I. INTRODUCTION

Although classical simulation of the quantum many-body problem is in general exponentially hard, many physically interesting, slightly entangled states can be efficiently simulated using tensor network methods [1–3]; in particular those obeying an entanglement “area law” [4, 5]. The most common approach for one-dimensional (1D) and quasi-two-dimensional (2D) systems is the matrix product state (MPS) ansatz. This forms the basis of the modern formulation [6–8] of White’s density matrix renormalization group (DMRG) algorithm [9] for computing ground states and low-lying excited states [10, 11].

The introduction of the MPS-based time-evolving block decimation (TEBD) algorithm [1, 2, 12] (and subsequent developments) allowed the short-time dynamics of local 1D quantum lattice models to be simulated with great success. In recent years, however, there has been a renewed interest in the dynamics of models with long-range interactions, driven by experimental advances in atomic, molecular, and optical physics. Interactions that decay as $1/r^\alpha$ are now realized in experiments with polar molecules ($\alpha = 3$) [13, 14] and Rydberg atoms ($\alpha = 6$) [15–17], whilst trapped ion experiments can simulate spin models with a tunable exponent ($0 \leq \alpha \leq 3$) [18–24].

In response, MPS algorithms have been developed that are able to simulate the time evolution of such models classically [25–37]. One of the most promising approaches is the time-dependent variational principle (TDVP) [31, 33–35], which has found widespread use in condensed matter physics, and which is beginning to find applications in quantum chemistry [38].

TDVP is a serial algorithm that uses sequential sweeps for numerical stability. Unfortunately, this means it cannot easily take advantage of multicore architectures or high-performance computing clusters. In fact the same is true of most MPS algorithms. Attempts to address this shortcoming include the use of parallel linear algebra operations [39–42], parallelization over quantum number blocks [39, 43], and parallelization over terms in the Hamiltonian [44]. More generally, it is desirable to parallelize over different parts of an MPS, but this network-level parallelization is nontrivial. To the best of our knowledge, the only such algorithms to date are nearest-neighbor TEBD [45–48], real-space parallel DMRG [49, 50], and parallel infinite DMRG [51], although network-level parallelization has also been proposed for projected entangled pair states (PEPS) [52, 53]. A parallel time evolution method for MPS capable of handling long-range interactions has remained an open problem.

Parallel time-dependent variational principle algorithm for matrix product states

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Combining the time-dependent variational principle (TDVP) algorithm with the parallelization scheme introduced by Stoudenmire and White for the density matrix renormalization group (DMRG), we present the first parallel matrix product state (MPS) algorithm capable of time evolving one-dimensional (1D) quantum systems with long-range interactions. We benchmark the accuracy and performance of our implementation by simulating quenches in the long-range Ising and XY models. We show that our code scales well up to 32 processes with parallel efficiencies as high as 86%. Finally, we calculate the dynamical correlation function of a 201-site Heisenberg XXX chain with $1/r^2$ interactions, which is challenging to compute sequentially. These results pave the way for the application of MPS to increasingly complex systems.
Given the close relationship between TDVP and DMRG established in Refs. [34, 35], it is natural to ask whether a parallel version of TDVP can be developed in a similar manner to real-space parallel DMRG. In this work we demonstrate that it can. Moreover, we show how the parallelization of the algorithm makes larger calculations possible that may otherwise be unfeasible. For example, in Sec. IV C, we calculate the dynamical spin-spin correlation function of a 201-site long-range Heisenberg model in a matter of days, rather than weeks.

The rest of the paper is organized as follows. We start with a background section, before moving on to introduce the parallel TDVP algorithm in Sec. III. We provide increasingly complex benchmark examples for quantum spin-chains in Sec. IV, and finally conclude and suggest directions for future research in Sec. V.

II. BACKGROUND

For completeness, we start by reviewing relevant background material, covering matrix product states, the inverse canonical gauge, matrix product operators, and the time dependent variational principle. We also establish the notation used in the rest of the paper.

A. Matrix product states

Any finite-dimensional, N-partite quantum state can be expressed in a given basis \(|\sigma_1\sigma_2\ldots\sigma_N\rangle\) as

\[
|\psi\rangle = \sum_{\sigma_1\ldots\sigma_N=1}^{d_1\ldots d_N} M_1^{\sigma_1}M_2^{\sigma_2}\ldots M_N^{\sigma_N} |\sigma_1\sigma_2\ldots\sigma_N\rangle, \tag{1}
\]

where the \(M_j^{\sigma_j}\) are matrices (\(M_1^{\sigma_1}\) and \(M_N^{\sigma_N}\) being row and column vectors, respectively). This decomposition is known as a tensor train [54] or matrix product state (MPS) [55]. To avoid index gymnastics we will often use the graphical tensor notation introduced by Penrose [56] to represent MPS as tensor networks (see e.g. Ref. [57]). In this notation, tensors are displayed as nodes in a network, with their connected edges representing pairs of dummy indices in the usual Einstein notation. A contractible edge is referred to as a bond and the dimension of the corresponding dummy index is the bond dimension. Free indices (which may represent physical degrees of freedom) are shown as disconnected edges. In this notation, Eq. (1) is written as

\[
|\psi\rangle = M_1^{\chi_1} \cdots M_N^{\chi_N}, \tag{2}
\]

where we have explicitly labeled the dimensions of all bonds \(\chi_j\), and physical edges \(d_j\) (for notational clarity, dimensions are suppressed in the rest of the paper).

Here we are interested in MPS in the context of finite 1D lattice models with open boundaries. In such a model there is a one-to-one correspondence between the lattice sites and the MPS “site tensors” \(M_j\). In quantum chemistry, the “sites” may instead be molecular orbitals [58]. In a lattice model, the physical dimensions \(d_j\) will often be independent of \(j\). For the spin-half chains considered in this paper, \(d_j = d = 2\). The bonds between sites capture the entanglement present. In general, \(\chi_j\) is not independent of \(j\). It is thus convenient to define \(\chi = \max(\chi_j)\). Exactly representing an arbitrary state as an MPS requires a \(\chi = \chi_{\text{exact}}\) that is exponential in the number of sites. However, physical states are often well approximated by MPS of lower bond dimension. We denote by \(\chi_{\text{max}}\) the maximum bond dimension chosen for a calculation, where typically \(\chi_{\text{max}} \ll \chi_{\text{exact}}\).

Even with all \(\chi_j\) fixed, an MPS representation is not unique, since

\[
\ldots M_j^{\sigma_j'}M_{j+1}^{\sigma_{j+1}}\ldots = \ldots \tilde{M}_j^{\sigma_j'}\tilde{M}_{j+1}^{\sigma_{j+1}}\ldots ,
\]

where \(\tilde{M}_j^{\sigma_j'} = M_j^{\sigma_j'}X\), and \(\tilde{M}_{j+1}^{\sigma_{j+1}} = X^{-1}M_{j+1}^{\sigma_{j+1}}\) for any invertible matrix \(X\). This “gauge freedom” can be exploited by algorithms for numerical stability. In particular, a canonical form is usually employed in which one or more tensors act as orthogonality centers [8]. The parts of the MPS to the left and right of an orthogonality center thus defines the quantum state with respect to these bases.

