Bounding the finite-size error of quantum many-body dynamics simulations

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Finite-size errors (FSEs), the discrepancies between an observable in a finite system and in the thermodynamic limit, are ubiquitous in numerical simulations of quantum many-body systems. Although a rough estimate of these errors can be obtained from a sequence of finite-size results, a strict, quantitative bound on the magnitude of FSE is still missing. Here we derive rigorous upper bounds on the FSE of local observables in real-time quantum dynamics initialized from a product state. In d-dimensional locally interacting systems with a finite local Hilbert space, our bound implies $|\langle \hat{S}(t) \rangle_L - \langle \hat{S}(t) \rangle_{\infty}| \leq C(2vt/L)^{d-\mu}$, with $v, C, c, \mu$ constants independent of $L$ and $t$, which we compute explicitly. For periodic boundary conditions (PBCs), the constant $c$ is twice as large as that for open boundary conditions (OBCs), suggesting that PBCs have smaller FSEs than OBCs at early times. The bound can be generalized to a large class of correlated initial states as well. As a byproduct, we prove that the FSE of local observables in ground-state simulations decays exponentially with $L$ under a suitable spectral gap condition. Our bounds are practically useful in determining the validity of finite-size results, as we demonstrate in simulations of the one-dimensional (1D) quantum Ising and Fermi-Hubbard models.

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I. INTRODUCTION

Numerical simulations are crucial to our understanding of many-body quantum matter, and are routinely applied in all fields of physics and in chemistry. Unfortunately, many numerical techniques popular in these fields incur significant FSEs when approximating properties of a large (potentially infinite) system by properties of a finite one. The most direct example is exact diagonalization, which exactly solves the finite system numerically [1–4]. Accessible system sizes are limited since the Hilbert space dimension grows exponentially with system size; for the simplest case of interacting spin-1/2s, a state-of-the-art ground-state calculation is limited to ~45 spins [5]. FSEs also significantly affect other techniques, such as density matrix renormalization group (DMRG) [6–9], many tensor network algorithms [10,11], quantum dynamical typicality-based algorithms [12–16], and quantum Monte Carlo [17], and they are a significant source of errors for simulating quantum systems on quantum computers [18] and for analog quantum simulations using ultracold matter [19], trapped ions [20], and other platforms [21].

It is often difficult to characterize FSEs. The standard method to assess them is to calculate and compare observables for different system sizes, ideally using finite-size scaling [3].

Although useful, this method has limitations. One is that it offers no guarantees. Two different system sizes may have results that closely agree, but at larger sizes the physics changes and observables deviate [22]. Another is that one may not be able to study multiple system sizes that are sufficiently large to get a good estimate of the convergence.

In this paper, we derive rigorous upper bounds on the error of approximating observables in a large, possibly infinite, quantum many-body system by results in a smaller one. The bounds are applicable to arbitrary Hamiltonians for which a Lieb-Robinson (LR) bound exists. For quantum dynamics simulations starting from product initial states and evolving under locally interacting Hamiltonians with a finite local Hilbert space, the bound for a local observable $\hat{S}$ is

$$|\langle \hat{S}(t) \rangle_L - \langle \hat{S}(t) \rangle_{\infty}| \leq C(2vt/L)^{d-\mu},$$

where $v, C, c, \mu$ are constants that can be computed explicitly and depend on the Hamiltonian, observable, and boundary condition.

Such dynamics is explored in a wide variety of ultracold matter experiments, such as quantum quenches and slow ramps in Rydberg atoms [23–28], molecules [29–31], Fermi gases [32], atoms in optical lattices [33–37], and optical clocks [38]. This dynamics can probe fundamental phenomena, such as many-body localization [39–43], prethermalization [44,45], and generation of topological defects near critical points [46].

This bound is then extended to a large family of correlated initial states satisfying an exponential clustering condition. While our main focus is on dynamics, we also show that the FSE of local observables in a many-body ground state decays as

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exponentially in system size, under a suitable spectral gap condition. The idea behind our bound is that locality—specifically, that one piece of a system does not instantly affect far-away pieces—imposes strong constraints on quantum dynamics [47, 48]. This can be seen by considering evolution under a Hamiltonian initiated from a product state (other scenarios can be understood by similar arguments). As illustrated in Fig. 1, an observable in a region X will be affected by FSEs only after a long enough time for information to propagate from the boundary to X. This idea is made precise by relating FSEs to unequal time correlation functions, which can then be bounded by a LR bound [49], a direct consequence of locality. Although similar ideas of applying LR bounds to analyze the performance of some numerical algorithms have been employed in Refs. [50–58], the connection to FSE has not been made explicit, and the practical utility of the bounds for numerics was not demonstrated. This idea has also been applied to estimate FSE in a nonrigorous way, for example, in Ref. [59].

