

Simulating adiabatic evolution of gapped spin systems

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We show that adiabatic evolution of a low-dimensional lattice of quantum spins with a spectral gap can be simulated efficiently. In particular, we show that as long as the spectral gap ΔE between the ground state and the first excited state is any constant independent of n , the total number of spins, then the ground-state expectation values of local operators, such as correlation functions, can be computed using polynomial space and time resources. Our results also imply that the local ground-state properties of any two spin models in the same quantum phase can be efficiently obtained from each other. A consequence of these results is that adiabatic quantum algorithms can be simulated efficiently if the spectral gap does not scale with n . The simulation method we describe takes place in the Heisenberg picture and does not make use of the finitely correlated state–matrix product state formalism.

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I. INTRODUCTION

The low-temperature physics of lattices of interacting quantum spins is typically very complex. The computational cost of even approximating basic properties, such as the ground-state energy eigenvalue, of these systems, is prohibitive. Indeed, for two-dimensional (2D) lattices of interacting spins, the task of computing an approximation to the ground-state energy eigenvalue correct to within some polynomial confidence interval is fantastically difficult—this problem is complete for the complexity class QMA (quantum Merlin-Arthur), which is the quantum version of the complexity class NP [1–3].

It might therefore seem that the computational task of approximating the low-temperature behavior of interacting quantum spins is entirely hopeless. However, for physically realistic models, this is not the case in practice. Many algorithms have been developed that appear to provide efficient approximations to a wide variety of local properties of physically realistic systems, such as correlators, at low temperature. Perhaps the most successful of these methods has been the family of algorithms based on the density matrix renormalization group (DMRG). (See [4] and references therein for a review of the DMRG and description of extensions.)

The DMRG is a remarkably flexible and adaptable algorithm, admitting a slew of generalizations. Applications include simulating dynamics [5,6], dissipative systems [7,8], disordered systems [9], and higher-dimensional lattices [10]. At least part of the flexibility of the DMRG is due to the fact that it is equivalent to a variational minimization over the space of finitely correlated states (FCSs) [11]. Hence, the methodology of the DMRG can be adapted to any situation where the principal object of study, be it an eigenstate or a propagator, can be approximated using a FCS vector on Hilbert space. An alternative to methods based on variations over FCSs has been recently proposed which appears to offer spectacular computational speedups over the DMRG and relatives [12].

In practice it appears that the DMRG and related algorithms can efficiently obtain arbitrarily accurate approximations to the local ground-state properties of a 1D collection of interacting quantum spins. However, at the current time, there is no satisfactory understanding of the correctness (i.e., will the DMRG always return a faithful approximation to the ground state and not some other eigenstate) and the complexity (i.e., assuming correctness, how many computational resources are required to obtain a good approximation to a ground state) of the DMRG.

The correctness of the DMRG is far from obvious. This is because the ground-state approximation obtained by the DMRG cannot be certified; the DMRG only returns an approximate ground-state eigenvector and cannot guarantee that this vector is close to the true ground state. It is therefore extremely desirable to determine *a priori* the class of systems for which the DMRG and relatives provably return faithful approximations to the ground state. The complexity¹ of the DMRG is also difficult to ascertain. Assuming we could prove correctness of the DMRG for a class of realistic physical systems, the actual complexity of the DMRG depends subtly on many detailed properties of the system, such as geometric entropy of the ground state, and nonconvexity of the objective function that is minimized.

Recently this situation is changing [13–15]. In [16] an analysis of the resource scaling of a DMRG-like algorithm to obtain approximations to the ground states of 1D gapped local models was undertaken. This paper provides the first general subexponential estimate for the time and space resource requirements of any provably correct method to compute approximations to the ground states of gapped models; it was found that if the model is gapped then resources scaling as $n^c \log n$, with c some constant, are sufficient to obtain and store a computational representation of the ground state

¹The complexity of the DMRG as an algorithm can be further refined into the spatial complexity, i.e., how much memory is required to store approximations to the ground state, and the temporal complexity, i.e., how much time the DMRG needs to run.

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of a gapped local model.² In [13] it was shown that the ground state of some³ critical 1D spin models can be stored efficiently. Unfortunately, there is currently no theoretical argument which implies that these approximations to the ground states can be obtained efficiently. Indeed, the results of this paper imply that if such approximations are obtained via adiabatic continuation then exponential computational resources may be required to obtain them. (Note, however, that we can say nothing about the other methods to obtain such FCS approximations.) Finally, in [14] it was shown that an approximation to the propagator for a 1D lattice of quantum spins can be obtained and stored (as a FCS vector) using polynomial resources in n and the error ϵ and exponential resources in the time $|t|$. (It is straightforward to extend the argument of [14] to show an analogous result in 2D.)

There is at least one solid reason why we believe that DMRG-like methods ought to provide a computationally efficient recipe to compute approximations to the ground states of gapped systems; namely, we know that the ground-state correlation functions for any gapped system are clustering or rapidly decaying with separation [19–21]. This result, which is the natural analog of Fredenhagen’s proof [22] of clustering for relativistic quantum field theories, is especially impressive given that it applies to an extremely wide class of quantum lattice systems in low dimensions. As a consequence of clustering results we conclude that gapped spin systems are essentially free—an intuition that is persuasively backed up by classical renormalization-group style argumentation—and thus can be modeled as noninteracting effective spins, which can be simulated easily.

Another way of arriving at this conclusion is to think of correlations as roughly “measuring” the degree of quantum correlation in the ground state. Since the amount of quantum correlation in a quantum state limits the extent to which a state can be approximated by a FCS [13], we are strongly encouraged to think that the clustering results may actually imply that DMRG-like algorithms may converge rapidly for at least some realistic gapped systems.

Unfortunately, knowing that the correlations decay is not enough information to infer that the eigenstates are finitely correlated. To understand this simply consider a generic quantum state [23] which is a quantum state chosen uniformly from the Haar measure induced on state space. A generic quantum state exhibits rapidly decaying correlations (indeed, all m -point correlation functions are essentially zero for $m < n/2$), yet such a state is extremely entangled and

cannot be efficiently represented as a finitely correlated state. Nevertheless, it might be argued that the results of [19–21] avoid this counterexample because they prove something stronger, namely, exponential clustering, which says that the reduced density operator ρ_{AB} of the ground state for two arbitrarily large separated regions A and B is indistinguishable from a product $\rho_A \otimes \rho_B$ when it is used to compute expectations for product observables $M_A M_B$. Interestingly, a naive attempt to exploit this exponential clustering runs into problems. The reason is that there exist highly entangled states σ_{AB} , called data-hiding states, which exhibit precisely these properties [24]. Thus, to prove that the ground state of a gapped local Hamiltonian is well approximated by a finitely correlated state with polynomial resources we appear to need more information than that given by correlation functions.

Despite some recent progress a solution to the fundamental problem, namely, to prove correctness of any algorithm that obtains approximations to local ground-state properties for gapped 1D models and to further provide a polynomial theoretical worst-case estimate on the resource requirements such an algorithm, still seems far away. Let us summarize the various approaches to finding approximations to the ground state of a spin model and the theoretical obstructions encountered in each of these approaches.

There are at least four ways to obtain an approximation to the ground state of a quantum system: (i) variation over a class of ansatz ground states; (ii) simulation of the thermalization process via imaginary time evolution or similar; (iii) approximation of the convex set of reduced density operators of translation-invariant quantum states; and (iv) adiabatic continuation from the ground states of classical spin models. The DMRG is an example of the first method, namely, it is a variation over the class of FCSs with fixed auxiliary dimension. Unfortunately this variation is, in general, nonconvex and it has been recently discovered [25] that hard instances for a closely related variation problem can be constructed. Thus it seems likely that the DMRG is not correct in general. The second approach, namely, imaginary time evolution, suffers from the shortcoming that an initial guess $|\Omega'\rangle$ for the ground state $|\Omega\rangle$ which has nontrivial overlap with the actual ground state is required. If such an initial guess is unavailable then the storage requirements of the imaginary time evolution approach could be, in the worst case, exponential.⁴ It seems plausible that obtaining such a guess could be as hard as solving the original problem. The third method requires an exponentially good characterization of the convex set of reduced density operators of translation-invariant quantum states in order to obtain $O(1)$ estimates for local operators. The final method, which is the focus of this paper, suffers from the limitation that it is not known if the ground

²While the analysis of [15] was carried out for 1D systems, it is clear how the calculations generalize to 2D systems and show a subexponential resource scaling to obtain a representation of the ground state as a 2D finitely correlated state [11,17] or projected-pair entangled state (PEPS) [10]. Note that it is currently an unsolved problem to determine the classes of 2D PEPSs for which it is computationally easy to extract local properties, such as correlators. Indeed, because of certain classical constructions [18], it must be at least an NP-hard problem in general.