Bipartitioning a system into sites \([1 : j]\) and \([j + 1 : N]\) allows us to write the Schmidt decomposition,

\[
|\psi\rangle = \sum_{k=1}^{\chi_1} \lambda_k |\Phi^{[1:j]}_{L,k}\rangle \otimes |\Phi^{[j+1:N]}_{R,k}\rangle. \tag{3}
\]

This can be expressed as an MPS with orthogonality center \(A_j = \text{diag}(\lambda_{1}\ldots \lambda_{\chi_j})\) [8],

\[
|\psi\rangle = \sum_{\sigma_1\ldots\sigma_N} \sum_{\sigma_{\Lambda_j}} A_1^{\sigma_1}\ldots A_{j-1}^{\sigma_{j-1}} A_j^{\sigma_j}B_{j+1}^{\sigma_{j+1}}\ldots B_N^{\sigma_N} |\sigma_1\ldots\sigma_N\rangle, \tag{4}
\]

where \(A_j^{\sigma_j} (1 \leq p \leq j)\) and \(B_q^{\sigma_q} (j + 1 \leq q \leq N)\) satisfy

\[
\sum_{\sigma_p} (A_p^{\sigma_p}) \Lambda_j = \sum_{\sigma_q} B_q^{\sigma_q} (B_q^{\sigma_q})^\dagger = 1. \tag{5}
\]

The orthogonality center can alternatively be made into a site tensor. For example, setting \(\Phi^{[j]}_j = A_j^{\sigma_j}A_j\) gives an MPS with orthogonality center at site \(j\),

\[
|\psi\rangle = \sum_{\sigma_1\ldots\sigma_N} \sum_{\sigma_{j-1}\ldots\sigma_{j+1}} A_1^{\sigma_1}\ldots A_{j-1}^{\sigma_{j-1}} \Psi_j^{\sigma_j}B_{j+1}^{\sigma_{j+1}}\ldots B_N^{\sigma_N} |\sigma_1\ldots\sigma_N\rangle. \tag{6}
\]

Eqs. (4) and (6) are known as the mixed canonical form [8]. This MPS gauge is useful for serial algorithms that update tensors sequentially, as the orthogonality center can be shifted by one site whilst maintaining the orthonormality of the state. For details of this approach we refer the reader to Ref. [8].
\section*{B. Inverse canonical gauge}

The key to parallelizing MPS algorithms is to use a gauge with multiple orthogonality centers. This allows different site tensors to be updated simultaneously, and to be merged back into the MPS consistently. The first such gauge was introduced by Vidal for TEBD. Any $N$-partite state can be written in Vidal’s canonical form [1, 2, 12],

\begin{equation}
|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_N} \Gamma_1^{\sigma_1} \Lambda_1 \Gamma_2^{\sigma_2} \Lambda_2 \ldots \Lambda_{N-1}^{\sigma_{N-1}} \Gamma_N^{\sigma_N} |\sigma_1 \ldots \sigma_N\rangle, \quad (7)
\end{equation}

where the $\Lambda_j$ are again diagonal matrices of singular values that serve as orthogonality centers. In graphical tensor notation we write this as

\begin{equation}
|\psi\rangle = \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc, \quad (8)
\end{equation}

where the $\Gamma_j$ are site tensors. The beauty of this canonical gauge is that it simultaneously gives the Schmidt decomposition of all bipartitions.

In this work we use the inverse canonical gauge due to Stoudenmire and White [49], which is given by

\begin{equation}
\Psi_1 V_1 \Psi_2 V_2 \Psi_3 V_3 \Psi_{N-1} V_N |\psi\rangle = \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc, \quad (9)
\end{equation}

where $V_j \equiv \Lambda_j^{-1}$. Although equivalent to the canonical gauge, it turns out to be a more natural choice for parallel TDVP and DMRG, as well as for TEBD, since it to the site tensors, rather than the diagonal matrices, being orthogonality centers. An MPS in canonical form is transformed into inverse canonical form by inserting $V_j \Lambda_j = I$ at each bond and then contracting the $\Lambda$ matrices with the $\Gamma$ site tensors, i.e.

\begin{align*}
\Gamma_1 & \Lambda_1 \Gamma_2 \Lambda_2 \Gamma_3 \Lambda_3 \Gamma_4 \Lambda_4 \Lambda_{N-1} \Gamma_N \\
= & \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \\
= & \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \\
= & \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \bigcirc \\
\Psi_1 V_1 \Psi_2 V_2 \Psi_3 V_3 \Psi_4 V_4 \Psi_{N-1} V_N
\end{align*}

As $\Lambda_j$ is diagonal, calculating $V_j$ simply requires taking the reciprocal of the singular values\footnote{Taking the reciprocal of a floating-point number should be “safe” as long as overflows and divisions by zero are avoided.}. The contractions $\Gamma_j V_j$ and $V_j \Gamma_{j+1}$ are similarly cheap. We find no issue with the inversion of $\Lambda_j$ as tiny singular values corresponding to numerical noise are discarded [8, 59].

\section*{C. Matrix product operators}

We represent $N$-site operators using the matrix product operator (MPO) construction,

\begin{equation}
O = \sum_{\sigma_1, \ldots, \sigma_N} O_1^{\sigma_1 \tau_1} O_2^{\sigma_2 \tau_2} \ldots O_N^{\sigma_N \tau_N} |\sigma_1 \ldots \sigma_N\rangle \langle \tau_1 \ldots \tau_N|, \quad (10)
\end{equation}

where the $O_j^{\sigma_j \tau_j}$ are matrices ($O_1^{\sigma_1 \tau_1}$ and $O_N^{\sigma_N \tau_N}$ being row and column vectors, respectively). In graphical tensor notation we write this as

\begin{equation}
\begin{array}{cccc}
O_1 & O_2 & O_3 & \cdots & O_N
\end{array}, \quad (11)
\end{equation}

where the $O_j$ are site operators (represented by squares). Site operators are analogous to MPS site tensors, but have an extra physical edge. The physical edges have the same dimensions $d_j$ as the MPS on which they act.

Local Hamiltonians are known to have a particularly compact MPO representation [60, 61], which means the maximum MPO bond dimension $m$ is independent of $N$. Exponentially decaying interactions can also be encoded efficiently [28, 62] as the same is not true of arbitrary long-range interactions, we follow Refs. [28, 62, 63] in approximating power laws by sums of exponentials, giving $m = n_H n_{\text{exps}} + 2$, where $n_H$ is the number of long-range terms in the Hamiltonian, and $n_{\text{exps}}$ is the number of exponentials used in the approximation. In this paper we use the algorithm described in Ref. [28]. An alternative method [64–66] is discussed in the Supplemental Material.