Our FSE bound not only shows the convergence of finite-size approximations in principle, but is tight enough to be useful in practice, which we demonstrate in simulations of some prototypical models. For example, in the dynamics following a sudden change of parameters in a 1D transverse Ising model (TFIM) with L = 21 sites, the error bounds for the transverse magnetization and nearest-neighbor correlations remain extremely small to times where they have evolved close to equilibrium. Furthermore, the bounds are reasonably tight: The time at which the error bound becomes significant is only 20–25% smaller than the time at which the actual FSE becomes noticeable. We similarly demonstrate this for the nonequilibrium relaxation of the Fermi-Hubbard model (FHM) from a checkerboard state, inspired by experiments and theory of Refs. [60–63]. The precision of these bounds is enabled by the major quantitative improvements offered by recent LR bounds [64, 65].

In addition to their quantitative utility, these bounds provide insight into the convergence of numerical methods and open the way to designing new algorithms. One immediate consequence of the bounds is to rigorously show that the FSE decays exponentially with the linear dimension of the system for periodic boundary conditions (PBCs), as well as for open boundary conditions (OBCs) provided that one measures observables only near the center of the system, as commonly employed in the DMRG community. If one instead averages the measurement over all sites in OBCs, then our bound indicates that the error decays only algebraically. Similar behavior at finite temperature has been observed and analyzed in Ref. [66]. Furthermore, if one compares PBCs to OBCs with center site measurements, our error bound for PBCs decays twice as fast with distance as the bound for OBCs at early times, suggesting that PBCs give more reliable results at early times [67]. These insights may lead to new methods; one example is that they show why the moving-average cluster expansion method of Ref. [30] converges exponentially faster than alternative schemes.

**A. A simple bound for both OBCs and PBCs**

Consider the dynamical evolution of a quantum many-body system on an infinite d-dimensional lattice, governed by a locally interacting Hamiltonian $\hat{H}$. For illustrative purposes, in Fig. 1 we draw the configuration for a 1D nearest-neighbor interacting lattice model. Let $|\psi\rangle$ be the initial product state, $\hat{S}$ be a local observable to be measured that acts on a finite region $X$ (center point in Fig. 1), and let $\Delta \hat{H} = \sum \hat{V}_i$ be the sum of all the interaction terms between the inner and outer parts of the system (red links in Fig. 1). If PBCs are used, we further subtract from $\Delta \hat{H}$ the interaction between the first and the last site (brown link in Fig. 1). Let $\hat{H}_t$ and $|\psi_t\rangle$ denote the Hamiltonian and the initial state of the finite-size simulation, respectively (i.e., the restriction of $\hat{H}$ and $|\psi\rangle$ to the $L$-site inner system). Denote $\hat{H}^i = \hat{H} - \Delta \hat{H}$, so $\hat{H}^i$ decouples into two commuting terms, one acting only on the inner system, the other acting only on the outer system. The FSE of the observable $\hat{S}$ is

$$\delta(\hat{S}(t))_\psi = \langle \epsilon^{i\hat{H}_t} \hat{S} e^{-i\hat{H}^i t} \rangle_{\psi} - \langle \epsilon^{i\hat{H}^i t} \hat{S} e^{-i\hat{H}^i t} \rangle_{\psi},$$

(2)

where $\langle A \rangle_\psi = \langle \psi | A | \psi \rangle$, and we set $\hbar = 1$ throughout. Since $\hat{H}^i$ decouples into two independent spatial regions (inner and outer) and $|\psi\rangle$ is a product state, the first term in Eq. (2) can be rewritten as $\langle \epsilon^{i\hat{H}^i t} \hat{S} e^{-i\hat{H}^i t} \rangle_{\psi}$. Inserted into Eq. (2), the two expectation values are taken in the same state $|\psi\rangle$, so their difference can be bounded by the operator norm $||\langle \psi | [A, \hat{S}] | \psi \rangle|| \leq ||[\hat{A}]||$. Using the unitary invariance of operator norm $||\hat{A}|| = ||\hat{U} \hat{A} \hat{V}^\dagger||$ for arbitrary unitary operators $\hat{U}, \hat{V}$, we have

$$\delta(\hat{S}(t))_\psi \leq ||\hat{U}_t(\hat{S}) \hat{V}_t(\hat{S})^\dagger - \hat{S}||,$$

