup B) \setminus B \). From the second layer, we only included terms which intersect the support of the terms considered from the first. We keep doing this recursively, when
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at each layer we include terms which intersect the support of the selected terms of the previous step (one can see this as a sort of light-cone, defined by the layer structure, generated by \((A \cup B) \setminus B\), as depicted in figure 3). The remaining \([gq/2]\) are treated similarly, but starting instead from the end of the product, and reversing the role of \(B\) and \(A\). At this point, it should be clear that by construction \(L^q = MA MB\), since every projector appearing in \(L\) has been assigned to either \(MA\) or \(MB\), and the two groups can be separated without breaking the multiplication order. If \(q \leq l\), then \(MB\) will be supported in \(B\), and \(MA\) will be supported on \(A\).

Denote with \(LA\) and \(LB\) the approximate ground state projections of \(PA\) and \(PB\) respectively, as in lemma 7. Then we have that
\[
\| PA - L^q_A \| \leq \epsilon_A^q
\]
and the same for \(B\). It should be clear that \(MA\) and \(MB\) contain strictly more projection terms than \(LA\) and \(LB\), and therefore \(PA MA = MA PA = PA\) and \(\| MA P_A \| \leq \epsilon_A\), and the same holds for \(B\).

Observe that we can write
\[
PA MB = PA MA MB := PA RL^q_B,
\]
where we have redistributed the projectors of \(MA\) in order to ‘fill’ the missing ones in \(MB\) to complete it to \(L^q_B\). What is left is put into \(R\), which can be reabsorbed into \(PA\). Therefore \(PA MB = PA L^q_B\), and this implies that
\[
\| PA(P_B - MB) \| = \| PA(P_B - L^q_B) \| \leq \epsilon_A^q.
\]
The same construction (but exchanging the roles of \(A\) and \(B\)) can be done in order to bound \(\|(PA - MA) MB\| \leq \epsilon_A^q\). □

With this construction, we can easily prove theorem 11.

**Proof of theorem 11.** We observe that
\[
PA PB - MA MB = PA(P_B - MB) + (PA - MA) MB.
\]
We can now apply lemma 12, and choose \(q = l\) to obtain
\[
\| PA PB - PA \cup B \| \leq \frac{1}{(1 + \lambda_A / g^2)^{l/2}}.\]

□

In the next section, we will show that condition 3 implies the spectral gap. Then theorem 11 allows us to prove the converse, therefore showing the equivalence stated in theorem 3.
4. Condition 3 implies spectral gap

4.1. Quasi-factorization of excitations

We will start with some useful inequalities regarding orthogonal projectors in Hilbert spaces.

**Lemma 13.** Let $P$ and $Q$ be two orthogonal projections on a Hilbert space $\mathcal{H}$. Then it holds that

$$\{P, Q\} \leq 1 - P - Q \leq \{P^\perp, Q^\perp\}$$  \hspace{1cm} (22)

where $\{P, Q\} = PQ + QP$ is the anti-commutator.

**Proof.** We start by observing that $-1 \leq P - Q \leq 1$, since $P$ and $Q$ are positive and bounded by 1, and therefore $0 \leq (P - Q)^2 \leq 1$. By observing that $(P - Q)^2 = P + Q - \{P, Q\}$, it immediately follows the l.h.s. of equation (22):

$$1 - P - Q \geq -\{P, Q\}.$$ \hspace{1cm} (23)

By algebraic manipulation we can show that

$$\{P, Q\} = (1 - P^\perp)(1 - Q^\perp) + (1 - Q^\perp)(1 - P^\perp) = 2(1 - P^\perp - Q^\perp) + \{P^\perp, Q^\perp\}.$$  

Applying equation (23) we obtain that

$$\{P^\perp, Q^\perp\} = \{P, Q\} + 2(1 - P - Q) \geq 1 - P - Q.$$ \hspace{1cm} \qed

We are now ready to prove the following quasi-factorization result.

**Lemma 14 (Quasi-factorization of excitations).** Let $A, B$ be subsets of $\Lambda$. Then it holds that

$$c\langle \varphi | P_{A\cup B}^\perp | \varphi \rangle \leq \langle \varphi | P_A^\perp | \varphi \rangle + \langle \varphi | P_B^\perp | \varphi \rangle,$$  \hspace{1cm} (24)

where $c = 1 - 2\delta(A, B)$.