³At least those which are equivalent to conformal models. Note that it is easy to construct models which are “critical” in the sense of vanishing spectral gap, but which require exponential resources to compute and store their ground states.

⁴Without a good initial guess one must store approximations to the full thermal density operator $\rho = e^{-\beta H} / \text{tr}(e^{-\beta H})$ which are close in trace norm. A recent counterexample due to Terhal and DiVincenzo [26] implies that, even for gapped systems, we need to approximate such states for $\beta = O(n)$. For large β no good estimates on the storage requirements of trace-norm close estimates for thermal states seem available with the current technology.

state of an arbitrary gapped spin model can be obtained via adiabatic continuation from a classical model without encountering a quantum phase transition. However, it has been recently proved [27–29] that in the neighborhood of a classical spin model adiabatic continuation will work. Thus, using this approach, we are able to provide polynomial estimates on the resource requirements of a correct method to obtain a representation of the ground state of at least a subclass of gapped models.

There is an intimate connection between simulating adiabatic continuation for quantum lattice models and simulating quantum computations [2,30]; namely, if adiabatic evolution for an arbitrary 2D lattice model with a gap that scales as an inverse polynomial of the system size could be simulated efficiently on a classical computer then⁵ $\text{BQP} \subseteq \text{P}$, thus obviating the need to design and engineer a quantum computer in the first place. Naturally, our results are nowhere near strong enough to show the complexity class inclusion $\text{BQP} \subseteq \text{P}$, but they do have implications for error correction methods for adiabatic quantum algorithms.

A complete theory of quantum error correction for adiabatic quantum algorithms [31] is still being developed. For example, for general thermalization decoherence, we really have no idea how to calculate a fault-tolerance threshold for adiabatic quantum algorithms (see [32,33] for a discussion of quantum error correction and fault tolerance). Presumably a general quantum error-correcting code for a quantum adiabatic algorithm would involve encoding the adiabatic evolution in a larger system such that the minimum spectral gap encountered along the evolution was larger.⁶ This would mean it would cost the environment more energy per unit time to induce a transition from the ground state during the evolution (an “error”). It is natural to assume that the gap could be boosted to a large constant, independent of the number n of spins, with a polynomial increase in size. Our results show that if this were possible then we could simulate adiabatic quantum algorithms efficiently on a classical computer. Thus, conditioned on the strict complexity class containment $\text{P} \subset \text{BQP}$, we obtain a bound on how large the gap could be made by encoding for adiabatic quantum algorithms.

The method we develop in this paper is very closely related to the method studied in [35]. In [35] the authors investigate the evolution of local operators under a quasiadiabatic change in a local Hamiltonian. As long as the Hamiltonian has a spectral gap throughout the evolution, it was found that local operators remained local, and thus it was possible to say that local gauge invariance remains when two Hamiltonians are in the same phase. Our task is similar: we wish to understand the expectation values of local operators in the ground state of a system that has undergone adia-

batic evolution. We wish to show that the computation of such expectation values can be done efficiently on a classical computer as long as the smallest gap encountered during the adiabatic evolution is $O(1)$. While this calculation can be treated using quasiadiabatic evolution and the methods developed in [35] to study such evolutions, we prefer to study exact adiabatic evolution. We do this primarily in anticipation of the application of these results to studying entropy-area laws for systems in the same phase.

We provide an efficient computational method to compute the expectation values of local operators in the ground states of Hamiltonians undergoing exact adiabatic evolution, a method that works equally well for Hamiltonians with spatially varying interactions. Our method does not make use of the FCS formalism. Rather, we develop our simulation method in the Heisenberg picture, where locality is manifest. Indeed, if we were to make use of state representations in the Schrödinger picture, i.e., the 2D FCS formalism (PEPS), we would be unable to apply our results because even if we could construct PEPS approximations to the adiabatically continued ground state it is currently unknown how to efficiently extract expectation values of local operators from the PEPS representation. We sidestep this issue by providing a ground-state certificate in the form of a specification of a local Hamiltonian that can be efficiently numerically simulated in the Heisenberg picture to extract local expectation values.

The outline of this paper is as follows. We begin in Sec. II by introducing the class of local Hamiltonians we consider and stating the problem we wish to solve. In Sec. III we then show how adiabatic evolution for quantum lattices of spins can be described by unitary dynamics of an effective local Hamiltonian. We use this effective dynamics in Sec. IV to construct an approximate local dynamics which can then be used to efficiently extract local properties of the adiabatically continued ground state. We conclude with some discussion of our results in Sec. V. We detail some simple properties of compactly supported C^∞ functions in the Appendix.

II. FORMULATION

In this section we introduce the Hilbert space and operator algebras for the systems we consider. We define what we mean by strictly local and approximately local Hamiltonians. Finally, we specify the computational task that will occupy us for the rest of this paper.

We consider quantum systems defined on a set of vertices V with a finite-dimensional Hilbert space \mathcal{H}_x attached to each vertex $x \in V$. We always assume that V is finite. (There are some minor theoretical obstructions which currently preclude a simple extension of our results to infinite lattices; we will discuss this in a further presentation.) For $X \subset V$, the Hilbert space associated with X is the tensor product $\mathcal{H}_X = \otimes_{x \in X} \mathcal{H}_x$, and the algebra of observables on X is denoted by $\mathcal{A}_X = \mathcal{B}(\mathcal{H}_X)$, where $\mathcal{B}(\mathcal{H}_X)$ denotes the C^* algebra of bounded operators on \mathcal{H}_X with norm

$$\|A\| = \sup_{|\psi\rangle \in \mathcal{S}(\mathcal{H}_X)} \|A|\psi\rangle\|, \quad (1)$$

and $\mathcal{S}(\mathcal{H}_X)$ is the state space for \mathcal{H}_X . We assume that V is equipped with a metric d . In the most common cases V is the

⁵The class BQP is the class of decision problems that can be decided in polynomial time on a quantum computer.

⁶This idea has been recently explored in [34], where it was found that quantum error-correcting codes against uncorrelated local noise can be constructed for adiabatic quantum algorithms. Note that the codes investigated in this paper do not increase the overall gap of the original Hamiltonian after the encoding.

vertex set of a graph, and the metric is given by the graph distance $d(x, y)$, which is the length of the shortest path of edges connecting x and y in the graph. Finally, by tensoring with the unit operators on $Y \setminus X$, we consider \mathcal{A}_X as a subalgebra of \mathcal{A}_Y , whenever $X \subset Y$.

We will, for the sake of clarity, introduce and describe our results for a collection of n distinguishable spin- $\frac{1}{2}$ particles. Thus, the Hilbert space \mathcal{H} for our system is given by $\mathcal{H} = \otimes_{j=0}^{n-1} \mathbb{C}^2$. We now fix the metric for our vertex set V to be that of a low-dimensional periodic lattice L of $n=m^\eta$ vertices, where $m \in \mathbb{N}$ and η is the dimension. Because the case $\eta=2$ is the only really nontrivial case that interests us, we fix $\eta=2$ from now on. We refer to vertices as sites and identify each site v with its coordinates $\mathbf{j}=(j_x, j_y)$. Because the lattice is periodic we identify coordinates $(j_x=m) \equiv (j_x=0)$ and $(j_y=m) \equiv (j_y=0)$. It is entirely straightforward to generalize our results to higher-dimensional lattices, higher dimensional spins, and more general lattices.

