Sample-efficient learning of quantum many-body systems

Anurag Srinivasan Tomotaka Mehdi Anshu* Arunachalam[†] Kuwahara[‡] Soleimanifar[§]

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Abstract

We study the problem of learning the Hamiltonian of a quantum many-body system given samples from its Gibbs (thermal) state. The classical analog of this problem, known as learning graphical models or Boltzmann machines, is a well-studied question in machine learning and statistics. In this work, we give the first sample-efficient algorithm for the quantum Hamiltonian learning problem. In particular, we prove that polynomially many samples in the number of particles (qudits) are necessary and sufficient for learning the parameters of a spatially local Hamiltonian in ℓ_2 -norm.

Our main contribution is in establishing the strong convexity of the log-partition function of quantum many-body systems, which along with the maximum entropy estimation yields our sample-efficient algorithm. Classically, the strong convexity for partition functions follows from the Markov property of Gibbs distributions. This is, however, known to be violated in its exact form in the quantum case. We introduce several new ideas to obtain an unconditional result that avoids relying on the Markov property of quantum systems, at the cost of a slightly weaker bound. In particular, we prove a lower bound on the variance of quasi-local operators with respect to the Gibbs state, which might be of independent interest. Our work paves the way toward a more rigorous application of machine learning techniques to quantum many-body problems.

^{*}Institute for Quantum Computing and Department of Combinatorics and Optimization, University of Waterloo, Canada and Perimeter Institute for Theoretical Physics, Canada. aanshu@uwaterloo.ca

[†]IBM Research. Srinivasan.Arunachalam@ibm.com

[‡]Mathematical Science Team, RIKEN Center for Advanced Intelligence Project (AIP), Japan and Interdisciplinary Theoretical & Mathematical Sciences Program (iTHEMS) RIKEN, Japan. tomotaka.kuwahara@riken.jp

[§]Center for Theoretical Physics, MIT. mehdis@mit.edu

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1 Introduction

The success of machine learning algorithms in analyzing high-dimensional data, has resulted in a surge of interest in applying these algorithms to study quantum many-body systems whose description requires dealing with an exponentially large state space. One important problem in this direction is the quantum Hamiltonian learning problem, which has been the focus of many recent theoretical and experimental works [BAL19, BGP+20, WGFC14b, WGFC14a, EHF19, WPS+17]. Here, one would like to learn the underlying Hamiltonian of a quantum system given multiple identical copies of its Gibbs (thermal) state. The classical analog of this problem is a central problem in machine learning and modern statistical inference, known as learning graphical models or Boltzmann machines (aka Ising models). Classically, understanding the learnability of Boltzmann machines was initiated by the works of Hinton and others in the 80s [AHS85, HS⁺86]. In the past few years, there has been renewed interest in this subject and has seen significant progress resulting in efficient provable learning algorithms for graphical models with optimal sample and time complexity especially for sparse and bounded-degree graphs [Bre15, KM17, VMLC16, HKM17, RWL+10]. Thus far, a rigorous analysis of the quantum Hamiltonian learning problem with guaranteed sample complexity has been lacking. The main contribution of this work is to provide the first sample-efficient algorithm for this task.

We now introduce the quantum Hamiltonian learning problem. Consider a κ -local Hamiltonian H acting on n qudits. In general, we can parameterize H by

$$H(\mu) = \sum_{\ell=1}^{m} \mu_{\ell} E_{\ell}$$

where $\mu_{\ell} \in \mathbb{R}$ and the operators E_{ℓ} are Hermitian and $\{E_{\ell}\}$ forms an orthogonal basis for the space of operators. For instance in the case of qubits, E_{ℓ} are tensor product of at most κ Pauli operators that act non-trivially only on spatially contiguous qubits. We let the vector $\mu = (\mu_1, \dots, \mu_m)^{\top}$ be the vector of *interaction coefficients*. In our setup, without loss of generality we assume the Hamiltonian is traceless, i.e., for the identity operator $E_{\ell} = \mathbb{1}$, the coefficient $\mu_{\ell} = 0$. At a *inverse-temperature* β , the qudits are in the *Gibbs state* defined as

$$\rho_{\beta}(\mu) = \frac{e^{-\beta H(\mu)}}{\operatorname{tr}[e^{-\beta H(\mu)}]}.$$

In the learning problem, we are given multiple copies of $\rho_{\beta}(\mu)$ and can perform arbitrary *local* measurements on them. In particular, we can obtain all the κ -local marginals of $\rho_{\beta}(\mu)$ denoted by

$$e_{\ell} = \operatorname{tr}[\rho_{\beta}(\mu)E_{\ell}] \quad \textit{for } \ell \in [m].$$

The goal is to learn the coefficients μ_{ℓ} of the Hamiltonian H using the result of these measurements. We call this the Hamiltonian Learning Problem. Before stating our main results, we provide further motivations for looking at this problem.

Physics perspective. Quantum many-body systems consist of many quantum particles (qudits) that *locally* interact with each other. The interactions between these particles are described by the Hamiltonian of the system. Even though the interactions in the Hamiltonian are local, the state of the whole system can be highly *entangled*. This is not only true at low temperatures when the

system is in the lowest energy eigenstate of its Hamiltonian (the ground state), but remains true even at finite temperatures when the state is a mixture of different eigenstates of the Hamiltonian known as the Gibbs or thermal state.

While the underlying fundamental interactions in these systems are long known to be given by Coulomb forces between electrons and nuclei, they are too complicated to be grasped in entirety. Physicists are primarily interested in "effective interactions" that, if accurately chalked out, can be used to describe a variety of properties of the system. How can such effective interactions be learned in a system as complicated as, for example, the high temperature superconductor? Algorithms for Hamiltonian learning can directly address this problem and provide a suitable approximation to the effective interactions.

Verification of quantum devices. The size of the available quantum computers is increasing and they are becoming capable of running more intricate quantum algorithms or preparing highly entangled states over larger number of qubits. Due to the noise in these devices, a major challenge that accompanies the scalable development of quantum devices is to efficiently *certify* their functionality. In recent times, one widely used subroutine in quantum algorithms is *quantum Gibbs sampling*. Preparing and measuring the Gibbs state of a given Hamiltonian is used in quantum algorithms for solving semi-definite programs [BS17, AGGW20, BKL+17, AG18, BKF19], quantum simulated annealing [Mon15b, HW20], metropolis sampling [TOV+11], quantum machine learning [WKS14], or quantum simulations at finite temperature [MST+20]. Given near term quantum devices will be noisy, an important problem when implementing these quantum subroutines is to certify the performance of the quantum Gibbs samplers and to calibrate them. More specifically, it would be ideal to have a *classical* algorithm that given samples from the output of a Gibbs sampler determines if the correct Hamiltonian has been implemented.

Quantum machine learning for quantum data. A popular family of models for describing classical distributions are graphical models or Markov random fields. These models naturally encode the causal structure between random variables and have found widespread applications in various areas such as social networks, computer vision, signal processing, and statistics (see [RWL $^+$ 10] for a survey). A simple and extremely well-studied example of such a family is the classical *Ising model* (also known as the *Boltzmann machine*) defined over a graph whose vertices correspond to the random variables x_i . A natural distribution that one can associate to this model is

$$\Pr[X = x] = \frac{1}{Z} \exp\left(\sum_{i \sim j} J_{ij} x_i x_j + \sum_i h_i x_i\right) \tag{1}$$

where J_{ij} , $h_i \in \mathbb{R}$ are real coefficients and the normalization factor Z is called the *partition function*. This distribution in Eq. (1) is also known as the *Gibbs distribution*. There is a rich body of work on learnability of Ising models given samples from the Gibbs distribution. Remarkably, a sequence of works concluded in showing a classical *efficient* algorithm with a running time quadratic in the number of vertices that outputs estimates of the coefficients J_{ij} and h_i [Bre15, KM17, VMLC16]. Similar results have been also proved for more general graphical models.

Considering these achievements in learning theory and the broad practical application of machine learning algorithms, there has been a rising interest in connecting these techniques to problems in quantum computing and many-body physics. This along with other related problems is loosely referred to as *quantum machine learning*. Is there a natural problem that we can rigorously

establish such a connection for it? Thus far, almost-all the proposals we are aware of in this direction are mostly based on heuristic grounds. One proposal that stands out due to its similarity to the classical case is the problem of learning quantum Ising model (aka quantum Boltzmann machine) or more generally the Hamiltonian Learning Problem.

In this paper, we rigorously show that by applying tools from statistics and machine learning such as maximum entropy estimation, one can get a sample complexity for the Hamiltonian Learning Problem that is *polynomial* in the number of qudits. To the best of our knowledge, this is the first such result that unconditionally obtains a non-trivial sample complexity. We believe our work opens the doors to further study of this problem using insight from machine learning and optimization theory.

2 Main result

Motivated by these applications, we now formally define the Hamiltonian learning problem.

Problem 1 (Hamiltonian learning problem). Consider a κ -local Hamiltonian $H(\mu) = \sum_{\ell=1}^m \mu_\ell E_\ell$ that acts on n qudits and consists of m local terms such that $\max_{\ell \in [m]} |\mu_\ell| \leq 1$. In the Hamiltonian Learning Problem, we are given N copies of the Gibbs state of this Hamiltonian

$$\rho_{\beta}(\mu) = \frac{e^{-\beta H(\mu)}}{\operatorname{tr}[e^{-\beta H(\mu)}]}$$

at a fixed inverse-temperature β . Our goal is to obtain an estimate $\hat{\mu} = (\hat{\mu}_1, \dots, \hat{\mu}_m)$ of the coefficients μ_k such that with probability at least $1 - \delta$,

$$\|\mu - \hat{\mu}\|_2 \le \varepsilon$$
,

where $\|\mu - \hat{\mu}\|_2 = \left(\sum_{\ell=1}^m |\mu_\ell - \hat{\mu}_\ell|^2\right)^{\frac{1}{2}}$ is the ℓ_2 -norm of the difference of μ and $\hat{\mu}$.

Our main result is a sample-efficient algorithm for the Hamiltonian Learning Problem.

Theorem 2 (Sample-efficient Hamiltonian learning). The Hamiltonian Learning Problem 1 can be solved using

$$N = \mathcal{O}\left(\frac{e^{\mathcal{O}(\beta^c)}}{\beta^{\tilde{c}} \varepsilon^2} \cdot m^3 \cdot \log\left(\frac{m}{\delta}\right)\right)$$
 (2)

copies of the Gibbs state $\rho_{\beta}(\mu) = e^{-\beta H(\mu)}/\mathrm{tr}[e^{-\beta H(\mu)}]$, where $c, \tilde{c} \geq 1$ are constants that depend on the geometry of the Hamiltonian.

As far as we are aware, our work is the first to establish unconditional and rigorous upper bounds on the sample complexity of the Hamiltonian Learning Problem. For spatially local Hamiltonians the number of interaction terms m scales as O(n). Hence, our result in Theorem 2 implies a sample complexity polynomial in the number of qudits.

The number of samples in (2) increases as $\beta \to \infty$ or $\beta \to 0$. As the temperature increases ($\beta \to 0$), the Gibbs state approaches the maximally mixed state independent of the choice of parameters μ . At low temperatures ($\beta \to \infty$), the Gibbs state is in the vicinity of the ground space,

which for instance, could be a product state $|0\rangle^{\otimes n}$ for the various choices of μ . In either cases, more sample are required to distinguish the parameters μ .

To complement our upper bound, we also obtain a $\Omega(\sqrt{m})$ lower bound for the Hamiltonian Learning Problem with ℓ_2 norm using a simple reduction to the state discrimination problem. The proof appears in Appendix F. Hence, our upper bound in Theorem 2 is tight up to polynomial factors.

Theorem 3. The number of copies N of the Gibbs state needed to solve the Hamiltonian Learning Problem and outputs a $\hat{\mu}$ satisfying $\|\hat{\mu} - \mu\|_2 \le \varepsilon$ with probability $1 - \delta$ is lower bounded by

$$N \ge \Omega\Big(\frac{\sqrt{m} + \log(1 - \delta)}{\beta \varepsilon}\Big).$$

3 Proof overview

In order to prove our main result, we introduce several new ideas. In this section, we provide a sketch of the main ingredients in our proof.

3.1 Maximum entropy estimation and sufficient statistics

In statistical learning theory, a conventional method for obtaining the parameters of a probability distribution from data relies on the concepts of *sufficient statistics* and the *maximum entropy estimation*. Suppose $p(x;\mu)$ is a family of probability distributions parameterized by μ that we want to learn. This family could for instance be various normal distributions with different mean or variance. Let $X_1,\ldots,X_m\sim p(x;\mu)$ be m samples from a distribution in this family. A sufficient *statistic* is a function T of these samples $T(X_1,\ldots,X_m)$ such that conditioned on that, the original date set X_1,\ldots,X_m does not depend on the parameter μ . For example, the sample mean and variance are well known sufficient statistic functions.

After obtaining the sufficient statistic of a given data set given classical samples, there is a natural algorithm for estimating the parameter μ : among all the distributions that match the observed statistic T(X) find the one that maximizes the Shannon entropy. Intuitively, this provides us with the least biased estimate given the current samples [Jay57a, Jay82]. This algorithm, which is closely related to the maximum likelihood estimation, is commonly used for analyzing the sample complexity of classical statistical problems.

Our first observation when addressing the Hamiltonian Learning Problem is that this method can be naturally extended to the quantum problem [Jay57b]. Indeed, the maximum entropy principle has already appeared in other quantum algorithms such as [BKL⁺17]. More formally, we first show that the marginals $\operatorname{tr}[E_{\ell}\rho]$ for $\ell \in [m]$ form a sufficient statistic for the Hamiltonian Learning Problem.

Proposition 4 (Matching local marginals implies global equivalence). *Consider the following two Gibbs states*

$$\rho_{\beta}(\mu) = \frac{e^{-\beta \sum_{\ell} \mu_{\ell} E_{\ell}}}{\operatorname{tr}[e^{-\beta \sum_{\ell} \mu_{\ell} E_{\ell}}]}, \quad \rho_{\beta}(\lambda) = \frac{e^{-\beta \sum_{\ell} \lambda_{\ell} E_{\ell}}}{\operatorname{tr}[e^{-\beta \sum_{\ell} \lambda_{\ell} E_{\ell}}]}$$
(3)

such that $\operatorname{tr}[\rho_{\beta}(\lambda)E_{\ell}] = \operatorname{tr}[\rho_{\beta}(\mu)E_{\ell}]$ for all $\ell \in [m]$, i.e. all the κ -local marginals of $\rho_{\beta}(\lambda)$ match that of $\rho_{\beta}(\mu)$. Then, we have $\rho_{\beta}(\lambda) = \rho_{\beta}(\mu)$, which in turns implies $\lambda_{\ell} = \mu_{\ell}$ for $\ell \in [m]$.

Similar to the classical case discussed above, one implication of Proposition 4 is a method for learning the Hamiltonian H: first measure all the κ -local marginals of the Gibbs state e_{ℓ} , then among all the states of the form (3), find the one that matches those marginals. Finding such a state can be naturally formulated in terms of an optimization problem known as the *maximum entropy problem*:

$$\max_{\sigma} \quad S(\sigma)$$
s.t. $\operatorname{tr}[\sigma E_{\ell}] = e_{\ell}, \quad \forall \ell \in [m]$

$$\sigma > 0, \quad \operatorname{tr}[\sigma] = 1.$$
(4)

where $S(\sigma) = -\text{tr}[\sigma \log \sigma]$ is the *von Neumann entropy* of the state σ . The optimal solution of this program is a quantum state with a familiar structure [Jay57b]. Namely, it is a Gibbs state $\rho(\lambda)$ for some set of coefficients $\lambda = (\lambda_1, \dots, \lambda_m)$. The coefficients λ are the *Lagrange multipliers* corresponding to the dual of this program. Indeed, we can write the dual program of Eq. (4) as follows:

$$\mu = \operatorname*{arg\,min}_{\lambda = (\lambda_1, \dots, \lambda_m)} \log Z_{\beta}(\lambda) + \beta \cdot \sum_{\ell=1}^m \lambda_{\ell} e_{\ell}, \tag{5}$$

where $Z_{\beta}(\lambda) = \operatorname{tr} \left(e^{-\beta \cdot \sum_{\ell} \lambda_{\ell} E_{\ell}} \right)$ is the *partition function* at inverse-temperature β . In principle, according to the result of Proposition 4, we could solve the Hamiltonian Learning Problem by finding the optimal solution of the dual program in (5). Of course, the issue with this approach is that since we have access to limited number of samples of the original Gibbs state $\rho_{\beta}(\mu)$, instead of the exact marginals e_{ℓ} , we can only *approximately* estimate the e_{ℓ} s. We denote these estimates by \hat{e}_{ℓ} . This means instead of solving the dual program (5), we solve its *empirical* version

$$\hat{\mu} = \underset{\lambda = (\lambda_1, \dots, \lambda_m)}{\operatorname{arg\,min}} \quad \log Z_{\beta}(\lambda) + \beta \cdot \sum_{\ell=1}^m \lambda_{\ell} \hat{e}_{\ell}. \tag{6}$$

The main technical problem that we address in this work is analyzing the robustness of the programs (4) and (5) to the statistical error in the marginals as appears in (6). This is an instance of a *stochastic optimization* which is a well-studied problem in optimization. In the next section, we review the ingredients from convex optimization that we need in our analysis.

3.2 Strong convexity

One approach to incorporate the effect of the statistical errors in the marginals e_{ℓ} into the estimates for μ_{ℓ} is to use Proposition 4. It is not hard to extend this proposition to show that if a Gibbs states $\rho_{\beta}(\lambda)$ approximately matches the marginals of $\rho_{\beta}(\mu)$ up to some error ε , then $\|\rho_{\beta}(\mu)-\rho_{\beta}(\lambda)\|_1^2 \leq \mathcal{O}(m\varepsilon)$ (see Section 5.2 for more details). This bound, however, is not strong enough for our purposes. This is because if we try to turn this bound to a one on the coefficients μ_{ℓ} of the Hamiltonian, we need to bound $\|\log \rho_{\beta}(\mu) - \log \rho_{\beta}(\lambda)\|$. Unfortunately, the function $\log(x)$ does not have a bounded gradient (i.e., it is not Lipschitz) over its domain and in general $\|\log \rho_{\beta}(\mu) - \log \rho_{\beta}(\lambda)\|$ can be exponentially worse than $\|\rho_{\beta}(\mu) - \rho_{\beta}(\lambda)\|_1$. In order to overcome the non-Lipschitz nature of the logarithmic function and bound $\|\log \rho_{\beta}(\mu) - \log \rho_{\beta}(\lambda)\|$, we prove a property of the dual objective function (5) known as the *strong convexity*, which we define now.

Definition 5. Consider a convex function $f : \mathbb{R}^m \to \mathbb{R}$ with gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ at a point x.¹ This function f is said to be α -strongly convex in its domain if it is differentiable and for all x, y,

$$f(y) \ge f(x) + \nabla f(x)^{\top} (y - x) + \frac{1}{2} \alpha ||y - x||_2^2,$$

or equivalently if its Hessian satisfies

$$\nabla^2 f(x) \succeq \alpha \mathbb{1}.^2 \tag{7}$$

In other words, for any vector $v \in \mathbb{R}^m$, it holds that $\sum_{i,j} v_i v_j \frac{\partial^2}{\partial x_i \partial x_j} f(x) \ge \alpha \|v\|_2^2$.

Roughly speaking, strong convexity puts a limit on how *slow* a convex function f(x) changes.³ This is particularly useful because given two points x, y and an upper bound on |f(y) - f(x)| and $\nabla f(x)^{\top}(y-x)$, it allows us to infer an upper bound on $|y-x||_2$.

For our application, we think of f as being $\log Z_{\beta}(\cdot)$. Then the difference |f(y) - f(x)| is the difference between the optimal solution of the original program in Eq. (5) and that of its empirical version in Eq. (6) which includes the statistical error. We apply this framework to our optimization (6) in two steps:

1) Proving the strong convexity of the objective function: This is equivalent to showing that the log-partition function (aka the free energy) is strongly convex, i.e., $\nabla^2 \log Z_\beta(\lambda) \succeq \alpha \mathbb{1}$ for some positive coefficient α . In particular, this means that the optimization (6) is a convex program. This result is the main technical contribution of our work and is stated in the following theorem:

Theorem 6 (Informal: strong convexity of log-partition function). Let $H = \sum_{\ell=1}^m \mu_\ell E_\ell$ be a κ -local Hamiltonian over a finite dimensional lattice with $\|\mu\| \le 1$. For a given inverse-temperature β , there are constants c, c' > 3 depending on the geometric properties of the lattice such that

$$\nabla^2 \log Z_{\beta}(\mu) \succeq e^{-\mathcal{O}(\beta^c)} \frac{\beta^{c'}}{m} \cdot \mathbb{1}, \tag{8}$$

i.e., for every vector $v \in \mathbb{R}^m$ we have $v^T \cdot \nabla^2 \log Z_\beta(\mu) \cdot v \ge e^{-\mathcal{O}(\beta^c)} \frac{\beta^{c'}}{m} \cdot \|v\|_2^2$.

2) Bounding the error in estimating μ in terms of the error in estimating the marginals e_{ℓ} : In this step we show that as long as the statistical error of the marginals is small, using the strong convexity property from step (1), we can still prove an upper bound on the difference between the solutions of the convex programs (5), (6).

We discuss this in more details later in Section 5.6. The result can be stated as follows:

Theorem 7 (Error bound from strong convexity). Let $\delta, \alpha > 0$. Suppose the marginals e_{ℓ} are determined up to error δ , i.e., $|e_{\ell} - \hat{e}_{\ell}| \leq \delta$ for all $\ell \in [m]$. Additionally assume $\nabla^2 \log Z_{\beta}(\lambda) \succeq \alpha \mathbb{1}$ and $\|\lambda\| \leq 1$. Then the optimal solution to the program (6) satisfies

$$\|\mu - \hat{\mu}\|_2 \leq \frac{2\beta\sqrt{m}\delta}{\alpha}$$

Combining Theorem 6 and Theorem 7, we obtain the main result of our paper. We now proceed to sketch the proof of Theorem 6.

 $^{^1}$ Recall that the entries of the Hessian matrix $\nabla^2 f(x)$ are given by $rac{\partial^2}{\partial x_i \partial x_j} f(x)$

²By $A \succeq B$ we mean A - B is positive semidefinite.

³This should not be confused with a related property called the smoothness which limits how fast the function grows.

3.3 Strong convexity of log-partition function: Review of the classical case

In order to better understand the motivation behind our quantum proof, it is insightful to start with the *classical* Hamiltonian learning problem. This helps us better describe various subtleties and what goes wrong when trying to adapt the classical techniques to the quantum case. We continue using the quantum notation here, but the reader can replace the Hamiltonian H, for instance, with the classical Ising model $H = \sum_{i \sim j} J_{ij} x_i x_j$ (where $x_i \in \{-1,1\}$ and $J_{ij} \in \mathbb{R}$).

The entries of the Hessian $\nabla^2 \log Z_{\beta}(\mu)$ for classical Hamiltonians are given by

$$\frac{\partial^2}{\partial \mu_i \partial \mu_j} \Big[\log Z_{\beta}(\mu) \Big] = \operatorname{Cov}[E_i, E_j] \tag{9}$$

where Cov is the covariance function which is defined as $\text{Cov}[E_i, E_j] = \langle E_i E_j \rangle - \langle E_i \rangle \langle E_j \rangle$ with the expectation taken with respect to the Gibbs distribution (i.e., $\langle E \rangle = \text{tr}[E \cdot \rho_{\beta}(\mu)]$). To prove the strong convexity of the log-partition function at a constant β , using (9) it suffices to show that for every vector v, we have

$$\sum_{i,j} v_i v_j \frac{\partial^2}{\partial \mu_i \partial \mu_j} \log Z_{\beta}(\mu) = \operatorname{Var} \left[\sum_{\ell=1}^m v_\ell E_\ell \right] \ge \Omega(1) \cdot \sum_{\ell=1}^m v_\ell^2. \tag{10}$$

Although the operator $\sum_{\ell} v_{\ell} E_{\ell}$ is a local Hamiltonian, note the mismatch between this operator and the original Hamiltonian in the Gibbs state $\sum_{\ell=1}^{m} \mu_{\ell} E_{\ell}$. Also note that compared to the inequality (8), the inequality (10) claims a stronger lower bound of $\Omega(1)$.

Before proving Eq. (10), we remark that an *upper bound* of $\operatorname{Var}[\sum_{\ell=1}^m v_\ell E_\ell] \leq \mathcal{O}(1)\|v\|_2^2$ is known in literature, under various conditions like the decay of correlations both in classical and quantum settings [Ara69, Gro79, PY95, Uel04, KGK+14, FU15]. This upper bound intuitively makes sense because the variance of the thermal state of a Hamiltonian and other local observables are expected to be *extensive*, i.e., they scale with the number of particles (spins) or norm of the Hamiltonian, which is replaced by $\|v\|_2^2$ in our setup. However, in the classical Hamiltonian learning problem, we are interested in obtaining a *lower bound* on the variance. To this end, a crucial property of the (classical) Gibbs distributions that allows us to prove the inequality (10) is the conditional independence or the *Markov property* of classical systems.