**Proof.** Notice that frustration freedom implies that $P_{A\cup B}^\perp P_A = P_A^\perp P_{A\cup B} = P_A^\perp$, and the same holds for $P_B^\perp$. Therefore if $P_{A\cup B}^\perp | \varphi \rangle = 0$, both sides of the equation reduce to 0, and we can restrict ourselves to the case in which $| \varphi \rangle$ is contained in the image of $P_{A\cup B}^\perp$. We can then apply equation (22) to $P_A^\perp$ and $P_B^\perp$ and we obtain:

$$\langle \varphi | P_{A\cup B}^\perp | \varphi \rangle \leq \langle \varphi | P_A^\perp | \varphi \rangle + \langle \varphi | P_B^\perp | \varphi \rangle + \langle \varphi | P_{A\cup B}^\perp \{P_A, P_B\} P_{A\cup B}^\perp | \varphi \rangle.$$  

To conclude the proof, we just need to observe that

$$P_{A\cup B}^\perp P_A P_B P_{A\cup B} = (P_A - P_{A\cup B})(P_B - P_{A\cup B}),$$

and that therefore by applying the Cauchy–Schwartz inequality
\[ \langle \varphi | P_{A \cup B}^+ P_A P_B P_{A \cup B}^- | \varphi \rangle \leq \| P_{A \cup B}^+ | \varphi \| (\langle P_A - P_{A \cup B} \rangle (P_B - P_{A \cup B}) P_{A \cup B}^+ | \varphi \| \|^2 \]
\[ = \| (P_A - P_{A \cup B}) (P_B - P_{A \cup B}) \| \langle \varphi | P_{A \cup B}^+ | \varphi \rangle. \]

Since the same holds for \( P_{A \cup B}^+ P_A P_B P_{A \cup B}^- \), and the operator norm is invariant under taking the adjoint, we obtain that
\[ \langle \varphi | P_{A \cup B}^+ \{ P_A, P_B \} P_{A \cup B}^+ | \varphi \rangle \leq 2 \| (P_A - P_{A \cup B}) (P_B - P_{A \cup B}) \| \langle \varphi | P_{A \cup B}^+ | \varphi \rangle, \]
which concludes the proof.

**Remark 6 (Comparison with the Converse DL).** A bound similar to what we have obtained in the previous lemma could also have been derived from the converse of the Detectability lemma \( 9 \). Indeed, if we apply it to the Hamiltonian \( P_A^+ + P_B^+ \), we obtain the following
\[ \| \varphi \|^2 - \| P_A P_B | \varphi \| \|^2 \leq 4 \langle \varphi | P_A^+ + P_B^+ | \varphi \rangle. \]
If we now choose \( | \varphi \rangle = P_{A \cup B}^+ | \varphi \rangle \), then a simple calculation shows that
\[ \| P_A P_B | \varphi \| \|^2 = \langle \varphi | P_B P_B P_A P_B | \varphi \rangle = \langle \varphi | P_{A \cup B}^+ P_B P_B P_{A \cup B}^+ | \varphi \rangle \]
\[ \langle \varphi | P_B (P_A - P_{A \cup B}) (P_B - P_{A \cup B}) P_B | \varphi \rangle \leq \| (P_A - P_{A \cup B}) (P_B - P_{A \cup B}) \| \langle \varphi | P_{A \cup B}^+ | \varphi \rangle. \]
We thus obtain the following bound
\[ \langle \varphi | P_{A \cup B}^+ | \varphi \rangle \leq \langle \varphi | P_A^+ | \varphi \rangle + \langle \varphi | P_B^+ | \varphi \rangle, \quad (25) \]
but now \( \delta' = \frac{1}{4} (1 - \delta(A, B)) \). While very similar to equation \( 24 \), the constant \( \delta' \) does not tend to 1 when \( \delta(A, B) \) goes to zero: as we will see next, this is a crucial property and it is for this reason that equation \( 25 \) will not be useful for our proof.