\section*{D. Time-dependent variational principle}

The McLachlan formulation of the Dirac-Frenkel-McLachlan time-dependent variational principle (TDVP) [67, 68] approximates the time evolution of a state $|\psi\rangle$ under the Hamiltonian $H$ by minimizing

\begin{equation}
\left\| \frac{d}{dt} |\psi(t)\rangle - H |\psi(t)\rangle \right\|_2^2, \quad (12)
\end{equation}

with $|\psi\rangle$ kept fixed while its derivative is varied (note that we set $\hbar = 1$ throughout this paper). Assuming the set of MPS with a given uniform bond dimension to be a smooth manifold (proven in Refs. [69–71]), Haegeman et al. used this variational principle to derive a novel algorithm for real and imaginary time evolution [31].

More recently, an improved TDVP algorithm was derived for finite MPS with open boundaries, which relies on the mixed canonical gauge [34, 35]. This approach leads to an effective Schrödinger equation for states constrained to the MPS manifold,

\begin{equation}
\frac{d}{dt} |\psi(t)\rangle = P_T |\psi\rangle H |\psi(t)\rangle, \quad (13)
\end{equation}

where
where $P_{T|\psi\rangle}$ is an orthogonal projector onto the tangent space of $|\psi(t)\rangle$. The essence of this method is that the tangent space projector can be decomposed as

$$P_{T|\psi\rangle} = \sum_{j=1}^{N} P_{L}^{[1:j-1]} \otimes \mathbb{1}_{j} \otimes P_{R}^{[j+1:N]} - \sum_{j=1}^{N-1} P_{L}^{[1:j]} \otimes P_{R}^{[j+1:N]}, \quad (14)$$

where

$$P_{L}^{[1:j-1]} = \sum_{k=1}^{\chi_{j-1}} \phi_{L,k}^{[1:j-1]} \langle \phi_{L,k}^{[1:j-1]} |,$$

$$P_{R}^{[j+1:N]} = \sum_{l=1}^{\chi_{j+1}} \phi_{R,l}^{[j+1:N]} \langle \phi_{R,l}^{[j+1:N]} |, \quad (15)$$

meaning

$$|\psi(t + \delta t)\rangle = \exp (-i P_{T|\psi\rangle} H \delta t) |\psi(t)\rangle \quad (16)$$

can be approximated by applying a Lie-Trotter-Suzuki decomposition [72] to the exponential. Consequently, one can sweep back and forth along the MPS (as in single-site DMRG [73–75]), time evolving one site tensor at a time. This algorithm, which we refer to as 1TDVP, is sympletic, so conserves the energy and norm of a state. However, it also restricts MPS to a fixed bond dimension.

To overcome this limitation, Haegeman et al. introduced a two-site variant (2TDVP) that similarly relies on the mixed canonical gauge [35]. In 2TDVP, the tangent space projector of Eq. (14) is replaced by

$$P_{T|\psi\rangle}^{[2]} = \sum_{j=1}^{N-1} P_{L}^{[1:j-1]} \otimes \mathbb{1}_{j} \otimes \mathbb{1}_{j+1} \otimes P_{R}^{[j+2:N]} - \sum_{j=2}^{N-1} P_{L}^{[1:j-1]} \otimes \mathbb{1}_{j} \otimes P_{R}^{[j+1:N]}, \quad (17)$$

Because MPS of different bond dimension do not belong to the same manifold, it is no longer possible to describe the time evolution of the entire MPS by a differential equation. Instead, Haegeman et al. use a symmetric second-order Lie-Trotter-Suzuki decomposition with a discrete timestep $\delta t$ to arrive at an algorithm with the same sweeping pattern as the original two-site DMRG. Being able to dynamically vary the bond dimension makes 2TDVP particularly convenient. It has also been shown to give accurate results for a range of problems [37, 76], so it is this variant we consider here.

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2 Higher-order decompositions entailing more sweeps are also possible [35].
time by another half a timestep. In our implementation we instead evolve the rightmost pair just once, by a full timestep (see Appendix A).

The one and two-site time evolution steps rely on “effective environments”, which are the same as in DMRG. Each site tensor $\Psi_j$ has a left and a right effective environment, labeled $\beta_j$ and $\gamma_j$, respectively. These are defined in Fig. 3. The leftmost and rightmost MPS environments ($\beta_1$ and $\gamma_N$) are trivial, corresponding to $1 \times 1$ identity matrices. It is important to note that the effective environments need not be created from scratch at every step since previous environments can be cached and updated. At the beginning of a simulation, all right-hand environments $\gamma_1 \ldots \gamma_N$ are created iteratively from right to left.

To time evolve two sites, $\Psi_j$ and $\Psi_{j+1}$, we construct an effective local state $\Theta^{(2)}$ and an effective two-site Hamiltonian $H^{(2)}_{\text{eff}}$. These are described in Fig. 4(a). Evolving $\Theta^{(2)}$ forwards in time means calculating

$$\Theta^{(2)\prime} = \exp \left( -i H^{(2)}_{\text{eff}} \delta t / 2 \right) \Theta^{(2)}. \quad (18)$$

Using the Lanczos exponentiation [77] method\(^3\) means that $H^{(2)}_{\text{eff}}$ is not explicitly required, only $H^{(2)}_{\text{eff}} \Theta^{(2)}$, so a more efficient tensor contraction pattern can be employed. Fig. 5 explains how $\Theta^{(2)\prime}$ is split back into two site tensors using the singular value decomposition (SVD). Here the smallest singular values are discarded to keep the bond dimension from growing too large. After this two-site update a new lefthand environment $\beta_{j+1}$ is created from the contraction of $\beta_j$, $\Psi_j$, $V_j$, $\Psi_j^\dagger$, $V_j$, and the Hamiltonian MPO tensor for site $j$, i.e.

$$\beta_{j+1} = \beta_j.$$

Time evolving one site $\Psi_{j+1}$ requires the construction of an effective one-site Hamiltonian $H^{(1)}_{\text{eff}}$ from $\beta_{j+1}$ and $\gamma_{j+1}$. This is described in Fig. 4(b). The local state $\Theta^{(1)}$ is now just the vectorization of $\Psi_{j+1}$. To time evolve

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\(^3\) An alternative is the recent algorithm from Al-Mohy and Higham based on truncated Taylor series [78].
\( \Theta^{(1)} \) backwards in time means calculating
\[
\Theta^{(1)\prime} = \exp \left( +iH^{(1)\text{eff}} \frac{\delta t}{2} \right) \Theta^{(1)},
\] (20)

but again only \( H^{(1)\text{eff}} \Theta^{(1)} \) is actually required by the Lanczos routine. After this one-site update, \( \gamma_{j+1} \) can be discarded.

A timestep in 2TDVP has the same time complexity as a sweep in two-site DMRG. The most expensive operation is the contraction of the network representing \( H^{(2)\text{eff}} \Theta^{(2)} \), giving a bound of
\[
O \left( N \chi^3 m^2 + N \chi^2 m^2 d^3 \right).
\] (21)

This means that systems with many degrees of freedom (e.g., bosonic systems) can be very demanding. Large systems with long-range interactions are also challenging because of the size of the bond dimension required by the Hamiltonian MPO (especially if it contains multiple long-range terms). These considerations motivate the need for a parallel algorithm.