(3)

where $\hat{U}_t(\hat{S}) = e^{-i\hat{H}_t / t} \hat{S} e^{i\hat{H}^i t}$ is the evolution operator in the interaction picture, which satisfies $\hat{U}_t(0) = 1$ and $i\partial_t \hat{U}_t(t) = \hat{U}_t(t) \Delta \hat{H}(t)$, where $\Delta \hat{H}(t) = e^{-i\hat{H}^i t} \Delta \hat{H} e^{i\hat{H}^i t}$. Now applying the fundamental theorem of calculus and the triangle inequality, we obtain a bound on the FSE:

$$\delta(\hat{S}(t))_\psi \leq \int_0^t \left| \frac{d}{dt} \langle \hat{U}_t(t) \hat{S} \hat{U}_t(t)^\dagger \rangle - \hat{S} \right| dt'$$

$$= \int_0^t ||\hat{U}_t(t') [\Delta \hat{H}(t'), \hat{S}] \hat{U}_t(t')^\dagger|| dt'$$

$$= \int_0^t ||[\Delta \hat{H}(t'), \hat{S}]|| dt'.$$

(4)

The integrand is the quantity bounded by LR bounds, so to upper bound the FSE, one can insert the relevant LR
bound. We focus on locally interacting systems, but Eq. (4) applies equally to long-range interactions by substituting the corresponding LR bounds [57,68–74] in those systems. For a locally interacting system, the currently tightest LR bound is obtained by computing the series in Eq. (S19) of the Supplemental Material (SM) [75], which is based on Refs. [64,65], although this may not be efficiently computable in general. A slightly looser but efficiently computable method is discussed in Ref. [65], in which one solves a system of first-order linear differential equations for a number of variables proportional to the system size. To see the qualitative features of the bound for large systems, we can insert the simple expression given in Eq. (3) of Ref. [65] into Eq. (4) to obtain

$$|\delta(\hat{S}(t))| \leq \sum_j c_j \left| \frac{v|t|}{d_{Xj}} \right| \frac{d\delta\hat{V}_j}{d\delta\hat{S}_j},$$  

(5)

where \(c_j\) are constants independent of \(t\) and \(d_{Xj}\), \(D(\hat{S}, \hat{V}_j)\) is the distance between the operators \(\hat{S}, \hat{V}_j\) in the commutativity graph (CG) as introduced in Ref. [65], and \(v\) is the LR speed. The distance in the CG is related to the distance in real space \(d_{Xj}\) by \(D(\hat{S}, \hat{V}_j) = \eta d_{Xj} - \mu\), where \(\eta, \mu\) are (straightforwardly determined) constants and \(d_{Xj}\) is the distance between \(X\) and \(j\) in real space. Therefore, the right-hand side of Eq. (5) is bounded by \(\left| v|t|/d_{Xj} \right| \eta d\hat{\delta}_{a\mu}\), where \(d_{Xj} = \min_{\mu \in B} d_{Xj}\). Despite its simplicity, the \(t\) dependence of this bound generically agrees with the exact error to lowest order in \(t\) in OBCs [75].

Besides its practical utility for bounding FSEs in calculations, as demonstrated below, this result has qualitative implications. One is to rigorously support the common practice of measuring observables close to the center site in OBC numerics (e.g., in the DMRG community), rather than averaging over all sites. This minimizes the error bound, since the center size maximizes \(d_{Xj}\). This choice yields our main result in Eq. (1) for the OBC case, with \(c = \eta/2\). Our bound allows one to extend this. For example, in dimensions greater than one, we can minimize FSEs by choosing an optimal cluster shape that minimizes the right-hand side of Eq. (5) and run simulations on the optimal shape.

As a side note, although we have restricted our discussion to a local observable \(\hat{S}\), our bounds can equally well be applied to nonlocal ones of finite extent, such as equal time correlation functions. To do this, one only needs to replace the local observable \(\hat{S}\) in Eq. (4) by a nonlocal one, and measure \(\hat{S}\) in the central region of the finite cluster so that \(\hat{S}\) is as far from the boundary as possible. The resulting FSE would be bigger than local observables, but for 1D finite-size simulation with ~20 sites, one can simulate a ~4 site correlation function with acceptably small error bounds. Such correlations are important for many experiments.

