Time evolution of matrix product operators with energy conservation

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(Dated: December 31, 2018)

We devise a numerical scheme for the time evolution of matrix product operators by adapting the time-dependent variational principle for matrix product states [J. Haegeman et al., Phys. Rev. B 94, 165116 (2016)]. A simple augmentation of the initial operator \( \mathcal{O} \) by the Hamiltonian \( H \) helps to conserve the average energy \( \text{tr}[H \mathcal{O}(t)] \) in the numerical scheme and increases the overall precision. As demonstration, we apply the improved method to a random operator on a small one-dimensional lattice, using the spin-1 Heisenberg XXZ model Hamiltonian; we observe that the augmentation reduces the trace-distance to the numerically exact time-evolved operator by a factor of 10, at the same computational cost.

I. INTRODUCTION

The real-time evolution of strongly correlated quantum systems poses a fundamental and computationally challenging task. Recent interest has been spurred by the question of how quantum information spreads in correlated systems, characterized by out-of-time-ordered correlation functions\(^1\)\(^–\)\(^4\). Another recent approach are hydrodynamic descriptions\(^5\)\(^–\)\(^10\), based on local conservation laws (in one dimension) of the form

\[
\frac{d}{dt} Q_n(t) + J_{n+1}(t) - J_n(t) = 0.
\]

(1)

Here \( n \) is the lattice site index, \( Q_n \) is a conserved field operator (like particle number or spin, or local energy) and \( J_n \) denotes the corresponding local current. Taking thermal averages \( \langle \cdot \rangle \equiv \frac{1}{Z} \text{tr}[\text{e}^{-\beta H}\cdot] \) and assuming slow variation on the scale of the lattice, Eq. (1) transforms into the Euler equation \( \partial_t q(x,t) + \partial_x j(x,t) = 0 \), where \( x \in \mathbb{R} \) is the continuum version of \( n \).

Abstractly, let \( \mathcal{O} \) be a linear operator (not necessarily Hermitian) acting on the quantum Hilbert space. Our goal is to approximate the time-evolved operator \( \mathcal{O}(t) = \text{e}^{iHt} \mathcal{O} \text{e}^{-iHt} \) (with \( H \) the Hamiltonian) by numerically solving the corresponding Heisenberg equation of motion

\[
\frac{d}{dt} \mathcal{O}(t) = i[H, \mathcal{O}(t)]
\]

(2)

while preserving the average energy \( \text{tr}[H \mathcal{O}(t)] \) in the numerical scheme.

For simulating quasi one-dimensional quantum systems on classical computers, density matrix renormalization group (DMRG) methods and modern formulations within the matrix product state (MPS) framework\(^11\)\(^–\)\(^12\) have emerged as one of the most successful methods. The time-dependent variational principle (TDVP) for matrix product states is the canonical approach for solving the Schrödinger equation \( i \frac{d}{dt} \Psi = H \Psi \) for a wavefunction \( \Psi \) projected onto the MPS manifold of given bond dimensions\(^13\). The desirable properties of the one-site integration scheme in Ref. 13 include the exact conservation of the norm \( \langle \Psi | \Psi \rangle ^{1/2} \) and the average energy \( \langle \Psi | H | \Psi \rangle \). In this work, we adapt the TDVP method to matrix product operators (MPO), and augment the initial operator \( \mathcal{O} \) to improve the numerical accuracy.

II. INTERPRETING OPERATORS AS STATES

We assume that \( \mathcal{O} \) is a MPO acting on a lattice with \( N \) sites (using open boundary conditions) of the form

\[
\mathcal{O}[A] = \sum_{s,s'} A^{s_1,s'_1}(1) A^{s_2,s'_2}(2) \cdots A^{s_N,s'_N}(N) |s\rangle \langle s'|.
\]

(3)

