

Spectral gaps in quantum computing

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Abstract. How does the spectral gap of a quantum many-body system scale with the system size? This turns out to be a very relevant question both in condensed matter physics and in quantum computing. However, there are very few available techniques to give bounds on that scaling. In the first part of this paper, we will review recent results which explain why it is undecidable to know if the spectral gap will vanish or not with the system size. In the second part, we will review complementary results which show that, despite this general impossibility result, one can still prove spectral gap estimates in a rather wide family of systems. As a consequence, one obtains new bounds on the lifetime of quantum memories.

1. Introduction

In this paper, we will review some recent results obtained in collaboration with different authors (J. Bausch, T. S. Cubitt, M. Kastoryano, A. Lucia, A. Pérez-Hernández and M. M. Wolf) regarding spectral gaps in lattice quantum spin systems [6, 15, 16, 22, 28, 38]. These results are steps in the larger program of understanding spectral gaps in interacting quantum systems. Both by the techniques and motivations, the focus will be located in the interconnection of the spectral gap problem with quantum computing.

The mathematical setup is the following. We consider “quantum particles” in a finite-size lattice, which for simplicity in the presentation we assume to be the square lattice in one or two dimensions. That is, we will consider the lattice $\Lambda_L = (\mathbb{Z} \cap [1, L])^\eta$ with $\eta = 1, 2$. We will usually consider periodic boundary conditions (i.e., a circle or a torus), though sometimes we will need to assume open boundary conditions.

We will be interested in the case $L \rightarrow \infty$, but we will study only the case of finite L and see how the relevant quantities behave asymptotically when $L \rightarrow \infty$. Note that in the mathematical physics literature, one usually considers directly the

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thermodynamic limit $L = \infty$ using operator algebraic techniques [31]. We will however consider the quantum information perspective of just looking at the asymptotic behavior of finite-size systems.

To make this presentation accessible to non-experts in quantum theory, we will start by quickly reviewing the main objects of interest.

Associated with each point v in the lattice Λ_L , there will be a complex Hilbert space $\mathcal{H}_v$, which we will take finite dimensional, and hence isomorphic to $\mathbb{C}^d$. The total Hilbert space of the system $\mathcal{H}_L$ will be $\bigotimes_{v \in \Lambda_L} \mathcal{H}_v$. Note that the dimension of the Hilbert space of the system grows exponentially with the system size L .

States on the system are semidefinite-positive operators ρ acting on the Hilbert space $\mathcal{H}_L$ and having $\text{tr}(\rho) = 1$. They encode all measurable properties of the system via Born's rule $\text{tr}(A\rho)$, which specifies the expected value of an observable A , when the system is in state ρ . Observables are modeled by self-adjoint operators on $\mathcal{H}_L$.

Pure states are the extreme points of the convex set of states and are therefore rank-one projectors associated with normalized vectors $|v\rangle \in \mathcal{H}_L$. In a slight abuse of notation, one usually identifies a pure state with the vector $|v\rangle$. Note that this is not a one-to-one correspondence since $\alpha|v\rangle$ ($|\alpha| = 1$) defines the same state as $|v\rangle$. We will use the standard *ket* notation $|\cdot\rangle$ for pure states. Non-pure states are called mixed states.

If the system is in state ρ but one is only interested in a subsystem, i.e., a subset $S \subset \Lambda_L$, one considers the *reduced state* ρ_S , which encodes all measurable properties of that subsystem and is defined as

$$\rho_S = (\mathbb{1}_S \otimes \text{tr}_{S^c})(\rho).$$

The operator $(\mathbb{1}_S \otimes \text{tr}_{S^c})$ is called partial trace and denoted by tr_{S^c} .

The behavior of the system is described by its *Hamiltonian* H_L , which is nothing but a self-adjoint operator that encodes the interactions between the particles and that is interpreted physically as the observable *energy*. Its eigenvalues $\lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots$ are the *energy levels* of the system. The smallest eigenvalue λ_0 is called *ground energy*, and the associated normalized eigenvectors are called *ground states*. The ground states encode all the observable properties of the system when the temperature of the system goes to 0. The difference between the two smallest eigenvalues $\gamma = \lambda_1 - \lambda_0$ is called the *spectral gap*. It can be interpreted as the energy one needs to pump into the system to change its properties from the ground state to some different *excited state*.

We will restrict our study to finite-range Hamiltonians with translation invariance. The motivation behind this is the fact that the interactions between particles usually do not depend on their position on the lattice and decay in many cases very fast with distance. Therefore, it is a sensible approximation to consider that those interactions are just 0 when the distance between the particles is larger than a given threshold R ,

which we call the interaction range. At the technical level, this hypothesis allows us to define easily the Hamiltonian H_L for all system sizes L (both with open and periodic boundary conditions) and hence to talk meaningfully about the case $L \rightarrow \infty$.

Formally, for any subset S of the lattice with diameter less than R , we will consider an interaction h_S , which is a self-adjoint operator on $\mathcal{H}_S = \bigotimes_{v \in S} \mathcal{H}_v$. In an abuse of notation, we will also call h_S its extension, tensoring with the identity operator, to the Hilbert space $\mathcal{H}_L$ of the full system. Any pair of sets S, S' which are related by a translation will have the same interaction ($h_S = h_{S'}$) under the identification by translation of the spaces $\mathcal{H}_S$ and $\mathcal{H}_{S'}$. The total Hamiltonian of the system will then be

$$H_L = \sum_{S, \text{diam}(S) \leq R} h_S.$$

1.1. The spectral gap problem and its importance

The spectral gap problem can be stated as follows. Given a family of short-range translational invariant Hamiltonians $\{H_L\}_L$, where each H_L is defined on the lattice Λ_L , how does the spectral gap γ_L behave as $L \rightarrow \infty$? In particular, we are interested in the case in which the system is *gapped*, i.e., there exists $\gamma > 0$ so that $\gamma_L \geq \gamma$ for all L .

The main historical motivation to study the spectral gap is due to the fact that it defines the notion of “quantum phase of matter” in condensed matter physics via the following informal definition: “two interactions are in the same phase if there is a smooth path of interactions connecting them so that the spectral gap remains uniformly bounded throughout the path” (see, e.g., [5] for a rigorous definition). Therefore, phase transition points are detected via a closure of the spectral gap with the system size. The intuitive idea is that the spectral gap *protects* the system from jumping into excited states with different properties, and hence one needs to *close the gap* in order to get relevant changes in the properties of the ground state. However, formalizing this intuition has turned out to be a very challenging task, particularly the crucial question of the stability of the spectral gap under small perturbations of the interactions [8, 29, 34].