Definition 8 (Markov property). Suppose the interaction graph is decomposed into three disjoint regions A, B, and C such that region B "shields" A from C, i.e., the vertices in region A are not connected to those in C. Then, conditioned on the sites in region B, the distribution of sites in A is independent of those in C. This is often conveniently expressed in terms of the conditional mutual information by I(A:C|B)=0.

It is known by the virtue of the Hammersley-Clifford theorem [HC71] that the family of distributions with the Markov property coincides with the Gibbs distributions. Using this property, we can lower bound $\operatorname{Var}\left[\sum_{\ell=1}^m v_\ell E_\ell\right]$ in terms of variance of local terms E_ℓ by *conditioning* on a subset of sites. To this end, we consider a partition of the interaction graph into two sets A and B. The set B is chosen, suggestively, such that the vertices in A are not connected (via any edges) to each other. We denote the spin configuration of sites in B collectively by S_B . Then using the concavity of the variance and the Markov property, we have

$$\operatorname{Var}\left[\sum_{\ell=1}^{m} v_{\ell} E_{\ell}\right] \overset{(1)}{\geq} \mathbb{E}_{s_{B}}\left[\operatorname{Var}\left[\sum_{\ell=1}^{m} v_{\ell} E_{\ell} \mid s_{B}\right]\right]$$

$$\overset{(2)}{=} \sum_{x \in A} \mathbb{E}_{s_{B}}\left[\operatorname{Var}\left[\sum_{\ell: E_{\ell} \text{ acts on } x} v_{\ell} E_{\ell} \mid s_{B}\right]\right]$$

$$\overset{(3)}{\geq} \Omega(1) \sum_{\ell=1}^{m} v_{\ell}^{2}, \tag{11}$$

where inequality (1) follows from the law of total variance, equality (2) can be justified as follows: by construction, the local terms E_ℓ either completely lie inside region B or intersect with only one of the sites in region A. In the former, the local conditional variance $\mathrm{Var}\left[E_\ell\,|\,s_B\right]$ vanishes, whereas in the latter, the interaction terms E_ℓ that act on different sites $x\in A$ become uncorrelated and the global variance decomposes into a sum of local variance. Finally, inequality (3) is derived by noticing that at any constant inverse-temperature β , the local variance is lower bounded by a constant that scales as $e^{-\mathcal{O}(\beta)}$. By carefully choosing the partitions A and B such that $|A| = \mathcal{O}(n)$, we can make sure that the variance in inequality (2) is a constant fraction of the $\sum_{\ell=1}^m v_\ell^2$ as in (11) (see [Mon15a, VMLC16] for details). This lower bound on variance results in a sample complexity $\mathcal{O}\left(e^{\mathcal{O}(\beta)}m(\log m)\varepsilon^{-2}\right)$, which compared to our result in Theorem 2 is more efficient (by only a polynomial factor in m).

3.4 Strong convexity of log-partition function: Proof of the quantum case

If we try to directly quantize the proof strategy of the classical case in the previous section, we immediately face several issues. We now describe the challenges in obtaining a quantum proof along with our techniques to overcome them.

3.4.1 Relating the Hessian to a variance

The first problem is that we cannot simply express the entries of the Hessian matrix $\nabla^2 \log Z_\beta(\mu)$ in terms of $\operatorname{Cov}[E_i, E_j]$ as in (9). This expression in (9) only holds for Hamiltonians with *commuting* terms, i.e., $[E_i, E_j] = 0$ for all $i, j \in [m]$. The Hessian for the non-commuting Hamiltonians takes a complicated form (see Lemma 29 for the full expression) that makes its analysis difficult. Our first contribution is to recover a similar result to (10) in the quantum case by showing that, for every v, we can still *lower bound* $v^\top \cdot \nabla^2 \log Z_\beta(\mu) \cdot v$ by the variance of a suitably defined *quasi-local* operator. We later define what we mean by "quasi-local" more formally (see Definition 14 in the body), but for now one can assume such an operator is, up to some small error, sum of local terms.

Lemma 9 (A lower bound on \nabla^2 \log Z_{\beta}(\mu)). For any vector $v \in \mathbb{R}^m$, we define a quasi-local operator $\widetilde{W} = \sum_{\ell=1}^m v_\ell \widetilde{E}_\ell$, where the operators \widetilde{E}_ℓ are defined by

$$\widetilde{E}_{\ell} = \int_{-\infty}^{\infty} f_{\beta}(t) \ e^{-iHt} \ E_{\ell} \ e^{iHt} dt. \tag{12}$$

Here $f_{\beta}(t) = \frac{2}{\beta\pi} \log \frac{e^{\pi|t|/\beta}+1}{e^{\pi|t|/\beta}-1}$ is defined such that $f_{\beta}(t)$ scales as $\frac{1}{\beta}e^{-\pi|t|/\beta}$ for large t and $f_{\beta}(t) \propto \log(1/t)$ for $t \to +0$. We claim that

$$\sum_{i,j} v_i v_j \frac{\partial^2}{\partial \mu_i \partial \mu_j} \log Z_{\beta}(\mu) \ge \beta^2 \operatorname{Var}[\widetilde{W}]$$
(13)

3.4.2 Lower bounding the variance

As a result of Lemma 9, we see that from here onwards, it suffices to lower bound the variance of the quasi-local operator $\widetilde{W} = \sum_{\ell=1}^m v_\ell \widetilde{E}_\ell$. One may expect the same strategy based on the Markov property in (11) yields the desired lower bound. Unfortunately, it is known that a natural extension of this property to the quantum case, expressed in terms of the *quantum conditional mutual information* (qCMI), does not hold. In particular, example Hamiltonians are constructed in [LP08] such that for a tri-partition A, B, C as in Definition 8, their Gibbs states have non-zero qCMI, i.e., I(A:C|B)>0. Nevertheless, it is *conjectured* that an *approximate* version of this property can be recovered i.e., $I(A:C|B) \leq e^{-\Omega(\text{dist}(A,C))}$. In other words, the approximate property claims that qCMI is exponentially small in the *width* of the shielding region B. Thus far, this conjecture has been proved only at sufficiently high temperatures [KKB19] and on 1D chains [KB19]. Even assuming this conjecture is true, we currently do not know how to recover the argument in (11). We get back to this point in Section 4.2. Given this issue we ask,

Can we obtain an unconditional lower bound on the variance of a quasi-local observable at any inverse-temperature β without assuming quantum conditional independence?

Our next contribution is to give an affirmative answer to this question. To achieve this, we modify the classical strategy as explained below.

From global to local variance. One ingredient in the classical proof is to lower bound the global variance $\operatorname{Var}[\sum_\ell v_\ell E_\ell]$ by sum of local conditional variances $\operatorname{Var}[E_\ell|s_B]$ as in (11). We prove a similar but slightly weaker result in the quantum regime. To simplify our discussion, let us ignore the fact that $\widetilde{W} = \sum_\ell v_\ell \widetilde{E}_\ell$ is a quasi-local operator and view it as (strictly) local. Consider a special case in which v is such that the operator \widetilde{W} is supported on a small number of sites. For instance, it could be that $v_1 > 0$ while $v_2, \ldots, v_m = 0$. Then the variance $\operatorname{Var}[\widetilde{W}]$ can be easily related to the local variance $\operatorname{Var}[E_1]$ and since $E_1^2 = 1$, $|\operatorname{tr}[E_1 \rho_\beta]| < 1$, we get

$$\operatorname{Var}[\widetilde{W}] = v_1^2 \cdot \left(\operatorname{tr}[E_1^2 \rho_\beta] - \operatorname{tr}[E_1 \rho_\beta]^2 \right) \ge \Omega(1) \cdot v_1^2$$

We show that even in the general case, where v_1, \ldots, v_m are all non-zero, we can still relate $\mathrm{Var}[\widetilde{W}]$ to the variance of a local operator supported on a constant region. Compared to the classical case in (11), where the lower bound on $\mathrm{Var}[W]$ includes a sum of $\mathcal{O}(m)$ local terms, our reduction to a *single* local variance costs "an extra factor of m" in the strong convexity bound in Theorem 6.

Our reduction to local variance is based on the following observation. By applying Haar-random local unitaries, we can remove all the terms of the operator \widetilde{W} except those that act on an arbitrary qudit at site i. We denote the remainder terms by $\widetilde{W}_{(i)}$ defined via

$$\widetilde{W}_{(i)} = \widetilde{W} - \mathbb{E}_{U_i \sim \text{Haar}}[U_i^{\dagger} \widetilde{W} U_i].$$

By using triangle inequality this relation implies

$$\operatorname{Var}[\widetilde{W}] \ge \frac{1}{2} \operatorname{tr}[\widetilde{W}_{(i)}^2 \rho_{\beta}] - \mathbb{E}_{U_i} \left[\operatorname{tr}[\widetilde{W}^2 \cdot U_i \rho_{\beta} U_i^{\dagger}] \right]. \tag{14}$$

Hence, if we could carefully analyze the effect of the term $\mathbb{E}_{U_i}[\operatorname{tr}[\widetilde{W}^2 \cdot U_i \rho_\beta U_i^{\dagger}]]$, this will allow us to relate the global variance $\operatorname{Var}[\widetilde{W}]$ to the local variance $\operatorname{tr}[\widetilde{W}_{(i)}^2 \rho_\beta]$. We discuss this next.

Bounding the effect of local unitaries. While applying the above reduction helps us to go to an easier local problem, we need to deal with the changes in the spectrum of the Gibbs state due to applying the random local unitaries U_i . Could it be that the unitaries U_i severely change the spectral relation between \widetilde{W} and ρ_{β} ? We show that this is not the case, relying on the facts: (1) local unitaries cannot mix up subspaces of \widetilde{W} and H that are energetically far away and (2) the weight given by the Gibbs state ρ_{β} to nearby subspaces of H are very similar at small H. Thus, (1) allows us to focus the subspaces that are close in energy and (2) shows that similar weights of these subspaces do not change the variance by much. In summary, we prove:

Proposition 10 (Invariance under local unitaries, informal). *Let* U_X *be a local unitary operator acting on region* X *that has a constant size. There exists a constant* $c \le 1$ *such that*

$$\operatorname{tr}\left[\widetilde{W}^{2}\cdot U_{X}\rho_{\beta}U_{X}^{\dagger}\right] \leq \left(\operatorname{Var}\left[\widetilde{W}\right]\right)^{c}.$$
 (15)

When combined with (14), the inequality (15) implies the following loosely stated local lower bound on the global variance:

$$\operatorname{Var}[\widetilde{W}] \ge \left(\operatorname{tr}\left[\widetilde{W}_{(i)}^2 \rho_{\beta}\right]\right)^{\frac{1}{c}}.$$

With this reduction, it remains to find a constant lower bound on $\operatorname{tr}[\widetilde{W}_{(i)}^2\rho_{\beta}]$. This can be done, again, by applying a local unitary U. Roughly speaking, we use this unitary to perform a "change of basis" that relates the local variance at finite temperature to its infinite-temperature version. The spectrum of ρ_{β} majorizes the maximally mixed state η . Hence, by applying a local unitary, we can rearrange the eigenvalues of $\widetilde{W}_{(i)}^2$ in the same order as that of ρ_{β} such that when applied to both ρ_{β} and η , we have $\operatorname{tr}[\widetilde{W}_{(i)}^2U\rho_{\beta}U^{\dagger}] \geq \operatorname{tr}[\widetilde{W}_{(i)}^2\eta]$. Formally, we show that

Proposition 11 (Lower bound on the local variance, informal). *There exists a unitary U supported on O*(1) *sites such that*

$$\operatorname{tr}\left[\widetilde{W}_{(i)}^{2}U\rho_{\beta}U^{\dagger}\right]\geq\operatorname{tr}\left[\widetilde{W}_{(i)}^{2}\eta\right],$$

where η is the maximally mixed state or the infinite temperature Gibbs state.

In summary, starting from (14) and following Proposition 10 and Proposition 11, the lower bound on the global variance takes the following local form:

$$\operatorname{tr}\left[\widetilde{W}^2\rho_{\beta}\right] \geq \left(\operatorname{tr}\left[\widetilde{W}_{(i)}^2\eta\right]\right)^{\mathcal{O}(1)}.$$

Lower bounding the quantity $\operatorname{tr}\left[\widetilde{W}_{(i)}^2\eta\right]$ by a constant is now an easier task, which we explain in more details later in Lemma 34 and Theorem 32.

4 Further discussions

4.1 Connection to previous work

A similar problem to Hamiltonian Learning Problem known as the shadow tomography has been considered before [Aar18a, AR19, BKL+17] where instead of the coefficients μ_ℓ , we want to find a state σ that approximately matches $\mathrm{tr}[E_\ell\sigma] \approx_\varepsilon \mathrm{tr}[E_\ell\rho]$ given multiple copies of an unknown state ρ . It was shown $\mathrm{poly}(\log m, \log d^n, 1/\varepsilon)$ copies of ρ are sufficient for tomography. The Hamiltonian Learning Problem differs from the shadow tomography problem. Our goal is to estimate the Hamiltonian (i.e. the coefficients μ_ℓ) within some given error bound. The shadow tomography protocol only concerns with estimating the marginals $\mathrm{tr}[E_\ell\rho]$ up to a fixed error and by itself does not imply a bound on the Hamiltonian. Moreover, since the Hamiltonians we consider are spatially local, we only need to measure local observables E_ℓ . This means we do not need to rely on the whole machinery of the shadow tomography which is applicable even when E_ℓ are non-local. We instead use a variant of this method introduced in [HKP20] or other approaches such as those in [CW20, BMBO19] to estimate $\mathrm{tr}[E_\ell\rho_\beta]$.

There have been a number of proposals for the Hamiltonian Learning Problem in the past. In [BAL19, EHF19, QR19] learning the Hamiltonian from local measurements is considered. Their approach is based on setting up a linear system of equations whose constraints (i.e., the matrix of coefficients) are determined from the measurement outcomes. The solution of these equations is the parameter μ_k of the Hamiltonian. The sample complexity in this approach depends inverse polynomially on the "spectral gap" of the matrix of coefficients which thus far has not been rigorously bounded. Another line of work considers learning the Hamiltonian using a trusted quantum simulator [WGFC14b, WGFC14a, VMN+19] which is analyzed using a combination of numerical evidence and heuristic arguments. Amin et al. [AAR+18b] quantized classical Boltzmann machines and proposed a method to train and learn quantum Boltzmann machines using gradient descent.

As mentioned earlier, there has been a fruitful series of works on the classical analog of the Hamiltonian Learning Problem (see e.g. [Bre15, KM17, VMLC16]). In our work, we assume it is a priori known that the interaction graph of the Hamiltonian is spatially local. We then estimate the parameters in ℓ_2 -norm using $\operatorname{poly}(n)$ samples which is polynomially tight even for classical Hamiltonians. If we instead consider estimation in ℓ_∞ -norm, the classical algorithms can achieve a stronger result. That is, given $\mathcal{O}(\log n)$ samples, they succeed in efficiently learning the structure of the underlying graph and its parameters in ℓ_∞ -norm. If we apply our current analysis to this setup, we cannot improve our $\operatorname{poly}(n)$ sample complexity to $\mathcal{O}(\log n)$. This is in part because the classical results devise a more efficient convex program that learns the parameters node-wise (this relies on the commutativity of the Hamiltonian terms), and partly because their required strong convexity assumptions is based on the Markov property, none of which are known to be quantizable.

4.2 Open questions

In Section 3.1 we explained our approach to analyzing the Hamiltonian Learning Problem based on reducing data to its sufficient statistics and using maximum entropy estimation. An issue with this approach is the blowup in the computationally complexity. It is shown in [Mon15a] that this approach basically requires approximating the partition function which is NP-hard. Ideally, one would like to have an algorithm for the Hamiltonian Learning Problem that requires small number

of samples, but also has an efficient running time. Satisfying both these constraints for all inverse-temperatures β even in the classical learning problems is quite challenge. It was only recently that more efficient algorithms are devised for learning graphical models [KM17, VMLC16]. In this work, we focus on the less demanding but still non-trivial question of bounding the sample complexity and leave obtaining an efficient running time for future work. Below we mention some of the open problems in this direction.

Our lower bound on the variance in Section 3.4.2 is obtained for any constant inverse-temperature β . It is an interesting open question to improve this bound, ideally to a constant independent of system size, assuming physically-motivated conditions such as the decay of correlations or the decay of conditional mutual information. Another approach might be to derive such a bound at high temperatures where powerful tools such as cluster expansions are available [KKB19]. We also expect our bounds can be improved for commuting Hamiltonians. Indeed, using structural results such as [BV03, AE11], one should be able to follow the same strategy as in Section 3.3 to find a constant lower bound on the variance of commuting Hamiltonians.

There are recent results on efficiently computing the partition function of quantum many-body systems under various assumptions [BG17, HMS19, KKB19]. We expect by combining these results with our maximum entropy estimation algorithm in Section 3.1, one can obtain efficient classical algorithms for the Hamiltonian Learning Problem. Another approach might be to use calibrated quantum computers (or Gibbs samplers) as in [BK16, BKL+17] to solve the maximum entropy optimization using multiplicative weight update method and learn the parameters of another quantum device.

Finally, an important future direction is to devise more refined objective functions for the Hamiltonian Learning Problem that matches the performance of the learning algorithms for the classical problem as discussed in Section 4.1. Given the non-commutative nature of quantum Hamiltonians, this seems to require substantially new ideas and advances in characterizing the information theoretic properties of the quantum Gibbs states.

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5 Preliminaries

5.1 Some mathematical facts

Here we summarize some of the basic mathematical facts used in the proof. Let A, B be arbitrary operator. The *operator norm* of A which is its largest singular value is denoted by ||A||. We also often use the *Frobenius norm* $||A||_F := \sqrt{\operatorname{tr}[A^{\dagger}A]}$ and more generally the Hilbert-Schmidt inner product

between A, B defined by $tr[A^{\dagger}B]$. Additionally using Hölder's inequality we have,

$$||AB||_F = \sqrt{\operatorname{tr}(B^{\dagger}AA^{\dagger}B)} \le \sqrt{||B||^2 \operatorname{tr}(AA^{\dagger})} = ||B|| \cdot ||A||_F.$$
 (16)

We define the von Neumann entropy of a quantum state σ by $S(\sigma) = -\text{tr}[\sigma \log \sigma]$ and the relative entropy between two states σ_1 and σ_2 by $S(\sigma_1 || \sigma_2) = -\text{tr}[\sigma_1 \log \sigma_2] - S(\sigma_1)$.

The gradient of a real function $f: \mathbb{R}^m \mapsto \mathbb{R}$ is denoted by $\nabla f(x)$ and its *Hessian* (second derivative) matrix by $\nabla^2 f(x)$. The entries of the Hessian matrix are given by $\frac{\partial^2}{\partial x_i \partial x_j} f(x)$.

We write $A \succeq 0$ to represent a *positive semi-definite* (PSD) operator A, one such example of a PSD operator is the Hessian matrix $\nabla^2 f(x)$.

For convenience, we will also gather a collection of infinite sums over exponentials. For t > 0, let

$$\Gamma(t) := \int_0^\infty x^{t-1} e^{-x} dx = \frac{1}{t} \int_0^\infty e^{-x} d\left(x^t\right) = \frac{1}{t} \int_0^\infty e^{-y^{\frac{1}{t}}} dy$$

be the gamma function. It holds that $\Gamma(t) \leq t^t$. This can be used to simplify several summations that we encounter later. Finally, we collect a few useful summations that we use in our proofs in the following fact. The proof is postponed until Appendix A.

Fact 12. Let a, c, p > 0 be reals and b be a positive integer. Then

- 1) $\sum_{j=0}^{\infty} e^{-cj} \le \frac{e^c}{c}.$
- 2) $\sum_{j=0}^{\infty} j^b e^{-cj^p} \le \frac{2}{p} \cdot \left(\frac{b+1}{cp}\right)^{\frac{b+1}{p}}.$
- 3) $\sum_{j=0}^{\infty} e^{-c(a+j)^p} \le e^{-\frac{c}{2}a^p} \left(1 + \frac{1}{p} \left(\frac{2}{cp}\right)^{\frac{1}{p}}\right).$

5.2 Local Hamiltonians and quantum Gibbs states

Local Hamiltonians. In this work, we focus on Hamiltonians that are *geometrically local*. That is, the interactions terms in the Hamiltonian act on a constant number of qudits that are in the neighborhood of each other. To describe this notion more precisely, we consider a D-dimensional lattice $\Lambda \subset \mathbb{Z}^D$ that contains n sites with a d-dimensional qudit (spin) on each site. We denote the dimension of the Hilbert space associated to the lattice Λ by \mathcal{D}_{Λ} . The Hamiltonian of this system is

$$H = \sum_{X \subset \Lambda} H_X.$$

Each term H_X acts only on the sites in X and X is restricted to be a connected set with respect to Λ . We also define the Hamiltonian restricted to a region $A\subseteq \Lambda$ by $H_A=\sum_{X\subseteq A}H_X$. Let $B(r,i):=\{j\in\Lambda|\mathrm{dist}(i,j)\leq r\}$ denotes a ball (under the Manhattan distance in the lattice) of size r centered at site i. For a given connected set $X\in\Lambda$, let $\mathrm{diam}(X):=\max\{\mathrm{dist}(i,j):i,j\in X\}$ denote the diameter of this set, $X^c:=\Lambda\setminus X$ denote the complement of this set and ∂X denote its boundary. Given two sets $X,Y\in\Lambda$, we define $\mathrm{dist}(X,Y):=\min\left(\mathrm{dist}(i,j):i\in X,j\in Y\right)$.

In order describe our Hamiltonians, we consider an orthogonal Hermitian basis for the space of operators acting on each qudit. For instance, for qubits this basis consists of the Pauli operators. By decomposing each local term H_X in terms of the tensor product of such basis operators, we find the following canonical form for the Hamiltonian H:

Definition 13 (Canonical representation for κ **-local Hamiltonians).** *A* κ *-local Hamiltonian H on a lattice* Λ *is sum of* m *Hermitian operators* E_{ℓ} *each acting non-trivially on* κ *qudits. That is,*

$$H = \sum_{\ell=1}^{m} \mu_{\ell} E_{\ell}. \tag{17}$$

where $\mu_\ell \in \mathbb{R}$ and we assume $||E_\ell|| \le 1$, $\mathrm{tr}[E_\ell^2] = \mathcal{D}_\Lambda$, $E_\ell^\dagger = E_\ell$ for $\ell \in [m]$, and

$$\operatorname{tr}[E_k E_\ell] = 0 \quad \text{for } k \neq \ell.$$
 (18)

Since H is geometrically local, it holds that $m = \mathcal{O}(|\Lambda|) = \mathcal{O}(n)$. As discussed earlier, we extensively use the notion of quasi-local operators, which we now formally define.

Definition 14 (Quasi-local operators). An operator A is said to be (τ, a_1, a_2, ζ) -quasi-local if it can be written as

$$A = \sum_{\ell=1}^{n} g_{\ell} \bar{A}_{\ell} \quad \text{with} \quad g_{\ell} \le a_{1} \cdot \exp(-a_{2}\ell^{\tau}),$$

$$\bar{A}_{\ell} = \sum_{|Z|=\ell} a_{Z}, \quad \max_{i \in \Lambda} \left(\sum_{Z:Z \ni i} \|a_{Z}\| \right) \le \zeta,$$
(19)

where the sets $Z \subset \Lambda$ are restricted to be balls.⁴

Although local operators are morally a special case of quasi-local operators (when $\tau=\infty$), we will reserve the above notation for operators with $\tau=\mathcal{O}(1)$. A useful tool for analyzing quasi-locality is the Lieb-Robinson bound, which shows a light-cone like behavior of the time evolution operator.

Fact 15 (Lieb-Robinson bound [LR72], [NS09]). Let P,Q be operators supported on regions X,Y of the D dimensional lattice Λ respectively. Let H be a (ζ,κ) -geometrically local Hamiltonian. There exist constants v_{LR} , f,c that only depend on ζ,κ and D such that

$$\|[e^{iHt}Ae^{-iHt},B]\| \leq f\|A\|\|B\| \cdot \min\left(|\partial X|,|\partial Y|\right) \cdot \min\left(e^{c(v_{\text{LR}}|t|-\text{dist}(X,Y))},1\right).$$

Gibbs states. At an *inverse-temperature* β , a quantum many-body system with the Hamiltonian $H(\mu)$ is in the Gibbs (thermal) state

$$\rho_{\beta}(\mu) = \frac{e^{-\beta H(\mu)}}{\operatorname{tr}[e^{-\beta H(\mu)}]}.$$
(20)

The partition function of this system is defined by $Z_{\beta}(\mu) = \text{tr}[e^{-\beta H(\mu)}]$.

