

Time-Dependent Variational Principle for Quantum Lattices

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We develop a new algorithm based on the time-dependent variational principle applied to matrix product states to efficiently simulate the real- and imaginary-time dynamics for infinite one-dimensional quantum lattices. This procedure (i) is argued to be optimal, (ii) does not rely on the Trotter decomposition and thus has no Trotter error, (iii) preserves all symmetries and conservation laws, and (iv) has low computational complexity. The algorithm is illustrated by using both an imaginary-time and a real-time example.

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The density-matrix renormalization group (DMRG) is arguably the most powerful tool available for the study of one-dimensional strongly interacting quantum lattice systems [1]. The DMRG—now understood as an application of the variational principle to matrix product states (MPSs) [2]—was originally conceived as a method to calculate ground-state properties. However, there has been a recent explosion of activity, spurred by insights from quantum information theory, in developing powerful extensions allowing the study of finite-temperature properties and non-equilibrium physics via time evolution [3]. The simulation of nonequilibrium properties with the DMRG was first attempted in Ref. [4], but modern implementations are based on the time-evolving block decimation algorithm (TEBD) [5] or the variational matrix product state approach [6].

At the core of a TEBD algorithm lies the Lie-Trotter decomposition for the propagator $\exp(it\hat{H})$, which splits it into a product of local unitaries. This product can then be dealt with in a parallelized and efficient way: When applied to an MPS, one obtains another MPS with a larger bond dimension. To proceed, one then truncates the MPS description by discarding irrelevant variational parameters. This is such a flexible idea that it has allowed even the study of the dynamics of infinite translation-invariant lattice systems via the infinite TEBD [7]. Despite its success, the TEBD has some drawbacks: (i) The truncation step may not be optimal; (ii) conservation laws, e.g., energy conservation, may be broken; and (iii) symmetries, e.g., translation invariance, are broken (although translation invariance by two-site shifts is retained for nearest-neighbor Hamiltonians). The problem is that when the Lie-Trotter step is applied to the state—stored as an MPS—it leaves the variational manifold and a representative from the manifold must be found that best approximates the new time-evolved state. There are a variety of

ways to do this based on diverse distance measures for quantum states, but implementations become awkward when symmetries are brought into account.

In this Letter, we introduce a new algorithm to solve the aforementioned problems—intrinsic to the TEBD—without an appreciable increase in computational cost. The resulting imaginary-time algorithm quickly converges towards the globally best uniform MPS (uMPS) approximation for translational-invariant ground states of strongly correlated lattice Hamiltonians, and the corresponding real-time evolution evolves an initial state without violating energy conservation for constant Hamiltonians or the conservation of any other quantities dictated by symmetry. The complexity of our approach can be made to scale as D^3 , comparable with current implementations, where D is the bond dimension of the uMPS. The low complexity of the algorithm developed here should have implications for related fields. For example, in the case of ultracold atoms moving in an optical lattice [8] it should be possible, via a straightforward truncation, to carry out accurate simulations of the atomic motion for systems involving large densities of strongly interacting particles. Another application is to the calculation of spectral functions $S(k, \omega)$ for interacting particle systems: The improved method described here will directly translate (via a double Fourier transform as in the second reference of [5]) to better estimates for these quantities.

We now introduce the variational manifold $\mathcal{M}_{\text{uMPS}}$ of uniform MPS for an infinite lattice of spin- $d/2$ degrees of freedom, parameterized via

$$|\psi(A)\rangle = \sum_{\{s_k\}=1}^d v_L^\dagger \left(\prod_{n \in \mathbb{Z}} A^{s_n} \right) v_R |s\rangle, \quad (1)$$

where $|s\rangle \equiv |\dots s_1 s_2 \dots\rangle$ and v_L and v_R are two D -dimensional vectors, which are presently argued to be irrelevant. The variational parameters A comprise the set of