### B. Parallelization

The intuition behind the parallel algorithm is the fact that local updates approximately preserve the inverse canonical gauge for small \( \delta t \). We thus parallelize 2TDVP by carrying out these local updates simultaneously on separate processes. More concretely, we split the \( N \)-site MPS into \( p \) partitions, which are updated in parallel. We use a message-passing parallel programming model and assign each partition to a separate process. A partition must contain a minimum of two site tensors, so we let \( p \) be an even number between 2 and \( N/2 \). The full sweeps of the serial algorithm are replaced by partial sweeps carried out in parallel; each process simultaneously sweeps along the tensors in its own partition following the pattern introduced by Stoudenmire and White for parallel DMRG \cite{49}. This is illustrated in Fig. 6 for two and four processes. Notice that the sweeping direction alternates for each neighboring partition. The two central processes always sweep away from the center of the MPS during the first half of a timestep.

At the start of a simulation, the necessary initial effective environments are computed sequentially, with each being assigned to the process owning the corresponding site tensor. Processes that start by sweeping right will require righthand environments and vice-versa for those that start by sweeping left.

When sweeps reach a partition boundary, it is necessary for neighboring processes to communicate. Firstly, the processes need to exchange boundary environments, and secondly, one of the processes needs the \( \Psi \) tensor belonging to its neighbor in order to carry out the two-site update. This communication involves sending \( O \left( \chi^2 (m + d) \right) \) floating-point numbers. We let the lefthand process update the boundary sites while the righthand process waits. The lefthand process then sends the updated tensors to the righthand process and both processes update their respective effective environments. Fig. 7 illustrates how the local updates proceed in parallel away from partition boundaries. We describe the algorithm formally in Appendix B.

### C. Error

Serial 2TDVP has four sources of error: the projection, the Lie-Trotter-Suzuki decomposition, the local integration, and the truncation of Schmidt coefficients. For a detailed discussion we refer the reader to Ref. [37].
dependence of the different errors on the MPS bond dimension and the choice of $\delta t$ is rather subtle [76] but, if these parameters are chosen with care, it is the truncation and projection errors that usually dominate due to the growth of bipartite entanglement [79]. The projection error can be prohibitively expensive to compute, especially for long-range models [37, 80], but the truncation error is simply calculated from the discarded singular values, as in TEBD [12].

To quantify the truncation error from the single SVD shown in Fig. 5 we use the discarded weight

$$w = \sum_{j=\chi+1}^{\chi'} \lambda_j^2,$$

(22)

where $\chi'$ is the full rank of the matrix $\Theta^{(2)'}$, $\lambda_j$ are its singular values (sorted in order of descending magnitude), and $\chi$ is the truncated rank. We choose $\chi$ as follows. First, we define a truncation error tolerance $w_{\text{max}}$, which is the maximum allowed discarded weight per SVD. We then find the minimum rank $\chi_w$ such that $w \leq w_{\text{max}}$. Finally, we set $\chi = \min(\chi_w, \chi_{\text{max}})$.

The total discarded weight $w_{\text{total}}$ is defined as the cumulative sum of $w$ over all SVDs, over all timesteps. In the worst case, $w_{\text{total}}$ will grow exponentially due to a linear growth of bipartite entanglement entropy [4]. However, long-range models can exhibit a logarithmic growth of entanglement entropy, even when this growth is linear in the corresponding local model [81–85], meaning $w_{\text{total}}$ will grow as a power law.

The parallelization of 2TDVP introduces two further sources of error:

i) Information about lattice sites propagates along the MPS at a finite speed meaning that each process will always be using at least one “out-of-date” local environment. For nonlocal 1D models, this induces an artificial locality, since instantaneous long-range interactions become effectively retarded. For $p$ parallel processes, we expect this error to be small if the characteristic velocity $v$ of the dynamics satisfies

$$v \ll (N/p)/\delta t,$$

(23)

where we have assumed that each parallel partition contains $\sim (N/p)$ sites.

ii) Like all parallel MPS algorithms, the local updates in p2TDVP formally break the global gauge conditions, meaning the inverse canonical form only holds approximately. In serial TDVP the inverse canonical gauge is also technically broken. However, the orthogonality of the state is preserved with respect to the last updated site, which remains an orthogonality center. In parallel TDVP this orthogonality may be lost, since different parts of the MPS are updated simultaneously. We discuss this issue further in Sec. IIIID and show how it can be addressed.

To quantify the error introduced by the parallelization, we run our benchmark simulations on a single process and calculate the difference in the observables of interest. We also compute the infidelity,

$$I (|\psi_1 \rangle, |\psi_2 \rangle) = 1 - \frac{|\langle \psi_1 | \psi_2 \rangle|}{\sqrt{\langle \psi_1 | \psi_1 \rangle \langle \psi_2 | \psi_2 \rangle}},$$

(24)

between the serial and parallel MPS at the end of the calculations, which bounds the error in all observables.

When truncation is the dominant source of error, $I \sim w_{\text{total}}$ [3, 54]. Under this condition $w_{\text{total}}$ can be used as a proxy for $I$. In general, however, we would expect $w_{\text{total}}$ to provide a lower bound as it does not account for the projection error.

D. Stability

The breaking of the gauge conditions at partition boundaries can cause the p2TDVP algorithm to become unstable if very small singular values are kept. To circumvent this, we define a relative SVD truncation tolerance $\varepsilon$. We discard singular values smaller than $\varepsilon \lambda_1$ (where $\lambda_1$ is the largest singular value), in addition to carrying out the truncation procedure described in Sec. III C.

If the error in the norm grows unacceptably large during a simulation, the MPS can also be reorthonormalized and the effective environments recomputed. As this is a serial procedure, it should be carried out infrequently to avoid affecting the algorithm’s parallel efficiency. Note that it is, however, important to ensure the initial state is orthonormal.

For the benchmark calculations described in Sec. IV, a value of $\varepsilon = 10^{-12}$ was sufficient, with no reorthonormalization necessary. However, the appropriate value...
FIG. 9 (color online). Density plots of the correlation function $C_{r,65}(t)$ for a 129-site chain evolved under the long-range Ising Hamiltonian for four values of $\alpha$. The data were calculated using p2TDVP with 32 processes. All values deviate from the serial calculations by less than 1% (less than 0.2% for the more accurate $\alpha = \infty$ case).

of $\varepsilon$ depends on the system and choice of timestep. In Fig. 8, we describe a p2TDVP simulation carried out on a 641-site spin chain using different values of $\delta t$, and $\varepsilon$. With $\delta t = 0.01$, and $\varepsilon = 10^{-8}$, the error in the norm is seen to blow up. However, reorthonormalization brings it back under control. In comparison, the calculation with $\delta t = 0.002$, and $\varepsilon = 10^{-12}$ remains stable.