The spectral gap also plays a key role in adiabatic quantum computation. In this model of quantum computation, the solution of a given problem is encoded in the ability to engineer the ground state of a target Hamiltonian. The system is initialized in the ground state of a trivial Hamiltonian, then the interactions are smoothly changed from the initial to the target one. The so-called “adiabatic theorems” show that if the parameters are changed slowly enough, then the system is kept close to the ground state throughout the path, and hence one obtains the desired solution to the computation. The total time required for the adiabatic algorithm scales as $\text{poly}(\frac{1}{\gamma_*})$,

where γ_* is the infimum of the spectral gaps of all Hamiltonians considered throughout the path. Therefore, the complexity of the algorithm is precisely characterized by the spectral gap.

We refer the reader to the review [3] for detailed information about adiabatic quantum computation, including references to several adiabatic theorems.

1.2. Content and structure

The manuscript will review two types of complementary results. In the first part, we will show that the spectral gap problem is as hard as one can imagine: it is undecidable in the sense of Turing. It will be based on [6, 15]. The proof of this negative result will strongly rely on quantum computing ideas. In the second part, we will turn to positive results. Despite being undecidable in the worst case, there are still interesting families of Hamiltonians for which the spectral gap can be decided. We will focus on a particularly interesting and wide family of models motivated by quantum information theory, the so-called *tensor networks* [13]. We will describe a sufficient condition which guarantees that the system is gapped [22] based on a holographic approach which dates back to [14]. A notable application of that result in the context of quantum computing is the proof that all Kitaev's quantum double models, despite being non-trivial topological phases of matter, are not self-correcting quantum memories in the presence of thermal noise, no matter how small the temperature is [28]. This constitutes an important step toward proving the conjecture that there cannot exist self-correcting quantum memories in 2D [9, 10, 26, 44].

Section 2 will be devoted to the undecidable results, Section 3 to the case of tensor network Hamiltonians, and finally, Section 4 to the problem of thermalization in topological quantum memories. We will introduce at the beginning of each section the necessary concepts and definitions to understand the statements of the results. We will also try to give some of the main ideas behind the proofs, but keep the presentation at a sufficiently non-technical level to be as accessible as possible for non-experts. We refer the reader to the corresponding papers for a technical exposition, including detailed proofs.

2. Undecidability of the spectral gap

2.1. Basics on computability theory

Let us recall the needed basic definitions of computability theory: Turing machines, undecidability and the halting problem.

Definition 2.1. A (deterministic) Turing machine (TM) is defined by a triple (Σ, Q, δ) , where Σ is a finite alphabet with an identified blank symbol, Q is a finite

set of internal control states with an identified initial state q_0 and final (or halting) state q_f , and δ is a transition function $\delta : Q \times \Sigma \rightarrow \Sigma \times Q \times \{L, R\}$.

The TM reads and writes in a two-way infinite tape of cells (identified with $\mathbb{Z}$) via a head which moves along the tape. The evolution of the machine is specified by its transition function δ . If the head is in a given position of the tape, δ takes as input the symbol read at that position and the internal state of the machine and specifies (i) which symbol from the alphabet Σ must be written on the tape in the current head position, (ii) which internal state from Q the machine must transition to, and (iii) where the head must move next, left (L) or right (R).

The machine keeps running until it enters the halting state. Then it stops, and the output is the set of non-blank symbols written on the tape.

We say that the TM halts on input x if, when initialized on input $x \in \Sigma^*$ written in positions $0, 1, 2, \dots$, with the head in cell 0 and internal state q_0 , it eventually enters the halting state.

It is a remarkable fact, already proven by [45], that there exist *universal* Turing machines (UTM). UTMs can simulate the behavior of any other TM T as follows. Given input x and a description of T , it halts if and only if T halts on input x , and, in that case, it produces as output the output of T when run on x .

An *undecidable problem* is a YES/NO decision problem which cannot be solved by any TM in the sense that there does not exist any TM which, given as input an instance of the problem, always halts and outputs the right answer YES or NO (identified with particular alphabet symbols).

The first and most important undecidable problem, to which most other undecidable problems reduce, is the *halting problem*, i.e., deciding whether a given TM halts or not. The undecidability of the halting problem was already proven by Turing in [45]. By the comments just made on UTMs, it is also undecidable to determine if a fixed UTM will halt on a given input x . In the following, we will fix a UTM and refer to it as *the* UTM.

2.2. Statements of results

We will state the undecidability of the spectral gap for 1D systems. In that case, we will consider the case of open boundary conditions for single-site and nearest neighbor interactions. That is, the overall Hamiltonian H_L will be given by two interaction terms $h^{(1)}$ and $h^{(2)}$, which are, respectively, operators on $\mathbb{C}^d$ and $\mathbb{C}^d \otimes \mathbb{C}^d$. The total Hamiltonian will be the sum of those local terms by translation:

$$H_L = \sum_{i=1}^{L-1} h_{i,i+1}^{(2)} + \sum_{i=1}^L h_i^{(1)}.$$

Note that we are in the open boundary condition case since we are not including the interaction $h_{L,1}^{(2)}$, which must be added for periodic boundary conditions.

The main result of [6] is a constructive proof of the following.

Theorem 2.2. *There exist (explicitly constructible) $d \times d$ matrices a, a', a'' and $d^2 \times d^2$ matrices b, b', b'', b''', b'''' with the following properties:*

- (1) *a and b are diagonal with entries in $\mathbb{Z}$, i.e., they correspond to a purely classical interaction.*
- (2) *a', a'', b', b'' are self-adjoint with entries in $\mathbb{Q}[\sqrt{2}]$, i.e., they are of the form $x + y\sqrt{2}$ with x and y being rational numbers.*
- (3) *b''', b'''' have entries in $\mathbb{Q}$.*
- (4) *For any $\eta \in \mathbb{N}$ and any rational number $0 < \beta \leq 1$ (which can be chosen arbitrarily small), define the following interaction terms with parameter η :*

$$\begin{aligned} h^{(1)}(\eta) &= a + \beta[2^{-2|\eta|}a' + a''], \\ h^{(2)}(\eta) &= b + \beta[2^{-2|\eta|}b' + b'' + e^{i\pi\phi(\eta)}b''' \\ &\quad + e^{-i\pi\phi(\eta)}b'''^\dagger + e^{i\pi 2^{-2|\eta|}}b'''' + e^{-i\pi 2^{-2|\eta|}}b''''^\dagger]. \end{aligned}$$