Here each \( A^{s_n,s'_n}(n) \) is a site-dependent complex matrix of dimension \( D_{n-1} \times D_n \) (with \( D_0 = 1 \) and \( D_N = 1 \)), and the components of the indices \( s_n \) and \( s'_n \) run from 1 to \( d \), with \( d \) the local Hilbert space dimension. To cast the time evolution into the form of a Schrödinger equation and render it amendable to the TDVP scheme for states, our first step is a “purification” of \( \mathcal{O} \) (see also Refs. 14–16); in our case combining the two physical dimensions per site into one large dimension \( d^2 \), as depicted in Fig. 1. We denote the resulting state by |\( \mathcal{O} \rangle \rangle ; its MPS representation literally agrees with (3) after grouping indices as...
\( \sigma_n = (s_n, s'_n) \) and formally replacing \(|s\rangle\langle s'| \) by \(|\sigma\rangle\). Consequently, the inner product of two linear operators \( O_1 \) and \( O_2 \) equals
\[
\langle O_1|O_2 \rangle = \text{tr}[O_1^\dagger O_2].
\] (4)

With the definition \( \tilde{H} = -[H, \cdot] \equiv -H \otimes 1 + 1 \otimes HT \) (where the second tensor factor corresponds to the primed indices), we can now formally express Eq. (2) as Schrödinger equation
\[
\frac{\text{d}}{\text{d}t} \langle \mathcal{O} \rangle = \hat{H}\langle \mathcal{O} \rangle.
\] (5)

Note that, by construction, \( \hat{H}|H\rangle = 0 \).

### III. MODIFIED TDVP METHOD

The TDVP method approximates Eq. (5) by projecting the evolution vector onto the MPS manifold (for fixed virtual bond dimensions) at the current state \( t = 1 \) and \( \tilde{H} |\mathcal{O}\rangle \) holds exactly at the initial \( |\mathcal{O}[\hat{A}]\rangle \), which follows from the block-diagonal structure of the MPS tensors representing the sum of the two states in (8). Thus, evaluated at the initial \( |\mathcal{O}[\hat{A}]\rangle \):
\[
\frac{\text{d}}{\text{d}t} \langle H|\mathcal{O}[\hat{A}] \rangle = -i\langle H|\tilde{P}_{\mathcal{T}|\mathcal{O}[\hat{A}]} \hat{H}|\mathcal{O}[\hat{A}] \rangle = 0.
\] (11)

One expects that this relation still holds approximately during the TDVP time evolution since \( e^{-i\hat{H}t}|\mathcal{O}[\hat{A}]\rangle = e^{-i\tilde{H}t}|\mathcal{O}[\hat{A}]\rangle + \gamma |H\rangle \), i.e., the form of (8) is preserved by the exact time evolution.

The \( \gamma \) parameter ensures that \(|\mathcal{O}[\hat{A}]\rangle \) is close to \(|\mathcal{O}[A]\rangle\), which we have found advantageous to increase the numerical precision of the time evolution. On the other hand, we observe that the resulting state \(|\mathcal{O}(t)\rangle\) only depends weakly on the precise value of \( \gamma \), as expected, such that a fine-tuning of \( \gamma \) is not required.

### IV. APPLICATION TO THE SPIN-1 XXZ HEISENBERG MODEL

To demonstrate and benchmark the numerical scheme, we consider the (non-integrable) spin-1 Heisenberg XXZ chain with Hamiltonian (setting \( \hbar = 1 \))
\[
H = J \sum_n \left( \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + \Delta S_n^z S_{n+1}^z \right)
\] (12)

where \( S_n^+ = S_n^x + i S_n^y \) and \( S_n^y, S_n^z \) are the usual spin-1 operators with eigenvalues \{\(-1, 0, 1\)\} acting on lattice site \( n \). The local Hilbert space dimension is thus \( d = 3 \). The time-evolved spin operator \( S_n^x(t) = e^{i\tilde{H}t} S_n^x e^{-i\tilde{H}t} \) obeys the microscopic conservation law
\[
\frac{\text{d}}{\text{d}t} S_n^z(t) + J_n^z(t) - J_n^z(t) = 0
\] (13)

with the local spin current
\[
J_n^z = J \left( S_{n-1}^z S_n^y - S_n^z S_{n-1}^y \right),
\] (14)