### IV. BENCHMARKS

In this section we describe the results of our numerical experiments. To test p2TDVP, we carried out benchmark calculations on spin-half models with one, two and three long-range interaction terms. We utilized up to 32 processes, with one process assigned per compute node. Each compute node used up to 16 threads (e.g. for linear algebra operations). Full details of the test platform [86], software used [87–100], and simulation parameters are provided in the Supplemental Material.

In the following, we define spin Hamiltonians in terms of Pauli-$X$, $-Y$, and -$Z$ operators $\sigma_i^x$, $\sigma_i^y$, and $\sigma_i^z$ (where $i$ is the index of the spin), and set the interaction strengths (and hence the energy and time scales) to unity.

#### A. Long-range Ising model

Our first benchmark follows Liu et al. [85] in simulating a global quench in the ferromagnetic phase of the transverse field Ising model with short to intermediate-range interactions ($\alpha > 2$). We track the evolution of an equal-time spin-spin correlation function to see how well p2TDVP can capture a nonlocal observable. Denoting the transverse magnetic field by $B$, the Hamiltonian is given by

$$H = -\sum_{i<j}^N \frac{1}{|i-j|^\alpha} \sigma_i^z \sigma_j^z - B \sum_{i=1}^N \sigma_i^z.$$  \hspace{1cm} (25)

Liu et al. use a Krylov space method [101, 102] to accurately simulate the global quench dynamics of a 19-site lattice with periodic boundaries. Starting from the ferromagnetic product state $|\psi(0)\rangle = |111\ldots1\rangle$, correlation confinement [103] is shown to arise due to the presence of long-range interactions. This confinement is stronger the longer the range of the interactions. Stronger confinement is also shown to decrease the bipartite entanglement present, meaning the maximal bond dimension required for our simulations should decrease for smaller $\alpha$.

The authors note that correlation confinement persists when the initial state is a ferromagnetic ground state of $H$. We observe this behaviour for lattices with open boundaries when applying a quench to the ground state of Eq. (25) with $\alpha = 3.0$ and $B = 0.1$. As in Ref. [85], we quench to $B = 0.27$ for various values of $\alpha$, and calculate the correlation function,

$$C_{r,k}(t) = \langle \psi(t) | \sigma_i^z \sigma_k^z | \psi(t) \rangle - \langle \psi(t) | \sigma_i^z | \psi(t) \rangle \langle \psi(t) | \sigma_k^z | \psi(t) \rangle,$$  \hspace{1cm} (26)

where $r$ is the lattice site index, $k$ is the index of the central lattice site, and $|\psi(t)\rangle$ is the state at time $t$ after the quench. As we consider chains with an odd number of spins, $k = (L+1)/2$.

In Fig. 9 we plot $C_{r,65}(t)$ for $\alpha = 2.3, 2.5, 3.0$, and for the nearest-neighbor case ($\alpha = \infty$). These results, computed using 32 processes, give excellent agreement with the serial calculations over many orders of magnitude. As in Ref. [85], we see that the correlation confinement disappears as $\alpha \to \infty$, and a linear lightcone [104–107] is recovered. In fact a linear lightcone also seems to be present in the $\alpha = 3.0$ case, consistent with Ref. [108]. The other striking difference between the local and nonlocal models is the existence of oscillatory power-law decaying correlations in the latter, consistent with Refs. [82, 109–113]. We find this power law to have an exponent approximately equal to $\alpha$.

### TABLE I. Summary of results for the 129-site long-range Ising model at the end of 1000 timesteps (corresponding to $t = 20$).

| $\alpha$ | $m$ | $\chi_{\text{max}}$ | $w_{\text{max}}$ | $w_{\text{total}}$ | Infidelity (1) | Speedup |
|---------|-----|---------------------|------------------|-------------------|----------------|---------|
| 2.3     | 15  | 128                 | $10^{-16}$       | 3.3 x $10^{-11}$  | 3.8 x $10^{-10}$ | 20.8    |
| 2.5     | 14  | 192                 | $10^{-16}$       | 3.1 x $10^{-11}$  | 3.4 x $10^{-10}$ | 23.0    |
| 3.0     | 13  | 256                 | $10^{-16}$       | 6.1 x $10^{-11}$  | 5.6 x $10^{-10}$ | 25.0    |
| $\infty$ | 3   | 512                 | $10^{-18}$       | 1.7 x $10^{-13}$  | 4.2 x $10^{-13}$ | 23.9    |
At the end of the simulations, we compute the infidelities $I$ between the serial and parallel calculations. In Table I we show these for 32 processes, along with the total discarded weights $w_{\text{total}}$ from the end of the serial calculations. We find that the ratio $I/w_{\text{total}}$ grows with decreasing $\alpha$, from 2.5 for the nearest-neighbor case, to 11.5 for $\alpha = 2.3$.

A strong scaling analysis for the $\alpha = 2.3$ case is shown in Fig. 1. A speedup of 20.8 was achieved using 32 processes, although by this point the parallel efficiency drops below 70%. We find greater speedups for the simulations with larger bond dimensions (summarized in Table I for 32 processes). This is to be expected as the computational complexity of the linear algebra operations asymptotically dominates over the parallel overheads.

**B. Long-range XY model**

We next simulate a local quench in the antiferromagnetic XY model,

$$H = \frac{1}{2} \sum_{i<j} N \left[ j \right]^{\alpha} \left( \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right),$$

(27)

with very long-range interactions ($\alpha < 1$). In this regime, information can spread through the system almost instantaneously [109–113]. This is an important test case as it is not a priori clear how accurately p2TDVP will capture the nonlocal [109] propagation of information from a single site.

Following Haegeman et al. [35, 114], we calculate the ground state $|\psi_0\rangle$ of $H$ for a 101-site spin chain and apply a U(1) symmetry-breaking perturbation,

$$U = \exp \left(i \pi \sigma_0^z / 4 \right),$$

(28)

to the central spin. We then examine the evolution of the single-site observable [35, 111]

$$C_{51,r}(t) = |\langle \psi(t) | \sigma^r | \psi(t) \rangle - \langle \psi_0 | \sigma^r | \psi_0 \rangle|,$$

(29)

**TABLE II.** Total discarded weights and infidelities for the 101-site long-range XY model at the end of 500 timesteps.

| Processes ($p$) | Total discarded weight ($w_{\text{total}}$) | Infidelity ($I$) |
|----------------|------------------------------------------|------------------|
| 1              | $6.0 \times 10^{-5}$                     | N/A              |
| 2              | $6.0 \times 10^{-5}$                     | $5.1 \times 10^{-4}$ |
| 8              | $6.5 \times 10^{-5}$                     | $5.3 \times 10^{-4}$ |
| 16             | $6.9 \times 10^{-5}$                     | $5.6 \times 10^{-4}$ |
| 32             | $7.9 \times 10^{-5}$                     | $6.1 \times 10^{-4}$ |

where the perturbed state at time $t$ is given by

$$|\psi(t)\rangle = e^{-iHtU} |\psi_0\rangle.$$  

(30)

Using p2TDVP we reproduce the results of Ref. [35] for $\alpha = 0.75$, which is the most interesting case as it illustrates the breakdown of lightcone dynamics. It is also the most numerically challenging due to large MPO bond dimension.