Remark 16. In our notation, we sometimes drop the dependency of the partition function or the Gibbs state on μ . We also often simply use the term local Hamiltonian H or quasi-local operator A when referring to Definition 13 and Definition 14.

⁴The assumption that Z is a ball suffices for us. Our results on quasi-local operators also generalize to the case where Z is an arbitrary *regular* shape, for example when the radii of the balls inscribing and inscribed by Z are of constant proportion to each other.

As discussed earlier, local marginals of the Gibbs states can be used to uniquely specify them. This provides us with "sufficient statistics" for learning the Hamiltonians from ρ_{β} . More precisely, we have:

Proposition 17 (Restatement of Proposition 4). Consider the following two Gibbs states

$$\rho_{\beta}(\mu) = \frac{e^{-\beta \sum_{\ell} \mu_{\ell} E_{\ell}}}{\operatorname{tr}[e^{-\beta \sum_{\ell} \mu_{\ell} E_{\ell}}]}, \quad \rho_{\beta}(\lambda) = \frac{e^{-\beta \sum_{\ell} \lambda_{\ell} E_{\ell}}}{\operatorname{tr}[e^{-\beta \sum_{\ell} \lambda_{\ell} E_{\ell}}]}$$
(21)

such that $\operatorname{tr}[\rho_{\beta}(\lambda)E_j] = \operatorname{tr}[\rho_{\beta}(\mu)E_j]$ for all $j \in [m]$, i.e. all the κ -local marginals of $\rho_{\beta}(\lambda)$ match that of $\rho_{\beta}(\mu)$. Then, we have $\rho_{\beta}(\lambda) = \rho_{\beta}(\mu)$, which in turns implies $\lambda_{\ell} = \mu_{\ell}$ for $\ell \in [m]$.

Proof. We consider the relative entropy between $\rho_{\beta}(\lambda)$ and the Gibbs state $\rho_{\beta}(\mu)$. We have

$$S(\rho_{\beta}(\mu) \| \rho_{\beta}(\lambda)) = \operatorname{tr} \left[\rho_{\beta}(\mu) \left(\log \rho_{\beta}(\mu) - \log \rho_{\beta}(\lambda) \right) \right]$$
$$= -S(\rho_{\beta}(\mu)) + \beta \cdot \operatorname{tr} \left[\rho_{\beta}(\mu) \sum_{\ell} \lambda_{\ell} E_{\ell} \right] + \log Z(\lambda)$$
(22)

$$\stackrel{(1)}{=} -S(\rho_{\beta}(\mu)) + \beta \sum_{\ell} \lambda_{\ell} \operatorname{tr}[\rho_{\beta}(\lambda) E_{\ell}] + \log Z(\lambda)$$
(23)

$$= -S(\rho_{\beta}(\mu)) + S(\rho_{\beta}(\lambda))$$

$$\stackrel{(2)}{\geq} 0,$$
(24)

where (1) follows because $\operatorname{tr}[\rho_{\beta}(\mu)E_{\ell}] = \operatorname{tr}[\rho_{\beta}(\lambda)E_{\ell}]$ for all $\ell \in [m]$ and (2) used the positivity of relative entropy. Similarly, we can exchange the role of $\rho(\mu)$ and $\rho(\lambda)$ in (24) and get

$$S(\rho_{\beta}(\lambda)||\rho_{\beta}(\mu)) = -S(\rho_{\beta}(\lambda)) + S(\rho_{\beta}(\mu)) \ge 0.$$
(25)

Combining these bounds imply $S(\rho_{\beta}(\mu)) = S(\rho_{\beta}(\lambda))$ and hence from Eq. (24), we get $S(\rho_{\beta}(\mu)\|\rho_{\beta}(\lambda)) = 0$. It is known that the relative entropy of two distribution is zero only when $\rho_{\beta}(\mu) = \rho_{\beta}(\lambda)$. Hence, we also have $\log \rho_{\beta}(\mu) = \log \rho_{\beta}(\lambda)$ or equivalently up to an additive term $\sum_{\ell=1}^{m} \mu_{\ell} E_{\ell} = \sum_{\ell=1}^{m} \lambda_{\ell} E_{\ell}$. Since the operators E_{ℓ} form an orthogonal basis (see Eq. (18)), we see that $\lambda_{\ell} = \mu_{\ell}$ for all $\ell \in [m]$.

Remark 18. When the marginals of the two Gibbs states only approximately match, i.e.,

$$|\operatorname{tr}[\rho_{\beta}(\mu)E_{\ell}] - \operatorname{tr}[\rho_{\beta}(\lambda)E_{\ell}]| \leq \varepsilon$$

for $\ell \in [m]$, then a similar argument to (24) shows that $S(\rho_{\beta}(\mu) \| \rho_{\beta}(\lambda)) \leq \mathcal{O}(m\varepsilon)$. By applying Pinsker's inequality, we get $\|\rho_{\beta}(\mu) - \rho_{\beta}(\lambda)\|_1^2 \leq \mathcal{O}(m\varepsilon)$.

5.3 Quantum belief propagation

Earlier we saw that we could express the Gibbs state of a Hamiltonian H by Eq. (20). Suppose we alter this Hamiltonian by adding a term V such that

$$H(s) = H + sV, \quad s \in [0, 1].$$
 (26)

⁵Pinsker's inequality states that for two density matrices ρ, σ , we have $\|\rho - \sigma\|_1^2 \le 2 \ln 2 \cdot S(\rho \|\sigma)$.

How does the Gibbs state associated with this Hamiltonian change? If the new term V commutes with the Hamiltonian H, i.e., [H, V] = 0, then the derivative of the Gibbs state of H(s) is given by

$$\frac{d}{ds}e^{-\beta H(s)} = -\beta e^{-\beta H(s)}V = -\frac{\beta}{2}\left\{e^{-\beta H(s)}, V\right\},\tag{27}$$

where $\{e^{-\beta H(s)},V\}=e^{-\beta H(s)}V+Ve^{-\beta H(s)}$ denotes the anti-commutator. In the non-commuting case though, finding this derivative is more complicated. The *quantum belief propagation* is a framework developed in [Has07, Kim17, KB19] for finding such derivatives in a way that reflects the locality of the system.

Definition 19 (Quantum belief propagation operator). For every $s \in [0,1]$, $\beta \in \mathbb{R}$, define H(s) = H + sV where $V = \sum_{j,k} V_{j,k} |j\rangle\langle k|$ is a Hermitian operator. Also let $f_{\beta}(t)$ be a function whose Fourier transform is

$$\tilde{f}_{\beta}(\omega) = \frac{\tanh(\beta\omega/2)}{\beta\omega/2},$$
(28)

i.e., $f_{\beta}(t) = \frac{1}{2\pi} \int d\omega \tilde{f}_{\beta}(\omega) e^{i\omega t}$. The quantum belief propagation operator $\Phi_{H(s)}(V)$ is defined by

$$\Phi_{H(s)}(V) = \int_{-\infty}^{\infty} dt f_{\beta}(t) e^{-iH(s)t} V e^{iH(s)t}.$$

Equivalently, in the energy basis of $H(s) = \sum_j \varepsilon_j(s) |j\rangle\langle j|$, we can write

$$\Phi_{H(s)}(V) = \sum_{j,k} |j\rangle\langle k| \ V_{j,k} \ \tilde{f}_{\beta}(\mathcal{E}_{j}(s) - \mathcal{E}_{k}(s)). \tag{29}$$

Proposition 20 (cf. [Has07]). *In the same setup as Definition* 19, *it holds that*

$$\frac{d}{ds}e^{-\beta H(s)} = -\frac{\beta}{2} \left\{ e^{-\beta H(s)}, \Phi_{H(s)}(V) \right\}. \tag{30}$$

5.4 Change in the spectrum after applying local operators

For a Hamiltonian H, let $P_{\leq x}^H$ and $P_{\geq y}^H$ be projection operators onto the eigenspaces of H whose energies are in $\leq x$ and $\geq y$, respectively (we use similar notation $P_{\leq x}^A$, $P_{\geq y}^A$ for the quasi-local operator A). Consider a quantum state $|\psi\rangle$ in the low-energy part of the spectrum such that $P_{\leq x}^H|\psi\rangle = |\psi\rangle$. Suppose this states $|\psi\rangle$ is perturbed by applying a local operator O_X on a subset $X\subset \Lambda$ of its qudits. Intuitively, we expect that the operator O_X only affects the energy of $|\psi\rangle$ up to $\mathcal{O}(|X|)$, i.e., $\|P_{\geq y}^HO_X|\psi\rangle\|\approx 0$ for $y\gg x+|X|$. A simple example is when $|\psi\rangle$ is the eigenstate of a classical spin system. By applying a local operation that flips the spins in a small region X, the energy changes at most by $\mathcal{O}(|X|)$. The following lemma rigorously formulates the same classical intuition for quantum Hamiltonians.

Lemma 21 (Theorem 2.1 of [AKL16]). *Let* H *be an arbitrary* κ *-local operator such that*

$$H = \sum_{|Z| < \kappa} h_Z,\tag{31}$$

and each $i \in \Lambda$ supports at most g terms h_Z . Then, for an arbitrary operator O_X which is supported on $X \subseteq \Lambda$, the operator norm of $P_{\geq y}^H O_X P_{\leq x}^H$ is upper-bounded by

$$||P_{\geq y}^H O_X P_{\leq x}^H|| \le ||O_X|| \cdot \exp\left(-\frac{1}{2g\kappa}(y - x - 2g|X|)\right).$$
 (32)

In our analysis, we need an different version of this lemma for *quasi-local* operators instead of κ -local operators. The new lemma will play a central role in lower-bounding the variance of quasi-local operators. The proof follows by the analysis of a certain moment function (as opposed to the moment generating function in [AKL16]). Due to formal similarities between the proofs, we defer the proof of the next lemma to Appendix C.

Lemma 22 (Variation of [AKL16] for quasi-local operators). *Let* A *be a* $(\tau, a_1, a_2, 1)$ -quasi-local operator, as given in Eq. (19), with $\tau \leq 1$. For an arbitrary operator O_X supported on a subset $X \subseteq \Lambda$ with $|X| = k_0$ and $||O_X|| = 1$, we have

$$||P_{\geq x+y}^A O_X P_{\leq x}^A|| \le c_5 \cdot k_0 \exp\left(-(\lambda_1 y/k_0)^{1/\tau_1}\right),$$
 (33)

where $\tau_1 := \frac{2}{\tau} - 1$, c_5 and λ_1 are constants depending on a_1 and a_2 as $c_5 \propto a_2^{2/\tau}$ and $\lambda_1 \propto a_2^{-2/\tau}$ respectively.

5.5 Local reduction of global operators

An important notion in our proofs will be a reduction of a global operator to a local one, which has influence on a site i. Fix a subset $Z \subseteq \Lambda$ and an operator O supported on Z. Define

$$O_{(i)} := O - \operatorname{tr}_i[O] \otimes \frac{\mathbb{1}_i}{d} \tag{34}$$

where operator $\mathbbm{1}_i$ is the identity operator on the ith site, d is the local dimension, tr_i is the partial trace operation with respect to the site i. Note that $O_{(i)}$ removes all the terms in O that do not act on the ith site. This can be explicitly seen by introducing a basis $\{E_Y^\alpha\}_{\alpha\in\mathbb{N},Y\in Z}$ of Hermitian operators, where Y labels the support of E_Y^α and α labels several possible operators on the same support. We can assume that $\operatorname{tr}[(E_Y^\alpha)^2] = 1$, $\operatorname{tr}_i[E_Y^\alpha] = 0$ for every $i \in Y$, and the orthogonality condition $\operatorname{tr}[E_Y^\alpha E_{Y'}^{\alpha'}] = 0$ holds if $\alpha \neq \alpha'$ or $Y \neq Y'$. These conditions are satisfied by the appropriately normalized Pauli operators. Expand

$$O = \sum_{\alpha, Y} g_{\alpha, Y} E_Y^{\alpha}.$$

Then

$$O_{(i)} = \sum_{\alpha,Y} g_{\alpha,Y} E_Y^{\alpha} - \sum_{\alpha,Y} g_{\alpha,Y} \operatorname{tr}_i[E_Y^{\alpha}] \otimes \frac{\mathbb{1}_i}{d} = \sum_{\alpha,Y:Y \ni i} g_{\alpha,Y} E_Y^{\alpha}.$$

Thus, $O_{(i)}$ is an operator derived from O, by removing all E_Y^{α} which act as identity on i. The following claim shows that the Frobenius norm of a typical $O_{(i)}$ is not much small in comparison to the Frobenius norm of O.

Claim 23. For every operator O and $O_{(i)}$ defined in Eq. (34), it holds that

$$\max_{i \in Z} \|O_{(i)}\|_F^2 \ge \frac{1}{|Z|} \sum_{i \in Z} \|O_{(i)}\|_F^2 \ge \frac{1}{|Z|} \|O\|_F^2, \tag{35}$$

Proof. Using the identities $\operatorname{tr}[E_Y^{\alpha}E_{Y'}^{\alpha'}]=0$ and $\operatorname{tr}[(E_Y^{\alpha})^2]=1$, we have

$$\|O\|_F^2 = \sum_{Y,\alpha} g_{\alpha,Y}^2 \le \sum_{i \in Z} \sum_{\alpha,Y:Y \ni i} g_{\alpha,Y}^2 = \sum_{i \in Z} \|O_{(i)}\|_F^2.$$

This completes the proof.

5.6 Stochastic convex optimization applied to Hamiltonian learning

Suppose we want to solve the optimization

$$\max_{x \in \mathbb{R}^m} f(x)$$

for a function $f: \mathbb{R}^m \to \mathbb{R}$ which is of the form $f(x) = \mathbb{E}_{y \sim \mathcal{D}}[g(x,y)]$. Here g(x,y) is some convex function and the expectation $\mathbb{E}_{y \sim \mathcal{D}}$ is taken with respect to an unknown distribution \mathcal{D} . Algorithms for this maximization problem are based on obtaining i.i.d. *samples* y drawn from the distribution \mathcal{D} . In practice, we can only receive finite samples y_1, y_2, \ldots, y_ℓ from such a distribution. Hence, instead of the original optimization, we solve an *empirical* version

$$\max_{x \in \mathbb{R}^m} \frac{1}{\ell} \sum_{k=1}^{\ell} g(x, y_k).$$

The natural question therefore is: How many samples ℓ do we need to guarantee the output of the empirical optimization is close to the original solution? One answer to this problem relies on a property of the objective function known as *strong convexity*.

Definition 24 (Restatement of Definition 5). Consider a convex function $f : \mathbb{R}^m \to \mathbb{R}$ with gradient $\nabla f(x)$ and Hessian $\nabla^2 f(x)$ at x. The function f is said to be α -strongly convex in its domain if it is differentiable and for all x, y, and

$$f(y) \ge f(x) + \nabla f(x)^{\top} (y - x) + \frac{1}{2} \alpha ||y - x||_2^2,$$

or equivalently if its Hessian satisfies

$$\nabla^2 f(x) \succeq \alpha \mathbb{1}. \tag{36}$$

In other words, for any vector $v \in \mathbb{R}^m$ it holds that $\sum_{i,j} v_i v_j \frac{\partial^2}{\partial x_i \partial x_j} f(x) \ge \alpha \|v\|_2^2$.

Next, we discuss how the framework of convex optimization and in particular strong convexity, can be applied to the Hamiltonian Learning Problem. To this end, we define the following optimization problems.

Definition 25 (Optimization program for learning the Hamiltonian). We denote the objective function in the Hamiltonian Learning Problem and its approximate version (equations (5) and (6) in Section 3.1) by $L(\lambda)$ and $\hat{L}(\lambda)$ respectively, i.e.,

$$L(\lambda) = \log Z_{\beta}(\lambda) + \beta \cdot \sum_{\ell=1}^{m} \lambda_{\ell} e_{\ell}, \quad \hat{L}(\lambda) = \log Z_{\beta}(\lambda) + \beta \cdot \sum_{\ell=1}^{m} \lambda_{k} \hat{e}_{\ell},$$
(37)

where the partition function is given by $Z_{\beta}(\lambda) = \operatorname{tr}(e^{-\beta \sum_{\ell=1}^{m} \lambda_{\ell} E_{\ell}})$. The parameters of the Hamiltonian that we intend to learn are $\mu = \arg\min_{\lambda \in \mathbb{R}^m: ||\lambda|| \le 1} L(\lambda)$. As before, we also define the empirical version of this optimization by

$$\hat{\mu} = \underset{\lambda \in \mathbb{R}^m: \|\lambda\| \le 1}{\arg \min} \hat{L}(\lambda). \tag{38}$$

We prove later in Lemma 30 that $\log Z_{\beta}(\lambda)$ is a convex function in parameters λ and thus, the optimization in (38) is a convex program whose solution can be in principle found. In this work, we do not constraint ourselves with the running time of solving (38). We instead obtain sample complexity bounds as formulated more formally in the next theorem.

Theorem 26 (Error in \mu from error in marginals e_{\ell}). Let $\delta, \alpha > 0$. Suppose the marginals e_{ℓ} are determined up to error δ , i.e., $|e_{\ell} - \hat{e}_{\ell}| \leq \delta$ for all $\ell \in [m]$. Additionally assume $\nabla^2 \log Z(\lambda) \succeq \alpha \mathbb{1}$ for $\|\lambda\| \leq 1$. Then the optimal solution to the program (38) satisfies

$$\|\mu - \hat{\mu}\|_2 \le \frac{2\beta\sqrt{m}\delta}{\alpha}$$

Proof. From the definition of $\hat{\mu}$ as the optimal solution of \hat{L} in (38), we see that $\hat{L}(\hat{\mu}) \leq \hat{L}(\mu)$. Thus, we get

$$\log Z_{\beta}(\hat{\mu}) + \beta \cdot \sum_{\ell=1}^{m} \hat{\mu}_{\ell} \hat{e}_{\ell} \leq \log Z_{\beta}(\mu) + \beta \cdot \sum_{\ell=1}^{m} \mu_{\ell} \hat{e}_{\ell}.$$

or equivalently,

$$\log Z_{\beta}(\hat{\mu}) \le \log Z_{\beta}(\mu) + \beta \cdot \sum_{\ell=1}^{m} (\mu_{\ell} - \hat{\mu}_{\ell}) \hat{e}_{\ell}. \tag{39}$$

We show later in Lemma 29 that for every $\ell \in [m]$, we have $\frac{\partial}{\partial \mu_\ell} \log Z_\beta(\mu) = -\beta e_\ell$. This along with the assumption $\nabla^2 \log Z(\mu) \succeq \alpha \mathbb{1}$ in the theorem statement, implies that for every μ' with $\|\mu'\| \leq 1$

$$\log Z_{\beta}(\mu') \ge \log Z_{\beta}(\mu) - \beta \cdot \sum_{\ell=1}^{m} (\mu'_{\ell} - \mu_{\ell}) e_{\ell} + \frac{1}{2} \alpha \|\mu' - \mu\|_{2}^{2}.$$
(40)

Hence, by choosing $\mu' = \hat{\mu}$ and combining (40) and (39), we get

$$\log Z_{\beta}(\mu) - \beta \cdot \sum_{\ell=1}^{m} (\hat{\mu}_{\ell} - \mu_{\ell}) e_{\ell} + \frac{1}{2} \alpha \|\hat{\mu} - \mu\|_{2}^{2} \leq \log Z_{\beta}(\mu) + \beta \cdot \sum_{\ell=1}^{m} (\mu_{\ell} - \hat{\mu}_{\ell}) \hat{e}_{\ell}$$

which further implies that

$$\frac{1}{2}\alpha \|\hat{\mu} - \mu\|_{2}^{2} \leq \beta \cdot \sum_{\ell=1}^{m} (\hat{\mu}_{\ell} - \mu_{\ell})(e_{\ell} - \hat{e}_{\ell}),
\leq \beta \cdot \|\hat{\mu} - \mu\|_{2} \cdot \|\hat{e} - e\|_{2}.$$

⁶In particular, see Eq. (44), where we showed $\frac{\partial}{\partial \mu_{\ell}} \log Z_{\beta}(\mu) = -\beta \cdot \text{tr}[E_{\ell} \rho_{\beta}(\mu)] = -\beta e_{\ell}$.

Hence, we have

$$\|\hat{\mu} - \mu\|_2 \le \frac{2\beta}{\alpha} \|\hat{e} - e\|_2 \le \frac{2\beta\sqrt{m}\delta}{\alpha}.$$

Corollary 27 (Sample complexity from strong convexity). Under the same conditions as in Theorem 26, the number of copies of the Gibbs state ρ_{β} that suffice to solve the Hamiltonian Learning Problem is

$$N = O\left(\frac{\beta^2 2^{\mathcal{O}(\kappa)}}{\alpha^2 \varepsilon^2} m \log m\right).$$

Proof. First observe that, using Theorem 26, as long as the error in estimating the marginals e_{ℓ} are

$$\delta \le \frac{\alpha \varepsilon}{2\beta \sqrt{m}},\tag{41}$$

we estimate the coefficients μ by $\hat{\mu}$ such that $\|\hat{\mu} - \mu\|_2 \leq \varepsilon$. The marginals e_{ℓ} can be estimated in various ways. One method considered in [CW20, BMBO19] is to group the operators E_{ℓ} into sets of mutually commuting observables and simultaneously measure them at once. Alternatively, we can use the recent procedure in [HKP20, Theorem 1] based on a variant of shadow tomography. In either case, the number of copies of the state needed to find all the marginals with accuracy δ is

$$N = O\left(\frac{2^{\mathcal{O}(\kappa)}}{\delta^2} \log m\right),\,$$

where recall that κ is the locality of the Hamiltonian. Plugging in Eq. (41) gives us the final bound

$$N = O\left(\frac{\beta^2 2^{\mathcal{O}(\kappa)}}{\alpha^2 \varepsilon^2} m \log m\right).$$

Strong convexity of $\log Z_{\beta}(\lambda)$

We now state our main theorem which proves the strong convexity of the logarithm of the partition function. Recall that for a vector $\lambda = (\lambda_1, \dots, \lambda_m) \in \mathbb{R}^m$, Hamiltonian $H(\lambda) = \sum_i \lambda_i E_i$ where E_i are tensor product of Pauli operators with weight at most κ and $\rho_{\beta}(\lambda) = \frac{1}{Z_{\beta}(\lambda)} e^{-\beta H(\lambda)}$, we defined the partition function as $Z_{\beta}(\lambda) = \operatorname{tr}(e^{-\beta H(\lambda)})$. We now prove our main theorem for this section.

Theorem 28 (Restatement of Theorem 6: log $Z(\lambda)$ is strongly convex). Let $H = \sum_{\ell=1}^m \mu_\ell E_\ell$ be a κ -local Hamiltonian over a finite dimensional lattice. For a given inverse-temperature β , there are constants c,c'>3 depending on the geometric properties of the lattice such that

$$\nabla^2 \log Z_{\beta}(\mu) \succeq e^{-\mathcal{O}(\beta^c)} \cdot \frac{\beta^{c'}}{m} \cdot \mathbb{1}, \tag{42}$$

i.e., for every vector $v \in \mathbb{R}^m$ we have $v^T \cdot \nabla^2 \log Z_{\beta}(\mu) \cdot v \geq \beta^{c'} e^{-\mathcal{O}(\beta^c)} / m \cdot \|v\|_2^2$

The proof of Theorem 28 is divided into multiple lemmas that we state and prove both in this and the following sections. We begin with finding an expression for the Hessian of $\log Z_{\beta}(\lambda)$.