$D \times D$ matrices A^s ($s = 1, 2, \dots, d$) and are denoted via a dD^2 vector with entries $A^i = A^s_{\alpha,\beta}$, with $i = (\alpha, s, \beta)$ a collective index. The uMPS variational manifold has a gauge invariance: Replacing $A^s \mapsto GA^sG^{-1}$ for invertible G results in an identical state. We do not fix the gauge and simply assume that A^s are completely general complex matrices. We do, however, assume that the transfer matrix $E = \sum_{s=1}^d A^s \otimes \bar{A}^s$ has precisely one eigenvalue 1 with corresponding left and right eigenvectors $|l\rangle$ and $|r\rangle$ of length D^2 , to which we can associate $D \times D$ matrices l and r , respectively, by simply reshaping them. These matrices are Hermitian and positive and assumed to have full rank. We choose the normalization so that $\langle l|r\rangle = \text{Tr}(lr) = 1$. In addition, we assume that all other eigenvalues of E lie strictly within the unit circle; i.e., the spectral radius of $E - |r\rangle\langle l|$ is smaller than 1. These conditions allow one to write for any local operator \hat{O} acting on n contiguous sites

$$\begin{aligned} O(\bar{A}, A) &= \langle \psi(\bar{A}) | \hat{O} | \psi(A) \rangle / \langle \psi(\bar{A}) | \psi(A) \rangle \\ &= (l | \sum_{s,t=1}^d O_{t_1 \dots t_n, s_1 \dots s_n} (A^{s_1} \dots A^{s_n}) \otimes (\bar{A}^{t_1} \dots \bar{A}^{t_n}) | r). \end{aligned}$$

The boundary vectors v_L and v_R do not feature in normalized expectation values and thus do not contain any variational degrees of freedom.

Denote a translation-invariant nearest-neighbor Hamiltonian as $\hat{H} = \sum_{n \in \mathbb{Z}} \hat{T}^n \hat{h} \hat{T}^{-n}$, where \hat{T} is the shift operator and \hat{h} acts nontrivially only on sites zero and one. We now try to approximate the time evolution generated by \hat{H} of a uMPS $|\psi(A)\rangle$ without ever leaving the variational manifold of uMPS with fixed bond dimension D , by introducing a time-dependent parameterization $A(t)$. Insertion into the time-dependent Schrödinger equation results in $\dot{A}^i |\partial_i \psi(A(t))\rangle = -i \hat{H} |\psi(A(t))\rangle$, where we denote ∂_i for $\partial/\partial A^i$. Whereas the left-hand side (LHS) is a linear combination of the tangent vectors $|\partial_i \psi(A(t))\rangle$ that span the tangent plane $T_A \mathcal{M}_{\text{uMPS}}$, the right-hand side (RHS) is a general vector in Hilbert space, and this equation does not have an exact solution for A^i . The best approximation is obtained by minimizing $\| \dot{A}^i |\partial_i \psi(A(t))\rangle + i \hat{H} |\psi(A(t))\rangle \|^2$. The minimizer \dot{A}^i is found by orthogonally projecting the evolution vector $\hat{H} |\psi(A(t))\rangle$ onto the tangent plane, as illustrated in Fig. 1, resulting in

$$\langle \partial_j \psi | \partial_i \psi \rangle \dot{A}^i = -i \langle \partial_j \psi | \hat{H} | \psi \rangle. \quad (2)$$

The LHS of Eq. (2) contains the $dD^2 \times dD^2$ Gram matrix of the tangent vectors $G_{\bar{i},j}(\bar{A}, A) = \langle \partial_{\bar{j}} \psi(\bar{A}) | \partial_j \psi(A) \rangle$. Expressions for this Gram matrix and the vector in the RHS of Eq. (2) are given by