We consider a distinguished basis, the standard product basis, for \mathcal{H}_V given by $|\mathbf{z}\rangle = \otimes_{j_x=0}^{m-1} \otimes_{j_y=0}^{m-1} |z_{(j_x, j_y)}\rangle$, $z_{\mathbf{j}} \in \mathbb{Z}/2\mathbb{Z}$. We will also have occasion to refer to a certain orthonormal basis for \mathcal{A}_V : we denote by $\sigma^\alpha = \otimes_{j_x=0}^{m-1} \otimes_{j_y=0}^{m-1} \sigma_{(j_x, j_y)}^\alpha$, $\alpha_{\mathbf{j}} \in \mathbb{Z}/4\mathbb{Z}$, the standard operator basis, where $\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, are the Pauli sigma matrices.

We define the support $\text{supp}(M) \subset V$ of an operator $M \in \mathcal{A}_V$ to be the smallest subset $\Lambda \subset V$ such that $M \in \mathcal{A}_\Lambda$, i.e., the smallest subset upon which M acts nontrivially. Let $M \subset L$ and $N \subset L$. We define the sumset $M+N \subset L$ of M and N by $M+N = \{\mathbf{x}+\mathbf{y} \mid \mathbf{x} \in M, \mathbf{y} \in N\}$ where the addition operation $\mathbf{x}+\mathbf{y}$ is inherited from the standard addition on $L \equiv (\mathbb{Z}/m\mathbb{Z}) \times (\mathbb{Z}/m\mathbb{Z})$. This operation is the natural generalization of the convolution operation on the real numbers to the finite group L . (It is fairly straightforward to generalize these operations to more general groups.)

We now introduce the family $H(s)$ of parameter-dependent Hamiltonians we are going to focus on. To define our family we will initially fix some parameter-dependent interaction term $h(s) \in \mathcal{A}_V$ which has bounded norm:⁷ $\|h(s)\| \leq O(1)$. We think of $h(s)$ as being ‘‘centered’’ on site $\mathbf{0}$, i.e., we demand that $\mathbf{0} \in \text{supp}[h(s)]$. Our family $H(s)$ of quantum systems is then defined by

$$H(s) = \sum_{\mathbf{j} \in L} \mathcal{T}_y^{\mathbf{j}}(\mathcal{T}_x^{\mathbf{j}}(h(s))) = \sum_{\mathbf{j} \in L} h_{\mathbf{j}}(s), \quad (2)$$

where \mathcal{T}_x (\mathcal{T}_y) is the unit translation operator which translates the subsystems one site across in the x (y) direction, e.g.,

$$\mathcal{T}_x \left(\otimes_{j_x=0}^{m-1} \otimes_{j_y=0}^{m-1} \sigma_{(j_x, j_y)}^\alpha \right) = \otimes_{j_x=0}^{m-1} \otimes_{j_y=0}^{m-1} \sigma_{(j_x+1, j_y)}^\alpha, \quad (3)$$

and $h_{\mathbf{j}}(s) = \mathcal{T}_y^{\mathbf{j}}(\mathcal{T}_x^{\mathbf{j}}(h(s)))$. While the Hamiltonian $H(s)$ generated by this construction is translation invariant, none of our subsequent calculations depend on this fact in any serious

way. Hence the results of this paper apply equally to Hamiltonians with spatially varying interactions.

We are going to make three simplifying assumptions about our Hamiltonian $H(s)$. The first is that $H(s)$ is assumed to be strictly local which means that $|\text{supp}[h(s)]|$ is an $O(1)$ constant. The second assumption we make is that the interaction $h(s)$ that generates $H(s)$ can be written as $h(s) = h_0 + sh'$, where h_0 and h' are two operators with $O(1)$ norm. The final assumption is that the ground state is unique and the spectral gap $\Delta E(s)$ between the ground and first excited states for $H(s)$ satisfies the inequality $\Delta E(s) \geq \Delta$, $\forall s \in [0, 1]$, where $\Delta E(s)$ is an $O(1)$ constant. Note that the first two assumptions can be lifted with a little extra work; however, the assumption that the gap $\Delta E(s)$ is an $O(1)$ constant cannot be relaxed: the simulation algorithm we present scales exponentially with $\Delta E(s)$.

We will also have occasion to discuss approximately local Hamiltonians. Such Hamiltonians are obtained in the same way as in (2), that is, we fix some initial interaction term $k(s)$ which we then average over translates to generate our Hamiltonian $K(s)$. In this case, however, the initial interaction term is allowed to have support equal to all of V . The only constraint we make is that $k(s)$ must decay rapidly, which means that $k(s)$ can be written as a sum:

$$k(s) = \sum_{\alpha=0}^{m-1} k_\alpha(s) \quad (4)$$

where $\text{supp}[k_\alpha(s)] = \Lambda_\alpha$, and Λ_α consists of all the sites within a distance α of site $\mathbf{0}$, i.e., $\Lambda_\alpha = \{\mathbf{j} \mid d(\mathbf{0}, \mathbf{j}) \leq \alpha\}$. As a result, $k_\alpha(s)$ is an operator with a support (or ‘‘radius’’) consisting of α sites centered on site $\mathbf{0}$. The rapid-decay condition is then that

$$\|k_\alpha(s)\| \leq f(\alpha), \quad 0 \leq \alpha < m, \quad (5)$$

where $f(\alpha)$ is some rapidly decreasing function of α .

We say that a Hamiltonian $K(s)$ constructed from the interaction $k(s)$ has rapid decay. We write the final Hamiltonian resulting from this construction as

$$K(s) = \sum_{\mathbf{j} \in L} \sum_{\alpha=0}^{m-1} k_{\mathbf{j}, \alpha}(s), \quad (6)$$

where $k_{\mathbf{j}, \alpha}(s) = \mathcal{T}_y^{\mathbf{j}}(\mathcal{T}_x^{\mathbf{j}}(k_\alpha(s)))$.

Finally, we set out the problem we aim to solve. We suppose $H(s)$ is a strictly local parameter-dependent Hamiltonian for a 2D lattice of the form (2), with interaction $h(s)$ having $O(1)$ norm and $O(1)$ support. We assume that the ground state $|\Omega(s)\rangle$ is unique and, further, that the spectral gap $\Delta E(s)$ between the ground state and first excited state satisfies $\Delta E(s) \geq \Delta$, $\forall s \in [0, 1]$, where Δ is a constant independent of n . Finally, we suppose that expectation values of arbitrary local operators $A \in \mathcal{A}_L$, with $O(1)$ support, in the initial ground state $|\Omega(0)\rangle$ can be computed efficiently, i.e., $\omega_0(A) = \langle \Omega(0) | A | \Omega(0) \rangle$ can be computed efficiently for all $A \in \mathcal{A}_L$. This would be the case when, for example, $H(0)$ is any regular classical Hamiltonian, that is, $[h_{\mathbf{j}}(s), h_{\mathbf{k}}(s)] = 0$, $\forall \mathbf{j}, \mathbf{k} \in L$. Alternatively, this occurs when $H(s)$ has a ground

⁷The order notation $O(\cdot)$ refers to the growth or decay of quantities with respect to the fundamental parameter of this paper: n , the number of spins.

state that is exactly a 2D finitely correlated state. [When $H(s)$ has spatially varying interactions we must require that the ground state of $H(0)$ is a known product state. We need to do this in order to avoid the constructions of [18], which show that computing the ground state of a disordered classical systems is at least NP hard.]

Our approximation problem is therefore the following. First fix some error ϵ . Then our problem is to find an efficient computational method to compute, for any local operator A with bounded support,⁸ uniform approximants $\omega'_s(A)$ to the exact expectation values $\omega_s(A) = \langle \Omega(s) | A | \Omega(s) \rangle$. That is, our problem is to efficiently compute $\omega'_s(A)$ so that $|\omega'_s(A) - \omega_s(A)| < \epsilon$ for all $s \in [0, 1]$ and for all bounded local operators A with bounded support.