Lemma 29. For every vector $v \in \mathbb{R}^m$, define the local operator $W_v = \sum_{i=1}^m v_i E_i$ (for notational convenience, later on we stop subscripting W by v). The Hessian $\nabla^2 \log Z_{\beta}(\lambda)$ satisfies

$$v^{\top} \cdot \left(\nabla^2 \log Z_{\beta}(\lambda)\right) \cdot v = \frac{\beta^2}{2} \operatorname{tr}\left[\left\{W_v, \Phi_{H(\lambda)}(W_v)\right\} \rho_{\beta}(\lambda)\right] - \beta^2 \left(\operatorname{tr}\left[W_v \rho_{\beta}(\lambda)\right]\right)^2, \tag{43}$$

Proof. Since the terms in the Hamiltonian are non-commuting, we use Proposition 20 to find the derivatives of $\log Z_{\beta}(\lambda)$. We get

$$\frac{\partial}{\partial \lambda_{j}} \log Z_{\beta}(\lambda) = \frac{1}{Z_{\beta}(\lambda)} \operatorname{tr} \left[-\frac{\beta}{2} \left\{ e^{-\beta H(\lambda)}, \Phi_{H(\lambda)}(E_{j}) \right\} \right]
= \frac{-\beta}{Z_{\beta}(\lambda)} \operatorname{tr} \left[e^{-\beta H(\lambda)} \int_{-\infty}^{\infty} dt f_{\beta}(t) e^{-iH(\lambda)t} E_{j} e^{iH(\lambda)t} \right]
= -\beta \operatorname{tr} \left[E_{j} \frac{e^{-\beta H(\lambda)}}{Z_{\beta}(\lambda)} \right],$$
(44)

where the second equality used the definition of the quantum belief propagation operator $\Phi_{H(\lambda)}(E_j) = \int_{-\infty}^{\infty} dt f_{\beta}(t) \ e^{-iH(\lambda)t} \ E_j \ e^{iH(\lambda)t}$ with f_{β} as given in Definition 19. The third equality used the fact that $e^{iH(\lambda)t}$ commutes with $e^{-\beta H(\lambda)}$. Similarly, we have

$$\frac{\partial^{2}}{\partial \lambda_{k} \partial \lambda_{j}} \log Z_{\beta}(\lambda) = -\beta \operatorname{tr} \left[E_{j} \cdot \frac{\partial}{\partial \lambda_{k}} \left(\frac{e^{-\beta H(\lambda)}}{Z_{\beta}(\lambda)} \right) \right]
= -\beta \operatorname{tr} \left[E_{j} \cdot \frac{1}{Z_{\beta}(\lambda)} \frac{\partial}{\partial \lambda_{k}} \left(e^{-\beta H(\lambda)} \right) \right] + \beta \operatorname{tr} \left[E_{j} \cdot \frac{e^{-\beta H(\lambda)}}{Z_{\beta}(\lambda)} \right] \cdot \frac{1}{Z_{\beta}(\lambda)} \frac{\partial}{\partial \lambda_{k}} Z_{\beta}(\lambda)
= \frac{\beta^{2}}{2} \operatorname{tr} \left[E_{j} \cdot \left\{ \rho_{\beta}(\lambda), \Phi_{H(\lambda)}(E_{k}) \right\} \right] - \beta^{2} \operatorname{tr} \left[E_{k} \rho_{\beta}(\lambda) \right] \operatorname{tr} \left[E_{j} \rho_{\beta}(\lambda) \right]
= \frac{\beta^{2}}{2} \operatorname{tr} \left[\left\{ E_{j}, \Phi_{H(\lambda)}(E_{k}) \right\} \cdot \rho_{\beta}(\lambda) \right] - \beta^{2} \operatorname{tr} \left[E_{k} \rho_{\beta}(\lambda) \right] \operatorname{tr} \left[E_{j} \rho_{\beta}(\lambda) \right].$$

One can see from this equation that $\nabla^2 \log Z_{\beta}(H)$ is a symmetric real matrix, ⁷ and hence its eigenvectors have real entries. Finally, we get

$$v^{\top} \cdot \left(\nabla^{2} \log Z_{\beta}(\lambda)\right) \cdot v = \sum_{j,k} v_{j} v_{k} \frac{\partial^{2}}{\partial \lambda_{k} \partial \lambda_{j}} \log Z_{\beta}(\lambda)$$

$$= \frac{\beta^{2}}{2} \operatorname{tr} \left[\left\{ W_{v}, \Phi_{H(\lambda)}(W_{v}) \right\} \rho_{\beta}(\lambda) \right] - \left(\beta \operatorname{tr} \left[W_{v} \rho_{\beta}(\lambda) \right] \right)^{2}.$$

$$(45)$$

⁷The terms $\operatorname{tr}[E_k \rho_\beta(\lambda)]$ and $\operatorname{tr}[E_j \rho_\beta(\lambda)]$ are real, being expectations of Hermitian matrices. Moreover, $\{E_j, \Phi_{H(\lambda)}(E_k)\}$ is a Hermitian operator, being an anti-commutator of two Hermitian operators. Hence $\operatorname{tr}\left[\{E_j, \Phi_{H(\lambda)}(E_k)\} \rho_\beta(\lambda)\right]$ is real too.

The statement of Lemma 29 does not make it clear that the Hessian is a variance of a suitable operator, or even is positive. The following lemma shows how to lower bound the Hessian by a variance of a quasi-local operator. The intuition for the proof arises by writing the Hessian in a manner that makes its positivity clear. This in particular, shows that $\log Z_{\beta}(\mu)$ is a convex function in parameters μ – we later improve this to being strongly convex.

Lemma 30 (A lower bound on \nabla^2 \log Z_{\beta}(\lambda)). For every $v \in \mathbb{R}^m$ and local operator $W_v = \sum_i v_i E_i$, define another local operator \widetilde{W} such that

$$\widetilde{W}_v = \int_{-\infty}^{\infty} f_{\beta}(t) e^{-iHt} W e^{iHt} dt, \tag{46}$$

where

$$f_{\beta}(t) = \frac{2}{\beta \pi} \log \frac{e^{\pi |t|/\beta} + 1}{e^{\pi |t|/\beta} - 1} \tag{47}$$

is defined such that $f_{\beta}(t)$ scales as $\frac{4}{\beta\pi}e^{-\pi|t|/\beta}$ for large t. We claim

$$\frac{1}{2} \operatorname{tr} \left[\left\{ W_v, \Phi_{H(\lambda)}(W_v) \right\} \rho_{\beta}(\lambda) \right] - \left(\operatorname{tr} \left[W_v \rho_{\beta}(\lambda) \right] \right)^2 \ge \operatorname{tr} \left[(\widetilde{W}_v)^2 \rho_{\beta}(\lambda) \right] - \left(\operatorname{tr} \left[\widetilde{W}_v \rho_{\beta}(\lambda) \right] \right)^2 \tag{48}$$

Remark 31. For the rest of the paper, we are going to fix an arbitrary $v \in \mathbb{R}^m$, in order to avoid subscripting W, \widetilde{W} by v.

Proof of Lemma 30. Let us start by proving a simpler version of Eq. (48), where we only show

$$\frac{1}{2} \operatorname{tr} \left[\left\{ W, \Phi_{H(\lambda)}(W) \right\} \rho_{\beta}(\lambda) \right] - \left(\operatorname{tr} \left[W \rho_{\beta}(\lambda) \right] \right)^{2} \ge 0. \tag{49}$$

Since v is an arbitrary vector, this shows that, as expected, $\nabla^2 \log Z_{\beta}(\lambda)$ is a positive semidefinite operator.

Consider the spectral decomposition of the Gibbs state $\rho_{\beta}(\lambda)$: $\rho_{\beta}(\lambda) = \sum_{j} r_{j}(\lambda)|j\rangle\langle j|$. Then observe that

$$\frac{1}{2} \operatorname{tr} \left[\left\{ W, \Phi_{H(\lambda)}(W) \right\} \rho_{\beta}(\lambda) \right] - \left(\operatorname{tr} \left[W \rho_{\beta}(\lambda) \right] \right)^{2}$$

$$= \frac{1}{2} \sum_{j} r_{j}(\lambda) \langle j | \left\{ W, \Phi^{H}(W) \right\} | j \rangle - \left(\sum_{j} r_{j}(\lambda) W_{j,j} \right)^{2}$$

$$= \frac{1}{2} \sum_{j,k} r_{j}(\lambda) \left(W_{j,k} \langle k | \Phi^{H}(W) | j \rangle + \langle j | \Phi^{H}(W) | k \rangle W_{k,j} \right) - \left(\sum_{j} r_{j}(\lambda) W_{j,j} \right)^{2}$$

$$\stackrel{(1)}{=} \frac{1}{2} \sum_{j,k} r_{j}(\lambda) \left(W_{j,k} W_{k,j} \tilde{f}_{\beta}(\mathcal{E}_{k} - \mathcal{E}_{j}) + W_{j,k} W_{k,j} \tilde{f}_{\beta}(\mathcal{E}_{j} - \mathcal{E}_{k}) \right) - \left(\sum_{j} r_{j}(\lambda) W_{j,j} \right)^{2}$$

$$\stackrel{(2)}{=} \sum_{j,k} r_{j}(\lambda) |W_{j,k}|^{2} \tilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|) - \left(\sum_{j} r_{j}(\lambda) W_{j,j} \right)^{2} .$$
(51)

In equality (1), we use Definition 19 and in equality (2) we use the facts that W is Hermitian and $\tilde{f}_{\beta}(t) = \tilde{f}_{\beta}(-t)$. Since $\tilde{f}_{\beta}(0) = 1$ and $\tilde{f}_{\beta}(t) > 0$ for all t, it is now evident from last equation that

$$\operatorname{tr}\left(\frac{1}{2}\{W,\Phi^{H}(W)\}\rho_{\beta}\right) - \operatorname{tr}\left(W\rho_{\beta}\right)^{2} \ge \sum_{j} r_{j}(\lambda)|W_{j,j}|^{2} - \left(\sum_{j} r_{j}(\lambda)W_{j,j}\right)^{2} \ge 0.$$

We can improve this bound by using the operator \widetilde{W} in (46). The function $f_{\beta}(t)$ in (46) is chosen carefully such that its Fourier transform satisfies $\widetilde{f}_{\beta}(\omega) = \widetilde{f}_{\beta}(|\omega|)$. Then, we have that

$$\widetilde{W} = \int_{-\infty}^{\infty} f_{\beta}(t) e^{-iHt} W e^{iHt} dt = \sum_{j,k} |j\rangle\langle k| W_{j,k} \, \widetilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|).$$
 (52)

Similar to (51) we get

$$\operatorname{tr}(\widetilde{W}^{2}\rho_{\beta}(\lambda)) - \left[\operatorname{tr}(\widetilde{W}\rho_{\beta}(\lambda))\right]^{2} = \sum_{j,k} r_{j}(\lambda)|W_{j,k}|^{2} \tilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|)^{2} - \left(\sum_{j} r_{j}(\lambda)W_{j,j}\right)^{2}$$

$$\leq \sum_{j,k} r_{j}(\lambda)|W_{j,k}|^{2} \tilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|) - \left(\sum_{j} r_{j}(\lambda)W_{j,j}\right)^{2}$$

$$= \operatorname{tr}\left(\frac{\{W, \Phi^{H}(W)\}}{2}\rho_{\beta}(\lambda)\right) - \left[\operatorname{tr}(W\rho_{\beta}(\lambda))\right]^{2}, \tag{53}$$

where the inequality is derived from $\tilde{f}_{\beta}(x)^2 \leq \tilde{f}_{\beta}(x)$ for arbitrary $-\infty < x < \infty$. Thus, we get

$$\left(\sum_{i=1}^{m} v_{i} \frac{\partial}{\partial \lambda_{i}}\right)^{2} \log Z_{\beta}(\lambda) \geq \operatorname{tr}(\widetilde{W}^{2} \rho_{\beta}(\lambda)) - \operatorname{tr}(\widetilde{W} \rho_{\beta}(\lambda))^{2}.$$

7 Lower bound on the variance of quasi-local operators

In the previous section, we showed how to give a lower bound on the Hessian of the logarithm of the partition function. To be precise, for a vector $\lambda=(\lambda_1,\ldots,\lambda_m)\in\mathbb{R}^m$ with $\|\lambda\|\leq 1$, Hamiltonian $H(\lambda)=\sum_i\lambda_i E_i$ and $\rho_\beta(\lambda)=\frac{1}{Z_\beta(\lambda)}e^{-\beta H(\lambda)}$ (where $Z_\beta(\lambda)=\operatorname{tr}(e^{-\beta H(\lambda)})$), we showed in Lemma 30 how to carefully choose a local operator \widetilde{W} such that for every v, we have

$$v^{\top} \cdot (\nabla^2 \log Z_{\beta}(\lambda)) \cdot v \ge \beta^2 \operatorname{Var}[\widetilde{W}].$$
 (54)

In this section, we further prove that the variance of \widetilde{W} with respect to $\rho_{\beta}(\lambda)$ can be bounded from below by a large enough quantity. Before looking at the highly non-trivial case of finite temperature, lets look at a simpler case of infinite temperature limit.

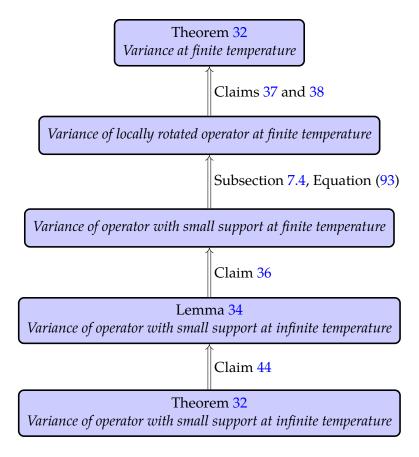


Figure 1: Flow of the argument in the proof of Theorem 33.

7.1 Warm-up: Variance at infinite temperature

Consider the infinite temperature state (i.e., the maximally mixed state) $\eta = \frac{\mathbb{1}_{\Lambda}}{\mathcal{D}_{\Lambda}}$. We have the following theorem, where we assume that the locality of W, namely $\kappa = \mathcal{O}(1)$.

Theorem 32. For \widetilde{W} as defined in Lemma 30, we have

$$\operatorname{tr}[(\widetilde{W})^{2}\eta] - \operatorname{tr}[\widetilde{W}\eta]^{2} \ge \frac{\Omega(1)}{(\beta \log(m) + 1)^{2}} \sum_{i=1}^{m} v_{i}^{2}.$$
(55)

The intuition behind the theorem is as follows. In the above statement, if \widetilde{W} is replaced by W, then the lower bound is immediate (see Eq. (56) below). Similarly, if H and W were commuting, then \widetilde{W} would be the same as W and the statement would follow. In order to show (55) for \widetilde{W} in general, we expand it in the energy basis of the Hamiltonian and use the locality of W to bound the contribution of cross terms (using Lemma 21). This accounts for the contributions arising due to non-commutativity of W and W.

Proof of Theorem 32. Recall from Lemma 30 that $W=\sum_i v_i E_i$. We first note that $\mathrm{tr}[\widetilde{W}\eta]=\mathrm{tr}[W\eta]=0$

0. From the definition, we have $\mathrm{tr}[(\widetilde{W})^2\eta] = \frac{1}{\mathcal{D}_\Lambda}\|(\widetilde{W})^2\|_F^2$. To begin with, we observe

$$||W||_F^2 = \mathcal{D}_{\Lambda} \sum_{i=1}^m v_i^2, \tag{56}$$

which holds since the basis E_i satisfies $||E_i||_F^2 = \mathcal{D}_{\Lambda}$ and $\operatorname{tr}[E_i E_j] = 0$ if $i \neq j$. Define P_s^H as the projection onto the energy range (s, s+1] of H.

$$P_s^H := \sum_{j:\mathcal{E}_j \in (s,s+1]} |j\rangle\langle j|. \tag{57}$$

Using the identity $\sum_s P_s^H = \mathbb{1}_{\Lambda}$ and the definition of \widetilde{W} , let us expand

$$||W||_{F}^{2} = \sum_{s,s'=-\infty}^{\infty} ||P_{s'}^{H}WP_{s}^{H}||_{F}^{2},$$

$$||\widetilde{W}||_{F}^{2} = \sum_{s,s'=-\infty}^{\infty} \left\| \int_{-\infty}^{\infty} dt P_{s'}^{H} f_{\beta}(t) e^{-iHt} W e^{iHt} P_{s}^{H} \right\|_{F}^{2}$$

$$= \sum_{s,s'=-\infty}^{\infty} \left\| \sum_{\substack{j:\mathcal{E}_{j} \in (s,s+1] \\ k:\mathcal{E}_{k} \in (s,s+1]}} W_{j,k} \widetilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|) P_{s'}^{H} |j\rangle \langle k| P_{s}^{H} \right\|_{F}^{2}.$$
(59)

By using the inequality

$$\tilde{f}_{\beta}(\omega) = \frac{\tanh(\beta\omega/2)}{\beta\omega/2} \ge \frac{1}{\frac{\beta}{2}|\omega|+1},$$

we have

$$\left\| \sum_{\substack{j:\mathcal{E}_{j} \in (s,s+1] \\ k:\mathcal{E}_{k} \in (s,s+1]}} W_{j,k} \tilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|) P_{s'}^{H} |j\rangle \langle k| P_{s}^{H} \|_{F}^{2} \right\|_{F}$$

$$= \sum_{j:\mathcal{E}_{j} \in (s,s+1]} \sum_{k:\mathcal{E}_{j} \in (s',s'+1]} [\tilde{f}_{\beta}(|\mathcal{E}_{j} - \mathcal{E}_{k}|)]^{2} |W_{j,k}|^{2}$$

$$\geq \frac{1}{\left(\frac{\beta}{2}(|s-s'|+1)+1\right)^{2}} \sum_{j:\mathcal{E}_{j} \in (s,s+1]} \sum_{k:\mathcal{E}_{j} \in (s',s'+1]} |W_{j,k}|^{2} = \frac{\|P_{s'}^{H}WP_{s}^{H}\|_{F}^{2}}{\left(\frac{\beta}{2}(|s-s'|+1)+1\right)^{2}}.$$
(60)

Plugging this lower bound in Eq. (59) gives the following lower bound for $\|\widetilde{W}\|_F^2$:

$$\|\widetilde{W}\|_{F}^{2} \ge \sum_{s,s'=-\infty}^{\infty} \frac{\|P_{s'}^{H}WP_{s}^{H}\|_{F}^{2}}{\left(\frac{\beta}{2}(|s-s'|+1)+1\right)^{2}} = \sum_{s_{0}=-\infty}^{\infty} \sum_{s_{1}=-\infty}^{\infty} \frac{\|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}}{\left(\frac{\beta}{2}(|s_{1}|+1)+1\right)^{2}}, \tag{61}$$

where we have introduced $s_0 = s + s'$, $s_1 = s - s'$. Let us consider the last expression for a fixed s_0 , introducing a cut-off parameter \bar{s} which we fix eventually:

$$\sum_{s_{1}=-\infty}^{\infty} \frac{\|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}}{\left[\frac{\beta}{2}(|s_{1}|+1)+1\right]^{2}}$$

$$\geq \frac{1}{\left(\frac{\beta}{2}(\bar{s}+1)+1\right)^{2}} \left(\sum_{|s_{1}|\leq \bar{s}} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}\right)$$

$$= \frac{1}{\left(\frac{\beta}{2}(\bar{s}+1)+1\right)^{2}} \left(\sum_{s_{1}=-\infty}^{\infty} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2} - \sum_{|s_{1}|>\bar{s}} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}\right). (62)$$

By combining the inequalities (61) and (62), we obtain

$$\|\widetilde{W}\|_{F}^{2} \ge \frac{\|W\|_{F}^{2}}{\left(\frac{\beta}{2}(\bar{s}+1)+1\right)^{2}} - \frac{1}{\left(\frac{\beta}{2}(\bar{s}+1)+1\right)^{2}} \sum_{s_{0}=-\infty}^{\infty} \sum_{|s_{1}|>\bar{s}} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}.$$
 (63)

Now, we will estimate the second term in (63). Since the subspaces $P^H_{(s_0+s_1)/2}$ and $P^H_{(s_0-s_1)/2}$ are sufficiently far apart in energy, we can use the exponential concentration on the spectrum [AKL16] (as stated in Lemma 21) to obtain the following: for $W = \sum_i v_i E_i$, we have

$$||P_{(s_0+s_1)/2}^H W P_{(s_0-s_1)/2}^H| \le \sum_{i=1}^m v_i ||P_{(s_0+s_1)/2}^H E_i P_{(s_0-s_1)/2}^H|$$

$$\le C e^{-\lambda(|s_1|-1-\kappa)} \sum_{i=1}^m |v_i| \le C m e^{-\lambda(|s_1|-1-\kappa)} \max_i |v_i|.$$
(64)

where we use the condition that E_i are tensor product of Pauli operators with weight at most κ , and the parameters C and λ are $\mathcal{O}(1)$ constants (see Lemma 21 for their explicit forms). Then, the second term in (63) can be upper-bounded by

$$\sum_{s_{0}=-\infty}^{\infty} \sum_{|s_{1}|>\bar{s}} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{F}^{2}$$

$$\stackrel{(1)}{\leq} \sum_{s_{0}=-\infty}^{\infty} \sum_{|s_{1}|>\bar{s}} \|P_{(s_{0}+s_{1})/2}^{H}WP_{(s_{0}-s_{1})/2}^{H}\|_{2}^{2} \cdot \|P_{(s_{0}+s_{1})/2}^{H}\|_{F}^{2}$$

$$\stackrel{(2)}{\leq} \sum_{|s_{1}|>\bar{s}} \sum_{s_{0}=-\infty}^{\infty} \|P_{(s_{0}+s_{1})/2}^{H}\|_{F}^{2} \cdot C^{2}m^{2}e^{-2\lambda(|s_{1}|-1-\kappa)} \max_{i} v_{i}^{2}$$

$$= \mathcal{D}_{\Lambda}C^{2}m^{2}e^{2\lambda(1+\kappa)} \max_{i} v_{i}^{2} \sum_{|s_{1}|\geq\bar{s}+1} e^{-2\lambda|s_{1}|}$$

$$\stackrel{(3)}{\leq} \mathcal{D}_{\Lambda} \max_{i} v_{i}^{2} \frac{C^{2}m^{2}e^{2\lambda(\kappa+1)}}{\lambda} e^{-2\lambda\bar{s}} \stackrel{(4)}{\leq} \mathcal{D}_{\Lambda} \frac{C^{2}m^{2}e^{2\lambda(\kappa+1)}}{\lambda} e^{-2\lambda\bar{s}} \left(\sum_{i} v_{i}^{2}\right), \tag{65}$$

where inequality (1) follows from Eq. (16), (2) follows from Eq. (64), (3) follows from Fact 12 and (4) follows from $\max_i v_i^2 \leq \sum_i v_i^2$. Therefore, by applying Eq. (56) and (65) to (63), we arrive at the lower bound as

$$\|\widetilde{W}\|_F^2 \ge \frac{\mathcal{D}_{\Lambda}}{[\beta(\bar{s}+1)/2+1]^2} \left(\sum_{i=1}^m v_i^2\right) \left(1 - \frac{C^2 m^2 e^{2\lambda(\kappa+1)}}{\lambda} e^{-2\lambda \bar{s}}\right). \tag{66}$$

Since $\lambda, C, \kappa = \mathcal{O}(1)$, by choosing $\bar{s} = \mathcal{O}(\log(m))$, we obtain the main inequality (55). This completes the proof. \square

7.2 Variance at finite temperature

Next, we show how to prove a variance lower bound at finite temperature. This is achieved by the following general theorem on the variance of arbitrary local operator, which will reduce the problem to estimating a "variance-like" quantity at the infinite temperature case (observe the occurrence of the maximally mixed state η in the theorem below).

Theorem 33. Let $\beta > 0$, H be a κ -local Hamiltonian on the lattice Λ and $\rho_{\beta} = \frac{e^{-\beta H}}{\operatorname{tr}(e^{-\beta H})}$. Let A be a $(\tau, a_1, a_2, 1)$ -quasi-local operator (see Eq. (19)) where $a_2 = \mathcal{O}(1/\beta), a_1 = \mathcal{O}(1)$ are constants and Z are restricted to be connected sets within Λ . Suppose $\operatorname{tr}[A\rho_{\beta}] = 0$ and $\tau \leq 1$. We have

$$\langle A^2 \rangle = \operatorname{tr}(A^2 \rho_\beta) \ge \left(\max_{i \in \Lambda} \operatorname{tr}[A_{(i)}^2 \eta] \right)^{\beta^{\Omega(1)}}.$$

We remark that the theorem statement above hides several terms that depend on the lattice, such as the lattice dimension, the degree of the graph and the locality of Hamiltonian (which we have fixed to be a constant). Additionally, the assumptions $a_2 = \mathcal{O}(1/\beta), a_1 = \mathcal{O}(1)$ are made in order to show that an operator A^* to which we apply the theorem, satisfies the assumptions of the theorem. Before proving the theorem, we first discuss how to use this theorem in order to prove a lower bound on the Hessian of $\log Z(\lambda)$.

For an arbitrary $v \in \mathbb{R}^m$, let $W = \sum_i v_i E_i$ and \widetilde{W} be the operators defined in Lemma 30. In Appendix \overline{D} we show that \widetilde{W} is a $(1/D, \mathcal{O}(1), \mathcal{O}(1/\beta), c_*\beta^{2D+1}(\max_{i\in\Lambda}|v_i|))$ -quasi-local operator, for $c_* = \mathcal{O}(1)$. Thus, the following operator

$$A^* = \frac{\beta^{-2D-1}}{c_* \max_{i \in \Lambda} |v_i|} (\widetilde{W} - \operatorname{tr}[\rho_{\beta} \widetilde{W}] \mathbb{1}),$$

is $(\mathcal{O}(1), \mathcal{O}(1), \mathcal{O}(1/\beta), 1)$ -quasi-local and satisfies $\operatorname{tr}[A\rho_{\beta}] = 0$. We now apply Theorem 33 to the operator A^* to prove Theorem 28. We need to estimate $\max_i \operatorname{tr}[A_{(i)}^{*2}\eta]$. Consider

$$\max_{i} \operatorname{tr}[(A_{(i)}^{*})^{2} \eta] = \frac{\beta^{-4D-2}}{c_{*}^{2} \left(\max_{i \in \Lambda} |v_{i}| \right)^{2}} \left(\max_{i} \operatorname{tr}[(\widetilde{W}_{(i)})^{2} \eta] \right).$$

The following lemma is shown in Appendix E.