Here, we denote by $|\eta|$ the number of digits in the binary expansion of η , $\eta = \eta_1\eta_2 \cdots \eta_{|\eta|}$, and we define $\phi(\eta)$ to be its binary fraction with interleaved 1's, i.e., $\phi(\eta) = 0.\eta_1 1 \eta_2 1 \cdots \eta_{|\eta|-1} 1 \eta_{|\eta|}$. Then $\|h^{(1)}(\eta)\| \leq 2$, $\|h^{(2)}(\eta)\| \leq 1$ and the family of Hamiltonians $\{H_L(\eta)\}_L$ defined on Λ_L by

$$H_L(\eta) = \sum_{i=1}^{L-1} h_{i,i+1}^{(2)}(\eta) + \sum_{i=1}^L h_i^{(1)}(\eta)$$

satisfies the following:

- (a) *If the UTM does not halt on input η , then $\{H_L(\eta)\}_L$ is gapped. Moreover, the spectral gap $\gamma_L(H_L(\eta)) \geq 1$ for all $L \in \mathbb{N}$.*
- (b) *If the UTM halts on input η , then $\{H_L(\eta)\}_L$ is gapless in the following strong sense. There exists a finite interval of size c above its ground energy such that the spectrum of $H_L(\eta)$ becomes dense therein as $L \rightarrow \infty$.*

By the undecidability of the halting problem, this immediately implies that the existence of a spectral gap is undecidable for 1D Hamiltonians.

There are some remarkable comments to be made. First of all, since the interactions given by a, b are classical, and β is arbitrarily small, the result holds for

arbitrarily small quantum perturbations of classical interactions. Moreover, the physical dimension and the interactions are fixed and explicitly constructed. The only dependency in η , the input of the UTM, is in the coupling constants. Finally, there is a completely analogous result for 2D, proven in [15] (the result was announced beforehand in [16]). The main difference is that in the 2D case, one can cover the case of periodic boundary conditions, and the roles of gap and gapless are interchanged with respect to the halting property of the UTM. That is, if the UTM does not halt on input η , then $\{H_L(\eta)\}_L$ is gapless; whereas, if the UTM halts, then $\{H_L(\eta)\}_L$ is gapped.

2.3. Idea of the proof

The proof has four main steps which are shared by the 1D and 2D cases, though the details of those ingredients change substantially between the two cases, and we refer the readers to the papers [6, 15] for full details.

Step 1: Writing η on the tape. In order to feed an arbitrary input $\eta \in \mathbb{N}$ to the UTM, we need to write η on the tape. A counting argument shows that this is impossible with a *classical* TM while keeping its size (alphabet size and number of internal states) constant. This is why it is the key *quantum* step in the construction, since this will be possible with a *quantum* Turing machine (QTM), concretely with a QTM associated with the *quantum phase estimation algorithm*. To construct such a QTM, we rely strongly on the seminal results and ideas of [7]. Formally, we construct a QTM with a fixed number of internal states such that, when fed with an input given by any sequence of 1's larger than the size of η , it writes η deterministically on the tape and halts. Then, we dovetail this QTM with the UTM, which then runs on the desired input η .

The quantum phase estimation algorithm is one of the most important basic sub-routines in quantum computing [35]. Given a black-box oracle access to a unitary of the form

$$U = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi\phi i} \end{pmatrix},$$

the goal is to obtain the binary expansion of the *phase* $\phi \in [0, 1)$. As in many other quantum algorithms, the key step is the quantum Fourier transform (QFT), which has only polynomial complexity [35]. This means that the QFT is a unitary operation acting on the space of n *qubits* $(\mathbb{C}^2)^{\otimes n}$ which can be decomposed into $\text{poly}(n)$ elementary unitaries which act non-trivially only in one or two of the qubits.

In order to define the QFT, we consider the canonical basis in the space of n qubits $(\mathbb{C}^2)^{\otimes n}$, given by $e_{i_1} \otimes \cdots \otimes e_{i_n}$, which we identify with $\tilde{e}_k$. Here, k is the natural number with binary expansion $i_n \cdots i_1$, i.e., $k = \sum_{j=1}^n i_j 2^{j-1}$, and $\tilde{e}_k$ is seen

as the canonical basis of the space $\mathbb{C}^N$, with $N = 2^n$. Note that, in the basis $\tilde{e}_k$, k runs from 0 to $N - 1$. The QFT is defined by its action on $\tilde{e}_k$ as

$$\text{QFT}(\tilde{e}_k) = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{\frac{2\pi j k}{N} i} \tilde{e}_j.$$

Let us assume for simplicity that ϕ has a binary rational expansion of size n , i.e., $\phi = \sum_{j=1}^n \phi_j 2^{-j}$ (otherwise the algorithm is not exact and has some error). Let us define $\tilde{\phi} = 2^n \phi = \sum_{j=1}^n \phi_j 2^{n-j}$, which is a natural number between 0 and $N - 1$.

The idea of the quantum phase estimation algorithm is to have n ancillary qubit systems which interact with the qubit on which U acts via so-called controlled U unitaries. After an appropriate initialization, this allows us to end up, in the ancillary qubits, precisely in the state $\text{QFT}(\tilde{e}_{\tilde{\phi}})$. Therefore, after applying the inverse QFT, one recovers the state $\tilde{e}_{\tilde{\phi}}$ in the ancillary qubits. One can obtain $\tilde{\phi}$ just by measuring the qubits in the canonical basis.

Step 2: A 1D Hamiltonian whose ground state energy depends on the behavior of the UTM on input η . For this step, we need a mapping from QTM to Hamiltonians so that the ground state reflects the evolution of the QTM. In this way, by applying that mapping to the QTM that first writes η on the tape and then runs the UTM on it, we can encode the halting problem in the ground state energy. This mapping was precisely done in a remarkable paper of Gottesman and Irani [20], though some non-trivial modifications are required to make it work here. The idea of constructing Hamiltonians whose ground state reflects quantum evolutions has a long history [2, 23, 25, 36], dating back to Feynman [19], and it is one of the most important techniques in quantum complexity theory.

After this step, we have, for each $\eta \in \mathbb{N}$, a 1D translational invariant Hamiltonian whose ground state energy for a chain of size L and open boundary conditions is different depending on the behavior of the UTM on η . Depending on whether, in the construction, one penalizes halting or non-halting in the energy (both things are possible), the energy is larger or smaller in the halting and non-halting cases. In the 2D construction, the ground state energy is larger for the halting case, and in the 1D construction, it is larger in the non-halting case. The problem is that the difference in energy between the two cases is exponentially small in L . This is why we need the next step.

Step 3: Amplifying the ground state energy difference between halting and non-halting cases. This step is implemented in completely different ways in 1D and 2D. The key ingredient is to have infinitely many well-identified segments of sufficiently large size so that the UTM has enough tape and time to halt (in the Hamiltonian

encoding of Step 2). Since the halting time is an uncomputable function, the easiest solution is to get segments of arbitrarily large lengths. This is the route taken in the 2D case, where we rely on an aperiodic tiling construction due to Robinson [40] to guarantee the existence of those segments.