**Remark 7.** For one dimensional systems, we expect the martingale condition to be implied by exponential decay of correlations, as has been shown in the commuting Gibbs sampler setting [16]. However, at this point we only know how to obtain this result if for any state \( | \psi \rangle \), there exists a (non-Hermitian) operator \( f_{A^c} \) on the complement of \( A \subseteq A \) such that
\[ P_A | \psi \rangle = f_{A^c} | \varphi \rangle, \quad (26) \]
and \( | \varphi \rangle \) is the unique ground state of \( H_A \). In that case, the proof is analogous to the one in [16]. Equation \( 26 \) does not hold in general, however it can be shown to hold for injective PEPS. Hence, for injective MPS correlation decay implies the martingale condition.

### 4.2. Spectral gap via recursion

As we have mentioned in the introduction, the strategy for proving a lower bound to the spectral gap will be a recursive one: given \( \Lambda \), we will decompose it into two overlapping subsets, so that \( \Lambda = A \cup B \) and we will be able to use lemma \( 14 \). This would lead to the following expression

\[ \frac{\| \psi \|^2}{\| \varphi \|^2} = \frac{\langle \varphi | P_{A \cup B}^+ | \varphi \rangle}{\langle \varphi | P_{A \cup B}^+ | \varphi \rangle} = \frac{\| (P_A - P_{A \cup B}) (P_B - P_{A \cup B}) \| \langle \varphi | P_{A \cup B}^+ | \varphi \rangle}{\langle \varphi | P_{A \cup B}^+ | \varphi \rangle} = \frac{\langle \varphi | P_{A \cup B}^+ | \varphi \rangle - \langle \varphi | P_{A \cup B}^- | \varphi \rangle}{\langle \varphi | P_{A \cup B}^+ | \varphi \rangle} = 1 - \delta(A, B), \quad (27) \]
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\[
(1 - 2\delta(A, B))\langle \varphi | P_A^+ | \varphi \rangle \leq \langle \varphi | P_A^+ | \varphi \rangle + \langle \varphi | P_B^+ | \varphi \rangle \leq \frac{1}{\min(\lambda_A, \lambda_B)} \langle \varphi | H_A + H_B | \varphi \rangle = \frac{1}{\min(\lambda_A, \lambda_B)} \langle \varphi | H_A + H_{A\cap B} | \varphi \rangle.
\] (27)

We now face the problem of what to do with the term \( \langle \varphi | H_{A\cap B} | \varphi \rangle \). Because of frustration freedom, we can bound it with \( \langle \varphi | H_A | \varphi \rangle \), leading to

\[
\lambda_{A\cup B} \geq \frac{1 - 2\delta(A, B)}{2} \min(\lambda_A, \lambda_B).
\] (28)

Then it is clear that, even in the case of \( \delta(A, B) = 0 \), this strategy is going to fail: at each step of the recursion our bound on \( \lambda_A \) is cut in half, so in the limit of \( \Lambda \to \Gamma \) we will obtain a vanishing lower bound. The way out of this obstacle is to observe that if we have \( s_k \) different ways of splitting \( \Lambda \) as \( A_i \cup B_i \), and if moreover the intersections \( A_i \cap B_i \) are disjoint for different \( i \), then we can average equation (27) and obtain

\[
\langle \varphi | P_A^+ | \varphi \rangle \leq \frac{1}{s_k} \sum_{i=1}^{s_k} \frac{(1 - 2\delta(A_i, B_i))^{-1}}{\min(\lambda_{A_i}, \lambda_{B_i})} \langle \varphi | H_{A_i} + H_{B_i} | \varphi \rangle \leq \frac{(1 - 2\delta_k)^{-1}}{\min\{\lambda_{A_i}, \lambda_{B_i}\}} \langle \varphi | H_A + \frac{1}{s_k} \sum_{i=1}^{s_k} H_{A_i \cap B_i} | \varphi \rangle \leq (1 - 2\delta_k)^{-1} \frac{1 + 1/s_k}{\min\{\lambda_{A_i}, \lambda_{B_i}\}} \langle \varphi | H_A | \varphi \rangle.
\] (29)

Then equation (28) becomes

\[
\lambda_A \geq \frac{1 - 2\delta_k}{1 + 1/s_k} \min\{\lambda_{A_i}, \lambda_{B_i}\}.
\] (30)

Now the problem is simply to check whether we can find a right balance between the number \( s_k \) of different ways to partition \( \Lambda \) (in order to make the product \( 1 + 1/s_k \) convergent in the recursion), the size of \( A_i \) and \( B_i \) (if one of them is similar in size to \( \Lambda \), then we will not have gained much from the recursion), and the size of their overlaps (in order to make \( \delta_k \) small). The geometrical construction presented in proposition 1 shows that such balance is obtainable, if we choose \( 1/s_k \) to be summable.