 $^{^{8}}$ We remark that we can also apply the theorem for other choices of a_{1}, a_{2} , with small modifications to the proof.

Lemma 34. It holds that

$$\max_{i \in \Lambda} (\operatorname{tr}[(\widetilde{W}_{(i)})^2 \eta]) = \frac{\Omega(1)}{(\beta \log(\beta) + 1)^{2D+2}} \left(\max_{i \in \Lambda} v_i^2 \right).$$

This implies

$$\max_{i} \operatorname{tr}[(A_{(i)}^*)^2 \eta] = \frac{\Omega(1)}{\beta^{4D+2} \left(\beta \log(\beta) + 1\right)^{2D+2} \left(\max_{i \in \Lambda} |v_i|\right)^2} \left(\max_{i \in \Lambda} v_i^2\right) = \frac{1}{\beta^{\Omega(1)}}.$$

Using this lower bound in Theorem 33, we find

$$\begin{split} \langle (\widetilde{W})^2 \rangle - \left(\langle \widetilde{W} \rangle \right)^2 &= \frac{\beta^{4D+2} \left(\max_{i \in \Lambda} |v_i| \right)^2}{c_*^2} \left(\langle (A^*)^2 \rangle - (\langle A^* \rangle)^2 \right) \\ &= \beta^{\Omega(1)} \left(\max_{i \in \Lambda} |v_i| \right)^2 \cdot \left(\max_{i} \operatorname{tr}[(A^*_{(i)})^2 \eta] \right)^{\beta^{\Omega(1)}} \\ &= \beta^{\Omega(1)} \cdot \left(\frac{1}{\beta^{\mathcal{O}(1)}} \right)^{\beta^{\mathcal{O}(1)}} \cdot \left(\max_{i \in \Lambda} |v_i| \right)^2 \\ &\stackrel{(1)}{=} \beta^{\Omega(1)} \cdot e^{-\beta^{\mathcal{O}(1)}} \left(\max_{i \in \Lambda} |v_i| \right)^2 \geq \beta^{\Omega(1)} \cdot \frac{e^{-\beta^{\mathcal{O}(1)}}}{m} \left(\sum_{i} v_i^2 \right), \end{split}$$

where we used $\beta^{-\mathcal{O}(1)} \geq e^{-\beta}$ in (1). Putting together the bound above with Eq. (54), we find that for every $v \in \mathbb{R}^m$,

$$v^{\top} \cdot (\nabla^2 \log Z_{\beta}(\lambda)) \cdot v \ge \beta^2 \operatorname{Var}[\widetilde{W}] \ge \beta^{\Omega(1)} \cdot \frac{e^{-\beta^{\mathcal{O}(1)}}}{m} \sum_{i=1}^m v_i^2.$$

This establishes Theorem 28.

7.3 Some key quantities in the proof and proof sketch

We now prove Theorem 33. For notational simplicity, let

$$H' := H - \frac{1}{\beta} \log Z_{\beta},\tag{67}$$

which allows us to write $\rho_{\beta}=e^{-\beta H'}$. We will interchangeably use the frobenius norm to write $\langle A^2\rangle=\mathrm{tr}(A^2\rho_{\beta})=\|A\sqrt{\rho_{\beta}}\|_F$. We now define the projection operator P_{γ}^A as follows (see Figure 2):

$$P_{\gamma}^{A} := \sum_{\omega \in [-\gamma, \gamma]} \Pi_{\omega},\tag{68}$$

where Π_{ω} is the projector onto the eigenspace of A with eigenvalue ω . We then define δ_{γ} by

$$\delta_{\gamma} := 1 - \|P_{\gamma}^A \sqrt{\rho_{\beta}}\|_F^2. \tag{69}$$

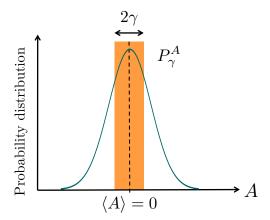


Figure 2: Plot of the probability distribution $\operatorname{tr}[\Pi_{\omega}\rho_{\beta}]$, where Π_{ω} is the projector onto the eigenvectors of A with eigenvalue ω . It is assumed that $\operatorname{tr}[A\rho_{\beta}]=0$. For a γ to be chosen in the proof, P_{γ}^{A} is the projector onto the subspace of eigenvectors of A with eigenvalue between $[-\gamma, \gamma]$. A lower bound on the variance of A follows if we can show that for a constant γ , the probability mass in the colored range is small (see Equation 70).

Using δ_{γ} , observe that we can lower bound $\langle A^2 \rangle$ as

$$\langle A^2 \rangle = \sum_{\omega} \omega^2 \langle \omega | \rho_{\beta} | \omega \rangle \ge \sum_{|\omega| \ge \gamma} \omega^2 \langle \omega | \rho_{\beta} | \omega \rangle \ge \gamma^2 \sum_{|\omega| \ge \gamma} \langle \omega | \rho_{\beta} | \omega \rangle \ge \gamma^2 \delta_{\gamma}. \tag{70}$$

Let $Q_{\gamma}^{A} = \mathbb{1} - P_{\gamma}^{A}$, then observe that from Eq. (69) that

$$||P_{\gamma}^{A}\sqrt{\rho_{\beta}} - \sqrt{\rho_{\beta}}||_{F}^{2} = ||Q_{\gamma}^{A}\sqrt{\rho_{\beta}}||_{F}^{2} = \delta_{\gamma}.$$

$$(71)$$

The proof is divided into the following subsections, each of which may be of independent interest on its own.

7.4 Reducing the global problem to a local problem

A main challenge in bounding the variance of the operator A is that it is a global operator and its properties may scale badly with the system size. But since it is a linear combination of local operators, it is related to operators supported in a local region by a simple linear transform. To this end, recall the definition of $A_{(i)}$ (the local operator which includes essentially the terms in A that have support on the ith site) from the subsection 5.5. Using Haar random unitaries, we obtain the integral representation of $A_{(i)}$ as

$$A_{(i)} = A - \frac{1}{d} [\operatorname{tr}_i(A)] \otimes \mathbb{1}_i = A - \int d\mu(U_i) U_i^{\dagger} A U_i, \tag{72}$$

where $\mu(U_i)$ is the Haar measure for unitary operator U_i which acts on the ith site. Since the $A_{(i)}$ is obtained from a quasi-local A_i , it is quasi-local itself. Next claim will approximate $A_{(i)}$ by a local operator.

Claim 35. For an integer R, let X_i be the radius-R ball around the site i, i.e., $X_i = B(R, i)$. There exists an operator A_{X_i} supported entirely on X_i , such that

$$||A_{(i)} - A_{X_i}|| \le 2a_1 \cdot \left(\frac{4}{a_2 \tau^2}\right)^{\frac{1}{\tau}} \cdot e^{-\frac{a_2}{2}(R)^{\tau}}.$$

Proof. Using the representation of A in Theorem 33 and the fact that local operators not containing i in their support are removed, we can write

$$A_{(i)} = \sum_{\substack{k,Z \subseteq \Lambda: \\ |Z| \le k, Z \ni i}} g_k \left(a_Z - \frac{1}{d} [\operatorname{tr}_i(a_Z)] \otimes \mathbb{1}_i \right),$$

Define

$$A_{X_i} = \sum_{\substack{k,Z \subseteq X_i: \\ |Z| \le k, Z \ni i}} g_k \left(a_Z - \frac{1}{d} [\operatorname{tr}_i(a_Z)] \otimes \mathbb{1}_i \right).$$

be the desired approximations of $A_{(i)}$ by removing all operators that are not contained in X_i . Observe that

$$||A_{(i)} - A_{X_{i}}|| \leq 2 \sum_{\substack{k,Z \subseteq \Lambda: \\ Z \not\subset X_{i}, |Z| \leq k, Z \ni i}} g_{k} ||a_{Z}|| \leq 2 \sum_{\substack{k,Z \subseteq \Lambda: \\ \operatorname{diam}(Z) \geq R, |Z| \leq k, Z \ni i}} g_{k} ||a_{Z}||$$

$$\stackrel{(2)}{\leq} 2 \sum_{k \geq R} g_{k} \left(\sum_{Z:Z \ni i} ||a_{Z}|| \right) \stackrel{(3)}{\leq} 2\zeta \sum_{k \geq R} g_{k}$$

$$\leq 2\zeta a_{1} \sum_{k \geq R} e^{-a_{2}k^{\tau}} \stackrel{(4)}{\leq} 2\zeta a_{1} \cdot a_{2}^{-\frac{1}{\tau}} \cdot \left(\frac{2}{\tau}\right)^{\frac{2}{\tau}} \cdot e^{-\frac{a_{2}}{2}(R)^{\tau}}.$$

$$(73)$$

For inequality (1), note that since $Z \not\subset X_i$ and $Z \ni i$, the diameter of Z (recall that Z is a ball) must be larger than the radius of X_i , which is R. Inequality (2) holds since $k \ge |Z| \ge \operatorname{diam}(Z)$, inequality (3) uses Definition 14 and inequality (4) uses Fact 12. Since $\zeta = 1$ for the given A (see the statement of Theorem 33), this completes the proof.

We now define i_0 as

$$i_0 := \arg\max_i \|A_i \sqrt{\eta}\|_F. \tag{74}$$

The set of unitaries U_{i_0} and the Haar measure $\mu(U_{i_0})$ are defined analogously. Plugging in

$$R = \left(\frac{2}{a_2} \log \frac{8 \cdot 4^{\frac{1}{\tau}} \cdot a_1}{\tau^{\frac{2}{\tau}} \cdot a_2^{\frac{1}{\tau}} \|A_{(i_0)} \sqrt{\eta}\|_F}\right)^{\frac{1}{\tau}}$$

in Claim 35 we get

$$||A_{(i_0)} - A_{X_{i_0}}|| \le \frac{1}{4} ||A_{(i_0)} \sqrt{\eta}||_F \tag{75}$$

Substituting $a_2 = \mathcal{O}(1/\beta), a_1 = \mathcal{O}(1), \tau = \mathcal{O}(1)$, we find that we can ensure the condition (75) for

$$R = \operatorname{diam}(X_{i_0}) = \left(\beta \log \left(\frac{1}{\|A_{(i_0)}\sqrt{\eta}\|_F}\right)\right)^{\Omega(1)}.$$
 (76)

7.5 Variance of operators with small support: finite temperature to infinite temperature

Having related A to the operator $A_{(i_0)}$ (which is essentially supported on a small number of sites in the lattice, up to a tail decaying sub-exponentially in the radius), we now argue that it is simpler to bound the variance of $A_{(i_0)}$ in terms of its variance at infinite temperature, as long as some local rotations are allowed. In particular, we will show the existence of a unitary U_{i_0} for which we can proceed in this fashion. The intuition here is that if rotations are allowed, then the eigenvectors of $A_{X_{i_0}}$ can be rearranged to yield largest possible variance with ρ_{β} . This turns out to be larger than the variance with η . To make this precise, we prove the following claim.

Claim 36. There exists $U_{X_{i_0}}$ such that

$$\|U_{X_{i_0}}^{\dagger}A_{(i_0)}U_{X_{i_0}}\sqrt{\rho_{\beta}}\|_F \ge \|A_{(i_0)}\sqrt{\eta}\|_F - 2\|A_{X_{i_0}} - A_{(i_0)}\| \ge \frac{1}{2}\|A_{(i_0)}\sqrt{\eta}\|_F,$$

where the second inequality uses Eq. (75).

Proof of Claim 36. Recall that the goal is to show the existence of a unitary $U_{X_{i_0}}$ satisfying

$$||U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F \ge ||A_{(i_0)} \sqrt{\eta}||_F - 2||A_{X_{i_0}} - A_{(i_0)}||.$$
(77)

We start from the following,

$$||U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F = ||U_{X_{i_0}}^{\dagger} [(A_{(i_0)} - A_{X_{i_0}}) + A_{X_{i_0}}] U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F$$

$$\geq ||U_{X_{i_0}}^{\dagger} A_{X_{i_0}} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F - ||A_{(i_0)} - A_{X_{i_0}}||$$
(78)

and lower-bound the norm of $\|U_{X_{i_0}}^{\dagger}A_{X_{i_0}}U_{X_{i_0}}\sqrt{\rho_{\beta}}\|_F$. For this, define

$$\rho_{\beta,X} := \operatorname{tr}_{X^{c}}(\rho_{\beta}), \tag{79}$$

where tr_{X^c} is the partial trace operation for the Hilbert space on X^c . We define the spectral decomposition of $A_{X_{i_0}}$ as

$$A_{X_{i_0}} = \sum_{s=1}^{\mathcal{D}_{X_{i_0}}} \varepsilon_s |\varepsilon_s\rangle \langle \varepsilon_s|, \tag{80}$$

where ε_s is ordered as $|\varepsilon_1| \ge |\varepsilon_2| \ge |\varepsilon_3| \ge \cdots$ and $\mathcal{D}_{X_{i_0}}$ is the dimension of the Hilbert space on X_{i_0} . Additionally, define the spectral decomposition of $\rho_{\beta,X_{i_0}}$ as

$$\rho_{\beta,X_{i_0}} = \sum_{s=1}^{\mathcal{D}_{X_{i_0}}} p_s |\mu_s\rangle \langle \mu_s|, \tag{81}$$

where p_s is ordered as $p_1 \geq p_2 \geq p_3 \geq \cdots$ and $|\mu_s\rangle$ is the sth eigenstate of $\rho_{\beta,X_{i_0}}$. We now choose the unitary operator $U_{X_{i_0}}$ such that

$$U_{X_{i_0}}|\mu_s\rangle = |\varepsilon_s\rangle \quad \text{for} \quad s = 1, 2, \dots, \mathcal{D}_{X_{i_0}}$$
 (82)

We then obtain

$$U_{X_{i_0}} \rho_{\beta, X_{i_0}} U_{X_{i_0}}^{\dagger} = \sum_{s=1}^{\mathcal{D}_{X_{i_0}}} p_s |\varepsilon_s\rangle \langle \varepsilon_s|.$$
(83)

This implies

$$||U_{X_{i_0}}^{\dagger} A_{X_{i_0}} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F^2 = \operatorname{tr}[U_{X_{i_0}}^{\dagger} A_{X_{i_0}}^2 U_{X_{i_0}} \rho_{\beta}]$$

$$= \operatorname{tr}[A_{X_{i_0}}^2 U_{X_{i_0}} \rho_{\beta} U_{X_{i_0}}^{\dagger}] = \operatorname{tr}_{X_{i_0}}[A_{X_{i_0}}^2 U_{X_{i_0}} \rho_{\beta, X_{i_0}} U_{X_{i_0}}^{\dagger}]$$

$$= \sum_{s=1}^{\mathcal{D}_{X_{i_0}}} p_s \varepsilon_s^2 \ge \frac{1}{\mathcal{D}_{X_{i_0}}} \sum_{s=1}^{\mathcal{D}_{X_{i_0}}} \varepsilon_s^2 = ||A_{X_{i_0}} \sqrt{\eta}||_F^2,$$
(84)

where the inequality used the fact that p_s, ε_s are given in descending order. Then, the minimization problem of $\sum_s p_s \varepsilon_s$ for p_{s_s} with the constraint $p_1 \geq p_2 \geq p_3 \geq \cdots$ has a solution of $p_1 = p_2 = \cdots = p_{D_{X_{in}}}$. Using the lower bound

$$||A_{X_{i_0}}\sqrt{\eta}||_F = ||(A_{X_{i_0}} - A_{(i_0)} + A_{(i_0)})\sqrt{\eta}||_F \ge ||A_{(i_0)}\sqrt{\eta}||_F - ||A_{X_{i_0}} - A_{(i_0)}||,$$
(85)

we can reduce inequality (84) to

$$||U_{X_{i_0}}^{\dagger} A_{X_{i_0}} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F \ge ||A_{(i_0)} \sqrt{\eta}||_F - ||A_{X_{i_0}} - A_{(i_0)}||.$$
(86)

By combining the inequalities (78) and (86), we obtain

$$\begin{aligned} \|U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F &\geq \|U_{X_{i_0}}^{\dagger} A_{X_{i_0}} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F - \|A_{(i_0)} - A_{X_{i_0}} \| \\ &\geq \|U_{X_{i_0}}^{\dagger} A_{X_{i_0}} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F - 2 \|A_{(i_0)} - A_{X_{i_0}} \| \end{aligned}$$

which proves the claimed statement.

7.6 Invariance under local unitaries

Recall that we reduced the problem of variance of A to that of the operator $A_{(i_0)}$ that is essentially supported on small number of sites. But in the process, we introduced several local unitaries (c.f. previous subsections). In order to handle the action of these unitaries, we will use two claims which show that local unitaries do not make much difference in the relative behavior of spectra of A and A'. To elaborate, consider any local operator A acting on constant number of sites A on the state A0. It is expected that the quantum state A1 is strongly concentrated for A2, one would expect this behavior to hold even for A3. We make this intuition rigorous in the following claim.

Claim 37. Let c_1, c_2, λ be universal constants. Let $X \subseteq \Lambda$. For every unitary U_X supported on X, we have

$$\|Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq \exp\left(\lambda|X|\right)\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}}.$$
(87)

Let us see a simple application of the claim. It allows us to control the variance of A even after local operations are applied to it. More precisely,

$$||AU_{X}\sqrt{\rho_{\beta}}||_{F}^{2} = ||AP_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}||_{F}^{2} + ||A(\mathbb{1} - P_{\gamma}^{A})U_{X}\sqrt{\rho_{\beta}}||_{F}^{2}$$

$$\leq \gamma^{2} + ||A||^{2} \cdot ||(\mathbb{1} - P_{\gamma}^{A})U_{X}\sqrt{\rho_{\beta}}||_{F}^{2}.$$
(88)

By Claim 37, the expression on the second line is upper bounded by $\gamma^2 + \|A\|^2 e^{\mathcal{O}(1)|X|} \delta_{\gamma}^{\mathcal{O}(1)/\beta}$. This upper bound on $\|AU_X\sqrt{\rho_\beta}\|_F$ suffices to provide an inverse-polynomial *lower bound* on the variance of A^2 , since we can lower bound δ_{γ} for an appropriate choice of γ . However we now show how one can polynomially improve upon this upper bound (thereby the lower bound on variance) using the following claim. This claim, along the lines of Claim 37, also shows that local unitaries U_X do not change the desired expectation values.

Claim 38. Let $X \subseteq \Lambda$. For every unitary U_X supported on X, we have

$$\|AQ_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq \frac{1}{\gamma} \cdot \exp\left(\mathcal{O}(1) \cdot |X|\right) \delta_{\gamma}^{\mathcal{O}(1)/\beta} + \mathcal{O}(1) \cdot |X|^{6} \cdot \langle A^{2} \rangle. \tag{89}$$

Proof of both the Claims 37, 38 appear in Section 7.8. An immediate corollary of this claim is the following, that improves upon Eq. (88).

Corollary 39. Let X be a subset of Λ of size $|X| = \mathcal{O}(1)$. For every unitary U_X supported on X, we have

$$||AU_X\sqrt{\rho_\beta}||_F^2 \le \gamma^2 + \frac{e^{\mathcal{O}(1)\cdot|X|}\delta_\gamma^{\mathcal{O}(1)/\beta}}{\gamma} + \mathcal{O}(1)|X|^6\langle A^2\rangle.$$
(90)

Proof. Similar to Eq. (88), we upper bound $\|AU_X\sqrt{\rho_\beta}\|_F^2$ as

$$||AU_X\sqrt{\rho_\beta}||_F^2 = ||AP_\gamma^A U_X\sqrt{\rho_\beta}||_F^2 + ||AQ_\gamma^A U_X\sqrt{\rho_\beta}||_F^2 \le \gamma^2 + ||AQ_\gamma^A U_X\sqrt{\rho_\beta}||_F^2, \tag{91}$$

since $Q_{\gamma}^{A} = \mathbb{1} - P_{\gamma}^{A}$. By combining this with Claim 38, the corollary follows.

7.7 Proof of the Theorem 33

We are now ready to prove the main theorem statement. The main idea of the proof is the following: if the spectrum of A is strongly concentrated for the Gibbs state ρ_{β} , the concentration can be proven to be protected to arbitrary local unitary operations (see Claims 37 and 38). On the other hand, by choosing local unitary operations appropriately, we can relate the variance of the operator A (rotated by certain local unitary U_{i_0} on the site i_0) to the variance of the operator $A_{(i_0)}$ and hence give a good lower bound to the variance (see Claim 36). Combining the two results allows us to lower bound the variance of A and hence prohibits the strong spectral concentration of the operator A. We formally prove this now.

Proof. Let $U_{X_{i_0}}$ be the unitary as chosen in Claim 36. Using Eq. (72), we obtain the following expression for $U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}}$

$$U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} = U_{X_{i_0}}^{\dagger} A U_{X_{i_0}} - \int d\mu(U_{i_0}) U_{X_{i_0}}^{\dagger} U_{i_0}^{\dagger} A U_{i_0} U_{X_{i_0}}.$$
(92)

⁹Explicit $\mathcal{O}(1)$ constants that appear in this inequality are made clear in the proof.