The constraint that the observables whose expectation values are to be simulated must have bounded support stems from the condition that in the large- n limit such operators should be elements of the quasilocal algebra \mathcal{A}_L . We lose no generality in this assumption when applying it to the simulation of quantum algorithms because the answer that the algorithm computes should be encoded in the ground state in such a way that it can be read out from the expectation value of a local operator. It is also worth noting that any correlation function involving a bounded number of subsystems satisfies our definition of having bounded support.

Before we end this section we introduce some notation for approximations. Because we have occasion to refer to functions for which only bounds on growth, derivatives, etc., are known it is convenient to adopt the following notation. If we have two quantities A and B then we use the notation $A \lesssim B$ to denote the estimate $A \leq CB$ for some constant C which depends only on unimportant quantities. In almost all the cases we consider the only important quantity to be n , the total number of spins. Thus, unless we indicate otherwise, $A \lesssim B$ means that $A \leq CB$ for some C independent of n . Because we will be interested in the consequences of allowing the minimum gap Δ to depend on n we will explicitly retain any dependence on Δ in our calculations.

III. EFFECTIVE LOCAL DYNAMICS FOR EXACT ADIABATIC EVOLUTION

In this section we study exact adiabatic evolution for quantum spin systems. We show that if there is a gap throughout the evolution then the exact adiabatic evolution is equivalent to unitary dynamics generated by an approximately local Hamiltonian.

We consider adiabatic quantum evolution generated by $H(s)$ as s is varied adiabatically from $s=0$ to 1. Thus we would like to understand the ground state $|\Omega(s)\rangle$ of $H(s)$. We do this by setting up a differential equation for $|\Omega(s)\rangle$:

$$\frac{d}{ds} |\Omega(s)\rangle = P'(s) |\Omega(s)\rangle, \quad (7)$$

where $P'(s) = (d/ds)(|\Omega(s)\rangle\langle\Omega(s)|)$ and we have set phases⁹ so that $\langle\Omega'(s)|\Omega(s)\rangle = 0$. Because $P'(s)$ is not anti-Hermitian the dynamics generated by this equation are not unitary.

There are at least two ways to set up differential equations for $|\Omega(s)\rangle$ that do generate unitary dynamics. The first is via exact adiabatic evolution (see [36,37] for a rigorous discussion of rather general results about exact adiabatic evolution):

$$\frac{d}{ds} |\Omega(s)\rangle = -[P(s), P'(s)] |\Omega(s)\rangle. \quad (8)$$

Because of the gap condition on $H(s)$, the ‘‘Hamiltonian’’ $[P(s), P'(s)]$ for this dynamics is given by first-order stationary perturbation theory:

$$[P(s), P'(s)] = |\Omega(s)\rangle\langle\Omega(s)| \frac{\partial H(s)}{\partial s} \frac{\mathbb{I}}{\Omega(s)\mathbb{I} - H(s)} - \frac{\mathbb{I}}{\Omega(s)\mathbb{I} - H(s)} \frac{\partial H(s)}{\partial s} |\Omega(s)\rangle\langle\Omega(s)|, \quad (9)$$

where $\Omega(s)$ is the ground-state energy of $H(s)$, and we define $\mathbb{I}/[\Omega(s)\mathbb{I} - H(s)]$ via the Moore-Penrose inverse $\{\mathbb{I}/[\Omega(s)\mathbb{I} - H(s)]\} |\Omega(s)\rangle = 0$.

The other way, which we call the effectively local exact adiabatic evolution, is obtained by rewriting $P'(s)$. We exploit the fact that $H(s)$ has a spectral gap to find

$$P(s) = \int_{-\infty}^{\infty} \chi_\gamma(t) e^{-it\Omega(s)} e^{itH(s)} dt, \quad (10)$$

where $\chi_\gamma(t)$ is an even real function whose Fourier transform $\hat{\chi}_\gamma$ is C^∞ , has compact support in $[-\gamma, \gamma]$, and is normalized so that $\hat{\chi}_\gamma(0) = 1$. (See the Appendix for a description of C^∞ cutoff functions and their properties.) We must set $\gamma < \Delta$ to ensure that only the ground state appears on the right-hand side of (10). The formula (10) for $P(s)$ may be verified by writing e^{itH} in its eigenbasis and exploiting the L_2 unitarity of the Fourier transform.

We next use the Duhamel formula

$$\frac{d}{ds} e^{itH(s)} = i \int_0^t e^{iuH(s)} \frac{\partial H(s)}{\partial s} e^{i(t-u)H(s)} du,$$

to rewrite (7),

⁸That is, we assume $|\text{supp}(A)|$ is any (arbitrarily large) $O(1)$ constant.

⁹Note that this choice precludes an extension of our analysis to study Berry phases in spin systems. We will relax this constraint in a future presentation.

$$\begin{aligned} \frac{d}{ds}|\Omega(s)\rangle &= -i\frac{d\Omega(s)}{ds}\int_{-\infty}^{\infty}t\chi_{\gamma}(t)dt|\Omega(s)\rangle + i\int_{-\infty}^{\infty}\chi_{\gamma}(t)e^{-it\Omega(s)} \\ &\times\left[\int_0^t\tau_u^{H(s)}\left(\frac{\partial H(s)}{\partial s}\right)du\right]e^{iH(s)}dt|\Omega(s)\rangle, \end{aligned} \quad (11)$$

where $\tau_u^{H(s)}(M)=e^{iuH(s)}Me^{-iuH(s)}$. Using the fact that $\chi_{\gamma}(t)$ is an even function of t and canceling phases we obtain

$$\frac{d}{ds}|\Omega(s)\rangle = i\int_{-\infty}^{\infty}\chi_{\gamma}(t)\left[\int_0^t\tau_u^{H(s)}\left(\frac{\partial H(s)}{\partial s}\right)du\right]dt|\Omega(s)\rangle. \quad (12)$$

By integrating this expression for $(d/ds)|\Omega(s)\rangle$ in the energy eigenbasis of $H(s)$ and using the assumed gap structure one can find that this expression is equivalent to the usual expression obtained from first-order perturbation theory,

$$\frac{d}{ds}|\Omega(s)\rangle = \frac{\mathbb{I}}{\Omega(s)\mathbb{I}-H(s)}\frac{\partial H(s)}{\partial s}|\Omega(s)\rangle. \quad (13)$$

Thanks to our assumed form of $H(s)=H_0+sH'$, with $H'=\sum_{j\in L}h'_j=\sum_{j\in L}\mathcal{T}_y^x(\mathcal{T}_x^y(h'))$, we notice that $\partial H(s)/\partial s=\sum_{j\in L}h'_j$, and we write

$$\frac{d}{ds}|\Omega(s)\rangle = i\sum_{j\in L}\mathcal{F}_s(h'_j)|\Omega(s)\rangle, \quad (14)$$

with initial condition that $|\Omega(0)\rangle$ is the ground state of $H(0)$ and where $\mathcal{F}_s(M)=\int_{-\infty}^{\infty}\chi_{\gamma}(t)\left[\int_0^t\tau_u^{H(s)}(M)du\right]dt$.

Equation (14) tells us that $|\Omega(s)\rangle$ can be obtained from $|\Omega(0)\rangle$ by unitary dynamics according to the time-dependent Hermitian Hamiltonian $K(s)=\sum_{j\in L}\mathcal{F}_s(h'_j)=\sum_{j\in L}k_j(s)$, where we write $k_j(s)=\mathcal{F}_s(h'_j)$. We also write $k(s)=\mathcal{F}_s(h')$ for the interaction term $k(s)$ which generates $K(s)$. Furthermore, we claim that $K(s)$ is approximately local for all $s\in[0,1]$.

The way to see that $K(s)$ is approximately local is to use the standard Lieb-Robinson bound [16,19,21,38]. The Lieb-Robinson bound reads

$$\|[\tau_t^{H(s)}(A),B]\| \leq |Y|e^{-v d(x,Y)}(e^{\kappa|t|}-1) \quad (15)$$

for any two norm-1 operators $A\in\mathcal{A}_x$ and $B\in\mathcal{A}_Y$, with $\{x\}\cap Y=\emptyset$, which are initially separated by a distance $d(x,Y)$. The constants v and κ are independent of n and depend only on $\|h(s)\|$, which is an $O(1)$ constant.