In 1D, aperiodic tilings do not exist, and hence one needs a different construction. The key technical lemma, which has interest on its own, is the construction of a 1D translational invariant Hamiltonian whose ground state has a periodic structure whose period is exactly the halting time of the UTM on input η . This is remarkable since the given 1D Hamiltonian is explicitly constructed, but the periodic structure in its ground state is uncomputable.

After this step, we manage to make the energy difference between halting and non-halting diverging to ∞ as $L \rightarrow \infty$.

Step 4: From ground state energy difference to spectral gap. The final step combines the *undecidable* Hamiltonian constructed in Step 3 with (i) a trivial Hamiltonian having product ground state and constant gap and (ii) a critical Hamiltonian having spectrum that becomes dense in $[0, \infty)$. It is not difficult to find a way to couple these Hamiltonians so that the resulting spectrum has the properties required by Theorem 2.2.

3. Spectral gap for tensor network parent Hamiltonians

The theory of tensor networks (TN) lies at the intersection of quantum information theory and condensed matter physics as an ansatz to describe accurately low-energy states of short-range quantum Hamiltonians. The origin of TN can be traced back to three seminal papers in the late 1980s and early 1990s: the definition of the *AKLT model* [1], its generalization via *finitely correlated states* [18], currently known as matrix product states (MPS), and the proposal of the *DMRG algorithm* [48], which turned out to be a variational optimization of the energy in the family of MPS.

Since then, TN theory has shown its power on two fronts. Numerically, it has motivated several algorithms to simulate quantum many-body systems that are now the state of the art in the field. Analytically, it has provided mathematically rigorous results in the study and classification of quantum phases of matter. Very recently, TN have started to find applications in a wide variety of other fields, ranging from machine learning to quantum gravity or quantum computing.

We refer the reader to the reviews [13, 37, 46] for more information about, respectively, the numerical aspects of TN, the application of TN in a wide number of different areas, and the mathematically rigorous results on TN, both regarding their

ability to approximate low-energy states of quantum Hamiltonians and their use to classify quantum phases of matter.

3.1. Basics on tensor networks

Here, we will restrict our attention to the family of tensor networks known as projected entangled pair states (PEPS), whose 1D version is precisely the family of MPS. There are several equivalent ways to define PEPS, and we refer to [13] for a deeper introduction to them. Here, we will mainly follow the presentation of [43]. Let us start with the 1D case, which is easier to describe.

Definition 3.1. Given a set of d matrices $A_1, \dots, A_d$ of dimension $D \times D$, we define its associated matrix product state (MPS) of size L , $|\Psi_A^L\rangle$, as the normalized pure state proportional to

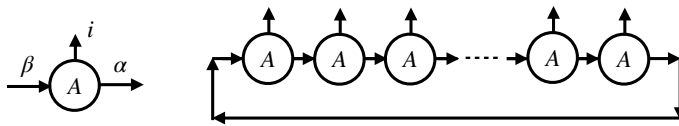
$$\sum_{i_1, \dots, i_L} \text{tr}(A_{i_1} A_{i_2} \cdots A_{i_L}) e_{i_1} \otimes e_{i_2} \otimes \cdots \otimes e_{i_L}$$

(where one is implicitly assuming that the last expression is non-zero).

The subindex A in the notation $|\Psi_A^L\rangle$ refers to the fact that the MPS is determined by the tensor

$$A = \sum_{i, \alpha, \beta} (A_i)_{\alpha, \beta} e_i \otimes e_\alpha \otimes e_\beta^*.$$

We will represent tensor A with the following graphical notation, where the arrow represents whether we are considering a Hilbert space or its dual, and different legs correspond to different tensor components. That is, we are looking at the tensor as a linear map from the ingoing systems to the outgoing ones. Indices α, β are called *virtual*, and D is called virtual or bond dimension. Index i is the *physical* index, and d is called the physical dimension of tensor A ; i.e., for each vertex v , $\mathcal{H}_v = \mathbb{C}^d$.



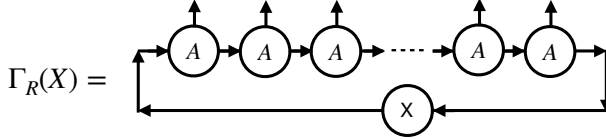
Given an MPS, one can define an associated *parent Hamiltonian* as follows. Take a region of R consecutive sites and define the space

$$\mathcal{G}_R = \left\{ \sum_{i_1, \dots, i_R} \text{tr}(X A_{i_1} A_{i_2} \cdots A_{i_R}) e_{i_1} \otimes e_{i_2} \otimes \cdots \otimes e_{i_R} : X \in \mathcal{M}_{D \times D} \right\}.$$

This is nothing but the image of $\Gamma_R : \mathcal{M}_{D \times D} \rightarrow \bigotimes_{v \in R} \mathcal{H}_v$ given by

$$X \mapsto \sum_{i_1, \dots, i_R} \text{tr}(X A_{i_1} A_{i_2} \cdots A_{i_R}) e_{i_1} \otimes e_{i_2} \otimes \cdots \otimes e_{i_R}.$$

One can understand Γ_R as a map between Hilbert spaces by considering in $\mathcal{M}_{D \times D}$ the Hilbert–Schmidt scalar product $\text{tr}(A^* B)$.



The interaction h_R is defined as the projection onto the orthogonal complement of $\mathcal{G}_R$. The parent Hamiltonian H_L is just the sum for all sets of R consecutive sites of those interactions h_R . It is clear from the definition that

- (1) each $h_R \geq 0$ (meaning semidefinite positive), and hence $H_L \geq 0$,
- (2) $h_R |\Psi_A^L\rangle = 0$ and hence $H |\Psi_A^L\rangle = 0$.

This implies immediately that $|\Psi_A^L\rangle$ is the ground state of H_L . It also implies that the Hamiltonian is frustration-free. That is, $|\Psi_A^L\rangle$ is the ground state of each one of the local interactions h_R defining the global Hamiltonian H_L .

It is a non-trivial question, related to quantum analogues of the classical Wielandt inequality [41] and the so-called *canonical form* of the tensor A , to determine the smallest R so that the MPS $|\Psi_A^L\rangle$ is the unique (or almost unique) ground state of H_L . We refer the reader to [12, 13] for further information. Here, we just state that if R_0 is the smallest size which makes the map Γ_{R_0} injective (assuming it exists), then taking $R > R_0$ is enough to guarantee that the given MPS is the unique ground state of its parent Hamiltonian. Such R_0 is usually called the injectivity length. In this case, one can also prove that the parent Hamiltonian is always gapped [18].