which follows from a straightforward evaluation of the commutator \( i[H, S_n^y] \). From Eq. (13) one concludes that \( \sum_n S_n^z \) is conserved in time (assuming periodic boundary conditions). Similarly, the local energy operator
\[
h_n = J \left( \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + \Delta S_n^z S_{n+1}^z \right)
\] (15)

obeys the microscopic conservation law
\[
\frac{\text{d}}{\text{d}t} h_n(t) + J_n^\prime(t) - J_n^\prime(t) = 0
\] (16)
with the energy current
\[
\mathcal{J}_n^x(t) = J_x J_y \left( S_{n-1}^y S_n^x S_{n+1}^z + S_{n-1}^x S_n^z S_{n+1}^y \right) + \text{cyclic permutations of } (x, y, z)
\]
and \( J_x = J_y = J, \ J_z = J \Delta \).

We consider a small system with \( N = 6 \) lattice sites and open boundary conditions, such that exact diagonalization is feasible for obtaining reference quantities. The Hamiltonian parameters are chosen as \( J = 1 \) and \( \Delta = 1.2 \). The nonzero complex entries of the tensors \( A(n) \) of the initial operator \( \mathcal{O}[A] \) are independently drawn from the standard normal distribution, separately for real and imaginary parts. We choose the small initial bond dimension \( 2 \), but zero-pad the tensors \( A(n) \) to accommodate a maximum bond dimension of \( 81 \), since the one-site TDVP method\(^{13} \) used for the time evolution leaves the bond dimensions invariant. Explicitly, the virtual bond dimensions \( D_n \) are \( (1, 9, 81, 81, 81, 9, 1) \). As last step of the initialization, the tensors \( A(n) \) are left-normalized by QR decompositions. Due to the sparsity pattern of the initial \( A(n) \) tensors, we can represent the sum in Eq. (8) without increasing the bond dimension. The tensors representing \( \mathcal{H} \) are temporarily scaled by \( 10^{-3} \) before adding it to \( \mathcal{O}[A] \), thus \( \gamma = 10^{-3}N = 10^{-18} \). The simulations are performed using the PyTeNet software package\(^{17} \).

We time-evolve up to \( t = \frac{1}{2} \) to ensure that the Schmidt coefficients of \( \mathcal{O}(t) \) (partitioning into left and right halves with \( N/2 \) sites) still decay fast, i.e., the exact \( \mathcal{O}(t) \) can in principle be well approximated by a matrix product operator of maximal bond dimension \( 81 \), see Fig. 2. The corresponding von Neumann entanglement entropy is 1.287 at \( t = \frac{1}{8} \). For comparison, it reads 0.9913 at \( t = 0 \).

We quantify the overall accuracy via the trace-distance (matrix 1-norm) of \( \mathcal{O}[A] \) and \( \mathcal{O}(t) \) from the numerically exact \( \mathcal{O}(t) \), respectively, see Fig. 4. Interestingly, the modified TDVP method reduces the error by a factor of 10, for the same bond dimensions used during the time evolution.

V. DISCUSSION AND OUTLOOK

While we have focused on energy conservation, the proposed modification of the TDVP method in Eqs. (8), (9)
and (10) works for any operator $K$ commuting with the Hamiltonian, since the corresponding conservation law can be written as

$$\frac{d}{dt} \langle K^\dagger |O(t)\rangle = \frac{d}{dt} \text{tr}[K \cdot O(t)] = \text{tr}[K \cdot i[H,O(t)]] = 0.$$  

(18)

Moreover, it is feasible to take several conservation laws simultaneously into account, by forming the sum

$$|X[\tilde{A}]\rangle = |O[A]\rangle + \sum_j \gamma_j |K_j\rangle.$$  

(19)

The effect of such a modification on the overall accuracy is an interesting question for future studies.

Considering practical implementations of the TDVP method for operators, we remark that the Hamiltonian $\hat{H} = -[H,\cdot] \equiv [-H \otimes 1 + 1 \otimes H^T]$ can be applied without explicitly forming the outer Kronecker product with identity matrices, in order to improve the computational efficiency.

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