Using triangle inequality, we have

$$||U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F \leq ||U_{X_{i_0}}^{\dagger} A U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F + \int d\mu(U_{i_0}) ||U_{X_{i_0}}^{\dagger} U_{i_0}^{\dagger} A U_{i_0} V_{X_{i_0}} \sqrt{\rho_{\beta}}||_F$$

$$= ||A U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F + \int d\mu(U_{i_0}) ||A U_{i_0} U_{X_{i_0}} \sqrt{\rho_{\beta}}||_F$$
(93)

This implies

$$\begin{aligned} \|U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F^2 &\leq \left(\|AU_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F + \int d\mu(U_{i_0}) \|AU_{i_0} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F \right)^2 \\ &\leq 2 \|AU_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F^2 + 2 \left(\int d\mu(U_{i_0}) \|AU_{i_0} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F \right)^2. \end{aligned}$$

Now, we can use Corollary 39 to obtain the upper bound

$$\|U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}}\|_F^2 \le 4\gamma^2 + \frac{e^{\mathcal{O}(1)|X_{i_0}|} \delta_{\gamma}^{\mathcal{O}(1)/\beta}}{\gamma} + \mathcal{O}(1)|X_{i_0}|^6 \langle A^2 \rangle. \tag{94}$$

Using Claim 36, we have

$$\|U_{X_{i_0}}^{\dagger} A_{(i_0)} U_{X_{i_0}} \sqrt{\rho_{\beta}} \|_F \ge \frac{1}{2} \|A_{(i_0)} \sqrt{\eta} \|_F. \tag{95}$$

Putting together the upper bound in Eq. (94) and the lower bound in Eq. (95), we have

$$4\gamma^{2} + \frac{e^{\mathcal{O}(1)|X_{i_{0}}|}\delta_{\gamma}^{\mathcal{O}(1)/\beta}}{\gamma} + \mathcal{O}(1)|X_{i_{0}}|^{6}\langle A^{2}\rangle \ge \frac{1}{4}||A_{(i_{0})}\sqrt{\eta}||_{F}^{2}.$$
 (96)

By choosing as $\gamma^2 = \|A_{(i_0)}\sqrt{\eta}\|_F^2/32 =: \gamma_0^2$, we obtain

$$\frac{e^{\mathcal{O}(1)|X_{i_0}|}\delta_{\gamma_0}^{\mathcal{O}(1)/\beta}}{\gamma_0} + \mathcal{O}(1)|X_{i_0}|^6 \langle A^2 \rangle \ge \gamma_0^2.$$
(97)

This inequality implies that either

$$\delta_{\gamma_0} \ge \left(\gamma_0^3 e^{-\mathcal{O}(1)|X_{i_0}|}\right)^{\beta \cdot \mathcal{O}(1)}$$

or

$$\langle A^2 \rangle \ge \frac{\Omega(1)\gamma_0^2}{|X_{i_0}|^6}.$$

Combining with Eq. (70), we conclude that

$$\langle A^2 \rangle \geq \min \Big\{ \gamma_0^2 \cdot \Big(\gamma_0^3 e^{-\mathcal{O}(1)|X_{i_0}|} \Big)^{\beta \cdot \mathcal{O}(1)}, \frac{\Omega(1)\gamma_0^2}{|X_{i_0}|^6} \Big\}.$$

Eq. (76) ensures that

$$|X_{i_0}| = \mathcal{O}(1)R^D = \beta^{\Omega(1)} \log \left(\frac{1}{\|A_{(i_0)}\sqrt{\eta}\|_F}\right)^{\Omega(1)},$$

where we have used the assumption that lattice dimension D is $\mathcal{O}(1)$. Plugging in this expression for $|X_{i_0}|$ with the choice of γ_0 , we find

$$\operatorname{tr}(A^{2}\rho_{\beta}) = \langle A^{2} \rangle \geq \min \left\{ \|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\beta \cdot \mathcal{O}(1)} \cdot e^{-\beta \mathcal{O}(1)|X_{i_{0}}|}, \frac{\Omega(1)\|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\Omega(1)}}{|X_{i_{0}}|^{6}} \right\}$$

$$\geq \min \left\{ \|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\beta^{\Omega(1)}}, \frac{\Omega(1)\|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\Omega(1)}}{\beta^{\mathcal{O}(1)}\log(\frac{1}{\|A_{(i_{0})}\sqrt{\eta}\|_{F}})^{\mathcal{O}(1)}} \right\}$$

$$\geq \min \left\{ \|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\beta^{\Omega(1)}}, \frac{\Omega(1)\|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\Omega(1)}}{\beta^{\mathcal{O}(1)}} \right\}$$

$$\geq \|A_{(i_{0})}\sqrt{\eta}\|_{F}^{\beta^{\Omega(1)}}.$$

Since we chose i_0 in Eq. (74) such that $||A_{(i_0)}\sqrt{\eta}||_F = \max_i ||A_{(i)}\sqrt{\eta}||_F$, this proves the theorem. \square

7.8 Proof of Claims 37 and 38

Proof of Claim 37. Recall that the goal is to show that for every $X \subseteq \Lambda$ and arbitrary unitaries U_X ,

$$\|Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \le c_{1}e^{\lambda|X|}\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}},\tag{98}$$

where $Q_{\gamma}^{A} = \mathbb{1} - P_{\gamma}^{A}$ and P_{γ}^{A} was defined in Eq. (68). To prove this inequality, we start from the following expression:

$$\|Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} = \left\|\sum_{m\in\mathbb{Z}}Q_{\gamma}^{A}U_{X}P_{m}^{H'}\sqrt{\rho_{\beta}}\right\|_{F}^{2} = \sum_{m\in\mathbb{Z}}\left\|Q_{\gamma}^{A}U_{X}P_{m}^{H'}\sqrt{\rho_{\beta}}\right\|_{F}^{2}$$
(99)

with

$$P_m^{H'} := \sum_{j: \mathcal{E}_j \in (m, m+1]} |j\rangle\langle j|, \tag{100}$$

where $|j\rangle$ is the eigenvector of the Hamiltonian H' with \mathcal{E}_j the corresponding eigenvalue. Note that $\sum_{m\in\mathbb{Z}}P_m^{H'}=\mathbb{1}$ and we have $P_m^{H'}=0$ for $m\notin[-\|H'\|,\|H'\|]$. For some $\Delta>0$ which we pick later, we now decompose $\left\|Q_\gamma^A U_X P_m^{H'} \sqrt{\rho_\beta}\right\|_F^2$ as a sum of the following quantities

$$\left\| Q_{\gamma}^{A} U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} = \left\| Q_{\gamma}^{A} \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} + P_{[m-\Delta,m+\Delta]}^{H'} \right) U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2}, \tag{101}$$

where

$$P^{H'}_{>m+\Delta} := \sum_{m'>m+\Delta} P^{H'}_{m'}, \quad P^{H'}_{< m+\Delta} := \sum_{m'< m+\Delta} P^{H'}_{m'}, \quad P^{H'}_{[m-\Delta,m+\Delta]} := \sum_{m-\Delta \leq m' \leq m+\Delta} P^{H'}_{m'}. \quad (102)$$

Summing over all $m \in \mathbb{Z}$ in Eq. (101) and using Eq. (99) followed by the triangle inequality gives us the following inequality

$$\|Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq 2 \sum_{\substack{m \in \mathbb{Z} \\ :=(1)}} \|Q_{\gamma}^{A}P_{[m-\Delta,m+\Delta]}^{H'}U_{X}P_{m}^{H'}\sqrt{\rho_{\beta}}\|_{F}^{2} + 2 \sum_{\substack{m \in \mathbb{Z} \\ :=(2)}} \|Q_{\gamma}^{A}(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'})U_{X}P_{m}^{H'}\sqrt{\rho_{\beta}}\|_{F}^{2}.$$
(103)

We first bound (1) in Eq. (103). Note that for every m,

$$\left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \leq \| P_{m}^{H'} \sqrt{\rho_{\beta}} \|^{2} \cdot \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \right\|_{F}^{2}$$

$$\leq e^{-\beta m} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \right\|_{F}^{2},$$

$$(104)$$

where the first inequality used Eq. (16). The expression in the last line can be upper bounded as

$$\begin{split} e^{-\beta m} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \right\|_{F}^{2} &= e^{-\beta m} \mathrm{tr} \left[Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \right] \\ &\leq e^{-\beta m} e^{\beta (m+\Delta+1)} \mathrm{tr} \left[Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \rho_{\beta} P_{[m-\Delta,m+\Delta]}^{H'} \right] \\ &= e^{\beta (\Delta+1)} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2}. \end{split}$$

where the inequality follows from

$$e^{-\beta(m+\Delta+1)}P_{[m-\Delta,m+\Delta]}^{H'} \preceq P_{[m-\Delta,m+\Delta]}^{H'}\rho_{\beta}P_{[m-\Delta,m+\Delta]}^{H'}.$$

Thus we conclude, from Equation 104, that

$$\begin{aligned} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} &\leq e^{\beta(\Delta+1)} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \\ &= e^{\beta(\Delta+1)} \sum_{m' \in [m-\Delta,m+\Delta]} \left\| Q_{\gamma}^{A} P_{m'}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2}. \end{aligned}$$

So the first term (1) in Eq. (103) can be bounded by

$$\sum_{m \in \mathbb{Z}} \left\| Q_{\gamma}^{A} P_{[m-\Delta,m+\Delta]}^{H'} U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \leq e^{\beta(\Delta+1)} \sum_{m \in \mathbb{Z}} \sum_{m' \in [m-\Delta,m+\Delta]} \left\| Q_{\gamma}^{A} P_{m'}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2}
\stackrel{(1)}{=} e^{\beta(\Delta+1)} \cdot 2\Delta \sum_{m'} \left\| Q_{\gamma}^{A} P_{m'}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2}
= 2\Delta e^{\beta(\Delta+1)} \left\| Q_{\gamma}^{A} \sqrt{\rho_{\beta}} \right\|_{F}^{2} = 2\Delta e^{\beta(\Delta+1)} \delta_{\gamma}, \tag{105}$$

where in (1) we use the fact that each m^\prime appears 2Δ times in the summation $\sum_{m\in\mathbb{Z}}\sum_{m'\in[m-\Delta,m+\Delta]}\cdot$ We now move on to upper bound (2) in Eq. (103) as follows. We have

$$\left\| Q_{\gamma}^{A} \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} \right) U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \leq \left\| \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} \right) U_{X} P_{m}^{H'} \right\| \cdot \| P_{m}^{H'} \sqrt{\rho_{\beta}} \|_{F}^{2}, \tag{106}$$

where we use $||Q_{\gamma}^{A}|| \leq 1$. Using Lemma 21, we obtain

$$\left\| \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} \right) U_X P_m^{H'} \right\| \le C e^{-\lambda(\Delta - |X|)},$$
 (107)

where C and λ are universal constants. Plugging Eq. (107) into Eq. (106), we get

$$\left\| Q_{\gamma}^{A} \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} \right) U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \le C e^{-\lambda(\Delta - |X|)} \| P_{m}^{H'} \sqrt{\rho_{\beta}} \|_{F}^{2}. \tag{108}$$

With this, we can bound (2) in Eq. (103) by

$$\sum_{m \in \mathbb{Z}} \left\| Q_{\gamma}^{A} \left(P_{>m+\Delta}^{H'} + P_{< m-\Delta}^{H'} \right) U_{X} P_{m}^{H'} \sqrt{\rho_{\beta}} \right\|_{F}^{2} \leq \sum_{m \in \mathbb{Z}} C e^{-\lambda(\Delta - |X|)} \| P_{m}^{H'} \sqrt{\rho_{\beta}} \|_{F}^{2} = C e^{-\lambda(\Delta - |X|)}, \quad (109)$$

where the equality used the fact that $\sum_{m \in \mathbb{Z}} \|P_m^{H'} \sqrt{\rho_\beta}\|_F^2 = \operatorname{tr}(\rho_\beta) = 1$. Putting together Eq. (105) and (109) into Eq. (103), we finally obtain the upper bound of

$$||Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}||_{F}^{2} \le 4\Delta e^{\beta(\Delta+1)}\delta_{\gamma} + 2Ce^{-\lambda(\Delta-|X|)}.$$
(110)

We let $\Delta = c\beta^{-1}\log(1/\delta_{\gamma})$, which gives

$$\|Q_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \le c_{1}e^{\lambda|X|}\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}},\tag{111}$$

for some universal constants c_1, c_2 . This proves the claim statement.

We now proceed to prove Claim 38.

Proof of Claim 38. Recall that the aim is to prove that for every $X \subseteq \Lambda$ and unitary U_X we have

$$\left\|AQ_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\right\|_{F}^{2} \leq \frac{e^{\mathcal{O}(1)|X|}\delta_{\gamma}^{\mathcal{O}(1)/\beta}}{\gamma} + \frac{\mathcal{O}(1)|X|^{5}}{\gamma^{5}}\langle A^{2}\rangle$$

We let c_5 , λ_1 , τ_1 be $\mathcal{O}(1)$ constants as defined in Lemma 22 and c_1 , c_2 , $\lambda = \mathcal{O}(1)$ be constants given by Claim 37. For the proof, we first decompose Q_{γ}^A as

$$Q_{\gamma}^{A} = \sum_{s=1}^{\infty} P_{s}^{A}, \quad P_{s}^{A} := P_{(s\gamma,(s+1)\gamma]}^{A} + P_{[-(s+1)\gamma,-s\gamma)}^{A}, \tag{112}$$

where $P_{[a,b]}^A$ is defined as $P_{[a,b]}^A := \sum_{a \leq \omega \leq b} \Pi_{\omega}$ (where Π_{ω} is the subspace spanned by the eigenvectors of A with eigenvalue ε). Using this notation, observe that $\|AQ_{\gamma}^A U_X \sqrt{\rho_{\beta}}\|_F$ can bounded by

$$\|AQ_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} = \sum_{s=1}^{\infty} \|AP_{s}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq \sum_{s=1}^{\infty} \|AP_{s}^{A}\|^{2} \cdot \|P_{s}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2}$$
$$\leq \gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} \|P_{s}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2}, \tag{113}$$

where we use $||AP_s^A|| \leq \gamma(s+1)$ from the definition (112) of P_s^A . The norm $||P_s^A U_X \sqrt{\rho_\beta}||_F$ is bounded from above by

$$\|P_{s}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F} = \|P_{s}^{A}U_{X}\sum_{s'=0}^{\infty}P_{s'}^{A}\sqrt{\rho_{\beta}}\|_{F} \le \sum_{s'=0}^{\infty}\|P_{s}^{A}U_{X}P_{s'}^{A}\sqrt{\rho_{\beta}}\|_{F},$$
(114)

where we use $\sum_{s'=0}^{\infty} P_{s'}^A = 1$ in the first equation and in the second inequality we use the triangle inequality for the Frobenius norm. Using Lemma 22 we additionally have

$$||P_s^A U_X P_{s'}^A|| \le c_5 |X| e^{-(\lambda_1 \gamma |s-s'|/|X|)^{1/\tau_1}}$$
 for every $s, s' \ge 0$, (115)

where c_5 , λ_1 are as given in Lemma 22. Using this, we have

$$\|P_{s}^{A}U_{X}P_{0}^{A}\sqrt{\rho_{\beta}}\|_{F} = \|P_{s}^{A}U_{X}P_{0}^{A}\sqrt{\rho_{\beta}}\|_{F}^{1/2} \cdot \|P_{s}^{A}U_{X}P_{0}^{A}\sqrt{\rho_{\beta}}\|_{F}^{1/2}$$

$$\stackrel{(1)}{\leq} \left(2c_{1}e^{\lambda|X|}\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}}\right)^{1/2} \cdot \|P_{s}^{A}U_{X}P_{0}^{A}\sqrt{\rho_{\beta}}\|_{F}^{1/2}$$

$$\stackrel{(2)}{\leq} \left(2c_{1}e^{\lambda|X|}\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}}\right)^{1/2} \cdot \|P_{s}^{A}U_{X}P_{0}^{A}\|^{1/2} \cdot \|\sqrt{\rho_{\beta}}\|_{F}^{1/2}$$

$$\stackrel{(3)}{\leq} \left(2c_{1}e^{\lambda|X|}\delta_{\gamma}^{\frac{c_{2}}{c_{2}+\beta}}\right)^{1/2} \cdot \left(c_{5}|X|e^{-(\lambda_{1}\gamma|s|/|X|)^{1/\tau_{1}}}\right)^{1/2} \cdot 1$$

$$\stackrel{(4)}{=} (\delta_{\gamma}')^{1/2} \cdot \left(c_{5}|X|e^{-(\lambda_{1}\gamma|s|/|X|)^{1/\tau_{1}}}\right)^{1/2},$$

$$(116)$$

where inequality (1) uses $\|P_s^A U_X P_0^A \sqrt{\rho_\beta}\|_F \le 2c_1 \delta_\gamma^{\frac{c_2}{c_2+\beta}}$ 10, inequality (2) uses Eq. (16), inequality (3) uses Eq. (115) and the fact that $\|\sqrt{\rho_\beta}\|_F = \operatorname{tr}(\rho_\beta) = 1$ and equality (4) defines $\delta_\gamma' := 2c_1 e^{\lambda|X|} \delta_\gamma^{\frac{c_2}{c_2+\beta}}$. Using Eq. (116), we obtain the following

$$\sum_{s'=0}^{\infty} \|P_s^A U_X P_{s'}^A \sqrt{\rho_{\beta}}\|_F \leq \|P_s^A U_X P_0^A \sqrt{\rho_{\beta}}\|_F + \sum_{s'=1}^{\infty} \|P_s^A U_X P_{s'}^A\| \cdot \|P_{s'}^A \sqrt{\rho_{\beta}}\|_F
\leq \delta'_{\gamma}^{1/2} c_5^{1/2} |X|^{1/2} e^{-(\lambda_1 \gamma s/|X|)^{1/\tau_1}/2}
+ \sum_{s'=1}^{\infty} c_5 |X| e^{-(\lambda_1 \gamma |s-s'|/|X|)^{1/\tau_1}} \|P_{s'}^A \sqrt{\rho_{\beta}}\|_F,$$
(117)

where the first term in the inequality was obtained from Eq. (116) and the second term was obtained from Eq. (115).

We now upper bound the summation in the second term of Eq. (117) by using the Cauchy–Schwarz inequality as follows:

$$\sum_{s'=1}^{\infty} e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}} \|P_{s'}^{A}\sqrt{\rho_{\beta}}\|_{F}$$

$$= \sum_{s'=1}^{\infty} e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}/2}} \cdot \left(e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}/2}} \|P_{s'}^{A}\sqrt{\rho_{\beta}}\|_{F}\right)$$

$$\leq \left(\sum_{s'=1}^{\infty} e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}}\right)^{1/2} \left(\sum_{s'=1}^{\infty} e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}} \|P_{s'}^{A}\sqrt{\rho_{\beta}}\|_{F}^{2}\right)^{1/2}$$

$$\stackrel{(1)}{\leq} \left(\frac{4\tau_{1}|X|}{\lambda_{1}\gamma} (2\tau_{1})^{\tau_{1}}\right)^{1/2} \cdot \left(\sum_{s'=1}^{\infty} p_{s'}^{A} e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}}\right)^{1/2}, \tag{118}$$

$$\left\|P_s^A U_X P_0^A \sqrt{\rho_\beta}\right\|_F \leq \left\|Q_\gamma^A U_X (\mathbb{1} - Q_\gamma^A) \sqrt{\rho_\beta}\right\|_F \leq \left\|Q_\gamma^A U_X \sqrt{\rho_\beta}\right\|_F + \left\|Q_\gamma^A U_X Q_\gamma^A \sqrt{\rho_\beta}\right\|_F \leq \left\|Q_\gamma^A U_X \sqrt{\rho_\beta}\right\|_F + \delta_\gamma \leq 2c_1 e^{\lambda |X|} \delta_\gamma^{\frac{c_2}{c_2 + \beta}},$$

where the first inequality used $P_s^A \leq Q_\gamma^A$ and the last inequality used $\|Q_\gamma^A U_X \sqrt{\rho_\beta}\|_F \leq c_1 e^{\lambda|X|} \delta_\gamma^{\frac{c_2}{c_2 + \beta}}$ from Claim 37.

 $^{^{10}}$ Since $Q_{\gamma}^{A} \leq \mathbb{1}$ and $P_{0}^{A} = P_{\gamma}^{A} = \mathbb{1} - Q_{\gamma}^{A}$, we have

where $p_{s'}:=\left\|P_{s'}^A\sqrt{\rho_\beta}\right\|_F^2$ and we used Fact 12 in inequality (1). Note that $\sum_{s'=1}^\infty p_{s'}=\|Q_\gamma^A\sqrt{\rho_\beta}\|_F^2$ because of $P_0^A=P_{(0,\gamma]}^A+P_{[-\gamma,0)}^A=P_\gamma^A$. We can obtain the following upper bound by combining the equations Eq. (114), (117) and (118):

$$\begin{split} & \left\| P_{s}^{A}U_{X}\sqrt{\rho_{\beta}} \right\|_{F}^{2} \\ & \leq \left(\sum_{s'=0}^{\infty} \left\| P_{s}^{A}U_{X}P_{s'}^{A}\sqrt{\rho_{\beta}} \right\|_{F} \right)^{2} \\ & \leq \left(\delta_{\gamma}^{\prime 1/2}c_{5}^{1/2}|X|^{1/2}e^{-(\lambda_{1}\gamma s/|X|)^{1/\tau_{1}/2}} + \sum_{s'=1}^{\infty}c_{5}|X|e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}} \left\| P_{s'}^{A}\sqrt{\rho_{\beta}} \right\|_{F} \right)^{2} \\ & \leq \left(\delta_{\gamma}^{\prime 1/2}c_{5}^{1/2}|X|^{1/2}e^{-(\lambda_{1}\gamma s/|X|)^{1/\tau_{1}/2}} + c_{5}|X| \left(\frac{4\tau_{1}|X|}{\lambda_{1}\gamma} \left(2\tau_{1} \right)^{\tau_{1}} \right)^{1/2} \cdot \left(\sum_{s'=1}^{\infty}p_{s'}^{A}e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}} \right)^{1/2} \right)^{2} \\ & \leq \underbrace{2c_{5}\delta_{\gamma}'|X|e^{-(\lambda_{1}\gamma s/|X|)^{1/\tau_{1}}}}_{:=f_{1}(s)} + \underbrace{\frac{8c_{5}^{2}\tau_{1}|X|^{3}}{\lambda_{1}\gamma} \left(2\tau_{1} \right)^{\tau_{1}} \cdot \left(\sum_{s'=1}^{\infty}p_{s'}^{A}e^{-(\lambda_{1}\gamma|s-s'|/|X|)^{1/\tau_{1}}} \right)}_{:=f_{2}(s)}. \end{split}$$

Recall that the goal of this claim was to upper bound Eq. (113), which we can rewrite now as

$$\|AQ_{\gamma}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq \gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} \|P_{s}^{A}U_{X}\sqrt{\rho_{\beta}}\|_{F}^{2} \leq \gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} f_{1}(s) + \gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} f_{2}(s).$$
 (119)

We bound each of these terms separately. In order to bound the first term observe that

$$\gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} f_{1}(s) = 2\gamma^{2} c_{5} \delta_{\gamma}' |X|^{2} \sum_{s=1}^{\infty} (s+1)^{2} e^{-(\lambda_{1} \gamma s/|X|)^{1/\tau_{1}}}$$

$$\stackrel{(1)}{\leq} 2\gamma^{2} c_{5} \delta_{\gamma}' |X| \cdot 8\tau_{1} \cdot \left(\frac{(3\tau_{1})^{\tau_{1}}|X|}{\lambda_{1} \gamma}\right)^{3} \leq \frac{16c_{5} \delta_{\gamma}' |X|^{4} \tau_{1} (3\tau_{1})^{3\tau_{1}}}{\lambda_{1}^{3} \gamma},$$

where inequality (1) uses Fact 12. We now bound the second term in Eq. (119) as follows

$$\gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} f_{2}(s) = \gamma^{2} \cdot \frac{8c_{5}^{2} \tau_{1} |X|^{3}}{\lambda_{1} \gamma} (2\tau_{1})^{\tau_{1}} \sum_{s=1}^{\infty} (s+1)^{2} \left(\sum_{s'=1}^{\infty} p_{s'}^{A} e^{-(\lambda_{1} \gamma |s-s'|/|X|)^{1/\tau_{1}}} \right).$$

$$= \frac{8 \gamma c_{5}^{2} \tau_{1} |X|^{3} (2\tau_{1})^{\tau_{1}}}{\lambda_{1}} \sum_{s'=1}^{\infty} p_{s'}^{A} \left(\sum_{s=1}^{\infty} (s+1)^{2} e^{-(\lambda_{1} \gamma |s-s'|/|X|)^{1/\tau_{1}}} \right)$$

$$\leq \frac{8 \gamma c_{5}^{2} \tau_{1} |X|^{3} (2\tau_{1})^{\tau_{1}}}{\lambda_{1}} \sum_{s'=1}^{\infty} p_{s'}^{A} (2s')^{2} \left(\sum_{s=1}^{\infty} (1+|s-s'|)^{2} e^{-(\lambda_{1} \gamma |s-s'|/|X|)^{1/\tau_{1}}} \right)$$

$$\stackrel{(1)}{\leq} \frac{8 \gamma c_{5}^{2} \tau_{1} |X|^{3} (2\tau_{1})^{\tau_{1}}}{\lambda_{1}} \cdot 16\tau_{1} \cdot \left(\frac{(3\tau_{1})^{\tau_{1}} |X|}{\lambda_{1} \gamma} \right)^{3} \sum_{s'=1}^{\infty} p_{s'}^{A} (2s')^{2},$$

$$(120)$$

where inequality (1) follows from Fact 12. Further upper bound this expression by simplifying the pre-factors, we get

$$\gamma^{2} \sum_{s=1}^{\infty} (s+1)^{2} f_{2}(s) \leq \frac{512 c_{5}^{2} |X|^{6} \tau_{1}^{2} (3\tau_{1})^{4\tau_{1}}}{\lambda_{1}^{4} \gamma^{2}} \sum_{s'=1}^{\infty} p_{s'}^{A}(s')^{2}
= \frac{512 c_{5}^{2} |X|^{6} \tau_{1}^{2} (3\tau_{1})^{4\tau_{1}}}{\lambda_{1}^{4}} \sum_{s'=1}^{\infty} (\gamma s')^{2} p_{s'}^{A}
= \frac{512 c_{5}^{2} |X|^{6} \tau_{1}^{2} (3\tau_{1})^{4\tau_{1}}}{\lambda_{1}^{4}} \sum_{s'=1}^{\infty} \|P_{s'}^{A} (\gamma s') \sqrt{\rho_{\beta}}\|_{F}^{2}
\stackrel{(2)}{\leq} \frac{512 c_{5}^{2} |X|^{6} \tau_{1}^{2} (3\tau_{1})^{4\tau_{1}}}{\lambda_{1}^{4}} \sum_{s'=0}^{\infty} \|P_{s'}^{A} A \sqrt{\rho_{\beta}}\|_{F}^{2} = \frac{512 c_{5}^{2} |X|^{6} \tau_{1}^{2} (3\tau_{1})^{4\tau_{1}}}{\lambda_{1}^{4}} \langle A^{2} \rangle,$$

In inequality (2), we used $P_{s'}^A(\gamma s') \leq P_{s'}^A$ from the definition (112) of $P_{s'}^A$. By combining the above inequalities altogether, we prove Eq. (89).

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A Proof of Fact 12

Here we restate and prove the following fact.