B. An improved bound for PBCs

In the previous section, we treated PBC in a way similar to OBCs. But it turns out that the resulting bound in Eqs. (4) and (5) is qualitatively loose at small \(t\) for PBCs. The reason for this can be intuitively understood as follows. The two terms on the right-hand side of Eq. (2) can be expanded in \(t\). As we discuss in greater detail in the SM [75], the FSE for \(\hat{S}(t)\) actually is only contributed by terms in \(e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\) whose spatial span is larger than \(L\) and terms in \(e^{i\hat{H}t}\hat{S}e^{-i\hat{H}t}\) that wrap around the whole periodic system. The leading order of these terms is proportional to \(t^2\), where \(L\) is the length of the shortest noncontractible loop on the PBC GC, which is roughly twice as large as the exponent \(D(\hat{S}, \hat{V}_j)\) in Eq. (5). The SM [75] extends methods developed in Refs. [64,65] to derive a rigorous upper bound for \(|\delta(\hat{S}(t))|\) that leads to this improved \(t^2\) scaling. The main result is

$$|\delta(\hat{S}(t))|_{(PBC)} \leq \sum_{l \leq p < d} C_p \left( \frac{2v_p d}{L_p} \right)^{L_p},$$  

(6)

where the constant \(C_p\) is given in Eq. (S52), \(v_p\) is the LR speed in the \(p\)th direction given in Eq. (S53), and \(L_p\) is the size of the periodic system in the \(p\)th direction in CG. \(L_p\) is related to the real space system size \(L\) by \(L_p = \eta_p L - \mu_p\) for constant integers \(\eta_p, \mu_p\). We note that while this bound improves the small-time exponent of the PBC bound by a factor of 2 compared to Eq. (5), the timescale \(\tau \approx \min_p L_p/2v_p\) on which the bound exponentially grows is still approximately the same as Eq. (5). Besides its quantitative utility, Eq. (6) shows that in anisotropic systems where \(v_p\) is different in each direction, one should choose \(L_p \propto v_p\) to minimize the FSE.

C. FSEs in nondegenerate gapped ground states

So far, we have been discussing FSEs of quantum dynamics simulations. We now derive a bound on FSEs of local observables in nondegenerate ground states under a gap assumption. This result is interesting in its own right, and will also be useful for our subsequent generalization of the dynamics error bound to correlated initial states.

The Hamiltonian \(\hat{H}\), observable \(\hat{S}\), boundary terms \(\Delta \hat{H}\), etc. are the same as before. For convenience, we suppose that the operator \(\hat{S} = \hat{S}_l\) has unit norm and acts nontrivially only within a region \(X = X_0\) of diameter \(l\) which sits on the center of the finite-size cluster. The difference now is that we consider the observable \(\langle \hat{S} \rangle = \text{Tr}[\hat{S}\hat{\rho}]\) given by the ground-state density matrix \(\hat{\rho}\). The numerical simulation approximates this thermodynamic quantity by the expectation value in the finite-size ground state \(\text{Tr}[\hat{\rho} \hat{S}]\), where \(\hat{\rho}\) is the ground-state density matrix of \(\hat{H}\). Our result relies on an assumption that the interpolated Hamiltonian \(\hat{H}(\lambda) \equiv \hat{H} - \lambda \Delta \hat{H}\) is nondegenerate for all \(0 \leq \lambda \leq 1\) and has a uniform spectral gap \(\min_{0 \leq \lambda \leq 1} \Delta(\lambda) = \Delta > 0\). When this condition is satisfied, then analogously to Eq. (1) we have [75]

$$|\text{Tr}[\hat{\rho} \hat{S}_l - \hat{\rho}_l \hat{S}_l]| \leq Ce^{-\left(\frac{L}{	au}\right)^2/24}.$$  

(7)

D. Bounds for correlated initial states

We now generalize our error bound to dynamics initiated from a class of (possibly mixed) initial states \(\hat{\rho}\), for which there exists a sufficiently good finite size approximation \(\hat{\rho}_L\), satisfying Eq. (7). This includes nondegenerate ground states (under the condition described above) but also includes translation invariant matrix product states (MPSSs) with a finite bond dimension [76] and finite-temperature thermal states [77] \(\hat{\rho} = e^{-\hat{H}/T}/\text{Tr}[e^{-\hat{H}/T}]\) above a certain tem-
perature, where \( \hat{\rho}_L = e^{-\beta \hat{H}_L}/\text{Tr}[e^{-\beta \hat{H}_L}] \), i.e., the thermal state of \( \hat{H}_L \).

