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Time-step targeting methods for real-time dynamics using the density matrix renormalization group

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We present a time-step targeting scheme to simulate real-time dynamics efficiently using the density matrix renormalization group. The algorithm works on ladders and systems with interactions beyond nearest neighbors, in contrast to existing Suzuki-Trotter-based approaches.

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Over the last ten years the density matrix renormalization group (DMRG) (Ref. 1) has proven to be remarkably effective at calculating static, ground-state properties of one-dimensional strongly correlated systems. During this period there has also been substantial progress made in calculating frequency dependent spectral functions.[2] However, the most significant progress in extending DMRG since its invention has occurred in the last year or two. Through a convergence of quantum information and DMRG ideas and techniques, a number of unique approaches are being developed. The first of these are highly efficient and accurate methods for real-time evolution, allowing both the calculation of spectral functions via Fourier transforming, and also time development studies of systems out of equilibrium.

The key real-time methods thus far developed[3–5] rely on the Suzuki-Trotter (S-T) breakup of the evolution operator. This approach has a number of important advantages: it is surprisingly simple and easy to implement in an existing ground-state DMRG program; the time evolution is very stable and the only source of nonunitarity is the truncation error; and the number of density matrix eigenstates needed for a given truncation error is minimal. It also has a notable weakness: it is limited to systems with nearest-neighbor interactions on a single chain. In the case of narrow ladders with nearest-neighbor interactions, one can avoid the problem by lumping all sites in a rung into a single supersite. Unfortunately, this approach becomes very inefficient for wider ladders, and is not applicable to general long-range interaction terms.

In this paper we propose a time evolution scheme which produces a basis that targets the states needed to represent one time step. Once this basis is complete enough, the time step is taken and the algorithm proceeds to the next time step. This targeting is intermediate to previous approaches:[6,7] the Trotter methods target precisely one instant in time at any DMRG step, while Luo *et al.*'s approach[7] targeted the entire range of time to be studied. Targeting a wider range of time requires that more density matrix eigenstates be kept, slowing the calculation. By targeting only a small interval of time, our approach is nearly as efficient as the Trotter methods. In exchange for the small loss of efficiency, we gain the ability to treat longer-range interactions, ladder systems, and narrow two-dimensional strips. In addition, the accuracy is much improved over the lowest-order Trotter method.

We want to find the solution to the time-dependent Schrödinger equation,

$$i\frac{d}{dt}|\psi(t)\rangle = (H(t) - E_0)|\psi(t)\rangle, \tag{1}$$

where the ground-state energy E_0 is introduced to reduce the amplitude of the oscillations by making the diagonal elements of H smaller.[6] We use a time-dependent Hamiltonian to include the case where a time-dependent perturbation $V(t)$ is added to the time-independent Hamiltonian H_0. The initial state $|\psi(t=0)\rangle$ is typically the ground state, or the ground state acted upon by an operator, but other possibilities are also interesting.

When the wave function of the system evolves in time, its density matrix samples a region of the Hilbert space that changes continuously. The DMRG basis is built to represent the states that are put into the density matrix

$$\rho = \sum_t w_t |\psi_t\rangle\langle\psi_t|, \tag{2}$$

where the target states $|\psi_t\rangle$ are weighted with a factor w_t, with $\Sigma_t w_t = 1$. Typically, some sweeps are needed to build self-consistency between the target states and the basis produced by the density matrix. A notable exception to this need for self-consistency are the Trotter-based time evolution methods: the bond time evolution operator is represented exactly in the current basis, and so the pretruncation density matrix is exact. Thus, the truncation error is an exact measure of the error in the basis produced at that step. In our time-step targeting approach, this ideal behavior is lost, and a sweep or two is needed to produce a good basis for the time step.

How do we produce a density matrix representing the wave function over an interval of time? Luo *et al.*[7] (see also Ref. 8) suggested targeting the wave function at a sequence of times spanning the interval, $\psi(t=0)$, $\psi(t=\tau)$, $\psi(t=2\tau), \ldots, \psi(t=n\tau)$, simultaneously. We argue that this choice is very close to ideal. Suppose that our basis includes $\psi(k\tau)$ and $\psi((k+1)\tau)$. Then, the basis includes any linear combination of these states, so that one could imagine using an interpolation formula to determine coefficients a and b to approximate the wave function at any time between $k\tau$ and $(k+1)\tau$ as $\psi(t) \approx a\psi(k\tau) + b\psi((k+1)\tau)$. This suggests that the error in the basis is at worst τ^2. If the basis includes more than two time points, one could imagine using higher-order interpolations, e.g., splines, putting a tighter bound on the

error in the basis. The key point is that we do not actually perform these interpolations; the basis is automatically good enough to allow whatever interpolation is most accurate given the set of time points. This suggests that the error in the basis varies as τ^{n+1}.