Fact 40 (Restatement of Fact 12). Let a, c, p > 0 be reals and b be a positive integer. Then

- 1) $\sum_{i=0}^{\infty} e^{-ci} \leq \frac{e^c}{c}$.
- 2) $\sum_{j=0}^{\infty} j^b e^{-cj^p} \le \frac{2}{p} \cdot \left(\frac{b+1}{cp}\right)^{\frac{b+1}{p}}.$
- 3) $\sum_{j=0}^{\infty} e^{-c(a+j)^p} \le e^{-\frac{c}{2}a^p} \left(1 + \frac{1}{p} \left(\frac{2}{cp}\right)^{\frac{1}{p}}\right).$

Proof. The first summation follows from

$$\sum_{i=0}^{\infty} e^{-cj} = \frac{1}{1 - e^{-c}} = \frac{e^c}{e^c - 1} \le \frac{e^c}{c}.$$

For the second sum, notice that the function $t^b e^{-ct^p}$ achieves the maximum at $t^* = \left(\frac{b}{cp}\right)^{\frac{1}{p}}$. Then

$$\begin{split} \sum_{j=0}^{\infty} j^b e^{-cj^p} & \leq t^* \left(t^* \right)^b e^{-c(t^*)^p} + \int_0^{\infty} t^b e^{-ct^p} dt \\ & = \left(\frac{b}{cp} \right)^{\frac{b+1}{p}} e^{-\frac{b}{p}} + \frac{1}{(b+1)c^{\frac{b+1}{p}}} \int_0^{\infty} e^{-y^{\frac{p}{b+1}}} dy \\ & = \left(\frac{b}{e^{\frac{b}{b+1}} cp} \right)^{\frac{b+1}{p}} + \frac{1}{pc^{\frac{b+1}{p}}} \Gamma \left(\frac{b+1}{p} \right) \\ & \leq \left(\frac{b}{e^{\frac{b}{b+1}} cp} \right)^{\frac{b+1}{p}} + \frac{1}{pc^{\frac{b+1}{p}}} \left(\frac{b+1}{p} \right)^{\frac{b+1}{p}} \leq \frac{2}{p} \cdot \left(\frac{b+1}{cp} \right)^{\frac{b+1}{p}}. \end{split}$$

For the third sum, we will use the identity

$$(a+j)^p \ge 2^{p-1} (a^p + j^p) \ge \frac{1}{2} (a^p + j^p).$$

This is clearly true if $p \ge 1$. For p < 1, we use concavity. Now, consider the following chain of inequalities and change of variables:

$$\begin{split} \sum_{j=0}^{\infty} e^{-c(a+j)^p} &\leq e^{-\frac{c}{2}a^p} \sum_{\ell=0}^{\infty} e^{-\frac{c}{2}\ell^p} \\ &\leq e^{-\frac{c}{2}a^p} \left(1 + \int_0^{\infty} e^{-\frac{c}{2}t^p} dt \right) \\ &= e^{-\frac{c}{2}a^p} \left(1 + \frac{2^{\frac{1}{p}}}{c^{\frac{1}{p}}} \int_0^{\infty} e^{-y^p} dy \right) \\ &= e^{-\frac{c}{2}a^p} \left(1 + \frac{2^{\frac{1}{p}}}{pc^{\frac{1}{p}}} \Gamma\left(\frac{1}{p}\right) \right) \leq e^{-\frac{c}{2}a^p} \left(1 + \frac{1}{pc^{\frac{1}{p}}} \left(\frac{2}{p}\right)^{\frac{1}{p}} \right). \end{split}$$

This completes the proof.

B Fourier transform of $\tanh(\beta\omega/2)/(\beta\omega/2)$

We here derive the Fourier transform of

$$\tilde{f}_{\beta}(\omega) = \frac{\tanh(\beta\omega/2)}{\beta\omega/2},$$

which is

$$f_{\beta}(t) := \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega.$$

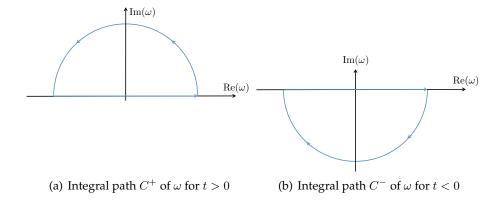


Figure 3: Cauchy's integral theorem for the calculation of the Fourier transform.

For the calculation of the Fourier transform, we first consider the case of t > 0. By defining C^+ as a integral path as in Fig. 3 (a), we obtain

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega = \frac{1}{2\pi} \int_{C^{+}} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega$$

$$= i \sum_{m=0}^{\infty} \operatorname{Res}_{\omega = i\pi + 2im\pi} [e^{i\omega t} \tilde{f}_{\beta}(\omega)]. \tag{122}$$

Note that the singular points of $[e^{i\omega t}\tilde{f}_{\beta}(\omega)]$ are given by $\beta\omega=i\pi(2m+1)$ with m integers. We can calculate the residue as

$$\operatorname{Res}_{\beta\omega=i\pi+2im\pi}[e^{i\omega t}\tilde{f}_{\beta}(\omega)] = \frac{4e^{-(2m+1)\pi t/\beta}}{\beta\pi} \frac{-i}{2m+1}$$
(123)

We thus obtain

$$f_{\beta}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega = \frac{4}{\beta\pi} \sum_{m=0}^{\infty} \frac{e^{-(2m+1)\pi t/\beta}}{2m+1}.$$
 (124)

for t > 0.

We can perform the same calculation for t < 0. In this case, we define C^- as a integral path as in Fig. 3 (b), and obtain

$$f_{\beta}(t) = \frac{1}{2\pi} \int_{C^{-}} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega = -i \sum_{m=0}^{\infty} \operatorname{Res}_{\omega = -i\pi - 2im\pi} [e^{i\omega t} \tilde{f}_{\beta}(\omega)].$$
 (125)

By using

$$\operatorname{Res}_{\omega=-i\pi-2im\pi}[e^{i\omega t}\tilde{f}_{\beta}(\omega)] = \frac{4e^{(2m+1)\pi t/\beta}}{\beta\pi} \frac{i}{2m+1},$$
(126)

we have

$$f_{\beta}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \tilde{f}_{\beta}(\omega) d\omega = \frac{4}{\beta\pi} \sum_{m=0}^{\infty} \frac{e^{(2m+1)\pi t/\beta}}{2m+1}.$$
 (127)

for t < 0. By combining the above expressions for $f_{\beta}(t)$, we arrive at

$$f_{\beta}(t) = \frac{4}{\beta\pi} \sum_{m=0}^{\infty} \frac{e^{-(2m+1)\pi|t|/\beta}}{2m+1}.$$
 (128)

The summation is calculated as

$$\sum_{m=0}^{\infty} \frac{e^{-(2m+1)x}}{2m+1} = \int_{x}^{\infty} \sum_{m=0}^{\infty} e^{-(2m+1)x'} dx' = \int_{x}^{\infty} \frac{1}{e^{x'} - e^{-x'}} dx' = \frac{1}{2} \log \frac{e^{x} + 1}{e^{x} - 1}$$
(129)

for x > 0, which yields

$$f_{\beta}(t) = \frac{2}{\beta \pi} \log \frac{e^{\pi |t|/\beta} + 1}{e^{\pi |t|/\beta} - 1}.$$
 (130)

Since

$$\log \frac{e^{\pi |t|/\beta} + 1}{e^{\pi |t|/\beta} - 1} \le \frac{2}{e^{\pi |t|/\beta} - 1},$$

 $f_{\beta}(t)$ shows an exponential decay in |t|.

C Derivation of the sub-exponential concentration

Recall that the goal in this appendix is to prove the following lemma.

Lemma 41 (Restatement of Lemma 22). Let A be a $(\tau, a_1, a_2, 1)$ -quasi-local operator with $\tau < 1$, as given in Eq. (19). For an arbitrary operator O_X supported on a subset $X \subseteq \Lambda$ with $|X| = k_0$ and $||O_X|| = 1$, we have

$$||P_{\geq x+y}^A O_X P_{\leq x}^A|| \le c_5 \cdot k_0 \exp\left(-(\lambda_1 y/k_0)^{1/\tau_1}\right),$$
 (131)

where $\tau_1 := \frac{2}{\tau} - 1$ and c_5 and λ_1 are constants which only depend on a_1 and a_2 . In particular, the a_2 dependence of c_5 and λ_1 is given by $c_5 \propto a_2^{2/\tau}$ and $\lambda_1 \propto a_2^{-2/\tau}$ respectively.

Before proving this lemma, let us elaborate upon the method. Recall that

$$P_{\leq x}^{A} = \sum_{\omega \leq x} \Pi_{\omega}, \quad P_{>y}^{A} = \sum_{\omega > y} \Pi_{\omega}, \tag{132}$$

where Π_{ω} is the projector onto the eigenvalue ω eigenspace of A. One way to prove the upper bound in the estimation of the norm (131) is to utilize the technique in Ref. [AKL16] (i.e., Lemma 21). The argument proceeds by considering

$$||P_{\geq x+y}^{A}O_{X}P_{\leq x}^{A}|| = ||P_{\geq x+y}^{A}e^{-\nu A}e^{\nu A}O_{X}e^{-\nu A}e^{\nu A}P_{\leq x}^{A}||$$

$$\leq ||P_{\geq x+y}^{A}e^{-\nu A}|| \cdot ||e^{\nu A}O_{X}e^{-\nu A}|| \cdot ||e^{\nu A}P_{\leq x}^{A}||$$

$$\leq e^{-\nu x}||e^{\nu A}O_{X}e^{-\nu A}||,$$
(133)

which reduces the problem to estimation of the norm $||e^{\nu A}O_Xe^{-\nu A}||$. Additionally, by definition of A in Theorem 33 we have

$$A = \sum_{\ell=1}^{n} g_{\ell} \bar{A}_{\ell},\tag{134}$$

where \bar{A}_ℓ is κ -local and g_ℓ is sub-exponentially decaying function for ℓ (as made precise in Eq. (19)), namely $g_\ell = \exp(-\mathcal{O}(\ell^{1/D}))$. In this case, for $\nu = \mathcal{O}(1)$, the norm of the imaginary time evolution can be finitely bounded only in the case D=1 [Kuw16]. That is, the norm $\|e^{\nu A}O_Xe^{-\nu A}\|$ diverges to infinity for $D\geq 2$. However, our main contribution in this section is that we are able to prove the lemma statement *without* going through the inequalities in (133) (which in turn used earlier results of [Kuw16, AKL16]). We now give more details.

C.1 Proof of Lemma 41

In order to estimate the norm, we need to take a different route from (133). Let I be any interval of the real line and P_I^A be the projector onto the eigenspace of A with eigenvalues in I. Using the operator inequality

$$P_{\geq z}^A (A - \omega \mathbb{1})^m \succeq (z - \omega)^m P_{\geq x+y}^A,$$

we obtain

$$\|(A - \omega \mathbb{1})^m O_X P_I^A\| \ge \|P_{>z}^A (A - \omega)^m O_X P_I^A\| \ge (z - \omega)^m \|P_{>z}^A O_X P_I^A\|, \tag{135}$$

hence

$$||P_{\geq z}^{A} O_{X} P_{I}^{A}|| \leq \frac{||(A - \omega)^{m} O_{X} P_{I}^{A}||}{(z - \omega)^{m}}.$$
(136)

Our strategy to establish Eq. (131) will be to expand

$$||P_{\geq x+y}^A O_X P_{\leq x}^A|| \le \sum_{j=0}^{\infty} ||P_{\geq x+y}^A O_X P_{I_j}^A||, \tag{137}$$

for carefully chosen intervals $I_j:=(x-a_1(j+1),x-a_1j]$ (the term a_1 is as given in the statement of Lemma 41). Towards this, let us fix an arbitrary ω , an interval $I:=(\omega-a_1,\omega]$ and prove an upper bound on $\|P_{>\omega+\theta}^A O_X P_{I_j}^A\|$ (for all θ). We show the following claim.

Claim 42. There is a constant c_6 such that

$$||P_{\geq \omega + \theta}^A O_X P_I^A|| \le \frac{1}{\tau} \exp\left[-[\theta/(ec_6 k_0)]^{1/\tau_1} + 1\right]. \tag{138}$$

The claim is proved in subsection C.2. Let us use the claim to establish the lemma. In the inequality (137), we need to estimate $\|P_{\geq x+y}^A O_X P_{I_j}^A\|$ with $I_j := (x-(j+1)a_1, x-ja_1]$. Setting $\omega = x-ja_1$ and $\theta = y+ja_1$ in Claim 42, we have

$$||P_{\geq x+y}^A O_X P_{I_j}^A|| \le \frac{1}{\tau} \exp\left\{-\left(\frac{y+a_1 j}{e c_6 k_0}\right)^{1/\tau_1} + 1\right\}.$$
(139)

In order to complete the bound on Equation 137, we need to take summation with respect to j. We have

$$\sum_{j=0}^{\infty} \|P_{\geq x+y}^{A} O_{X} P_{I_{j}}^{A}\| \leq \sum_{j=0}^{\infty} \frac{1}{\tau} \exp\left\{-\left(\frac{y+a_{1}j}{ec_{6}k_{0}}\right)^{1/\tau_{1}} + 1\right\} \leq \frac{1}{\tau} e^{-\frac{1}{2}\left(\frac{y}{ec_{6}k_{0}}\right)^{1/\tau_{1}}} \left(1 + \frac{ec_{6}k_{0}\tau_{1}}{a_{1}} \left(4/\tau\right)^{1/\tau_{1}}\right),\tag{140}$$

where in last inequality we used Fact 12 (3) with $c = (ec_6k_0/a_1)^{-1/\tau_1}$, $p = 1/\tau_1$ and $a = y/a_1$. This gives the form of (131) and completes the proof.

C.2 Proof of Claim 42

From Equation 136, it suffices to upper bound $\|(A-\omega)^m O_X P_I^A\|$. Abbreviate $\tilde{A} := A - \omega \mathbb{1}$. Introduce the multi-commutator

$$\operatorname{ad}_{\tilde{A}}^{s}(O_{X}) := \underbrace{[\tilde{A}, \dots [\tilde{A}, [\tilde{A}, O_{X}]] \dots]}_{s \text{ times}}.$$

Consider the following identity,

$$\tilde{A}^m O_X P_I^A = \sum_{s=0}^m \binom{m}{s} \operatorname{ad}_{\tilde{A}}^s (O_X) \tilde{A}^{m-s} P_I^A. \tag{141}$$

This shows that

$$\|\tilde{A}^{m}O_{X}P_{I}^{A}\| \leq \sum_{s=0}^{m} {m \choose s} \|\operatorname{ad}_{\tilde{A}}^{s}(O_{X})\| \cdot \|\tilde{A}^{m-s}P_{I}^{A}\| \leq \sum_{s=0}^{m} {m \choose s} a_{1}^{m-s} \|\operatorname{ad}_{\tilde{A}}^{s}(O_{X})\|, \tag{142}$$

where we use $\|\tilde{A}^{m-s}P_I^A\|=\|(A-\omega)^{m-s}P_I^A\|\leq a_1^{m-s}$. The remaining task is to estimate the upper bound of $\|\operatorname{ad}_{\tilde{A}}^s(O_X)\|=\|\operatorname{ad}_A^s(O_X)\|$. This is done in the following claim.

Claim 43. Let A be an operator that is given by the form (19). Then, for an arbitrary operator O_X which is supported on a subset X ($|X| = k_0$), the norm of the multi-commutator $\operatorname{ad}_A^s(O_X)$ is bounded from above by

$$\|\operatorname{ad}_{A}^{s}(O_{X})\| \le \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2s}{\tau}} \cdot (s^{\tau_{1}})^{s} \quad \text{for} \quad s \le m,$$
 (143)

where the constants a_1 and a_2 have been defined in Eq. (19), and $\Gamma(\cdot)$ is the gamma function.

By applying the inequality (143) to (142), we obtain

$$\begin{split} \|\tilde{A}^{m}O_{X}P_{I}^{A}\| &\leq \sum_{s=0}^{m} \binom{m}{s} a_{1}^{m-s} \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2s}{\tau}} \cdot (s^{\tau_{1}})^{s} \\ &\leq \sum_{s=0}^{m} \binom{m}{s} (2a_{1})^{m} \frac{(2ek_{0})^{m}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2m}{\tau}} \cdot (m^{\tau_{1}})^{m} \\ &= (4a_{1})^{m} \frac{(2ek_{0})^{m}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2m}{\tau}} \cdot (m^{\tau_{1}})^{m} = \frac{1}{\tau} \left[8ea_{1}k_{0}[2/(a_{2}\tau)]^{2/\tau}m^{\tau_{1}}\right]^{m}. \end{split}$$

Therefore, setting $z = \omega + \theta$ in the inequality (136), we obtain

$$\|P_{\geq \omega + \theta}^{A} O_{X} P_{I}^{A}\| \leq \frac{\|\tilde{A}^{m} O_{X} P_{I}^{A}\|}{\theta^{m}} \leq \frac{1}{\tau} \left[8ea_{1}k_{0} [2/(a_{2}\tau)]^{2/\tau} \frac{m^{\tau_{1}}}{\theta} \right]^{m}$$
(144)

$$\leq \frac{1}{\tau} \left(\frac{c_6 k_0 m^{\tau_1}}{\theta} \right)^m, \tag{145}$$

where $c_6 := 8ea_1[2/(a_2\tau)]^{2/\tau}$. Let us choose $m = \tilde{m}$ with \tilde{m} the minimum integer such that

$$\frac{c_6 k_0 \tilde{m}^{\tau_1}}{\theta} \le 1/e. \tag{146}$$

The above condition is satisfied by $\tilde{m}^{\tau_1} \leq \theta/(ec_6k_0)$, which implies

$$\tilde{m} = \left[\left[\theta / (ec_6 k_0) \right]^{1/\tau_1} \right], \tag{147}$$

where $|\cdot|$ is the floor function. From this choice, the claim concludes.

C.3 Proof of Claim 43

Recall that we need to show, for an arbitrary operator O_X which is supported on k_0 sites, the norm of the multi-commutator $\operatorname{ad}_A^s(O_X)$ is bounded by

$$\|\operatorname{ad}_{A}^{s}(O_{X})\| \leq \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2s}{\tau}} \cdot (s^{\tau_{1}})^{s} \quad \text{for} \quad s \leq m.$$

We start from the following expansion:

$$\operatorname{ad}_{A}^{s}(O_{X}) = \sum_{k_{1}, k_{2}, \dots, k_{s}} g_{k_{1}} g_{k_{2}} \cdots g_{k_{s}} [\bar{A}_{k_{s}}, [\bar{A}_{k_{s-1}}, \cdots [\bar{A}_{k_{1}}, O_{X}] \cdots].$$

By using Lemma 3 in Ref. [KMS16] and setting $\zeta = 1$ (see Definition 19) we obtain

$$\|[[\bar{A}_{k_s}, [\bar{A}_{k_{s-1}}, \cdots [\bar{A}_{k_1}, O_X] \cdots]]\| \le 2^s k_0 (k_0 + k_1) (k_0 + k_1 + k_2) \cdots (k_0 + k_1 + k_2 + \cdots + k_{s-1}).$$
(148)

Recall that we set $||O_X|| = 1$ and $|X| = k_0$. The norm of $\operatorname{ad}_A^s(O_X)$ is bounded from above by

$$\|\operatorname{ad}_{A}^{s}(O_{X})\|$$

$$\leq \sum_{k_{1},k_{2},\dots,k_{s}=1}^{\infty} 2^{s} g_{k_{1}} g_{k_{2}} \cdots g_{k_{s}} k_{0}(k_{0}+k_{1})(k_{0}+k_{1}+k_{2}) \cdots (k_{0}+k_{1}+k_{2}+\dots+k_{s-1})$$

$$= \sum_{K \geq s} \sum_{\substack{k_{1}+k_{2}+\dots+k_{s}=K\\k_{1}\geq 1,k_{2}\geq 1,\dots,k_{s}\geq 1}} 2^{s} g_{k_{1}} g_{k_{2}} \cdots g_{k_{s}} k_{0}(k_{0}+k_{1})(k_{0}+k_{1}+k_{2}) \cdots (k_{0}+k_{1}+k_{2}+\dots+k_{s-1}),$$

$$(149)$$

where the summation over K starts from s because each of $\{k_j\}_{j=1}^s$ is larger than 1. Now, using the expression $\log[g_k/a_1] = -a_2k^{\tau}$ for $\tau \leq 1$, we have $\sum_{j=1}^s \log(g_{k_j}/a_1) \leq \log(g_{k_1+k_2+\cdots+k_s}/a_1)$. This

follows from $\sum_{j=1}^{s} k_j^{\tau} \ge (k_1 + k_2 + \dots + k_s)^{\tau}$. Thus, using $k_1 + k_2 + \dots + k_s = K$, the summand in the inequality (149) is upper-bounded by

$$g_{k_1}g_{k_2}\cdots g_{k_s}k_0(k_0+k_1)(k_0+k_1+k_2)\cdots(k_0+k_1+k_2+\cdots+k_{s-1}) \le a_1^s(g_K/a_1)k_0(k_0+K)^{s-1},$$
(150)

where we use the inequality $k_1 + k_2 + \cdots + k_j \le K$ for $j = 1, 2, \dots, s - 1$. By combining the two inequalities (149) and (150), we obtain

$$\|\operatorname{ad}_{A}^{s}(O_{X})\| \leq \sum_{K \geq s} \sum_{\substack{k_{1}+k_{2}+\ldots+k_{s}=K\\k_{1}\geq 1,k_{2}\geq 1,\ldots,k_{s}\geq 1}} (2a_{1})^{s}(g_{K}/a_{1})k_{0}(k_{0}+K)^{s-1}$$

$$\stackrel{(1)}{\leq} \sum_{K \geq s} \left(\binom{s}{K-s}\right) (2a_{1})^{s}(g_{K}/a_{1})k_{0}(k_{0}+K)^{s-1}$$

$$= \sum_{K \geq s} \binom{K-1}{s-1} (2a_{1})^{s}(g_{K}/a_{1})k_{0}(k_{0}+K)^{s-1}$$

$$\stackrel{(2)}{\leq} (2a_{1})^{s}(2k_{0})^{s} \sum_{K \geq s} \frac{e^{s}K^{s}}{s^{s}} (g_{K}/a_{1})(K)^{s-1}$$

$$\stackrel{(3)}{=} \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{s^{s}} \sum_{K \geq s} K^{2s-1}e^{-a_{2}K^{\tau}} \leq \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{s^{s}} \sum_{K \geq 0} K^{2s-1}e^{-a_{2}K^{\tau}}$$

$$\stackrel{(4)}{\leq} \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{s^{s}\tau} \cdot \left(\frac{2s}{a_{2}\tau}\right)^{\frac{2s}{\tau}} = \frac{(2a_{1})^{s}(2k_{0})^{s}e^{s}}{\tau} \cdot \left(\frac{2}{a_{2}\tau}\right)^{\frac{2s}{\tau}} \cdot \left(s^{\frac{2}{\tau}-1}\right)^{s}.$$

where in (1), (()) denotes the multi-combination, namely $\binom{n}{m} = \binom{n+m-1}{n-1}$, in 2 we upper bound $\binom{K-1}{s-1} \leq \frac{e^s K^s}{s^s}$, $k_0 + K \leq 2k_0 K$, in (3) we use the sub-exponential form of g_K in Eq. (19) and in (4) we use Fact 12. Since $\tau_1 = \frac{2}{\tau} - 1$, this proves the statement.