As shown in Fig. 1, this calculation scales well up to 32 processes with an efficiency $\geq 86\%$. For 32 processes this corresponds to a speedup of 27.4. The scaling is near optimal because the MPS saturates our chosen $\chi_{\text{max}}$ after just one timestep. We have excluded the time taken to compute expectation values, but note here that we were also able to compute these in parallel, as discussed in Ref. [49], since $C_{51,r}$ depends on $\sigma^r$, which is a single-site observable.

The time evolution of $C_{51,r}(t)$, calculated using 32 processes, is shown in Fig. 10(a). The results deviate from the serial calculation by less than 1%, except for small values at the start of the simulation ($t < 0.8$). The spatial profile of $C_{51,r}$ is seen most clearly in Fig. 10(b). Its value oscillates, but appears to decay algebraically with $r$, in excellent agreement with Fig. 5 of Ref. [35].

In Fig. 10(c) we show the maximum absolute deviation in $C_{51,r}(t)$ from the serial calculation for 2, 16, and 32 processes, along with the discarded weight from the serial calculation. The deviation has a weak dependence on the
FIG. 11 (color online). Left panel: density plot of $|C(x, t)|$ in the $t$-$x$ plane for the 201-site long-range XXX spin chain. At the edges, $|C(x, t)|$ drops to $1.2 \times 10^{-3}$. Right panel: the relative difference $\eta_{\infty}$ from the exact thermodynamic limit result. Towards the edges, $\eta_{\infty}$ grows to 0.78. The calculation was carried out using p2TDVP on 32 processes with $m = 38$, $\delta t = 0.025$, $\varepsilon = 10^{-12}$, and $w_{\max} = 10^{-16}$. $w_{\text{total}}$ at the end of the calculation was $7.4 \times 10^{-11}$.

number of processes $p$, but appears to be approximately bounded by $w_{\text{total}}$ (except at the beginning of the simulation where the parallelization error seems to dominate). The infidelities $I$ and total discarded weights $w_{\text{total}}$ from the end of the calculations are shown in Table II. These also depend weakly on $p$, with $I$ being less than an order of magnitude larger than $w_{\text{total}}$.

C. Long-range XXX model

In our final benchmark, we test p2TDVP with a U(1) symmetric MPS [89, 115] by simulating the long-range isotropic Heisenberg (XXX) Hamiltonian with $\alpha = 2$,

$$H = \frac{1}{4} \sum_{i<j}^{N} \frac{1}{|i-j|^{2}} \left(\sigma_{i}^{x} \sigma_{j}^{x} + \sigma_{i}^{y} \sigma_{j}^{y} + \sigma_{i}^{z} \sigma_{j}^{z}\right).$$

(31)

In the thermodynamic limit this is equivalent to the exactly solvable spin-half Haldane-Shastry model [116, 117], which was argued in Ref. [30] to provide a stringent test case as it is both long-ranged and critical. Here we instead use p2TDVP to time evolve a 201-site spin chain with open boundaries in order to calculate the dynamical spin-spin correlation function,

$$C(r-k, t) = \langle \psi_{0} | \sigma_{z}^{k}(t) \sigma_{z}^{k}(0) | \psi_{0}\rangle,$$

(32)

where $|\psi_{0}\rangle$ is the ground state of Eq. (31), and $k$ is the central lattice site (i.e. $k = 101$). As a $\sigma^{z}$ perturbation does not break the U(1) symmetry of $|\psi_{0}\rangle$, the Z-component of spin is conserved. This allows us to take advantage of symmetric block-sparse tensors [89, 115], and hence use a relatively large bond dimension of $\chi_{\max} = 1024$.

In the thermodynamic limit, the dynamical spin-spin correlation function is given by [118]

$$C_{\infty}(x, t) = \frac{(-1)^{x}}{4} \int_{-1}^{1} d\lambda_{1} \int_{-1}^{1} d\lambda_{2} e^{i(Qx-Et)},$$

$$Q = \pi \lambda_{1} \lambda_{2},$$

$$E = \frac{\pi^{2}}{4}(\lambda_{1}^{2} + \lambda_{2}^{2} - 2\lambda_{1}^{2}\lambda_{2}^{2}).$$

(33)

In Fig. 11 we show the magnitude of $C(x, t)$ calculated using p2TDVP on 32 processes. We also show the relative difference $\eta_{\infty}$ from $C_{\infty}(x, t)$, where

$$\eta_{\infty} = \frac{|C(x, t) - C_{\infty}(x, t)|}{|C_{\infty}(x, t)|}.$$  

(34)

There is quantitative difference between the calculations, but they agree well qualitatively (except towards the edges where $|C(x, t)|$ drops off exponentially in the finite system due to the open boundaries). In Fig. 12 we plot the real and imaginary parts of $C(x, t)$ for $x = 0, 2, 4, 6$. Again, we see good qualitative agreement with the analytic result, and with Fig. 4 of Ref. [30].

The simulation took 3.4 days to run, excluding the calculation of $C(x, t)$, although a different partitioning of the MPS should give a slight speedup (see Supplemental Material). The same computation would likely take weeks to run on a single compute node with serial 2TDVP, making a full scaling analysis impractical.

As we cannot easily calculate the error introduced by the parallel splitting for this system, we repeat the simulation on a smaller lattice of 65 sites with $\chi_{\max} = 512$. Denoting the results calculated on 1 and 32 processes
by \( C_s \) and \( C_p \), respectively, we find a maximum relative difference of \( \max(\eta_p) = 3.1 \times 10^{-5} \), where

\[
\eta_p = \frac{|C_p(x, t) - C_s(x, t)|}{|C_s(x, t)|}.
\]

(35)

In contrast, \( \min(\eta_{\infty}) = 5.3 \times 10^{-4} \) for both the serial and parallel simulations. At least for this smaller system then, the parallelization error is negligible compared to the deviation from the thermodynamic limit (see Fig. 13).

V. DISCUSSION

We have introduced a parallel version of the two-site TDVP algorithm (p2TDVP) and applied it to quenches in paradigmatic spin-half models with power law decaying interactions. To assess our algorithm’s accuracy we calculated onsite expectation values, equal-time two-point correlation functions, and a dynamical spin-spin correlation function. Remarkably, we have shown that demanding calculations can be accelerated at the cost of very little additional error. Though the parallel splitting can potentially lead to instability, we have explained how this can be worked around. Speedups are system dependent, but we have demonstrated parallel efficiencies of 65–86% with 32 processes. This suggests that it should be possible to use our algorithm to simulate systems in a week that would otherwise take many months. The use of a dynamical load balancer may further improve this efficiency.