If τ is small enough and n big enough, and enough self-consistency sweeps are made, the error in the basis is given by the truncation error. This is the ideal situation for a DMRG calculation. Since this truncation error is often miniscule we shall say that an approximate algorithm is "quasiexact" when the error is strictly controlled by the DMRG truncation error ϵ (with some properties proportional to ϵ and others to $\epsilon^{1/2}$). For example, the infinite system method applied to a finite system is *not* quasiexact, even though the error goes to zero as the number of states kept m increases. If enough sweeps are taken, and absent any "sticking" problems with metastable ground states, the finite system ground-state DMRG method is quasiexact. Non-quasi-exact algorithms seem to be the source of most DMRG "mistakes." The procedure below is nearly quasiexact: it has a small separate time-step error, perhaps of order τ^4, in addition to the truncation error.

Our procedure consists of taking a tentative time step at each DMRG step, the purpose of which is to generate a good basis. The standard fourth-order Runge-Kutta (R-K) algorithm is very convenient for this purpose. This is defined in terms of a set of four vectors,

$$|k_1\rangle = \tau\tilde{H}(t)|\psi(t)\rangle,$$

$$|k_2\rangle = \tau\tilde{H}(t+\tau/2)[|\psi(t)\rangle + 1/2|k_1\rangle],$$

$$|k_3\rangle = \tau\tilde{H}(t+\tau/2)[|\psi(t)\rangle + 1/2|k_2\rangle],$$

$$|k_4\rangle = \tau\tilde{H}(t+\tau)[|\psi(t)\rangle + |k_3\rangle], \quad (3)$$

where $\tilde{H}(t)=H(t)-E_0$. The state at time $t+\tau$ is given by

$$|\psi(t+\tau)\rangle \approx \frac{1}{6}[|k_1\rangle + 2|k_2\rangle + 2|k_3\rangle + |k_4\rangle] + O(\tau^5). \quad (4)$$

We choose to target the state at times t, $t+\tau/3$, $t+2\tau/3$, and $t+\tau$. The R-K vectors have been chosen to minimize the error in $|\psi(t+\tau)\rangle$, but they can also be used to generate $|\psi\rangle$ at other times. The states at times $t+\tau/3$ and $t+2\tau/3$ can be approximated, with an error $O(\tau^4)$, as

$$|\psi(t+\tau/3)\rangle \approx |\psi(t)\rangle + \frac{1}{162}[31|k_1\rangle + 14|k_2\rangle + 14|k_3\rangle - 5|k_4\rangle],$$

$$|\psi(t+2\tau/3)\rangle \approx |\psi(t)\rangle + \frac{1}{81}[16|k_1\rangle + 20|k_2\rangle + 20|k_3\rangle - 2|k_4\rangle]. \quad (5)$$

In practice we proceed as follows: each half sweep corresponds to one time step. At each step of the half sweep, we calculate the R-K vectors (3), but without advancing in time. The density matrix is then obtained by using the formula (2) with the target states $|\psi(t)\rangle$, $|\psi(t+\tau/3)\rangle$, $|\psi(t+2\tau/3)\rangle$, and $|\psi(t+\tau)\rangle$. Advancing in time is done on the last step of a half sweep. However, we may choose to advance in time only every other half sweep, or only after several half sweeps, in order to make sure the basis adequately represents the time step. Our tests show that one half-sweep is adequate and most efficient for the systems studied here. The method used to advance in time in the last step need not be the R-K method used in the previous tentative steps. In fact, the computation time involved in the last step of a sweep is typically miniscule, so a more accurate procedure is warranted. A simple way which keeps the time-integration errors much smaller than the basis errors is by performing 10 R-K iterations with step $\tau/10$. We usually use this method. Alternatively, one can evolve using the exponential of the the Hamiltonian in the Lanczos tridiagonal representation, which is exactly unitary. However, the truncation to a finite number of density matrix eigenstates introduces nonunitarity anyway, so the Lanczos procedure has no special advantage. In practice, we find comparable overall accuracy in the two methods.[9]

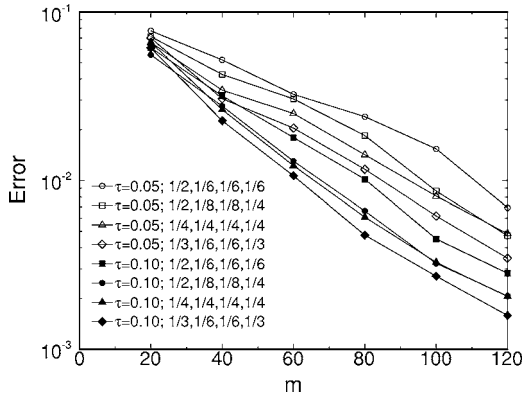

FIG. 1. Error $E(t=8)$ for the Haldane chain ($L=32$), according to Eq. (6), as a function of the number of states kept m. We show results of simulations using the Runge-Kutta algorithm, for different time steps and distributions of weights.