D Quasi-locality of \widetilde{W}

We here aim to obtain (τ, a_1, a_2, ζ) -quasi-locality of the operator \widetilde{W} , where $\{\tau, a_1, a_2, \zeta\}$ defined in Definition 14. In particular, we will show that

$$\left(\tau, a_1, a_2, \zeta\right) = \left(1/D, \mathcal{O}(1), \mathcal{O}(1/\beta), \mathcal{O}(\beta^{2D+1}) \left(\max_{j \in \Lambda} v_j\right)\right)$$

suffices to prove the quasi-locality of \widetilde{W} . Recall the definition of \widetilde{W} :

$$\widetilde{W} = \int_{-\infty}^{\infty} f_{\beta}(t) e^{-iHt} W e^{iHt} dt,$$

where

$$f_{\beta}(t) = \frac{2}{\beta \pi} \log \frac{e^{\pi |t|/\beta} + 1}{e^{\pi |t|/\beta} - 1}$$

and

$$W = \sum_{i \in \Lambda} v_i E_i.$$

We write

$$\widetilde{W} = \sum_{i} v_{i} \int_{-\infty}^{\infty} f_{\beta}(t) e^{-iHt} E_{i} e^{iHt} dt.$$

Abbreviate

$$\tilde{E}_i(t) := e^{-iHt} E_i e^{iHt}$$

and recall that $\tilde{E}_i = \int_{\infty}^{\infty} f_{\beta}(t) \tilde{E}_i(t)$. Moreover, (with some abuse of notation) let B(r,i) denote the ball of radius r such that: the centre of B(r,i) coincides with the the center of the smallest ball containing E_i . We assume that r ranges in the set $\{m_i, m_i + 1, \dots, n_i\}$, where m_i is the radius of the smallest ball containing E_i and n_i is the number such that $B(n_i,i) = \Lambda$. Define

$$\tilde{E}_{i}^{r}(t) := \operatorname{tr}_{B(r,i)^{c}}[\tilde{E}_{i}(t)] \otimes \frac{\mathbb{1}_{B(r,i)^{c}}}{\operatorname{tr}[\mathbb{1}_{B(r,i)^{c}}]}, \quad \tilde{E}_{i}^{0}(t) = 0,$$

i.e., $\tilde{W}_i^r(t)$ traces out all the qudits in $\tilde{E}_i(t)$ that are at outside the B(r,i)-ball around \tilde{E}_i^r . From [BHV06], we have

$$\|\tilde{E}_i(t) - \tilde{E}_i^r(t)\| \le \|E_i\| \min \left\{1, c_3 r^{D-1} e^{-c_4(r - v_{LR}|t|)}\right\}$$

which in particular implies

$$\|\tilde{E}_i^r(t) - \tilde{E}_i^{r-1}(t)\| \le 2 \min \left\{ 1, c_3 r^{D-1} e^{-c_4(r - v_{LR}|t|)} \right\},$$

where we use $||E_i||=1$, v_{LR} is the Lieb-Robinson velocity (as defined in Fact 15) and c_3, c_4 are constants. We note that the $2\min\{1,\cdot\}$ is derived from the trivial upper bound $||\tilde{E}_i^r(t) - \tilde{E}_i^{r+1}(t)|| \le 2$. This allows us to write the following quasi-local expression:

$$\tilde{E}_i(t) = \sum_{r=m_i}^{n_i} \left(\tilde{E}_i^r(t) - \tilde{E}_i^{r-1}(t) \right).$$

Using this, we can now write the quasi-local representation of \tilde{E}_i as follows.

$$\int_{-\infty}^{\infty} f_{\beta}(t)\tilde{E}_{i}(t)dt = \int_{-\infty}^{\infty} f_{\beta}(t) \sum_{r=m_{i}}^{n_{i}} \left(\tilde{E}_{i}^{r}(t) - \tilde{E}_{i}^{r-1}(t) \right).$$

To see that it is quasi-local, observe that the term with radius r has norm

$$\int_{-\infty}^{\infty} f_{\beta}(t) \left\| \tilde{E}_{i}^{r}(t) - \tilde{E}_{i}^{r-1}(t) \right\| \\
\leq c_{3} r^{D-1} e^{-c_{4}r} \cdot \int_{-r/v_{LR}}^{r/v_{LR}} e^{c_{4}v_{LR}|t|-\pi|t|/\beta} dt + \int_{r/v_{LR}}^{\infty} e^{-\pi|t|/\beta} dt + \int_{-\infty}^{-r/v_{LR}} e^{-\pi|t|/\beta} dt \\
\leq 2c_{3} r^{D-1} e^{-c_{4}r} \frac{e^{|c_{4}v_{LR}-\pi/\beta|r/v_{LR}} - 1}{|c_{4}v_{LR} - \pi/\beta|} + 2 \frac{e^{-\pi r/(\beta v_{LR})}}{\pi/\beta} \\
\leq 2c_{3} r^{D-1} (r/v_{LR}) e^{-\min(\pi r/(\beta v_{LR}), c_{4}r)} + 2(\beta/\pi) e^{-\pi r/(\beta v_{LR})},$$

where we use $(e^{xy}-1)/x \le ye^{xy}$ for $x \ge 0$ and $y \ge 0$. Define

$$a_{B(r,i)} := e^{\pi r/(2\beta v_{\text{LR}})} \int_{-\infty}^{\infty} f_{\beta}(t) \left(\tilde{E}_i^r(t) - \tilde{E}_i^{r-1}(t) \right).$$

Here, the operator $a_{B(r,i)}$ is supported on the subset B(r,i). Then, from $|B(r,i)| = \mathcal{O}(r^D)$, the quasi-local representation of \widetilde{W} is given as

$$\widetilde{W} = \sum_{i \in \Lambda} v_i \sum_{r=m_i}^{n_i} e^{-\pi r/(2\beta v_{LR})} a_{B(r,i)} = \sum_{i \in \Lambda} \sum_{r=m_i}^{n_i} e^{-\mathcal{O}(|B(r,i)|^{\frac{1}{D}})} v_i a_{B(r,i)},$$

with $e^{-\mathcal{O}(|B(r,i)|^{\frac{1}{D}})}$ decaying sub-exponentially with rate $\tau=1/D$, for all $i\in\Lambda$. We also obtain the parameter ζ in Eq. (19) by

$$\begin{split} \sum_{r,j:B(r,j)\ni i} v_j \|a_{B(r,j)}\| &\leq \sum_r c_5 r^D \sum_{j:B(r,j)\ni i} v_j e^{-\pi r/(2\beta v_{\mathrm{LR}})} \leq \left(\max_{j\in\Lambda} v_j\right) \sum_r c_5 c_B r^{2D} e^{-\pi r/(2\beta v_{\mathrm{LR}})} \\ &\leq 2c_B c_5 \left(\frac{2D+1}{\pi/(2\beta v_{\mathrm{LR}})}\right)^{2D+1} \left(\max_{j\in\Lambda} v_j\right), \end{split}$$

where we define c_B such that $|B(r,j)| \leq c_B r^D$ and we used Fact 12 (2) with p=1, b=2D and $c=\pi/(2\beta v_{\rm LR})$. This completes the representation and shows that \widetilde{W} is a $\left(1/D,\mathcal{O}(1),\mathcal{O}(1/\beta),\mathcal{O}(\beta^{2D+1})\left(\max_{j\in\Lambda}v_j\right)\right)$ -quasi-local.

E Proof of Lemma 34

Recall that the goal in this section is to prove that for \widetilde{W} defined in Lemma 30 we have

$$\max_{i \in \Lambda} \operatorname{tr}[(\widetilde{W}_{(i)})^2 \eta] = \frac{\Omega(1)}{(\beta \log(\beta) + 1)^{2D + 2}} \left(\max_{i \in \Lambda} v_i^2 \right),$$

where η is the maximally mixed state. In this direction, we will now prove that

$$\max_{i \in \Lambda} \|\widetilde{W}_{(i)} \sqrt{\eta}\|_F \ge \frac{c_7}{(\beta \log(\beta) + 1)^{D+1}} \max_{i \in \Lambda} (|v_i|), \tag{151}$$

for a constant $c_7 = \mathcal{O}(1)$. For convenience, let us define $\arg\max_{i \in \Lambda} |v_i| = i_+$, or equivalently $|v_{i_+}| = \max_{i \in \Lambda} |v_i|$. We denote the ball region $B(r,i_+)$ by B_r for the simplicity, where r is fixed later. Let us consider $\widetilde{W}[B_r]$ which is defined as follows:

$$\widetilde{W}[B_r] := \int_{-\infty}^{\infty} f_{\beta}(t)e^{-iHt}W[B_r]e^{iHt}dt, \quad W[B_r] := \sum_{i \in B_r} v_i E_i.$$
(152)

Since $\widetilde{W}[B_r]$ is obtained from $W[B_r]$ in an equivalent manner as \widetilde{W} is obtained from W, the following claim follows along the same lines as Theorem 32. We skip the very similar proof.

Claim 44. It holds that

$$\|\widetilde{W}[B_r]\|_F^2 \ge \frac{\mathcal{D}_{\Lambda}}{c_5[\beta \log(r) + 1]^2} \sum_{i \in B_r} v_i^2,$$

where c_5 is a constant of $\mathcal{O}(1)$.

Since the new operator $\widetilde{W}[B_r]$ well approximates the property of \widetilde{W} around the site i_+ , as long as r is sufficiently large, we expect that $\widetilde{W}[B_r]_{(i_+)}$ and $\widetilde{W}_{(i_+)}$ are close to each other. The claim below makes this intuition rigorous:

Claim 45. It holds that

$$\|\widetilde{W}_{(i_{+})} - \widetilde{W}[B_{r}]_{(i_{+})}\| \le c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta},\tag{153}$$

where c_1, c_2 are constants of $\mathcal{O}(1)$.

This claim implies that the contribution of all the terms in $\widetilde{W}_{(i_+)}$ which are not included in the B_r ball around i_+ decays exponentially with r. Hence,

$$\|\widetilde{W}_{(i_{+})}\|_{F} = \|\widetilde{W}_{(i_{+})} - \widetilde{W}[B_{r}]_{(i_{+})} + \widetilde{W}[B_{r}]_{(i_{+})}\|_{F} \ge \|\widetilde{W}[B_{r}]_{(i_{+})}\|_{F} - \|\widetilde{W}_{(i_{+})} - \widetilde{W}[B_{r}]_{(i_{+})}\|_{F}$$

$$\ge \|\widetilde{W}[B_{r}]_{(i_{+})}\|_{F} - \sqrt{\mathcal{D}_{\Lambda}}\|\widetilde{W}_{(i_{+})} - \widetilde{W}[B_{r}]_{(i_{+})}\|_{F}$$

$$\ge \|\widetilde{W}[B_{r}]_{(i_{+})}\|_{F} - \sqrt{\mathcal{D}_{\Lambda}}c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta}, \quad (154)$$

where we use $\|\widetilde{W}_{(i_+)} - \widetilde{W}[B_r]_{(i_+)}\|_F \le \sqrt{\mathcal{D}_\Lambda} \|\widetilde{W}_{(i_+)} - \widetilde{W}[B_r]_{(i_+)}\|$ in the second inequality. Second, we consider the approximation of $\widetilde{W}[B_r]$ by $\widetilde{W}[B_r, B_{r'}]$ which are supported on $B_{r'}$:

$$\widetilde{W}[B_r, B_{r'}] := \operatorname{tr}_{B_{r'}^c}(\widetilde{W}[B_r]) \otimes \frac{\mathbb{1}_{B_{r'}^c}}{d^{|B_{r'}^c|}}.$$
(155)

Because of the quasi-locality of \widetilde{W} , we expect $\widetilde{W}[B_r,B_{r'}]\approx \widetilde{W}[B_r]$ for $r'\gg r$. This is shown in the following lemma:

Claim 46. The norm difference between $\widetilde{W}[B_r, B_{r'}]$ and $\widetilde{W}[B_r]$ is upper-bounded as

$$\|\widetilde{W}[B_r] - \widetilde{W}[B_r, B_{r'}]\| \le c_3 |v_{i_+}| r^D \beta e^{-c_4|r'-r|/\beta}$$
(156)

and

$$\|\widetilde{W}[B_r]_{(i_+)} - \widetilde{W}[B_r, B_{r'}]_{(i_+)}\| \le 2c_3|v_{i_+}|r^D\beta e^{-c_4|r'-r|/\beta},\tag{157}$$

where c_3, c_4 are constants of $\mathcal{O}(1)$.

The claim reduces the inequality (154) to

$$\|\widetilde{W}_{(i_{+})}\|_{F} \geq \|\widetilde{W}[B_{r}]_{(i_{+})}\|_{F} - \sqrt{\mathcal{D}_{\Lambda}}c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta}$$

$$\geq \|\widetilde{W}[B_{r}, B_{r'}]_{(i_{+})}\|_{F} - \sqrt{\mathcal{D}_{\Lambda}}\|\widetilde{W}[B_{r}]_{(i_{+})} - \widetilde{W}[B_{r}, B_{r'}]_{(i_{+})}\| - \sqrt{\mathcal{D}_{\Lambda}}c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta}$$

$$\geq \|\widetilde{W}[B_{r}, B_{r'}]_{(i_{+})}\|_{F} - \sqrt{\mathcal{D}_{\Lambda}}c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta} - 2\sqrt{\mathcal{D}_{\Lambda}}c_{3}|v_{i_{+}}|r^{D}\beta e^{-c_{4}(r'-r)/\beta}. \tag{158}$$

Next, we relate the norm of $\widetilde{W}[B_r,B_{r'}]_{(i_+)}$ to that of $\widetilde{W}[B_r,B_{r'}]$ using Claim 23. By recalling that $\widetilde{W}[B_r,B_{r'}]_{(i_+)}$ is supported on $B_{r'}$, this gives

$$\|\widetilde{W}_{(i_{+})}[B_{r}, B_{r'}]\|_{F} \ge \frac{1}{|B_{r'}|} \|\widetilde{W}[B_{r}, B_{r'}]\|_{F}, \tag{159}$$

which reduces the inequality (158) to

$$\|\widetilde{W}_{(i_{+})}\|_{F} \geq \frac{1}{|B_{r'}|} \|\widetilde{W}[B_{r}, B_{r'}]\|_{F} - \sqrt{\mathcal{D}_{\Lambda}} c_{1} |v_{i_{+}}| \beta^{D} e^{-c_{2}r/\beta} - 2\sqrt{\mathcal{D}_{\Lambda}} c_{3} |v_{i_{+}}| r^{D} \beta e^{-c_{4}(r'-r)/\beta}$$

$$\geq \frac{1}{|B_{r'}|} \|\widetilde{W}[B_{r}]\|_{F} - \sqrt{\mathcal{D}_{\Lambda}} c_{1} |v_{i_{+}}| \beta^{D} e^{-c_{2}r/\beta} - (2 + 1/|B_{r'}|) \sqrt{\mathcal{D}_{\Lambda}} c_{3} |v_{i_{+}}| r^{D} \beta e^{-c_{4}(r'-r)/\beta},$$
(160)

where in the second inequality we apply Claim 46 to $\|\widetilde{W}[B_r,B_{r'}]\|_F$. Finally, we use the lower bound given in Claim 44 and the inequality $\sum_{i\in B_r}v_i^2\geq v_{i_+}^2$ (since $i_+\in B_r$) to obtain

$$\|\widetilde{W}[B_r]\|_F^2 \ge \frac{\mathcal{D}_{\Lambda}}{c_5[\beta \log(r) + 1]^2} v_{i_+}^2.$$

This reduces the inequality (160) to the following:

$$\frac{\|\widetilde{W}_{(i_{+})}\|_{F}}{\sqrt{\mathcal{D}_{\Lambda}}} \geq \frac{|v_{i_{+}}|}{c_{8}\left(r'\right)^{D}\sqrt{c_{5}}[\beta\log(r)+1]} - c_{1}|v_{i_{+}}|\beta^{D}e^{-c_{2}r/\beta} - 3c_{3}|v_{i_{+}}|r^{D}\beta e^{-c_{4}(r'-r)/\beta},$$

where we used $|B_{r'}| \le c_8 (r')^D$, for some constant c_8 . By choosing r' = 2r and $r = \mathcal{O}(1) \cdot D\beta \log(\beta) + 1$, we have

$$\frac{\|\widetilde{W}_{(i_{+})}\|_{F}}{\sqrt{\mathcal{D}_{\Lambda}}} = \|\widetilde{W}_{(i_{+})}\sqrt{\eta}\|_{F} \ge \frac{c_{7}|v_{i_{+}}|}{(\beta\log(\beta)+1)^{D+1}},\tag{161}$$

for some constant c_7 . By using the inequality $\max_{i\in\Lambda}\|\widetilde{W}_{(i)}\|_F\geq \|\widetilde{W}_{(i_+)}\|_F$, we obtain the main statement. This completes the proof. \square

E.1 Proof of Claims 45, 46

Proof of Claim 45. Recall that the goal is to prove

$$\|\widetilde{W}_{(i_+)} - \widetilde{W}[B_r]_{(i_+)}\| \le c_1 |v_{i_+}| \beta^D e^{-c_2 r/\beta}$$

for constants c_1, c_2 . We start from the integral representation of $\widetilde{W}_{(i_+)}$:

$$\widetilde{W}_{(i_{+})} = \widetilde{W} - \int \mu(U_{i_{+}}) U_{i_{+}}^{\dagger} \widetilde{W} U_{i_{+}}, \tag{162}$$

where $\mu(U_{i_+})$ is the Haar measure for unitary operator U_{i_+} which acts on the i_+ th site. This yields

$$\widetilde{W}_{(i_+)} - \widetilde{W}[B_r]_{(i_+)} = \widetilde{W}[B_r^{\mathrm{c}}] - \int \mu(U_{i_+}) U_{i_+}^{\dagger} \widetilde{W}[B_r^{\mathrm{c}}] U_{i_+}. \tag{163}$$

We thus obtain

$$\|\widetilde{W}_{(i_{+})} - \widetilde{W}[B_{r}]_{(i_{+})}\| \leq \sup_{U_{i_{+}}} \|[U_{i_{+}}, \widetilde{W}[B_{r}^{c}]]\|$$

$$\leq \int_{-\infty}^{\infty} f_{\beta}(t) \sum_{j \in B_{r}^{c}} |v_{j}| \sup_{U_{(i)}} \|[U_{i_{+}}, e^{-iHt} E_{j} e^{iHt}]\| dt$$

$$\leq |v_{i_{+}}| \sum_{j \in B_{r}^{c}} \int_{-\infty}^{\infty} f_{\beta}(t) \min(e^{-c(\operatorname{dist}(i_{+}, j) - v_{\operatorname{LR}}t)}, 1) dt, \tag{164}$$

where we use $|v_j| \le |v_{i_+}|$ and the Lieb-Robinson bound (Fact 15) for the last inequality. Because the function $f_\beta(t)$ decays as $e^{-\mathcal{O}(t/\beta)}$ and $\operatorname{dist}(i_+,j) \ge r$ for $j \in B_r^c$, we have

$$|v_{i_{+}}| \sum_{j \in B^{c}} \int_{-\infty}^{\infty} f_{\beta}(t) \min(e^{-c(\operatorname{dist}(i_{+},j)-v_{LR}t)}, 1) dt \le c_{1}|v_{i_{+}}|\beta^{D} e^{-c_{2}r/\beta}.$$
(165)

This completes the proof.

Proof of Claim 46. Recall that we wanted to show

$$\|\widetilde{W}[B_r] - \widetilde{W}[B_r, B_{r'}]\| \le c_3 |v_{i\perp}| r^D \beta e^{-c_4 |r'-r|/\beta}$$

In order to prove this, we also utilize the integral representation of $\widetilde{W}[B_r, B_{r'}]$:

$$\widetilde{W}[B_r, B_{r'}] := \int \mu(U_{B_{r'}^c}) U_{B_{r'}^c}^{\dagger} \widetilde{W}[B_r] U_{B_{r'}^c}, \tag{166}$$

which yields an upper bound of $\|\widetilde{W}[B_r] - \widetilde{W}[B_r, B_{r'}]\|$ as

$$\|\widetilde{W}[B_r] - \widetilde{W}[B_r, B_{r'}]\| \le \int \mu(U_{B_{r'}^c}) \|[\widetilde{W}[B_r], U_{B_{r'}^c}]\|.$$
(167)

From the definition (152) of $\widetilde{W}[B_r]$ and the Lieb-Robinson bound (Fact 15), we obtain

$$\int \mu(U_{B_{r'}^{c}}) \| [\widetilde{W}[B_{r}], U_{B_{r'}^{c}}] \| \leq \int \mu(U_{B_{r'}^{c}}) \int_{-\infty}^{\infty} f_{\beta}(t) \sum_{j \in B_{r}} |v_{j}| \cdot \| [e^{-iHt} E_{j} e^{iHt}, U_{B_{r'}^{c}}] \| \\
\leq |v_{i+}| \int_{-\infty}^{\infty} f_{\beta}(t) \sum_{j \in B_{r}} \min(e^{-c(r'-r-v_{LR}t)}, 1) dt \\
\leq c'_{3} |v_{i+}| \cdot |B_{r}| \cdot \beta e^{-c_{4}r/\beta}, \tag{168}$$

where $\partial B_{r'}^c$ is the surface region of $B_{r'}^c$. Since $|B_r| \propto r^D$, we obtain the main inequality (156). Now, since

$$\widetilde{W}[B_r]_{(i_+)} = \widetilde{W}[B_r] - \int \mu(U_{i_+}) U_{i_+}^{\dagger} \widetilde{W}[B_r] U_{i_+}$$

and

$$\widetilde{W}[B_r, B_{r'}]_{(i_+)} = \widetilde{W}[B_r, B_{r'}] - \int \mu(U_{i_+}) U_{i_+}^{\dagger} \widetilde{W}[B_r, B_{r'}] U_{i_+},$$

we obtain the second inequality (157) due to

$$\|\widetilde{W}[B_r]_{(i_+)} - \widetilde{W}[B_r, B_{r'}]_{(i_+)}\| \le 2\|\widetilde{W}[B_r] - \widetilde{W}[B_r, B_{r'}]\|.$$

This completes the proof.

F Proof of Theorem 3

For convenience of the reader, we restate the theorem here.

Theorem 47 (Restatement of Theorem 3). The number of copies N of the Gibbs state needed to solve the Hamiltonian Learning Problem and outputs a $\hat{\mu}$ satisfying $\|\hat{\mu} - \mu\|_2 \le \varepsilon$ with probability $1 - \delta$ is lower bounded by

$$N \ge \Omega\Big(\frac{\sqrt{m} + \log(1 - \delta)}{\beta \varepsilon}\Big).$$

Proof. In order to prove the lower bound, we consider learning the parameters $\mu \in \mathbb{R}^m$ of the following class of one-local Hamiltonians on m qubits:

$$H(\mu) = \sum_{i=1}^{m} \mu_i |1\rangle\langle 1|_i.$$

Let $T_m: \{\mu \in \mathbb{R}^m_+: \sum_i \mu_i^2 \leq 100\varepsilon^2\}$ be an orthant of the hypersphere of radius θ in \mathbb{R}^m_+ . We have the following claim.

Claim 48. There exists a collection of 2^m points in T_m , such that the ℓ_2 distance between each pair is $\geq \varepsilon$.

Proof. Pick 2^m points uniformly at random in T_m . By union bound, the probability that at least one pair is at a distance of at most ε is at most $(2^m)^2$ times the probability that a fixed pair of points is at a distance of at most ε . But the latter probability is upper bounded by the ratio between the volume of a hypersphere of radius ε and the volume of T_m , which is $\frac{\varepsilon^m}{(10\varepsilon)^m/2^m} = \frac{1}{5^m}$. Since $(2^m)^2 \frac{1}{5^m} < 1$, the claim concludes.

Let these set of 2^m points be S. For some temperature $\beta>0$ and unknown $\mu\in S$, suppose $\mathcal A$ is an algorithm that is given N copies of $\rho_\beta(\mu)$ and, with probability $1-\delta$, outputs μ' satisfying $\|\mu'-\mu\|_2\leq \varepsilon$. We now use $\mathcal A$ to assign the estimated $\hat\mu$ to exactly one of the parameters μ . Once the learning algorithm obtains an output μ' , we can find the closest point in S (in ℓ_2 distance) as our estimate of μ , breaking ties arbitrarily. With probability $1-\delta$, the closest $\mu\in S$ to μ' is the correct μ since by the construction of S, $\|\mu'-\mu\|_2\leq \varepsilon$. Thus, the algorithm $\mathcal A$ can be used to solve the problem of estimating the parameters μ themselves (not only approximating it). We furthermore show that the number of samples required to estimate $\mu\in S$ is large using lower bounds in the quantum state discrimination. We will directly use the lower bound from [HKK08] (as given in [HW12]). Before we plug in their formula, we need to bound the maximum norm of $\rho_\beta(\mu)$ for

 $\mu \in S$. That is,

$$\begin{aligned} \max_{\mu \in S} \{2^m \| \rho_{\beta}(\mu) \| \} &= \max_{\mu \in S} 2^m \left(\bigotimes_{i=1}^m \left\| \frac{1}{1 + e^{-\beta \mu_i}} |0\rangle \langle 0| + \frac{e^{-\beta \mu_i}}{1 + e^{-\beta \mu_i}} |1\rangle \langle 1| \right\| \right) \\ &= \max_{\mu \in S} \left(\bigotimes_{i=1}^m \left| \frac{2}{1 + e^{-\beta \mu_i}} \right| \right) \\ &= \max_{\mu \in S} \left(\bigotimes_{i=1}^m \left| \frac{2e^{\beta \mu_i}}{e^{\beta \mu_i} + 1} \right| \right) \\ &\leq \max_{\mu \in S} \left(\bigotimes_{i=1}^m \left| \frac{2e^{\beta \mu_i}}{2} \right| \right) \\ &= \max_{\mu \in S} \left(e^{\beta \sum_{i=1}^m \mu_i} \right) \leq e^{\beta \sqrt{m} \sqrt{\sum_{i=1}^m \mu_i^2}} \leq e^{\beta \sqrt{m} \cdot 10\varepsilon}, \end{aligned}$$

since $\sum_i \mu_i^2 \le 100\varepsilon^2$ for all $i \in S$. Thus, the lower bound for state identification of $\{H(\mu) : \mu \in S\}$ in [HW12, Equation 2] (cf. [HKK08] for the original statement) implies that

$$N \ge \frac{\log|S| + \log(1 - \delta)}{\log(\max_{\mu \in S} \{2^m \|\rho(\mu)_{\beta}\|\})} = \frac{m\log 2 + \log(1 - \delta)}{10\sqrt{m}\beta\varepsilon} = \mathcal{O}\Big(\frac{\sqrt{m} + \log(1 - \delta)}{\varepsilon\beta}\Big).$$

This establishes the lower bound.