What we do is define

$$k_0(s)=\mathcal{F}_s^{H_{\Lambda_0}(s)}(h') \quad (16)$$

and

$$k_{\alpha}(s)=\mathcal{F}_s^{H_{\Lambda_{\alpha}}(s)}(h')-\mathcal{F}_s^{H_{\Lambda_{\alpha-1}}(s)}(h'), \quad 0<\alpha<m, \quad (17)$$

where we define

$$\mathcal{F}_s^{H_{\Lambda_{\alpha}}(s)}(M)=\int_{-\infty}^{\infty}\chi_{\gamma}(t)\left(\int_0^t\tau_u^{H_{\Lambda_{\alpha}}(s)}(M)du\right)dt, \quad (18)$$

with

$$H_{\Lambda_{\alpha}}(s)=\sum_{j\in\Lambda_{\alpha}}h_j(s), \quad (19)$$

where $\Lambda_{\alpha}=\{j|d(\mathbf{0},j)\leq\alpha\}$. Obviously $k_{\alpha}(s)$ has support $\text{supp}[k_{\alpha}(s)]=\Lambda_{\alpha}+\text{supp}(h')$. Also note that $k(s)=\sum_{\alpha=0}^{m-1}k_{\alpha}(s)$ (recall that m is the diameter of the lattice).

We now show how the Lieb-Robinson bound provides an estimate on the decay of $\|k_{\alpha}(s)\|$. First, we rewrite the Lieb-Robinson bound (15) so that it is more useful:

$$\begin{aligned} &\|\tau_t^{H_{\Lambda_{\alpha}}(A)}-\tau_t^{H_{\Lambda_{\alpha-1}}(A)}\| \\ &= \left\|\int_0^t dt' \frac{d}{dt'}(\tau_{t-t'}^{H_{\Lambda_{\alpha-1}}(\tau_{t-t'}^{H_{\Lambda_{\alpha}}(A)})}\right\| \\ &= \left\|\int_0^t dt' \tau_{t-t'}^{H_{\Lambda_{\alpha-1}}}\{[H_{\Lambda_{\alpha}}-H_{\Lambda_{\alpha-1}},\tau_{t-t'}^{H_{\Lambda_{\alpha}}(A)}]\}\right\| \\ &\leq \int_0^{|t|} dt' \| [H_{\Lambda_{\alpha}}-H_{\Lambda_{\alpha-1}},\tau_{t-t'}^{H_{\Lambda_{\alpha}}(A)}] \| \\ &\leq 2\int_0^{|t|} dt' \| [H_{\Lambda_{\alpha}}-H_{\Lambda_{\alpha-1}}] \| e^{-v\alpha+\kappa|t'|} \leq \alpha e^{\kappa|t|-v\alpha}, \end{aligned} \quad (20)$$

where we used the fundamental theorem of calculus to get the first line, the triangle inequality and unitary invariance of the norm to get the third line, we substituted the Lieb-Robinson bound (15) in the fourth line, and we integrated the bound to get the fifth line. The α term in the one fifth line comes from the fact that the operator $H_{\Lambda_{\alpha}}-H_{\Lambda_{\alpha-1}}$ consists of α terms (the number of terms crossing the boundary). The Lieb-Robinson bound, in this form, says that the evolution of A with respect to $H_{\Lambda_{\alpha}}$ is almost the same as that for $H_{\Lambda_{\alpha-1}}$, i.e., the boundary effects are unimportant for short times.

Now consider

$$\begin{aligned} \|k_{\alpha}(s)\| &= \left\|\int_{-\infty}^{\infty}\chi_{\gamma}(t)\left(\int_0^t[\tau_u^{H_{\Lambda_{\alpha}}(s)}(h')-\tau_u^{H_{\Lambda_{\alpha-1}}(s)}(h')]du\right)dt\right\| \\ &\leq 2\int_0^{\infty}|\chi_{\gamma}(t)|\left(\int_0^t\|\tau_u^{H_{\Lambda_{\alpha}}(s)}(h')-\tau_u^{H_{\Lambda_{\alpha-1}}(s)}(h')\|du\right)dt \\ &\leq 2\int_0^{\infty}|\chi_{\gamma}(t)|\left(\int_0^t\min\{2\|h'\|,c\alpha e^{\kappa|u|-v\alpha}\}du\right)dt \\ &\leq \alpha\int_0^{c\alpha}|\chi_{\gamma}(t)|e^{\kappa|t|-v\alpha}dt + \int_{c\alpha}^{\infty}|\chi_{\gamma}(t)|t|dt \\ &\leq \alpha\int_0^{c\alpha}e^{\kappa t-v\alpha}dt + \int_{c\alpha}^{\infty}\frac{1}{\gamma|t|^{l-1}}dt, \quad \forall l>1, \\ &\leq \alpha e^{(\kappa c-v)\alpha} + \frac{1}{c\gamma\alpha^{l-1}}, \quad \forall l>1, \end{aligned} \quad (21)$$

where to get the second line we applied the triangle inequality, to get the third line we applied the Lieb-Robinson bound in the form (20) with $\alpha=\text{diam}(\Lambda_{\alpha})+\text{const}$ [we have dropped the dependence of the interactions $H_{\Lambda_{\alpha}}(s)$ on the parameter s

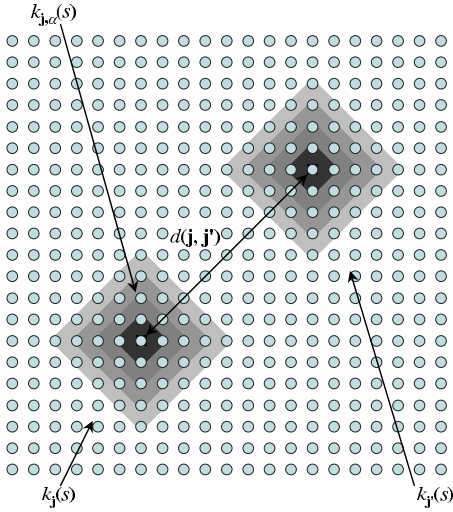


FIG. 1. (Color online) Illustration of the rapidly decaying interactions for the effectively local Hamiltonian for exact adiabatic evolution.

because for these inequalities the evolution is independent of the parameter s], in the fourth line we have broken the integral into two pieces and applied the different regimes of the Lieb-Robinson bound separately with c some constant¹⁰ to be chosen later, and in the final line we applied the decay estimates on $\chi_\gamma(t)$ (see the Appendix for a derivation of these estimates). Thus, by choosing $c < v/\kappa$ we see that $\|k_\alpha(s)\|$ is decaying faster than the inverse of any polynomial in α for $\alpha \geq 1/\gamma$, i.e., for $\alpha > c/\Delta$, where c is some constant. In this way we see that exact adiabatic evolution can be thought of as unitary dynamics according to the parameter-dependent Hamiltonian $K(s)$ which is approximately local with respect to the metric d on the lattice. For an illustration of the interactions of $K(s)$ see Fig. 1.

IV. EFFICIENT SIMULATION OF ADIABATIC EVOLUTION

In this section we apply a Lieb-Robinson bound to show that the dynamics according to effectively local exact adiabatic evolution keeps local operators approximately local, and hence show that expectation values of local operators in adiabatically evolved ground states can be computed efficiently.

Recall that we can write the ground state $|\Omega(s)\rangle$ by integrating (14) as

$$|\Omega(s)\rangle = \mathcal{U}(s;0)|\Omega(0)\rangle, \quad (22)$$

where

$$\mathcal{U}(s;0) = \mathcal{T} \exp\left(i \int_0^s K(s') ds'\right), \quad (23)$$

and \mathcal{T} denotes the time-ordering operation. Our objective is to uniformly approximate

¹⁰Because of our \leq notation we will reuse the symbol c by systematically redefining it.

$$\omega_s(A) = \langle \Omega(0) | \mathcal{U}^\dagger(s;0) A \mathcal{U}(s;0) | \Omega(0) \rangle, \quad (24)$$

for all $s \in [0, 1]$. The way we do this is to show that the operator $A(s) \equiv \mathcal{U}^\dagger(s;0) A \mathcal{U}(s;0)$ remains approximately local for all $s \in [0, 1]$ and use the assumed fact that $\omega_0(B)$ can be computed efficiently for all local operators B . For simplicity we assume that the operator A is located at the origin and has support $|\text{supp}(A)| = 1$. It is easy to extend the results of this section to apply to operators with bounded support on disconnected regions, such as correlators.