Given that we have an initial state \( \hat{\rho}_L \) satisfying Eq. (7), we can bound the dynamics FSE as
\[
\delta(\hat{S}(t))_\rho = \{[\hat{S}_L(t)]_\rho - \langle \hat{S}(t) \rangle_\rho\}
\leq \{\text{Tr}[\{\hat{\rho}_L - \hat{\rho}_L\} \hat{S}_L(t)]\} + \|\hat{S}_L(t) - \langle \hat{S}(t) \rangle_\rho\|,
\]
where \( \hat{S}_L(t) = e^{\hat{H}_L t} \hat{S} e^{\hat{H}_L t}, \hat{\rho}_L \) is the reduced density matrix of \( \hat{\rho} \) on the finite cluster, and in the second line we used the triangle inequality. The second term can be bounded using the same method as in Eq. (2), since Tr\(|\hat{A}\| \leq \|\hat{A}\| \) for any density matrix \( \hat{\rho} \). To bound the first term, we insert the expansion \( \hat{S}_L(t) = \hat{S}_0(t) + \sum_{\ell=1}^{L} \hat{S}_{\ell}(t) - \hat{S}_{\ell-1}(t) \) into Eq. (8) and notice that \( \hat{S}_\ell(t) - \hat{S}_{\ell-1}(t) \) is an operator acting on \( \chi_\ell \), whose norm is bounded by Eqs. (4) and (5) to be \( \|\hat{S}_\ell(t) - \hat{S}_{\ell-1}(t)\| \leq C(2\sqrt{\ell}\eta)^{\ell/2} \) for some constant \( C \). For initial states satisfying Eq. (7), this implies [75]
\[
\delta(\hat{S}_\ell(t))_\rho \leq C_1 e^{(\ell - L)/\xi} + C_2 e^{\ell\eta - L/4},
\]
where \( C_1 \) and \( C_2 \) are model-dependent constants that can be explicitly determined.

E. Example: 1D TFIM

We test our dynamics error bounds in simulations of prototypical models for quantum many-body physics, starting with the TFIM,
\[
\hat{H} = -J \sum_{\ell=1}^{L} \delta_{\ell+1} \delta_{\ell-1} - \hbar \sum_{\ell=1}^{L} \delta_{\ell}.
\]
This is a canonical model for quantum phase transitions [78,79] and occurs in materials like CoNb_2O_6 [80], cold atom [26,46,81] and trapped ion [82–86] experiments, and superconducting circuits [87,88]. We numerically study the dynamics of this model at the critical point \( J = \hbar \) for several \( L \) and calculate the exact evolution for \( L = \infty \). Specifically, we study the dynamics of \( \langle \hat{\sigma}_x(t) \rangle \) starting from \( |\psi(0)\rangle = |\downarrow \rangle \rightarrow |\rightarrow \rangle \). Analogous dynamics in the 2D TFIM has been explored in Rydberg atom experiments [26,27].

Figure 2(a) shows \( \langle \hat{\sigma}_x(t) \rangle \) for \( L = 5 \) to 21 using PBCs, along with the exact \( L = \infty \) solution [89]. To obtain a FSE bound for \( \langle \hat{\sigma}_x(t) \rangle \), we use the LR bound given in Eq. (S24) of the SM [75] [obtained from the general bound Eq. (S20)], which, after inserting into Eq. (4), yields
\[
\langle \delta(\hat{\sigma}_x(t)) \rangle \leq \frac{\sqrt{2}}{\sqrt{\hbar(2L - 1)}} + 2\sqrt{\hbar(2L - 2)}.
\]
As Fig. 2(a) shows, this error bound provides a guarantee of the numerical calculations’ accuracy out to interesting and useful timescales. For the \( L = 21 \)-site calculation, the bound guarantees that the results are accurate (within \( 10^{-2} \)) up to times \( Jt \sim 3.5 \), where the observable has nearly reached equilibrium. Furthermore, this time is in reasonable accord with the true time at which FSE becomes important (within 20%).