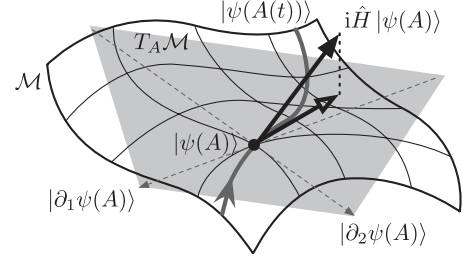


FIG. 1. A sketch of the manifold $\mathcal{M} = \mathcal{M}_{\text{uMPS}}$ (wire frame) embedded in state space. The tangent plane $T_A \mathcal{M}$ to \mathcal{M} (rotated gray square) in a uMPS $|\psi(A)\rangle$ (black dot) is spanned by generally nonorthogonal coordinate axes $|\partial_1 \psi(A)\rangle$ and $|\partial_2 \psi(A)\rangle$ (dotted lines). The direction $i\hat{H}|\psi(A)\rangle$ of time evolution (arrow with solid head) is best approximated by its orthogonal projection into the tangent plane (arrow with open head). The optimal path $|\psi(A(t))\rangle$ (gray curve) follows the vector field generated by these orthogonally projected vectors throughout \mathcal{M} .

$$\begin{aligned} \bar{B}^i G_{\bar{i},j} B^j &= |Z| [(l | E_{B'}^B | r) + (l | E_{B'}^A (1-E)^{-1} E_A^B | r) \\ &\quad + (l | E_A^B (1-E)^{-1} E_{B'}^A | r) \\ &\quad + (|Z| - 1) (l | E_{B'}^A | r) (l | E_A^B | r)], \end{aligned}$$

$$\begin{aligned} B^i \langle \partial_i \psi | \hat{H} | \psi \rangle &= |Z| [(l | H_{AB}^{AA} | r) + (l | H_{BA}^{AA} | r) \\ &\quad + (l | H_{AA}^{AA} (1-E)^{-1} E_B^A | r) \\ &\quad + (l | E_B^A (1-E)^{-1} H_{AA}^{AA} | r) \\ &\quad + (|Z| - 2) (l | E_B^A | r) (l | H_{AA}^{AA} | r)], \end{aligned}$$

where $E_B^A = \sum_{s=1}^d A^s \otimes \bar{B}^s$ (note the identity $E = E_A^A$) and $H_{CD}^{AB} = \sum_{s,t,u,v=1}^d \langle s, t | \hat{h} | u, v \rangle (A^u B^v) \otimes (\bar{C}^s \bar{D}^t)$. In these expressions, $(1-E)^{-1}$ should be interpreted as the pseudoinverse of $(1-E)$; i.e., it produces zero when acting on the left or right eigenvector of E with eigenvalue 1: $(l | (1-E)^{-1} = 0 = (1-E)^{-1} | r)$. The overall factors $|Z|$ are a consequence of the infinite volume of our system and cancel, as they appear in both the LHS and RHS of Eq. (2). The additional divergent terms on the last line of the brackets disappear if we restrict ourselves to tangent vectors that are orthogonal to the uMPS itself, so that $\langle \psi(A) | \partial_i \psi(A) \rangle B^i = |Z| (l | E_A^B | r) = 0$. The evolution along $|\psi(A)\rangle$ changes the norm or phase of the state, which is not a desired effect.

This construction can also be derived from an action principle and is known as the time-dependent variational principle (TDVP) [9,10]. The resulting TDVP equations [Eq. (2)] can be shown to be symplectic [11]. Hence, they respect energy conservation as well as conservation of all constants of motion, such as the expectation value of generators of symmetries. Since only expectation values occur in the equations of motion, one can use techniques familiar from DMRG, including the decomposition of the matrices A^i into irreducible representations of the relevant symmetry group. Furthermore, this approach is manifestly translation-invariant. For time-reversal-invariant operators,

the TDVP equations are also invariant under time reversal (see [12] for a Trotter-based approach that recovers time-reversal invariance). This approach does not require any truncation and is thus globally optimal within the manifold $\mathcal{M}_{\text{uMPS}}$.