We now study the locality of $A(s)$. What we do is first show that $A(s)$ can be uniformly approximated in operator norm by the series of approximants

$$A_\alpha(s) \equiv \mathcal{V}_{\Lambda_\alpha}^\dagger(s;0) A \mathcal{V}_{\Lambda_\alpha}(s;0), \quad (25)$$

where $\mathcal{V}_{\Lambda_\alpha}(s;0)$ satisfies the differential equation

$$\frac{d}{ds} \mathcal{V}_{\Lambda_\alpha}(s;0) = i \sum_{\mathbf{j} \in \Lambda_\alpha} \mathcal{F}_s(h_{\mathbf{j}}) \mathcal{V}_{\Lambda_\alpha}(s;0) = i K_{\Lambda_\alpha}(s) \mathcal{V}_{\Lambda_\alpha}(s;0), \quad (26)$$

with $\mathcal{V}_{\Lambda_\alpha}(0;0) = \mathbb{I}$ and where $K_{\Lambda_\alpha}(s) = \sum_{\mathbf{j} \in \Lambda_\alpha} \mathcal{F}_s(h_{\mathbf{j}}')$ and $\Lambda_\alpha = \{\mathbf{j} | d(\mathbf{0}, \mathbf{j}) \leq \alpha\}$. In words, the approximation $A_\alpha(s)$ is that operator obtained by evolving A with respect to only those interaction terms in $K(s)$ whose centers are within a distance α of A . Naturally this means that $A_{m-1}(s) = A(s)$. We use a Lieb-Robinson bound to show that $\|A(s) - A_\alpha(s)\|$ is rapidly decaying.

To show this we prove that $\|\tau_{s;0}^{K(s)}(A) - \tau_{s;0}^{K_{\Lambda_\alpha}(s)}(A)\|$ is small for $|s| \leq 1$ and large constant α where $\tau_{s;s'}^{K(s)}(M) = \mathcal{U}^\dagger(s;s') M \mathcal{U}(s;s')$. To make this expression easier to deal with, and to more explicitly relate it to group-velocity bounds, we rewrite it:

$$\begin{aligned} \|\tau_{s;0}^{K(s)}(A) - \tau_{s;0}^{K_{\Lambda_\alpha}(s)}(A)\| &= \left\| \int_0^s ds' \frac{d}{ds'} [\tau_{s';0}^{K_{\Lambda_\alpha}(s')} (\tau_{s;s'}^{K(s)}(A))] \right\| \\ &= \left\| \int_0^s ds' \tau_{s';0}^{K_{\Lambda_\alpha}(s')} \{ [K_{\Lambda_\alpha^c}(s'), \tau_{s;s'}^{K(s)}(A)] \} \right\| \\ &\leq \int_0^{|s|} ds' \| [K_{\Lambda_\alpha^c}(s'), \tau_{s;s'}^{K(s)}(A)] \|, \quad (27) \end{aligned}$$

where $K_{\Lambda_\alpha^c}(s) = \sum_{\mathbf{j} \in \Lambda \setminus \Lambda_\alpha} k_{\mathbf{j}}(s)$.

We now apply a general Lieb-Robinson bound recently proved in [16]. In order to apply the Lieb-Robinson bound of [16] we need to establish that our Hamiltonian $K(s)$ satisfies the conditions of Assumption 2.2 of [16], which in our case reads

$$\sum_{\alpha=0}^{m-1} \|k_\alpha\| [1 + 2\alpha(\alpha+1)]^2 (2 + 2\alpha)^\eta \leq s_1, \quad (28)$$

where η is a positive constant and s_1 is some constant. We need to ensure that the sum on the left evaluates to a constant instead of diverging. The only flexibility we have is to choose a decay estimate for $\|k_\alpha\|$ that is strong enough to overwhelm the polynomial in α it is multiplied by. The high-

est power of α appearing in this sum is $\alpha^{4+\eta}$. Thus we use the decay estimate (21) and choose $l \geq 7 + \eta$, and so we find that this constant s_1 equates to

$$s_1 = \sigma(l)/\gamma^l, \quad (29)$$

where

$$\sigma(l) = c_l \sum_{\alpha=1}^{m-1} \frac{[1 + 2\alpha(\alpha + 1)]^2 (2 + 2\alpha)^\eta}{\alpha^{l-1}}, \quad (30)$$

c_l is the constant arising from the estimate (21), and l is any chosen power $l \geq 7 + \eta$. [The proof of the general Lieb-Robinson bound described in [16] is easily extended to cover parameter-dependent Hamiltonians such as $K(s)$.] This reads

$$\|[\tau_s^{K(s)}(A), B]\| \leq \frac{\rho(l)|Y|(e^{[\sigma(l)/\gamma^l]|s|} - 1)}{[1 + d(x, Y)]^l}, \quad \forall l > 7 + \eta, \quad (31)$$

for any two norm-1 operators $A \in \mathcal{A}_x$ and $B \in \mathcal{A}_Y$, with $\{x\} \cap Y = \emptyset$, which are initially separated by a distance $d(x, Y)$, and $\rho(l)$ a constant that depends only on l . The constant v is independent of n and depends only on $\|h(s)\|$. We isolate the dependence of this bound on the minimum gap γ by defining

$$g(\gamma, l) = \rho(l)(e^{[\sigma(l)/\gamma^l]|s|} - 1). \quad (32)$$

Note that we are going to systematically redefine this function in our subsequent derivations to absorb extra constants and occurrences of γ . With this bound we first obtain an upper bound on $\|[\tau_{s,s'}^{K(s)}(A), k_{j,\alpha}(s')]\|$ [recall that the operators $k_{j,\alpha}(s)$ are defined via Eq. (6)]:

$$\| [A(s), k_{j,\alpha}(s)] \| \leq \begin{cases} \frac{g(\gamma, l)[1 + 2\alpha(\alpha + 1)] \|k_\alpha(s)\|}{(1 + \delta - \alpha)^l}, & \alpha < \delta, \\ 2\|A\| \|k_\alpha(s)\|, & \alpha \geq \delta, \end{cases} \quad (33)$$

where $\delta = d(\mathbf{0}, \mathbf{j})$ and $[1 + 2\alpha(\alpha + 1)] = |\Lambda_\alpha(\mathbf{j})| = \{|\mathbf{x}| | d(\mathbf{j}, \mathbf{x}) \leq \alpha\}$. We use the estimate (21) and redefine $g(\gamma, l)$ to find the upper bound

$$\| [A(s), k_{j,\alpha}(s)] \| \leq \begin{cases} \frac{g(\gamma, l)[1 + 2\alpha(\alpha + 1)]}{\alpha^{l+2}(1 + \delta - \alpha)^l}, & \alpha < \delta, \\ 2\|A\| \|k_\alpha(s)\|, & \alpha \geq \delta. \end{cases} \quad (34)$$

We next find the minimum of the denominator $\alpha^{l+2}(1 + \delta - \alpha)^l$ on the interval $1 \leq \alpha \leq \delta$, which is δ^l , and redefine $g(\gamma, l)$ to arrive at the final upper bound

$$\| [A(s), k_{j,\alpha}(s)] \| \leq \begin{cases} \frac{g(\gamma, l)}{\delta^l}, & \alpha < \delta, \\ \frac{2c_l \|A\|}{\gamma^{l+1} \alpha^l}, & \alpha \geq \delta. \end{cases} \quad (35)$$

Thus, by choosing the center \mathbf{j} far enough away from the center $\mathbf{0}$ of $A(s)$ we find the behavior

$$\| [A(s), k_{j,\alpha}(s)] \| \leq \frac{g(\gamma, l)}{d(\mathbf{0}, \mathbf{j})^l}, \quad \forall l > 1, \quad (36)$$

i.e., the quantity $\| [A(s), k_{j,\alpha}(s)] \|$ decays faster than any polynomial in $d(\mathbf{0}, \mathbf{j})$.