By formalizing this idea, we can finally prove the main theorem of this section.

**Theorem 15 (Spectral gap recursion bound).** Fix an increasing sequence of positive integers \( (s_k)_k \) such that \( \sum_k \frac{1}{s_k} \) is summable. Let \( k_k \) and \( F_k \) be as in definition 3, and \( \delta_k = \delta_k^s \) as in equation (6) and

\[
\lambda_k = \inf_{\Lambda \in F_k} \lambda_{A_k}.
\]

Let \( k_0 \) be the smallest \( k \) such that \( \delta_k < 1/2 \) for all \( k \geq k_0 \). Then there exists a constant \( C > 0 \), depending on \( \Gamma \) and on the sequence \( (s_k)_k \) but not on \( k \), such that

\[
\lambda_k \geq \lambda_{k_0} C \prod_{j=k_0+1}^{k} (1 - 2\delta_j).
\] (31)

In particular, if condition 3 is satisfied, the Hamiltonian is gapped.

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Proof. Fix a \( \Lambda \in \mathcal{F}_k \setminus \mathcal{F}_{k-1} \) and let \( (A_i, B_i)_{i=1}^{s_k} \) be an \( s_k \)-decomposition of \( \Lambda \) as in proposition 1. We can then apply lemma 14 to each pair \( (A_i, B_i) \), average over the resulting bounds, and obtain as in equation (30)

\[
\lambda_{A} \geq \frac{1 - 2\delta_k}{1 + 1/s_k} \min_i \{\lambda_{A_i}, \lambda_{B_i}\} \geq \frac{1 - 2\delta_k}{1 + 1/s_k} \lambda_{k-1}.
\]

Since \( \Lambda \) was arbitrary, we have obtained that

\[
\lambda_k \geq \frac{1 - 2\delta_k}{1 + 1/s_k} \lambda_{k-1}.
\] (32)

By iterating equation (32) \( k - k_0 \) times, we obtain

\[
\lambda_k \geq \prod_{j=k_0+1}^{k} \frac{1 - 2\delta_j}{1 + 1/s_j} \lambda_{k_0}.
\]

We want to show now that this gives rise to the claimed expression. Notice that if we denote \( C^{-1} := \prod_{j=1}^{\infty} (1 + 1/s_k) \) then

\[
1 \leq C^{-1} \leq \prod_{j=1}^{\infty} [1 + \frac{1}{s_k}] < \infty.
\]

This can be seen by observing that the series \( \log \prod_{j=1}^{\infty} (1 + \frac{1}{s_k}) = \sum_{j=1}^{\infty} \log (1 + \frac{1}{s_k}) \) is summable, since by comparison it has the same behavior as \( \sum_{j=1}^{\infty} \frac{1}{s_k} \), which is summable by assumption. This implies in particular that \( \prod_{j=1}^{k} (1 + 1/s_k) \geq C > 0 \) for all \( k \).

Finally, in order to prove that the Hamiltonian is gapped, we only need to show that condition 3 implies

\[
K := \prod_{j=k_0+1}^{\infty} (1 - 2\delta_j) > 0.
\] (33)

This again is equivalent to the fact that \( (\delta_j)_{j=k_0+1}^{\infty} \) is a summable sequence, which is imposed by condition 3.