Constructing the relevant quantities and solving Eq. (2) for \dot{A}^i involve operations with a computational complexity of $\mathcal{O}(D^6)$. Using an iterative method to implement $(1 - E)^{-1}$ and then solving for \dot{A}^i can reduce this to $\mathcal{O}(D^3)$. However, the matrix $G_{\bar{i},j}$ is not invertible: Because of the gauge invariance in the (u)MPS parameterization, not all dD^2 tangent vectors are linearly independent. Defining the action of a 1-parameter group of gauge transformations $G(\varepsilon) = \exp(\varepsilon X)$ as $A^s(\varepsilon) = G(\varepsilon)A^sG(\varepsilon)^{-1}$, we obtain that $dA^s/d\varepsilon = XA^s - A^sX$. Because of gauge invariance, there is no corresponding change in $|\psi(A(\varepsilon))\rangle$ and thus $d|\psi(A(\varepsilon))\rangle/d\varepsilon = (dA^i/d\varepsilon)|\partial_i\psi\rangle = 0$. Indeed, any vector B_X^i defined by $B_X^s = XA^s - A^sX$ produces a zero norm state, evident when introducing it into the explicit form of $B^i|\partial_i\psi(A)\rangle$. The vectors B_X^i thus span the null space of $G_{\bar{i},j}$. Any vector B in the tangent plane is gauge equivalent to $B' = B + B_X$, $\forall X \in \mathbb{C}^{D \times D}$. There are $D^2 - 1$ linearly independent choices of B_X , as we can easily prove by noting that $B_X = 0$ requires that $\sum_{s=1}^d (A^s)^\dagger B_X^s = 0 = \sum_{s=1}^d (A^s)^\dagger I X A^s - I X$. Since E has a single eigenvalue 1, and l has full rank, the only solution to this equation is $X = 1$. In order to invert $G_{\bar{i},j}$, we fix the gauge which eliminates $D^2 - 1$ components of B . Norm preservation $[(l|E_A^B|r) = 0]$ fixes one more component, resulting in a $(d - 1)D^2$ -dimensional tangent plane.

Different choices for fixing the gauge of tangent vectors result in different effective Gram matrices with different condition numbers. By using the gauge-fixing condition $(l|E_A^B = 0$ —which also includes norm preservation and imposes the condition that the eigenvalue and left eigenvector of the transfer matrix do not change to first order—the effective Gram matrix reduces to $\overline{B}^i G_{\bar{i}} B^j = |\mathbb{Z}|(l|E_A^B|r)$ and all nonlocal contributions are effectively canceled. Let us now explain how to exploit this result even further. We start by defining the $D \times dD$ matrix $L_{\alpha,(s\beta)} = [(A^s)^\dagger l^{1/2}]_{\alpha\beta}$. Clearly, the null space of this matrix is $D(d - 1)$ -dimensional. Let the $Dd \times D(d - 1)$ matrix V_L with entries $[V_L]_{(\alpha s),\gamma}$ be a matrix of orthonormal basis vectors for this null space, which can be obtained from, e.g., the singular value decomposition of L and thus satisfies $L V_L = 0$ and $V_L^\dagger V_L = 1$. We also introduce the notation V_L^s for the $D \times D(d - 1)$ matrix with components $[V_L^s]_{\alpha,\gamma} = [V_L]_{(\alpha s),\gamma}$. If we now group the $(d - 1)D^2$ independent components of B in a $D(d - 1) \times D$ matrix x , we can use a parameterization $B(x)$ given by $B^s(x) = l^{-1/2} V_L^s x r^{-1/2}$. One can check that this parameterization satisfies the left gauge-fixing constraint $(l|E_A^{B(x)} = 0$, since V_L contains only null vectors of L , and that $\overline{B}^i(x) G_{\bar{i}} B^j(y) = |\mathbb{Z}| \text{tr}[x^\dagger y]$, since the vectors in V_L are

orthonormal. Up to the overall diverging factor $|\mathbb{Z}|$ that cancels in the LHS and RHS of Eq. (2), we have found a linear parameterization $B(x)$ for which the effective Gram matrix is the unit matrix. This same parameterization cancels the last two terms in $\langle \partial_{\bar{i}} \psi | \hat{H} | \psi \rangle$. The third term is still nonlocal and requires the inversion of $1 - E$. This is a pseudoinverse as E has a single eigenvalue 1 and $1 - E$ is thus singular. Let $(K| = (l|H_{AA}^{AA}(1 - E)^{-1}$. We can safely replace $(l|H_{AA}^{AA}$ by $(l|H_{AA}^{AA} - h(l|$, where $h = (l|H_{AA}^{AA}|r)$, since $(l|(1 - E)^{-1} = 0$. Then, by replacing $1 - E$ with the nonsingular matrix $1 - E + |r)(l|$, we iteratively solve for the $D \times D$ matrix K from