Given an MPS associated with tensor A and a region R , one can also consider the important concept of *boundary state*, as $\rho_{\partial R} = \Gamma_R^* \Gamma_R$. By its very definition, ρ_R is a semidefinite-positive operator on the Hilbert space $\mathcal{M}_{D \times D}$ associated with the boundary of region R . Note that $\rho_{\partial R}$ lives in the virtual degrees of freedom of the MPS.

The definition of PEPS in two (and higher) dimensions is analogous. For simplicity, we will restrict just to the 2D case.

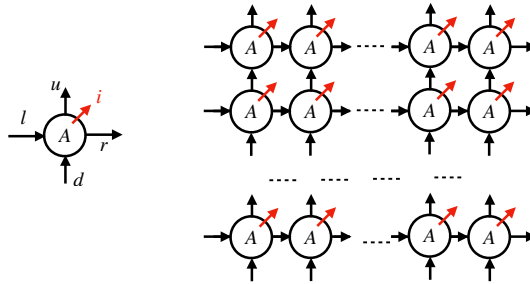
Definition 3.2. Given a set of d tensors $A_1, \dots, A_d$ of degree 4 and dimension $D \times D \times D \times D$, we define its associated projected entangled pair state (PEPS) of

size L as the normalized state $|\Psi_A^L\rangle$ of $\mathcal{H}_L = \bigotimes_{v \in \Lambda_L} \mathcal{H}_v$ proportional to the vector obtained by contracting the tensor

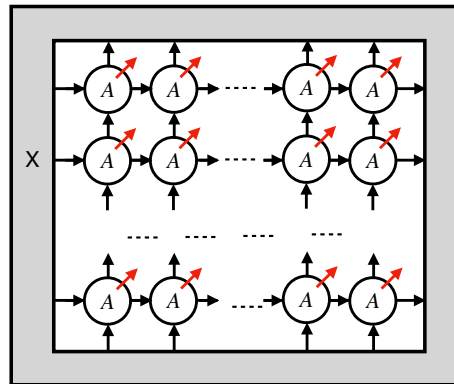
$$A = \sum_{i,u,l,d,r} (A_i)_{\alpha,\beta} e_i \otimes e_u \otimes e_r \otimes e_d^* \otimes e_l^* \quad (3.1)$$

on the square lattice Λ_L , where one takes periodic boundary conditions (assuming such a vector is non-zero).

The indices u, r, d, l stand for up, right, down, left, indicating the leg they refer to in the following diagrammatic notation, where, as in the 1D case, joining legs indicate the implementation of the duality mapping between one space and its dual.



Given a region $R \in \Lambda_L$, which we take to be a square for simplicity, we define, as in the 1D case above, the map $\Gamma_R : \bigotimes_{e \in \partial R} (\hat{\mathcal{H}}_e) \rightarrow \bigotimes_{v \in R} \mathcal{H}_v$ assigning to a boundary condition X in the virtual boundary of R the corresponding vector (or unnormalized state) in R . (Here, $\hat{\mathcal{H}}_e$ denotes the Hilbert space isomorphic to $\mathbb{C}^D$ corresponding to edge e .) Diagrammatically, $\Gamma_R(X)$ is given as follows.



Following the MPS case, we define $\mathcal{G}_R$ as the image of Γ_R and h_R as the interaction given by the projection onto the orthogonal complement of $\mathcal{G}_R$. The associated,

frustration-free, parent Hamiltonian is obtained by translating h_R throughout the lattice Λ_L , where we are taking periodic boundary conditions.

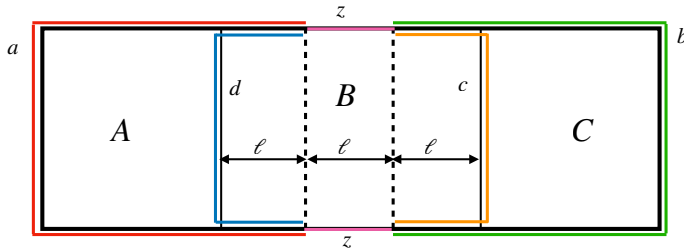
As in the 1D case, if R_0 is a square region of size $L_0 \times L_0$, where Γ_{R_0} is injective (assuming it exists), and if one defines the parent Hamiltonian interaction h_R by taking R of size $(L_0 + 1) \times (L_0 + 1)$, then the given PEPS $|\Psi_A^L\rangle$ will be the unique ground state [39]. We will refer to this situation as the “injective case”.

One can also define in this case the boundary state of a region R by $\rho_{\partial R} = \Gamma_R^* \Gamma_R$, which is an unnormalized mixed state in the virtual Hilbert space of the boundary of R , $\bigotimes_{e \in \partial R} \mathcal{H}_e$.

3.2. Sufficient condition for gap in PEPS parent Hamiltonians

Unfortunately, even if one restricts to PEPS parent Hamiltonians, the spectral gap problem remains undecidable [42]. This forces one to restrict to particular subfamilies of PEPS and/or to aim at just the necessary or sufficient conditions for the existence of gap.

Among the most important necessary conditions for gap is the property that correlations in the ground state must decay exponentially with the distance [21, 33]. This already shows that, in the 2D case, parent Hamiltonians of PEPS are not always gapped, even in the injective case, since there exist PEPS with power-law decaying correlations [47]. Here, we will focus on a sufficient condition for gap at the level of the boundary state $\rho_{\partial R}$. The holographic perspective in PEPS, where global properties, like the gap, are characterized by properties of the boundary, which is 1D and hence simpler, has been very successful, as illustrated extensively in the recent review [13]. For the particular case of the gap, it was conjectured by numerical evidence in [14] that gap should be related to some form of *locality* of the boundary state. This was later formalized in [22] via the notion of *approximate factorization*. For that, we consider regions of the form given by the following figure.