To test the method we first studied the $S=1$ Heisenberg chain.[10] Since it is a single chain system, the Suzuki-Trotter methods are also applicable. In addition to our method, we have used both the traditional first-order Suzuki-Trotter decomposition[4] and the fourth-order Forest-Ruth breakup.[11] In order to compare the results, we calculated the error as

$$E(t) = \sqrt{\frac{1}{L}\sum_{x=1}^{L}(S^z(x,t) - S^z_{Exact}(x,t))^2}, \quad (6)$$

where S^z_{Exact} is obtained using fourth-order Suzuki-Trotter with $m=200$ and $\tau=0.02$, which keeps the truncation error under 10^{-12}.

The target states (5) can be weighted equally, or unequally. We have performed several test runs with different distributions of weights. In Fig. 1 we show the error (6) at time $t=8$ as function of the number of states kept m, for various weightings. The best weighting we have found is $w_1=w_3=1/3$, $w_2=w_3=1/6$. The calculations described below, unless otherwise noted, use this choice of weights.

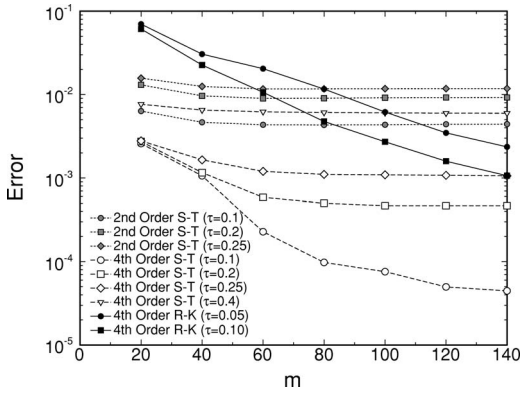

FIG. 2. Same as in Fig. 1, using first-order Suzuki-Trotter breakup (gray symbols), fourth-order Suzuki-Trotter (empty symbols), and fourth-order Runge-Kutta (filled symbols).

In Fig. 2 we compare results by using our method and Suzuki-Trotter evolution. The Suzuki-Trotter simulations converge when the error reaches a plateau and remains constant with increasing number of states m. This occurs generally for a relatively small m, after which the accuracy of the simulation is completely controlled by the Trotter error, and not by the truncation error. Gobert *et al.*[12] argue that the truncation error accumulates in time and eventually starts dominating over the Trotter error. However, in the time intervals studied, this does not occur. In Fig. 3(a) we verify that the quantity E is proportional to τ, τ^2, and τ^4 for the three Suzuki-Trotter breakups considered.[11] In the R-K simulations, convergence is slower with the number of states m because we need the basis to be optimized for four states at slightly different times. The accuracy improves steadily with the size of the basis, and also with the size of the time step τ, as it can be seen in Fig. 3(b), although the method breaks down for time steps larger than $\tau \simeq 0.25$. These results may look counterintuitive, since the R-K error is expected to be proportional to τ^4. The reason for this behavior is that smaller time steps require more iterations, with a consequent accumulation of error due to the truncation. Therefore, unlike the S-T case, the simulation is now dominated by the truncation error, which can be reduced by increasing the size of the DMRG basis.

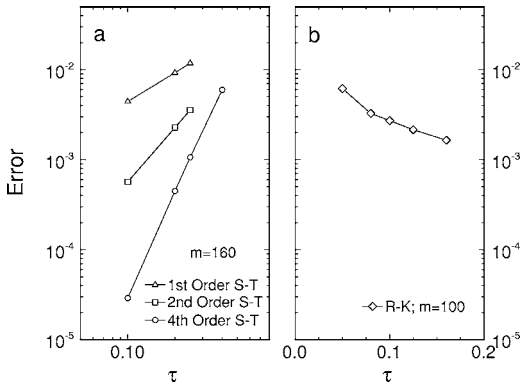

FIG. 3. Error $E(t=8)$ for the Haldane chain for different time steps τ: (a) First-, second-, and fourth-order Suzuki-Trotter breakups and $m=160$; (b) Runge-Kutta and $m=100$. Time is in units of the Heisenberg exchange J.