$$K - \sum_{s=1}^d (A^s)^\dagger K A^s + \text{tr}[K r] l = [(l|H_{AA}^{AA}) - h l$$

with $[(l|H_{AA}^{AA}) = \sum_{stuv} \langle st|\hat{h}|uv\rangle (A^s A^t)^\dagger l (A^u A^v)$. Tracing this equation shows that $\text{tr}[K r] = (K|r) = 0$ as required. Finally, we define the $D(d - 1) \times D$ tensor F

$$F = \sum_{s,t=1}^d d(V_L^s)^\dagger l^{1/2} C^{st} r (A^t)^\dagger r^{-1/2} + \sum_{s=1}^d (V_L^s)^\dagger l^{-1/2} \left(\sum_{t=1}^d (A^t)^\dagger l C^{ts} + K A^s \right) r^{1/2},$$

where $C^{st} = \sum_{uv} \langle st|\hat{h}|uv\rangle A^u A^v$. This definition allows us to write $\|B^i(x)|\partial_i\psi\rangle - \hat{H}|\psi^2\rangle\|^2 = |\mathbb{Z}| \text{tr}[x^\dagger x - x^\dagger F - F^\dagger x + \text{const}]$. This expression is minimized by choosing $x = x^* = F$ and thus $\dot{A}^i = -iB(x^*)$. Note that, thanks to the iterative solver, all steps can be performed in $\mathcal{O}(D^3)$ computation time.

Having now an explicit construction of \dot{A}^i , the simulation of time evolution with the TDVP now boils down to integrating a set of nonlinear coupled differential equations. The simplest numerical integrator is built on the Euler method and proceeds as follows. (i) Construct $x^* = F$ from the previous paragraph. (ii) Set $A(t + dt) = A(t) - idtB(x^*)$. (iii) Fix the gauge and norm of A by rescaling A . (iv) Calculate the energy and evaluate the step, change the time step dt if necessary.

Step (iii) is required since the gauge-fixing condition only fixes the norm and left eigenvector up to first order, and higher-order corrections are generally present. This simple implementation is already useful for finding ground states through imaginary-time evolution ($dt \rightarrow -id\tau$). The TDVP produces the best approximation to a gradient descent in the full Hilbert space, in contrast to a pure gradient descent in parameter space (see [13]). For real-time evolution, a simple first-order Euler integrator does not inherit the symplectic properties of the differential equations, and a more advanced integrator (see [10]) should be used.

We now illustrate the power of our approach. Using imaginary-time evolution with the Euler implementation, we have obtained a uMPS approximation for the ground state of the $S = 1$ Heisenberg antiferromagnet. The TDVP

TABLE I. First 24 Schmidt values of the $D = 128$ uMPS approximation for the ground state of the $S = 1$ Heisenberg antiferromagnet. The degeneracy in the Schmidt spectrum as a result of $SU(2)$ symmetry manifests itself, not by exploiting the symmetry, but rather by converging up to “state tolerance” $\eta = 10^{-10}$. (Roman type, $S = 1/2$; bold type, $S = 3/2$; italic type, $S = 5/2$.)

0.696 198 978 2	0.005 770 050 5	<i>0.001 487 766 9</i>
0.696 198 978 2	0.005 770 050 5	<i>0.001 487 766 9</i>
0.086 098 881 5	0.005 770 050 5	<i>0.001 487 766 9</i>
0.086 098 881 5	0.005 770 050 5	<i>0.001 487 766 9</i>
0.086 098 881 5	0.001 665 909 3	<i>0.001 487 766 9</i>
0.086 098 881 5	0.001 665 909 3	<i>0.001 487 766 9</i>
0.020 013 261 6	0.001 665 909 3	<i>0.001 106 527 3</i>
0.020 013 261 6	0.001 665 909 3	<i>0.001 106 527 3</i>