5. Local gap threshold

Equivalence between conditions 3 and 1 can be seen as a ‘self-improving’ condition on \( \delta_k \), where assuming that it decays faster than some threshold rate implies that it is actually decaying exponentially. This type of argument is reminiscent of ‘spectral gap amplification’ as described in [4]. The same type of self-improving statement can be obtained for the spectral gap of \( H \).
Lemma 16. Fix an increasing sequence of integers $s_k$ such that $\sum \frac{1}{s_k} < \infty$ and $\sum_k \frac{s_k}{l_k} < \infty$. Let $H$ be a local Hamiltonian, and let (as in theorem 15) $\lambda_k = \inf_{\Lambda \in \mathcal{F}_k} \lambda_{\Lambda}$, where $\lambda_{\Lambda}$ is the spectral gap of $H_{\Lambda}$. If there exist a $C > 0$ and a $k_0$ such that

$$\lambda_k > C \frac{s_k}{l_k}, \quad \forall k \geq k_0,$$

then system is gapped (and $\inf_k \lambda_k > 0$).

Proof. Since for every $s_k$-decomposition $A_i, B_i$ of $\Lambda \in \mathcal{F}_k$ the overlap $A_i \cap B_i$ has size at least $l_k s_k^{-1}$, by theorem 11, we have that

$$\delta_k \leq (1 + \frac{\lambda_k}{g^2})^{- \frac{l_k}{16 s_k}}.$$

We now need to check that $\delta_k$ is summable. By the root test, it is sufficient that

$$\limsup \left(1 + \frac{\lambda_k}{g^2}\right)^{- \frac{l_k}{16 s_k}} = \left(\liminf \left(1 + \frac{\lambda_k}{g^2}\right)^{\frac{l_k}{16 s_k}}\right)^{-1} < 1,$$

i.e. that

$$\liminf \left(1 + \frac{\lambda_k}{g^2}\right)^{\frac{l_k}{16 s_k}} = \exp \left(\liminf \frac{\lambda_k l_k}{16 l_k s_k} \log \left(1 + \frac{\lambda_k}{g^2}\right) \frac{1}{s_k}\right) > 1.$$

If $\liminf \lambda_k = 0$, then $\liminf (1 + \frac{\lambda_k}{g^2})^{\frac{l_k}{s_k}} = e^{\frac{l_k}{g^2}} > 1$ (and if $\liminf \lambda_k > 0$ there is nothing left to prove, since then we already know that the system is gapped), and therefore we can reduce to check that

$$\liminf \frac{\lambda_k l_k}{K s_k} > 0,$$

which is implied by equation (34). \qed

If we now read the condition of equation (34) in terms of the length of the sides of the sets in $\mathcal{F}_k$, we obtain a proof of corollary 4.

Proof of corollary 4. Let $\Lambda \in \mathcal{F}_k$: then its diameter will be at most a constant times $l_k$. If we denote it by $n$, then $k \geq q \log(n)$ for some $q > 0$. If we choose $s_k = k^{1+\varepsilon}$ for some $\varepsilon > 0$, we see that equation (34) is satisfied if we can find $\varepsilon$ and $C > 0$ such that

$$\lambda_\Lambda > C \frac{\log(n)^{2+\varepsilon}}{n}$$

holds for all rectangles $\Lambda$ with sides bounded by $n$. If the Hamiltonian is gapless, then necessarily $\lambda_\Lambda = o\left(\frac{\log(n)^{2+\varepsilon}}{n}\right)$ for every $\varepsilon > 0$. \qed

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This result has to be compared with similar results obtained in [12, 17] in the specific case of nearest-neighbor interactions in 1D chains and in 2D square and hexagonal lattices. In all these cases, the authors obtain a local gap threshold which implies a spectral gap in the limit in the following sense: denoting \( \lambda_n \) the spectral gap of a finite system defined on a subset of ‘side-length’ \( n \) (where the exact definition depends on the dimension and the geometry of the lattice, but the general idea is that such a subset has \( \mathcal{O}(n^D) \) sites), there exists a sequence \( \gamma_n \) (the local gap threshold) such that, if for some \( n_0 \) it holds that \( \lambda_{n_0} > \gamma_{n_0} \), then the system is gapped in the limit. The converse is that, if the Hamiltonian is gapless, then \( \lambda_n = \mathcal{O}(\gamma_n) \). The values of \( \gamma_n \) present in [12, 17] are recalled in table 1.