We next use our upper bound (35) to obtain an upper bound on $\| [A(s), k_j(s)] \|$:

$$\begin{aligned} \| [A(s), k_j(s)] \| &\leq \sum_{\alpha=0}^{m-1} \| [A(s), k_{j,\alpha}(s)] \| \leq \frac{g(\gamma, l)}{\delta^{l-1}} + \sum_{\alpha=\delta}^{m-1} \frac{2c_{l+1} \|A\|}{\gamma^{l+1} \alpha^l} \\ &\leq \frac{g(\gamma, l)}{\delta^{l-1}}, \end{aligned} \quad (37)$$

where we have redefined $g(\gamma, l)$ in the last line.

Now we use the decay estimate (37) in (27) to provide an upper bound for $\|A(s) - A_\alpha(s)\|$:

$$\begin{aligned} \|A(s) - A_\alpha(s)\| &\leq \sum_{\mathbf{j} \in L \setminus \Lambda_\alpha} \int_0^1 ds \| [A(s), k_j(s)] \| \\ &\leq \sum_{\delta=\alpha}^{m-1} \frac{[1 + 2\delta(\delta + 1)] g(\gamma, l)}{\delta^{l-1}} \leq \frac{g(\gamma, l)}{\alpha^{l-4}}, \end{aligned} \quad (38)$$

where we have redefined $g(\gamma, l)$.

So, as long as α is chosen to be so large that it overwhelms the $O(1)$ constant $g(\gamma, l)$ we find that $\|A(s) - A_\alpha(s)\|$ can be made to decay faster than any polynomial in α , and hence can be made as small as desired. Thus there exists some constant α such that $\|A(s) - A_\alpha(s)\| < \epsilon$. Note that, because $k(s)$ has support throughout L , $A_\alpha(s)$ has support throughout L .

In order to provide a simulation method to compute approximations to ground-state expectation values $\omega_s(A)$ we need to show that $A_\alpha(s)$ can be approximated by an operator with support only on a constant number of sites around $\text{supp}(A) = \mathbf{0}$. The way we do this is to show that $A_\alpha(s)$ is operator-norm close to

$$\tilde{A}_{\alpha,\beta}(s) = \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}^\dagger(s) A \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s), \quad (39)$$

where $\tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}$ satisfies the differential equation

$$\frac{d}{ds} \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s) = i \sum_{\mathbf{j} \in \Lambda_\alpha} \tilde{\mathcal{F}}_{\mathbf{j},s}^{H_{\Lambda_{\alpha,\beta}}(\mathbf{j})}(h_{\mathbf{j}}) \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s) = i \tilde{K}_{\Lambda_{\alpha,\beta}}(s) \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s), \quad (40)$$

and

$$\tilde{\mathcal{F}}_{\mathbf{j},s}^{H_{\Lambda_{\alpha,\beta}}(\mathbf{j})}(h_{\mathbf{j}}) = \int_{-\infty}^{\infty} \chi_\gamma(t) \left(\int_0^t \tau_u^{H_{\Lambda_{\alpha,\beta}}(\mathbf{j})}(h_{\mathbf{j}}) du \right) dt, \quad (41)$$

with $\Lambda_\beta(\mathbf{j}) = \{\mathbf{x} | d(\mathbf{j}, \mathbf{x}) \leq \beta\}$.

To show that $\tilde{A}_{\alpha,\beta}(s)$ is close to $A_\alpha(s)$ we first exploit the general inequality

$$\|\mathcal{V}_{\Lambda_\alpha}(s) - \tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s)\| \leq \int_0^{|s|} \|K_{\Lambda_\alpha}(s') - \tilde{K}_{\Lambda_{\alpha,\beta}}(s')\| ds', \quad (42)$$

which is proved, for example, by exploiting the Lie-Trotter expansion, and then taking the upper bound of the right-hand side using the triangle inequality by

$$\begin{aligned} & \int_0^{|s|} \|K_{\Lambda_\alpha}(s') - \tilde{K}_{\Lambda_{\alpha,\beta}}(s')\| ds' \\ & \leq \sum_{\mathbf{j} \in \Lambda_\alpha} \int_0^{|s|} \|k_{\mathbf{j}}(s') - \tilde{k}_{\mathbf{j},\beta}(s')\| ds', \end{aligned} \quad (43)$$

where $\tilde{k}_{\mathbf{j},\beta}(s) = \tilde{\mathcal{F}}_{\mathbf{j},s}^{H_{\Lambda_\alpha}(\mathbf{j})}(h'_{\mathbf{j}})$. We can upper-bound the integral on the right-hand side by using an argument identical to the one used to show (21). We thus obtain

$$\sum_{\mathbf{j} \in \Lambda_\alpha} \int_0^{|s|} \|k_{\mathbf{j}}(s') - \tilde{k}_{\mathbf{j},\beta}(s')\| ds' \leq \sum_{\mathbf{j} \in \Lambda_\alpha} \frac{1}{\gamma \beta^{l-1}} \leq \frac{\alpha^2}{\gamma \beta^{l-1}}, \quad (44)$$

where l is any power, and we have used the fact that the number of sites in Λ_α is given by $1 + 2\alpha(\alpha + 1)$. By choosing $\beta \geq \alpha$ we find that $\mathcal{V}_{\Lambda_\alpha}(s)$ can be made as close as desired to $\tilde{\mathcal{V}}_{\Lambda_{\alpha,\beta}}(s)$.

To obtain closeness of our final approximation $\tilde{A}_{\alpha,\beta}(s)$ to $A(s)$ we use the triangle inequality

$$\begin{aligned} \|A(s) - \tilde{A}_{\alpha,\beta}(s)\| & \leq \|A(s) - A_\alpha(s)\| + \|A_\alpha(s) - \tilde{A}_{\alpha,\beta}(s)\| \\ & \leq \frac{g(\gamma, l)}{\alpha^l} + \frac{\alpha^2}{\gamma' \beta'^{l-1}}, \end{aligned} \quad (45)$$

where we have used the upper bound (38) with an adjusted value of l and we have also used (44) with an appropriate choice of power l' . We therefore find that it is sufficient, for a given constant ϵ to choose large [but $O(1)$] α and β so that

$$\|A(s) - \tilde{A}_{\alpha,\beta}(s)\| \leq \epsilon. \quad (46)$$

The actual values of α and β required to reduce the error (46) to below ϵ scale better than linearly with $w = \max[g(\gamma, l), 1/\gamma]$, where γ is a constant multiplied by the minimum energy ΔE encountered along the adiabatic path. Thus the support of the final approximation $\tilde{A}_{\alpha,\beta}(s)$ is given, in the worst case, by $\text{supp}[\tilde{A}_{\alpha,\beta}(s)] \leq w$. Note that w depends, via $g(\gamma, l)$, exponentially on $1/\gamma$, i.e., the inverse energy gap.

Because the final approximation $\tilde{A}_{\alpha,\beta}(s)$ can be computed via integrating (40), and by noticing that this integration can be performed by restricting our attention to the finite-dimensional subalgebra \mathcal{A}_w , where $W = \text{supp}[\tilde{A}_{\alpha,\beta}(s)]$, we see that $\tilde{A}_{\alpha,\beta}(s)$ can be computed using resources that scale as 2^{cw} , with c some constant.

V. DISCUSSION

In this paper we have shown how to efficiently calculate the ground-state expectation values of local operators with constant support for gapped adiabatically evolving spin systems. In order to provide our simulation method we reduced the problem to showing that under exact adiabatic evolution the expectation value of a local operator can be computed from the expectation value of an approximately local operator in the unevolved ground state. Given this observation we then argued that if it is easy to compute expectation values of local operators in the original ground state then one could approximate the desired expectation values arbitrarily well by using time and space resources that scale with the inverse gap.