We emphasize that the FSE bound never made use of the TFIM’s exact solution. The bound Eq. (4) can be applied to any system, including in dimensions greater than one. As we will now demonstrate in the 1D FHM, the bound still provides a useful guarantee of the finite-size results when no exact solution is available.

F. Example: FHM

The 1D FHM describes spin-1/2 fermions in a lattice whose Hamiltonian is
\[
\hat{H} = -J \sum_{\langle \ell, \sigma = \uparrow, \downarrow \rangle} (\hat{a}_\ell^\dagger \hat{a}_{\ell+1} + \text{H.c.}) + U \sum_{\ell} \hat{n}_\ell \hat{n}_\ell^\dagger.
\]
The FHM exhibits rich behavior, such as a metal-Mott insulator transition, and potentially high-temperature superconductivity. It is a reasonable approximation of some real materials, such as FeO, NiO, CoO [90], and has been realized in ultracold atoms [91–95].

We numerically study the relaxation dynamics of a charge density wave state \( |\psi(0)\rangle = |\uparrow \rangle \rightarrow |\rightarrow \rangle \), analogous to previous theory [96] and experiments [97], where \( |\uparrow \rangle \) means a doubly occupied (empty) site. We run the finite-size simulations in OBCs and measure the density imbalance \( \hat{M}(t) = \langle \hat{N}_\uparrow(t) - \hat{N}_\downarrow(t) \rangle / L \) [96]. To get a FSE bound for \( \hat{M}(t) \), we use the currently tightest LR bound, obtained by numerically summing the series in Eq. (S19) of the SM [75] and inserting the result into Eq. (4), Figure 2(b) shows the results.

Our error bound can be compared to estimates of FSE obtained from comparing calculations of different sizes. For example, one can take the difference between the \( L = 10 \) and \( L = 12 \) as a rough estimate of the FSE of the \( L = 12 \) calculation. Our bound is comparable in its guaranteed timescale of convergence to this conventional estimate. For example, we can guarantee that the FSE in \( \langle \hat{M}(t) \rangle \) of the \( L = 12 \) result is less than \( 1% \) for \( Jt \lesssim 1.2 \), comparable to the time \( Jt \sim 1.6 \) where the \( L = 10 \) and 12 results differ noticeably.

II. CONCLUSIONS

We have presented a rigorous upper bound on the FSE of local observables measured in numerical simulations of quantum dynamics starting from a large class of initial states.
For product initial states, the bounds show an advantage of using PBCs at early times. We also presented a generalization to simulations of local observables in nondegenerate gapped ground states. In all the cases we considered, the bounds decay exponentially in system size and guarantee the accuracy of finite-size dynamics simulation up to a timescale $t_e \sim L^2/\nu$. These insights into FSE can motivate better algorithms.

The quantitative utility of the bounds is demonstrated in the 1D TFIM and 1D FHM. In both cases, the error bounds are extremely small up to timescales where there is interesting physics and even equilibration, and they are reasonably tight compared to the actual FSEs. We expect these bounds to provide useful tools to researchers going forward, providing FSE bounds on numerical calculations and suggesting new numerical methods that minimize this error.

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[75] See Supplemental Material at https://link.aps.org/supplemental/10.1103/PhysRevResearch.3.L032047 for the comparison of the error bounds to perturbation theory at early times, the derivation of the PBC error bound in Eq. (6), and the detailed proof of Eqs. (7) and (9). The PBC error bound Eq. (6) is derived from an important intermediate result Eq. (S18), for which we introduce three different methods to bound its right-hand side. The numerically tightest one is given in Eq. (S20), a more efficiently computable one is given in Eq. (S39), and the constants for the simplest one Eq. (6) are given in Eqs. (S52), (S53), and (S55). The PBC error bound for TFIM in Eq. (11) is derived in Eqs. (S22-S25), and the OBC error bound for FHM is obtained by numerically summing the series in Eq. (S19) on the CG shown in Figure S2.

[76] For translation invariant MPS with a finite bond dimension, $\beta_t$ can be taken as the $L$-site periodic version of $\beta$. That $\beta_t$ satisfies the condition in Eq. (7) can be proved using the transfer operator method which is used to prove that MPS has finite correlation length, see, e.g., Refs. [8,10,11]. The parameter $2\xi$ can simply be taken as the correlation length of the MPS.
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