The obvious downside of lemma 16 over the results in [12, 17] is that these only require a single \( n_0 \) satisfying \( \lambda_{n_0} > \gamma_{n_0} \), while equation (34) is a condition to be satisfied for each \( n \). On the other hand, it can be applied in more general settings than nearest neighbor interactions, as well as in dimensions higher than 2, and can be easily generalized to regions with different shapes. The upper bound on \( \lambda_n \) for a gapless Hamiltonian which we derive is worse by a polynomial factor than the ones obtained in 1D and in the 2D square lattice, and it is only off by a logarithmic factor in the 2D hexagonal lattice case. While the logarithmic factor in our bound is probably just an artifact of the proof, it is an interesting open question whether the optimal scaling for the general case is \( \mathcal{O}(1/n^2) \).

One should also mention the Lieb–Schultz–Mattis theorem [18] and its generalization to higher dimensions [14, 24], which proves that a class of half-integer spin models (not necessarily frustration free) with translational invariance, continuous symmetry and unique ground state is gapless. For this class of models the gap is bounded by \( \mathcal{O}(\log n/n) \) (the \( \log n \) factor can be removed in 1D), which is slightly better than the general upper bound we have obtained.

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### Appendix. Geometrical construction

#### Proof of proposition 1.

Let \( d_k = l_k/s_k \). For \( i = 1, \ldots, s \), we define

\[
A_i = ([0, l_{k+1}] \times \cdots \times [0, l_{k+D-1}] \times [0, l_{k+D}/2 + 2i d_k]) \cap \Lambda;
\]

\[
B_i = ([0, l_{k+1}] \times \cdots \times [0, l_{k+D-1}] \times [(l_{k+D}/2) + (2i - 1)d_k, l_{k+D}]) \cap \Lambda.
\]
Let us start by proving that $A_i$ and $B_i$ are in $\mathcal{F}_{k-1}$. In order to do so, we need to show that up to translations and permutations of the coordinates, they are contained in $R(k-1)$. If we look at coordinate $j = 1, \ldots, D – 1$, then their sides are contained in $[0, l_{k+1}]$, so it is enough to show that across the $D$th coordinate they are not more than $l_k$ long, $A_i$ has a larger side than $B_i$, so we can focus on it only. Then we see that

$$\frac{1}{2}l_{k+D} + 2i d_k \leq \frac{1}{2} (3/2)^{\frac{k+D}{2}} + 2s d_k = \frac{3}{4} l_k + \frac{1}{4} l_k = l_k.$$

So that $A_i$ and $B_i$ belong to $\mathcal{F}_{k-1}$ for every $i$. If either $A_i$ or $B_i$ were empty for a given $i$, then $\Lambda$ would be contained in a set belonging to $\mathcal{F}_{k-1}$, and thus it would itself belong to $\mathcal{F}_{k-1}$, but we have excluded this by assumption. So $A_i$ and $B_i$ are not empty. Clearly $\Lambda = A_i \cup B_i$, and $\text{dist} (\Lambda \setminus A_i, \Lambda \setminus B_i) \geq d_k – 2$. Finally, we see that

$$A_i \cap B_i = \left( [0, l_{k+1}] \times \cdots \times [0, l_{k+D-1}] \times \left[ \frac{l_{k+D}}{2} + (2i-1)d_k, \frac{l_{k+D}}{2} + 2i d_k \right] \right) \cap \Lambda,$$

so that $A_i \cap B_i \cap A_j \cap B_j = \emptyset$ for all $i \neq j$. \hfill \square