Definition 3.3. A given PEPS has factorizable boundary if there exists a function $\xi(\ell)$ which decays to 0 at least polynomially fast (i.e., $\xi(\ell) \leq C \ell^{-\alpha}$ for constants $C, \alpha > 0$) so that for regions ABC as in the figure, there exist states $\sigma_{\partial AB}$, $\sigma_{\partial B}$,

$\sigma_{\partial BC}, \sigma_{\partial ABC}$ which factorize as follows:

$$\sigma_{\partial AB} = \Omega_{zc} \Delta_{az}, \quad \sigma_{\partial B} = \Omega_{zc} \Omega_{dz}, \quad \sigma_{\partial BC} = \Delta_{zb} \Omega_{dz}, \quad \sigma_{\partial ABC} = \Delta_{zb} \Delta_{az},$$

with $\Delta_{az}, \Delta_{zb}, \Omega_{dz}, \Omega_{zc}$ invertible matrices, and such that they approximate the true boundary states $\rho_{\partial AB}, \rho_{\partial B}, \rho_{\partial BC}, \rho_{\partial ABC}$ as follows:

$$\begin{aligned} \left\| \rho_{\partial R}^{\frac{1}{2}} \sigma_{\partial R}^{-1} \rho_{\partial R}^{\frac{1}{2}} - \mathbb{1} \right\| &\leq \xi(\ell) \quad \text{for } R \in \{AB, BC, ABC\}, \\ \left\| \rho_{\partial B}^{-\frac{1}{2}} \sigma_{\partial B} \rho_{\partial B}^{-\frac{1}{2}} - \mathbb{1} \right\| &\leq \xi(\ell). \end{aligned}$$

One of the main theorems of [22] is as follows.

Theorem 3.4. *In the injective case, the parent Hamiltonian of a PEPS has gap if the PEPS has factorizable boundary.*

Versions of this theorem also apply beyond the injective case; examples include the so-called MPO-injective PEPS (proven in [22]), which are generalizations of the G -isometric PEPS considered in Section 4.1, as well as the general case where the boundary states have a stronger form of approximate factorization: the operators $\sigma_{\partial R}$ appearing in Definition 3.3 have tensor product form and are full rank in the support of the corresponding boundary states $\rho_{\partial R}$ (see [28] for details). This latter case is the one that will be used in Section 4; there, we will refer to it simply as Theorem 3.4.

The proof of Theorem 3.4 is done by reducing to the so-called *martingale condition*, which in turn implies gap as proven in [32]. The reason that the boundary state is so closely related to the Hamiltonian can be easily understood from the fact that, in the injective case, the Hamiltonian is defined precisely via the boundary state:

$$h_R = \mathbb{1} - k_R, \quad \text{with } k_R = \Gamma_R \rho_{\partial R}^{-1} \Gamma_R^*.$$

To see it, just observe that, by definition, k_R , and hence h_R , is self-adjoint. Moreover,

$$k_R^2 = \Gamma_R \rho_{\partial R}^{-1} \underbrace{\Gamma_R^* \Gamma_R}_{\rho_{\partial R}} \rho_{\partial R}^{-1} \Gamma_R^* = k_R.$$

So k_R , and hence h_R , is a projector. Finally, it is clear from the definition that the support of k_R (and hence the kernel of h_R) is exactly the image of Γ_R .

4. Thermalization in topological quantum memories

4.1. Topological order in PEPS

One of the main advantages of PEPS as a way to represent low-energy quantum states is that they allow the characterization of global properties of interest in the

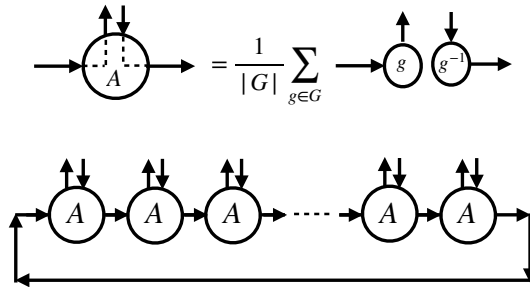
local tensor A (3.1) which defines the state. This has been particularly successful for topological order, which turns out to emerge from symmetries of the tensor A . In the most general case, those symmetries come from finite-dimensional weak Hopf algebras [11, 30]. Here, we will restrict to the particular, and simpler, case of finite groups G , leading to the notion of G -isometric PEPS defined in [43].

In topologically ordered systems, the dimension of the subspace of ground states (called ground space) in the torus is strictly larger than one. On top of that, the key feature is that all ground states are locally indistinguishable, meaning that they have exactly the same reduced state ρ_S in all contractible regions S of the torus Λ_L .

This makes those systems good candidates for quantum memories, where the encoded Hilbert space is the ground space. Topological order implies that only global operations, acting non-trivially in non-contractible regions of the torus, can affect the information encoded in the memory.

A good proxy to understand G -isometric PEPS and why they have topological order is their 1D analogue, the family of G -isometric MPS.

Definition 4.1. Given a finite group G , define the tensor $A = \frac{1}{|G|} \sum_{g \in G} L_g \otimes L_{g^{-1}}$, where L_g stands for the left regular representation. Note that now both the virtual and physical systems are seen as matrix spaces endowed with the Hilbert–Schmidt scalar product as in the figure (for simplicity, we use the notation g to represent the operator L_g). The associated MPS is called the G -isometric MPS.



For each $g \in G$, we define the (unnormalized) MPS with g -boundary condition as

$$|\Psi_A^g\rangle = \sum_{i_1, \dots, i_L} \text{tr}(L_g A_{i_1} A_{i_2} \cdots A_{i_L}) e_{i_1} \otimes e_{i_2} \otimes \cdots \otimes e_{i_L}.$$

Those states are also translational invariant since the operator L_g can be pulled through the tensor A .

$$\begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} \begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} A \begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} = \begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} A \begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} g \begin{array}{c} \uparrow \downarrow \\ \circlearrowleft \end{array} \quad (4.1)$$

Proposition 4.2. *The family of G -isometric MPS fulfills the following properties:*

(i) *The parent Hamiltonian is nearest neighbor, and the interaction between consecutive sites $i, i + 1$ is given by $\mathbb{1}_i \otimes \mathbb{1}_{i+1} - k_{i,i+1}$, where, for a given region R , $k_R = \Gamma_R \Gamma_R^*$.*

(ii) *The terms of the parent Hamiltonian commute. Moreover,*

$$k_{i,i+1} k_{i+1,i+2} = k_{i+1,i+2} k_{i,i+1} = k_{i,i+1,i+2}.$$

(iii) *The set of ground states of the global Hamiltonian H_L is spanned by the set $\{|\Psi_A^g\rangle : g \in G\}$, where $|\Psi_A^g\rangle$ and $|\Psi_A^h\rangle$ are equal if g and h are in the same conjugacy class and are orthogonal otherwise.*

It is instructive to prove this proposition, since the more interesting 2D case follows along similar ideas, but proofs are easier to illustrate in 1D. The proof also shows the power of the graphical notation.