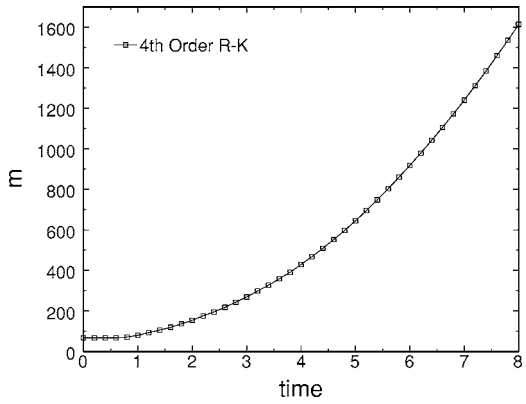

FIG. 4. Number of states required to keep a truncation error of 10^{-8}, as a function of time. The results correspond to a R-K simulation of a Haldane chain with $L=32$.

The R-K method requires more operations per DMRG step—multiplying by a Hamiltonian several times—but progresses one time step in one-half DMRG sweep, whereas the fourth-order S-T method requires seven half sweeps. In our implementation for the $S=1$ chain, for a fixed number of states m, one R-K DMRG step takes three times as long as a S-T step, but one R-K time step (one half sweep) takes half as long as one fourth-order S-T time step. However, this difference is overwhelmed by requiring a fixed accuracy. For instance, in order to obtain an error of the order of 10^{-3} at $t=8$ we could use first-order S-T with $\tau=0.016$ and $m=40$, fourth-order S-T with $\tau=0.25$ and $m=40$, or R-K with $\tau=0.10$ and $m=140$. In this case, the difference in m makes the fourth-order S-T method 15 times as fast as R-K for the same accuracy.

In Fig. 4 we show how the number of states m required to keep a fixed, very small truncation error of 10^{-8}, grows with time. This rapid growth in m for a fixed accuracy is not surprising. At $t=0$, an operator is applied to the ground state, creating $|\psi(0)\rangle$. For small t, $|\psi(t)\rangle$ is still closely related to the ground state, and so requires a comparable number of states to represent it. For larger t, $|\psi(t)\rangle$ becomes more com-

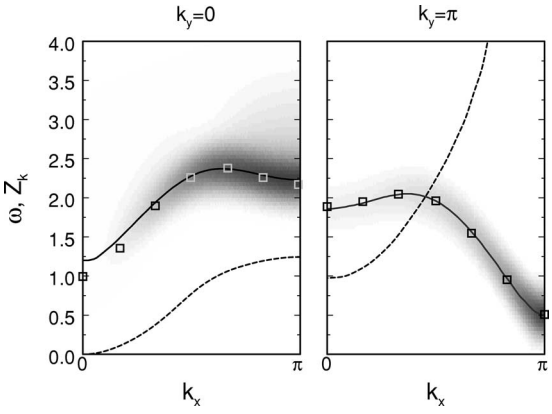

FIG. 5. Structure factor $A(\mathbf{k},\omega)$ for the Heisenberg ladder using fourth-order Runge-Kutta, $m=256$ states, and time step $\tau=0.1$. The solid line is centered at the quasiparticle peak. The tones of gray are proportional to the quasiparticle weight (dashed curve). The symbols are Lanczos results for $L=12$ from Ref. 14.

plicated as each excited eigenstate evolves with a different frequency and becomes independent of the others.

As an application of the R-K method we calculated the spin structure factor for a $2 \times L$ Heisenberg ladder with spin $S=1/2$, $A(\mathbf{k},\omega)=-(1/\pi)\mathrm{Im}\, G(\mathbf{k},\omega)$, obtained by Fourier transforming the time-dependent spin-spin correlation function[4]

$$G(\mathbf{x},t) = \langle S^-(\mathbf{x},t)S^+(0,0)\rangle.$$

In this case, besides targeting the four states at different times (5), we also need to target the ground state at $t=0$. We have used a weight $w_0=1/2$ for the ground state, and all the other weights equal to $1/8$. In Fig. 5 we show the results for $L=32$ using a time step $\tau=0.1$ and $m=256$, which kept the truncation error under 10^{-7} for times up to $t=30$. The result for the spin gap is $\Delta=0.506$, which should be compared to the very precise DMRG value $\Delta_{\mathrm{exact}}=0.502\,49$ in the thermodynamic limit.[13] We also show for comparison the exact diagonalization results for the singlet-triplet excitations for $L=12$ from Ref. 14. A continuum of excitations can be observed above the magnon band for $k_y=0$. It becomes more difficult to resolve the band for $k_y=0$ in the proximity of $k_x \to 0$ because the quasiparticle weight tends to zero in this limit. This is not the case for $k_y=\pi$, where the band is well defined in the entire range of momenta.

To summarize, we have presented a unique method for simulating time evolution of quantum systems. Unlike methods that rely on Suzuki-Trotter breakups, our algorithm can be applied to systems with arbitrary geometry and interactions beyond first neighbors. We demonstrated its application by calculating the excitation spectrum of the Heisenberg ladder.

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