As a next step, p2TDVP could be applied to fermionic models. It is not yet clear how accurately p2TDVP can simulate 2D systems, but fermionic models in two dimensions can be especially challenging for all numerical methods [11, 119], underlining the need for a parallel algorithm. Targeting larger 1D systems should be more straightforward. Large system sizes are important for the study of transport properties [120], and to distinguish between many-body localized and thermal phases [121, 122].

In Ref. [50] it was established that single-site DMRG can be parallelized. We therefore expect that a parallel variant of one-site TDVP (p1TDVP) could be developed using the same approach. This would enable a parallel version of the hybrid method discussed in Refs. [37, 79, 123], whereby a simulation starts with 2TDVP and switches to 1TDVP when \( \chi_{\text{max}} \) is saturated. 1TDVP is faster, and can give more accurate results for some observables [79]. A parallel version should scale well as the fixed bond dimension would allow for optimal load balancing. It may similarly be possible to apply the parallelization scheme presented here to other related MPS-local time-evolution methods [26, 37, 42].

We have focused on real time evolution, but p2TDVP can also be used for imaginary time evolution. This might prove beneficial for cases where parallel DMRG fails to converge. As this evolution is non-unitary, however, one has to pay particularly careful attention to the orthonormality of the MPS.

An obvious extension to this work would be the combination of parallel TDVP with established MPS techniques such as non-Abelian symmetries [60], different local bases [124–128], and infinite boundary conditions [129]. A code combining these features would be of great benefit to the research community. Generalizing to other tensor network types is a further avenue to explore. TDVP can be extended to tree tensor network states [35, 130], so it would be worthwhile to see if our algorithm can be modified to work with these or other networks that admit a canonical form [131, 132].

Finally, a promising future application for parallel TDVP is the solution of general partial differential equations (PDEs). MPS-based PDE solvers, such as the multigrid renormalization method [133], can be exponentially faster than standard PDE solvers. It is exciting to anticipate an additional speedup for such methods via the parallelization technique reported here.

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APPENDIX A: SERIAL ALGORITHM

We use unified modelling language (UML) activity diagrams to describe a single timestep in the serial 2TDVP algorithm for an MPS in the inverse canonical gauge. Figs. 14(a) and 14(b) describe the left-to-right sweep (illustrated schematically in Fig. 2) and right-to-left sweep, respectively. For each two-site update, the left and right site tensors are labeled $\Psi_L$ and $\Psi_R$, with $V$ being the diagonal matrix sandwiched between them.

As noted in Section III A, we evolve the rightmost pair of sites at the end of the first sweep by a single full timestep. This means that the second sweep does not need to carry out a forwards time evolution step for the rightmost two sites. We use this same approach in the parallel version of the algorithm (see Fig. 15).

APPENDIX B: PARALLEL ALGORITHM

Here we use UML activity diagrams to describe a single timestep in the p2TDVP algorithm. Figs. 15 and 16 describe the first and second sweeps, respectively. For concreteness we show four parallel processes (illustrated schematically in Fig. 6b). This case contains all the logic necessary to generalize to $p$ processes.

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FIG. 15. UML activity diagram describing the first half of a p2TDVP timestep on four processes. Dashed lines represent message-passing communication, and “site” is shorthand for “site tensor.”
FIG. 16. UML activity diagram describing the second half of a p2TDVP timestep on four processes. The sweep on each partition occurs in the opposite direction to the corresponding sweep in Fig. 15.

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Parallel time-dependent variational principle algorithm for matrix product states
(Supplemental Material)

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In this Supplemental Material we present technical information aimed at practitioners wishing to use the parallel two-site time dependent variational principle algorithm. We compare two different methods of approximating power laws by sums of exponentials, which should prove useful for calculations on larger systems. We also provide details of the software, settings, and parameters used to carry out our numerical experiments, in order to aid reproducibility.

S1. IMPLEMENTATION

The parallel two-site time-dependent variational principle (p2TDVP) code was built on top of the Tensor Network Theory (TNT) Library [S1–S4] – a C code that implements OpenMP [S5] shared memory parallelism [S2], and which supports multithreaded linear algebra libraries. p2TDVP was implemented using the Message Passing Interface (MPI) standard [S6]. This allowed us to target distributed memory architectures, hence increasing the total amount of random-access memory (RAM) available for simulations. For our benchmark calculations we employed a hybrid parallel approach in which the MPI network-level parallelism was combined with existing shared memory parallelism.

S2. APPROXIMATING POWER LAWS

The Hamiltonian matrix product operators (MPOs) used in our calculations were defined using a MATLAB [S10] interface written by Coulthard [S4]. This employs the method described by Pirvu et al. in the Appendix of Ref. [S7] to approximate power laws by sums of exponentials. Henceforth, when we refer to the MPO error, we mean the error in this approximation.

Although the approach suggested by Pirvu et al. seems particularly fast and stable, it does not necessarily give optimal results. Instead a nonlinear least-squares fit can be employed. In Fig. S1 we compare the method from Ref. [S7] to the Levenberg-Marquardt nonlinear least-squares algorithm [S8, S9], by approximating 1/r² as a sum of nine exponentials.

The Levenberg-Marquardt fit was calculated in MATLAB using the lsqnonlin() function [S11] with the options shown in Table S1. We find that the Levenberg-Marquardt method is slower but gives better results, comparable to those in Ref. [S12]. Using this method should thus allow for smaller MPO bond dimensions, and hence slight speedups. More importantly, it seems better at representing interactions over longer distances, making it valuable for simulations with larger sized systems.

| Option                  | Value     |
|-------------------------|-----------|
| Algorithm               | levenberg-marquardt |
| MaxFunctionEvaluations  | 10000     |
| MaxIterations           | 1000      |
| StepTolerance           | 1E-6      |
| FunctionTolerance       | 1E-14     |

TABLE S1. Options used for the MATLAB lsqnonlin() function when calculating the fit shown in Fig. S1.

S3. TEST PLATFORM

We carried out our benchmarks on the Balena high performance computing (HPC) cluster [S13] at the University of Bath. We had access to a maximum of 32 compute nodes, with a maximum runtime per job of 5 days. All simulations were run on Dell PowerEdge C8220 nodes, which have two Intel E5-2650 v2 CPUs (20 MB Cache, 2.60 GHz base frequency), giving a total of 16 cores per node. Each node has a memory of 64 GB (8 GB × 8) DDR3 (1866 MHz).

S4. SIMULATION DETAILS

We linked the TNT Library to ARPACK-NG [S14], and the multithreaded Intel Math Kernel Library (MKL) [S15]. We used the same version of the Intel MPI Library [S16] and compiler, compiling with the -O2 and -xHost optimization flags. We set the OpenMP/MKL environment variables shown in Table S2 to allow dynamic adjustment of the number of threads used (up to a maximum of 16), whilst also disabling nested threading.