Proof. From the definition, it is clear that $k_{i,i+1}$ is self-adjoint. That it is a projector and leaves the G -isometric MPS invariant is a trivial consequence of the following graphical equation:

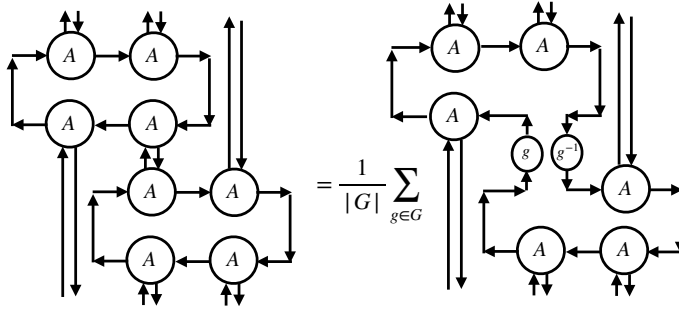
$$\begin{aligned}
 & \text{Diagram 1: A } 2 \times 2 \text{ grid of circles labeled } A. \text{ The top two circles are enclosed in a red box labeled } k_{i,i+1}. \text{ Arrows connect the circles horizontally and vertically.} \\
 & = \frac{1}{|G|^2} \sum_{g,h \in G} \text{Diagram 2: A diagram with two rows of } A \text{ circles. The top row has two } A \text{ circles. The bottom row has three circles: } g, h, h^{-1}. \text{ The } g \text{ and } h \text{ circles are enclosed in a red box labeled } \delta_{g,h}. \text{ Arrows connect the } A \text{ circles and the } g, h, h^{-1} \text{ circles.} \\
 & = \frac{1}{|G|} \sum_{g \in G} \text{Diagram 3: A diagram with two } A \text{ circles. The first } A \text{ circle is preceded by a } g \text{ circle and followed by a } g^{-1} \text{ circle. Arrows connect the } A \text{ circles and the } g, g^{-1} \text{ circles.} \\
 & = \text{Diagram 4: A diagram with two } A \text{ circles. Arrows connect the } A \text{ circles.}
 \end{aligned} \tag{4.2}$$

where in the last equality, we have used the pulling through equation (4.1), and in the first equality, we are using the orthogonality properties of the left regular representation

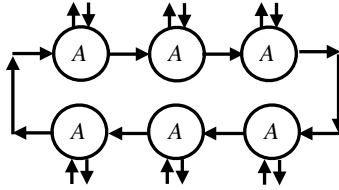
$$\frac{1}{|G|} \text{tr}(L_{g^{-1}} L_h) = \delta_{g,h}.$$

Note that, in particular, this argument shows that the boundary state of a region R of consecutive spins is exactly given by $\rho_{\partial R} = \frac{1}{|G|} \sum_{g \in G} L_g \otimes L_{g^{-1}}$, where the tensor product structure now refers to the left and right boundaries of the region.

That $k_{1,2}k_{2,3} = k_{1,2,3}$ is proven as follows. Diagrammatically, the operator $k_{1,2}k_{2,3}$ can be written as follows.



By using the pulling through equation (4.1), this equals



which is nothing but $k_{1,2,3}$. A similar argument shows that $k_{2,3}k_{1,2} = k_{1,2,3}$.

A similar argument proves that $K_L = \prod_{i=1}^L k_{i,i+1}$ equals $\sum_{g \in G} |\Psi_A^g\rangle \langle \Psi_A^g|$. Since the set of states stabilized by K_L is exactly the set of ground states of H_L , one concludes the first part of (iii). The pulling through equation (4.1) enforces that if g and h are in the same conjugacy class, $|\Psi_A^g\rangle$ and $|\Psi_A^h\rangle$ define the same state. That they are orthogonal otherwise can be seen as follows. By employing similar arguments with the graphical notation, it is not difficult to see that

$$\langle \Psi_A^h | \Psi_A^k \rangle = \frac{1}{|G|} \sum_g \text{tr}(L_g L_{h^{-1}} L_{g^{-1}} L_k)$$

which is 0 if h and k are not in the same conjugacy class. ■

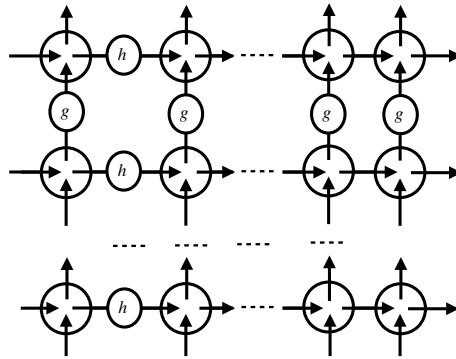
We can now turn to the definition of G -isometric PEPS.

Definition 4.3. Given a finite group G , define the tensor as follows.

$$A = \frac{1}{|G|} \sum_{g \in G} L_g \otimes L_g \otimes L_{g^{-1}} \otimes L_{g^{-1}} = \text{---} \bigcirc \text{---} = \frac{1}{|G|} \sum_{g \in G} \text{---} \bigcirc \text{---}$$

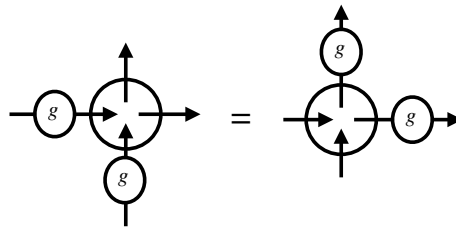
As in the 1D case, both the virtual and physical systems are seen as matrix spaces endowed with the Hilbert–Schmidt scalar product. In this case, the arrows in the interior of the circle correspond to the physical degrees of freedom. The associated PEPS are called the G -isometric PEPS.

The following theorem, proven in [43], summarizes some of the properties of G -isometric PEPS. Note the extra property (iv) with respect to Proposition 4.2, which is the one associated with topological order. In the theorem, $|\Psi_A^{(g,h)}\rangle$ refers to the state associated with the following diagram with periodic boundary conditions.



As shown in [43], states $|\Psi_A^{(g,h)}\rangle$, with $gh = hg$, are precisely the ground states of Kitaev's quantum double model associated with group G [24].

Similarly to the 1D case, the pulling through equation associated with tensor A



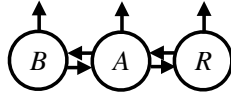
together with the fact that g commutes with h implies that the positions of strings associated with g and h in the definition of $|\Psi_A^{(g,h)}\rangle$ can be moved freely.