stops when $\langle \partial_{\bar{t}} \psi | \hat{H} | \psi \rangle = 0$, which indeed signals a minimum in the energy expectation value. Since the gradient has zero length at the minimum, it automatically decreases in size as we approach it, and there is typically no need to reduce the size of the time step. This should be compared with the (infinite)TEBD case, where reduction of the time step, and thus automatic slowing-down, is necessary to overcome the Trotter error. An ordinary laptop or PC allows one to find the ground state up to $D = 1024$ in less than 1 h (without exploiting symmetries), resulting in a ground-state energy density $e = -1.401\,484\,038\,971\,2(2)$ obtained with step size $dt = 0.1$. Since we can easily calculate the norm of the gradient as $\eta = \|\chi^*\|$, we can continue the evolution until η has converged below a specified tolerance level. The convergence of the energy density can be shown to be $\mathcal{O}(\eta^2)$ and can already be far beyond machine precision. This allows a much more accurate localization of the energy minimum than with the ordinary variational principle based on convergence of the energy and is useful to, e.g., obtain an accurate convergence in the entanglement spectrum. The entanglement spectrum can offer valuable information but is not converged very accurately by other approaches (see [14] for an example). Table I shows how the first Schmidt values of the uMPS ground state for the Heisenberg chain at $D = 128$ at $\eta = 10^{-10}$ accurately reproduce the degeneracy according to half-integral spin representations. We can also assess the error of being confined to the manifold and derive from this a construction to optimally increase the bond dimension. Rather than starting from a random state at $D = 1024$, we can progressively build better approximations at larger D [10].

Using the time-reversal-invariant numerical integrator discussed in Ref. [10], we can simulate a real-time evolution using the TDVP equations. We start with the $D = 128$ uMPS ground-state approximation of the XX model with magnetic field $\mu = 1/2$ along the z axis, which is a critical model with nonzero magnetization $\langle \hat{S}^z \rangle \neq 0$, whereas $\langle \hat{S}^x \rangle = \langle \hat{S}^y \rangle = 0$ due to the $U(1)$ symmetry. We evolve

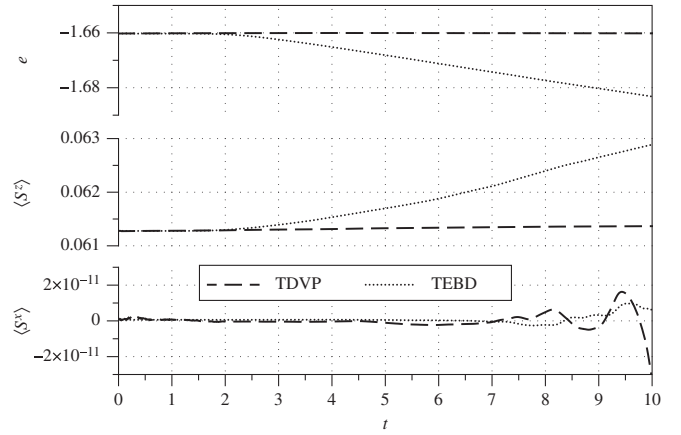


FIG. 2. Comparison of real-time simulation results at $D = 128$ with time step $dt = 5 \times 10^{-3}$ for conserved quantities e (energy density), $\langle \hat{S}^x \rangle$, and $\langle \hat{S}^z \rangle$ with TDVP (dashed lines) and TEBD (dotted lines).

this state according to the critical $S = 1/2$ Heisenberg antiferromagnet, so the expectation values $\hat{S}^{x,y,z}$ should be conserved due to the $SU(2)$ symmetry. Comparative results for the TDVP implementation and a second-order, translation-invariant TEBD implementation based on Ref. [15] are shown in Fig. 2 and illustrate that TDVP is much more capable of describing the evolution of conserved quantities.

In this Letter, we have introduced a new algorithm for simulating real- and imaginary-time evolution with (uniform) matrix product states. The algorithm is shown to be globally optimal within the variational manifold while conserving all symmetries in the system.

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