Our approach has several shortcomings. The first is that the scaling of the simulation resources with the error ϵ scales faster than $2^{1/\epsilon}$. This means that if the expectation value of an operator which is a sum of many local operators is desired then our simulation method may require superpolynomial resources. For example, if the expectation value of the total magnetization $M = \sum_{j \in L} \sigma_j^z$ (as opposed to the more traditional average magnetization $m = M/n$) is required to some accuracy ϵ then our simulation method will require superpolynomial resources. This is not entirely unexpected; after all, in the thermodynamic limit such operators are unbounded and cannot be approximated at all. Another manifestation of this shortcoming is that if the expectation values of the local operators are required to an accuracy which scales as $\epsilon < 1/n$ then our method may require superpolynomial resources. These problems do not manifest themselves for the applications we have in mind; namely, when applied to the calculation of average properties of two states in the same quantum phase we only require accuracy to some small constant ϵ which does not scale with the system size, and when applied to simulating adiabatic quantum algorithms we only need ϵ to scale as a constant in order to read out the answer of the algorithm.

The second shortcoming of our method is that, by the current method, we are unable to directly approximate the scaling of the geometric entropy¹¹ S_Λ with Λ . The reason for this is that our current method approximates $\rho_\Lambda(s)$ by calculating approximations to all the expectation values of a basis of operators for \mathcal{A}_Λ . Because we are computing approximations to expectation values we end up computing only an approximation $\tilde{\rho}_\Lambda(s)$ to $\rho_\Lambda(s)$. The best continuity result available for the von Neumann entropy is the Fannes inequality (see, for example, [32]) for a derivation) which implies that the error in the approximation \tilde{S}_Λ calculated from $\tilde{\rho}_\Lambda(s)$ grows larger as Λ increases. We will describe an

¹¹Recall that the geometric entropy S_Λ is equal to the von Neumann entropy of the restriction of the ground state $\rho(s) = |\Omega(s)\rangle\langle\Omega(s)|$ to a contiguous block of Λ spins: $S_\Lambda = S(\rho_\Lambda(s))$, where $S(\rho) = -\text{tr}[\rho \log_2(\rho)]$ and $\rho_\Lambda(s) = \text{tr}_{\hat{\Lambda}}[\rho(s)]$, with $\text{tr}_{\hat{\Lambda}}$ denoting the partial trace over all spins except those in Λ .

approach to this problem using exact adiabatic evolution in a future presentation.

The principle characteristic of our approach is that approximations are made in the Heisenberg picture. What we mean here is that instead of approximating the evolved quantum state of the spin system in operator norm we instead compute approximations to the evolved local operators. We should expect this strategy to be successful because the locality of the interactions in the Hamiltonian does not manifest itself in the Schrödinger picture but, thanks to the Lieb-Robinson bound, it is precisely clear what locality implies for local operators in the Heisenberg picture. Because in the thermodynamic limit we are only able to physically access local operators (such as average magnetization and correlators) this approach does not lead to any loss of generality over computations carried out in the Schrödinger picture.

It is possible that our analysis actually applies to all gapped spin models. This is because it is possible that any gapped spin model is adiabatically connected¹² to a classical spin model with trivial ground state. Classical renormalization-group style argumentation certainly seems to back this statement up: after all, we know that the RG fixed points are either trivial (classical) or quantum critical points. However, there is as yet no rigorous general proof of this statement for quantum spin systems.

We would like to suggest that the following description of the space of local (translation-invariant) spin models is correct. First, in this space there are many distinguished points, classical spin systems, where the ground state can be calculated trivially. Around each of these points is a small region in Hamiltonian space of Hamiltonians which are provably adiabatically connected to the classical spin model points [27–29]. In these regions we have shown that the local ground-state properties can be determined efficiently. Outside these small regions there are other regions which may or may not be adiabatically connected to the classical spin model points where the Hamiltonians are gapped. In these regions it is known that the local ground-state properties can be calculated using subexponential resources [16]. On the boundaries between the quantum phases there are quantum critical walls. For these points, in 1D, it is known that an approximation to the ground state as a finitely correlated state can be stored using polynomial space [13]. It is not known if these approximations can be obtained efficiently. This picture is summarized in Fig. 2.

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¹²What we mean here is that there exists some adiabatic path of local Hamiltonians from a local classical spin model to the desired gapped spin model where there is a constant gap along the entire path.

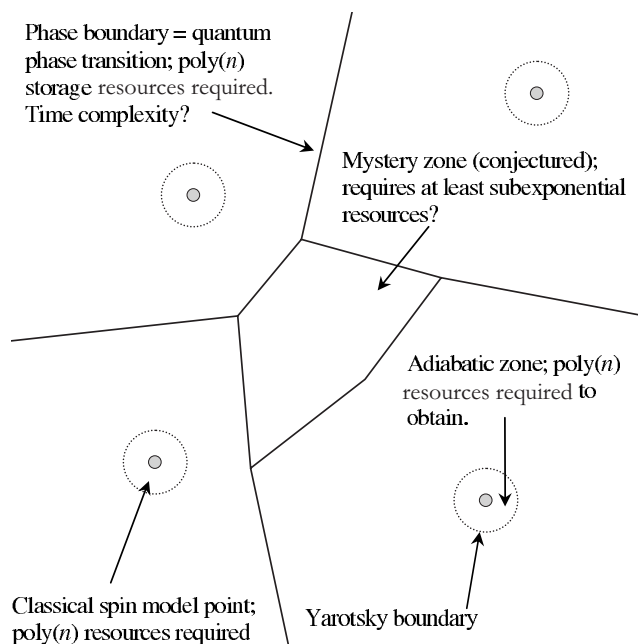


FIG. 2. Conjectured diagram of the space of local spin models and the associated computational resources required to compute approximations to local ground-state properties.

APPENDIX: PROPERTIES OF SMOOTH CUTOFF FUNCTIONS

In this appendix we briefly review the properties of compactly supported C^∞ cutoff functions.

Of fundamental utility in our derivations is a class of functions known as compactly supported C^∞ bump functions. These functions are defined so that their Fourier transform $\hat{\chi}_\gamma(\omega)$ is compactly supported on the interval $[-\gamma, \gamma]$, and equal to 1 on the middle third of the interval. Such functions satisfy the following derivative bounds:

$$\frac{d^j \hat{\chi}_\gamma(\omega)}{d\omega^j} \lesssim \gamma^{-j}, \quad (\text{A1})$$

for all j with the implicit constant depending on j . This is just about the best estimate possible given Taylor's theorem with remainder and the constraints that $\hat{\chi}_\gamma(\omega)$ is equal to 1 at $\omega=0$ and $\hat{\chi}_\gamma(\omega)$ is compactly supported.

The function $\chi_\gamma(t)$ has support throughout \mathbb{R} but it is decaying rapidly. To see this, consider

$$\chi_\gamma(t) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{it} e^{-it\omega} \frac{d}{d\omega} \hat{\chi}_\gamma(\omega) d\omega, \quad (\text{A2})$$

which comes from integrating by parts. Continuing in this fashion allows us to arrive at

$$\chi_\gamma(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(-\frac{1}{it}\right)^j e^{-it\omega} \frac{d^j}{d\omega^j} \hat{\chi}_\gamma(\omega) d\omega. \quad (\text{A3})$$

Since $\hat{\chi}_\gamma(\omega)$ has all its derivatives bounded, according to (A1), and using the compact support of $\hat{\chi}_\gamma(\omega)$ we find

$$\begin{aligned} |\chi_\gamma(t)| &\leq \left| \int_{-\gamma}^{\gamma} \left(\frac{1}{it}\right)^j e^{-it\omega} \gamma^{-j} d\omega \right| \\ &\leq \int_0^\gamma \frac{1}{|\gamma t|^j} d\omega \leq \frac{1}{\gamma^{j-1} |t|^j}, \end{aligned} \quad (\text{A4})$$

for all $j \in \mathbb{N}$. Thus we find that $\chi_\gamma(t)$ decays to 0 faster than the inverse of any polynomial in t with characteristic “width” $1/\gamma$. The existence and construction of such functions is discussed, for example, in [39,40].

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