Theorem 4.4. *The set of G -isometric PEPS enjoys the following properties:*

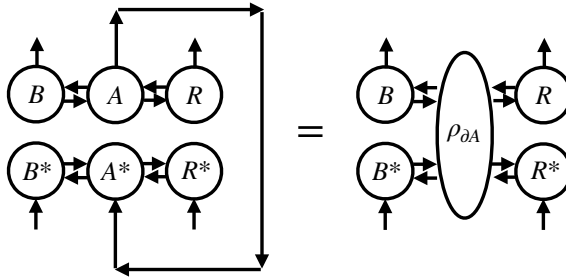
- (i) *The parent Hamiltonian acts on plaquettes, and the interaction on a plaquette p is given by $\mathbb{1} - k_p$, where, for a region R , we define $k_R = \Gamma_R \Gamma_R^*$.*
- (ii) *The terms of the parent Hamiltonian commute with each other. Indeed, for overlapping plaquettes p, q , $k_p k_q = k_q k_p = k_{p \cup q}$.*

- (iii) The set of ground states of the global Hamiltonian H_L is spanned by the set $\{|\Psi_A^{(g,h)}\rangle : (g, h) \in G, gh = hg\}$, where $|\Psi_A^{(g,h)}\rangle$ and $|\Psi_A^{(g',h')}\rangle$ are equal if (g, h) and (g', h') are in the same pair-conjugacy class, meaning that there exists $k \in G$ with $g' = kgk^{-1}$, $h' = khk^{-1}$, and they are orthogonal otherwise.
- (iv) All states $|\Psi_A^{(g,h)}\rangle$ are indistinguishable in the bulk, in the sense that they have the same reduced state in any contractible region of the torus Λ_L .

The proof of (i)–(iii) is identical to the corresponding 1D cases of Proposition 4.2. Item (iv) can be proven by the following argument. Take a contractible region R and assume it to be a square for simplicity. One can pull the strings of g and h out of the region R . Let us separate the lattice Λ_L into three regions, R , the sites in the annulus next to R , call it A , and the rest of the lattice B . By blocking the tensors in each region of the PEPS, we have the following tripartite tensor network.



The reduced density matrix associated with region $R \cup B$ is given by the following diagram:



where the middle tensor corresponds precisely to the boundary state of region A , which is easily seen to be

$$\frac{1}{|G|} \sum_g \tilde{L}_g^{\text{out}} \otimes \tilde{L}_g^{\text{in}}.$$

Here, $\tilde{L}_g^{\text{out}}$ is a tensor product over all edges connecting A with B of elements of the form L_g (or $L_{g^{-1}}$ depending on the orientation of the edge). The operator $\tilde{L}_g^{\text{in}}$ is defined analogously for the edges connecting A with R . The operator $\tilde{L}_g^{\text{in}}$ can be pulled through region R and disappears, exactly as it happened in figure (4.2). Therefore, the reduced density matrix for region $R \cup B$ is of the form $\rho_B \otimes \rho_R$, where ρ_R is exactly proportional to $k_R = \Gamma_R \Gamma_R^*$ and therefore the same for all ground states.

4.2. Lifetime of quantum memories

Motivated by the possibility of having a self-correcting quantum memory, i.e., one for which there is no need to implement active error correction, there has been an intensive search for topologically ordered quantum systems which could keep the quantum information stored in the ground state subspace for times which scale exponentially with the system size. One usually considers the case of thermal noise, where the temperature is low enough, but finite and independent of the system size.

It has been conjectured, based on arguments about energy barriers, that in 2D, self-correcting quantum memories cannot exist [9, 27]. However, this has only been rigorously proven for particular models [4, 26, 44]. We refer to [10] for a review on the topic.

The standard model for thermal noise is given by Davies dynamics [17]. This is a semigroup of completely positive trace-preserving maps $e^{\mathcal{L}_\beta t}$ defined on the set of states of the system. As usual, β corresponds to the inverse temperature. The specific form of the infinitesimal generator $\mathcal{L}_\beta$, called Lindbladian, is irrelevant for this paper. Its explicit form can be found in [28], where one considers, instead of the parent Hamiltonian of the G -isometric PEPS, the original Kitaev's Hamiltonian [24] which has the same ground space and similar properties.

The Lindbladian $\mathcal{L}_\beta$ is in our case finite range and translational invariant, so one can define the semigroup $e^{\mathcal{L}_\beta t}$ for all Λ_L . The semigroup $e^{\mathcal{L}_\beta t}$ has as a unique fixed point the thermal state of Kitaev's Hamiltonian H at inverse temperature β , i.e.,

$$\sigma_\beta = \frac{e^{-\beta H}}{\text{tr}[e^{-\beta H}]}.$$

In the thermal state, all information encoded in the ground space is washed out. Therefore, understanding the lifetime of the quantum memory given by G -isometric PEPS (when considering Kitaev's Hamiltonian on them) boils down to estimating the mixing time of the associated Davies semigroup. By standard arguments [28], it is enough to give a bound on the spectral gap of $-\mathcal{L}_\beta$, independently of the system size, to ensure that the system is not a self-correcting quantum memory, since this would imply that, for any fixed ε , the time needed to guarantee that

$$\sup_{\rho_0} \|e^{\mathcal{L}_\beta t}(\rho_0) - \sigma_\beta\|_1 \leq \varepsilon \quad (4.3)$$

scales only polynomially with the size of the system L . The norm considered in (4.3) is the trace norm $\|A\|_1 = \text{tr}[(AA^*)^{\frac{1}{2}}]$, which is the natural norm to measure distances between quantum states. Note that if two states are ε -close in trace norm, by the duality between trace and operator norms and Born's rule, both give ε -close expectation values for every observable which is normalized in operator norm.

The spectral gap for $-\mathcal{L}_\beta$ was proven so far only for the case of abelian groups [4, 26, 44], but the case of non-abelian ones remained open. Note that only non-abelian groups allow for universal topological quantum computation. The main contribution of [28] is precisely to extend the result to all finite groups.

Theorem 4.5. *For any finite group G , and any inverse temperature β , there exists a constant γ so that for any Λ_L , the spectral gap of $-\mathcal{L}_\beta$ is lower bounded by γ .*

The proof goes as follows. If we consider σ_β as a vector in $\bigotimes_{v \in \Lambda_L} \mathcal{M}_{d \times d}$ with the Hilbert–Schmidt scalar product in each $\mathcal{M}_{d \times d}$, the fact that the terms in the Hamiltonian commute with each other implies that σ_β is a PEPS, which we call $|\sigma_\beta\rangle$. One can then consider its parent Hamiltonian H_β . Note that this is very different from the parent or Kitaev Hamiltonians for the original G -isometric PEPS. In particular, the interaction terms of this Hamiltonian H_β do not commute with each other. The key insight, which somehow traces back to [47], is the following.

Lemma 4.6. *The operator $-\mathcal{L}_\beta$ has gap if H_β has gap.*

One can then use Theorem 3.4 to reduce the problem to proving that the boundary states of the PEPS $|\sigma_\beta\rangle$ have the appropriate approximate factorization property (see comments below Theorem 3.4). This is the technical part of the proof of Theorem 4.5.

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