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FIG. S1. Approximation of $1/r^2$ (dashed lines) by a sum of 9 exponentials (solid lines) using (left panel) the method described by Pirvu et al. in Ref. [S7], and (right panel) the Levenberg-Marquardt nonlinear least-squares algorithm [S8, S9] discussed in the main text. The broken lines show the absolute error in the approximations, and the insets show the relative error.

| Environment variable       | Value                                      |
|----------------------------|--------------------------------------------|
| OMP_NUM_THREADS            | 16                                         |
| MKL_NUM_THREADS            | 16                                         |
| OMP_NESTED                 | FALSE                                      |
| OMP_DYNAMIC                | TRUE                                       |
| MKL_DYNAMIC                | TRUE                                       |
| KMP_AFFINITY               | compact,1,0,granularity=fine               |

TABLE S2. Environment variables used to control OpenMP threading in the TNT Library and Intel MKL.

The linear algebra settings used for all calculations were as follows. We used the TNT Library default zero tolerance of $10^{-14}$ for the automatic blocking of matrices [S2]. We set a relative truncation tolerance of $\varepsilon = 10^{-12}$ for singular value decompositions (SVDs), and used the LAPACK [S17] dense matrix divide-and-conquer [S18–S20] routine (as implemented in Intel MKL). For the Lanczos exponentiation in p2TDVP, we created the Krylov subspace using ARPACK-NG with a maximum of 8 basis vectors, and a convergence tolerance of $10^{-6}$. Density matrix renormalization group (DMRG) calculations used the ARPACK-NG sparse eigenvalue solver [S14, S21] with these same settings.

A. Long-range Ising model

All Hamiltonian MPOs had a maximum absolute error $\lesssim 10^{-8}$. The other parameters are as described in the main text. The ground state matrix product state (MPS) was calculated using two-site DMRG, and was found to have a maximum bond dimension of $\chi = 22$. For the p2TDVP calculations, the 129-site MPS was partitioned as described in Table S3.

| $p$ | Number of sites owned by first process | Number of sites owned by central processes | Number of sites owned by last process |
|-----|--------------------------------------|-------------------------------------------|-------------------------------------|
| 8   | 17                                    | 16                                        | 16                                  |
| 16  | 9                                     | 8                                         | 8                                   |
| 24  | 10                                    | 5                                         | 9                                   |
| 32  | 5                                     | 4                                         | 4                                   |

TABLE S3. Partitioning of the 129-site MPS in the long-range Ising model simulations for $p$ parallel processes.

B. Long-range XY model

The ground state of the antiferromagnetic XY Hamiltonian is twofold degenerate when there are an odd number of lattice sites. To break this degeneracy we added a small perturbation to the Hamiltonian, so that we actually considered the ground state of

$$H = \frac{1}{2} \sum_{i<j} \frac{1}{|i-j|^\alpha} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \frac{\delta B}{2} \sum_k \sigma_k^x,$$  

(S1)

with $\delta B = 10^{-6}$. We calculated this ground state using parallel two-site DMRG with 16 processes. As in Ref. [S22], we used a maximum MPS bond dimension of $\chi = 128$ [S23], and a Hamiltonian MPO with maximum absolute error $<10^{-8}$.
### C. Long-range XXX model

To calculate the thermodynamic limit results, we numerically integrated the exact expression for $C_\infty(x, t)$ (given in the main text) using the integral2() function in MATLAB with the iterated option [S24].

For the 201-site p2TDVP calculation we approximated the $1/r^2$ power law by a sum of 12 exponentials, giving an MPO bond dimension of 38 with a maximum absolute error of $1.5 \times 10^{-7}$ and a maximum relative error of $5.3 \times 10^{-3}$. As shown in Fig. S1, it is possible to use the Levenberg-Marquardt nonlinear least-squares algorithm to approximate the power law more efficiently using just 9 exponentials, albeit with a slightly larger error. This would give an MPO bond dimension of 29, and hence a potential speedup of $\approx 1.3$.

The ground state of the model $|\psi_0\rangle$ was found using two-site DMRG with a U(1) symmetric MPS of maximum bond dimension $\chi = 512$. The energy per site converged to

$$E_0/N = -0.410611165931,$$

with a total discarded weight of $2.1 \times 10^{-9}$. In Fig. S2 we show the magnitude of the ground state correlation function $\langle \sigma_r^z \sigma_k^z \rangle$ for $k = 101$. This appears to follow a power law with exponent equal to 1 (dashed line), except towards the edges where the correlations decay exponentially due to the open boundaries.

The initial state for our p2TDVP calculation was $|\psi\rangle = \sigma_{101}^z |\psi_0\rangle$. We time evolved $|\psi\rangle$ on 32 processes, using a truncation error tolerance of $w_{\text{max}} = 10^{-16}$, and a maximum bond dimension of $\chi_{\text{max}} = 1024$. The MPS was partitioned as shown in Table S5. As in Ref. [S25], we used a timestep of $\delta t = 0.025$ and computed the dynamical spin-spin correlation function,

$$C(r - k, t) = e^{-iE_0t} \langle \psi_0 | \sigma_r^z | \psi(t) \rangle,$$

every eight timesteps.

Although a full scaling analysis was impractical for this simulation, we used different numbers of processes to time evolve the final state at the end of the simulation for an additional timestep. With one process, this took 71.6 minutes; with 32 processes, it took 7.8 minutes – a speedup of 9.1 (in comparison, the 65-site simulation gave a speedup of 11.0 on 32 processes). This suggests that our partitioning of the MPS was not optimal. By looking at the final bond dimensions we were able to devise a better partitioning scheme, which gave a speedup of 15.4 with 32 processes. The scaling results are shown in Fig. S3, with the corresponding partitions described in Table S6. We see close to ideal scaling up to 4 processes, with reasonable scaling up to 16 processes. A speedup of 15.1 was achieved with 24 processes, after which it tails off due to load imbalance. The reason for this is that the dynamics of the system are fairly localized, so the relatively large bond dimension is only saturated by the central tensors.
| Process ID(s)   | 0 1 | 0 1–2 3 | 0 1–6 7 | 0 1 2–21 22 23 | 0 1 2–13 14 15 | 0 1 2–6 7 8 9 10 | 0 1 2–10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 | 0 1 2–10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 |
|----------------|-----|---------|---------|----------------|----------------|-----------------|------------------|------------------|
| No. of sites owned | 101 100 | 85 16 84 | 77 8 76 | 60 11 3 11 59 | 65 12 4 12 64 | 60 11 3 11 59 | 33 32 6 2 6 32 | 33 32 6 2 6 32 |

This example highlights the fact that the choice of partitioning scheme and number of processes is nontrivial for simulations in which the MPS bond dimensions $\chi_j$ grow inhomogeneously. Unless necessitated by memory requirements, using “too many” compute nodes is a waste of resources. On the other hand, sub-optimal partitioning is a performance issue. It should be possible to address this using a dynamic load balancer, as has previously been done for the parallel time-evolving block decimation algorithm [S26].

TABLE S6. (top to botttom) MPS partitions for 2, 4, 8, 16, 24, and 32 processes, corresponding to the single timestep scaling shown in Fig. S3.