References

[1] Aharonov D, Arad I and Vidick T 2013 Guest column: the quantum PCP conjecture ACM SIGACT News \textbf{44} 47
[2] Aharonov D, Arad I, Vazirani U and Landau Z 2011 The detectability lemma and its applications to quantum Hamiltonian complexity \textit{New J. Phys.} \textbf{13} 113043
[3] Aharonov D, Arad I, Landau Z and Vazirani U 2009 The detectability lemma and quantum gap amplification \textit{Proc. 41st Annual ACM Symp. on Theory of Computing} (ACM, New York, NY) 417–26
[4] Anshu A, Arad I and Vidick T 2013 Guest column: the quantum PCP conjecture
[5] Bachmann S, Michalakis S, Nachtergaele B and Sims R 2011 Automorphic equivalence within gapped phases of quantum lattice systems \textit{Commun. Math. Phys.} \textbf{309} 835–71
[6] Bachmann S, Hamza E, Nachtergaele B and Young A 2015 Product vacua and boundary state models in d-dimensions \textit{J. Stat. Phys.} \textbf{160} 636–58
[7] Bishop M, Nachtergaele B and Young A 2016 Spectral gap and edge excitations of d-dimensional PVBS models on half-spaces \textit{J. Stat. Phys.} \textbf{162} 1485–521
[8] Cesà F 2001 Quasi-factorization of the entropy and logarithmic Sobolev inequalities for Gibbs random fields \textit{Probab. Theory Relat. Fields} \textbf{120} 569–84
[9] Cubitt T S, Perez-Garcia D and Wolf M M 2015 Undecidability of the spectral gap \textit{Nature} \textbf{528} 207–11
[10] Farhi E \textit{et al} 2000 Quantum computation by adiabatic evolution (arXiv:quant-ph/0001106)
[11] Gao J 2015 Quantum union bounds for sequential projective measurements \textit{Phys. Rev. A} \textbf{92} 052331
[12] Gosset D and Mozgunov E 2016 Local gap threshold for frustration-free spin systems. \textit{J. Math. Phys.} \textbf{57} 091901
[13] Hastings M B 2007 An area law for one-dimensional quantum systems \textit{J. Stat. Mech.} \textbf{P08024}
[14] Hastings M B 2004 Lieb–Schultz–Mattis in higher dimensions \textit{Phys. Rev. B} \textbf{69} 104431
[15] Hastings M B and Koma T 2006 Spectral gap and exponential decay of correlations \textit{Commun. Math. Phys.} \textbf{265} 781–804
[16] Kastoryano M J and Brandão F G S L 2016 Quantum gibbs samplers: the commuting case \textit{Commun. Math. Phys.} \textbf{344} 915–57
[17] Knabe S 1988 Energy gaps and elementary excitations for certain VBS-quantum antiferromagnets \textit{J. Stat. Phys.} \textbf{52} 627–38
[18] Lieb E, Schultz T and Mattis D 1961 Two soluble models of an antiferromagnetic chain \textit{Ann. Phys.} \textbf{16} 407–66
[19] Martinelli F and Olivieri E 1994 Approach to equilibrium of Glauber dynamics in the one phase region. I. The attractive case \textit{Commun. Math. Phys.} \textbf{161} 447–86

https://doi.org/10.1088/1742-5468/aaa793
Divide and conquer method for proving gaps of frustration free Hamiltonians

[20] Martinelli F and Olivieri E 1994 Approach to equilibrium of Glauber dynamics in the one phase region. II. The general case Commun. Math. Phys. 161 487–514
[21] Martinelli F, Olivieri E and Schonmann R H 1994 For 2D lattice spin systems weak mixing implies strong mixing Commun. Math. Phys. 165 33–47
[22] Martinelli F 1999 Lectures on Glauber dynamics for discrete spin models Lectures on Probability Theory and Statistics (Lecture notes in Mathematics vol 717) ed P Bernard (Berlin: Springer) pp 93–191
[23] Nachtergaele B 1996 The spectral gap for some spin chains with discrete symmetry breaking Commun. Math. Phys. 175 565–606
[24] Nachtergaele B and Sims R 2007 A multi-dimensional Lieb–Schultz–Mattis theorem Commun. Math. Phys. 276 437–72
[25] Nachtergaele B and Sims R 2006 Lieb–Robinson bounds and the exponential clustering theorem Commun. Math. Phys. 265 119–30
[26] Pra P D, Paganoni A M and Posta G 2002 Entropy inequalities for unbounded spin systems Ann. Probab. 30 1959–76
[27] Sachdev S 2012 The quantum phases of matter (arXiv:1203.4565 [hep-th])
[28] Schuch N, Cirac I and Pérez-García D 2010 PEPS as ground states: degeneracy and topology Ann. Phys. 325 2153–92
[29] Schwarz M, Temme K, Verstraete F, Perez-Garcia D and Cubitt T S 2013 Preparing topological projected entangled pair states on a quantum computer Phys. Rev. A 88 032321