# Real-Time Evolution Using the Density Matrix Renormalization Group

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We describe an extension to the density matrix renormalization group method incorporating real-time evolution. Its application to transport problems in systems out of equilibrium and frequency dependent correlation functions is discussed and illustrated in several examples. We simulate a scattering process in a spin chain which generates a spatially nonlocal entangled wave function.

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The density matrix renormalization group (DMRG) [1] is perhaps the most powerful method for simulating one-dimensional quantum lattice systems. DMRG was originally formulated as a ground state method. Later, it was generalized to give frequency dependent spectral functions [2,3]. The best spectral method, Jeckelmann's dynamical DMRG [4], yields extremely accurate spectra. However, it is limited to only one momentum and one narrow frequency range at a time. Constructing an entire spectrum for a reasonable grid in momentum and frequency space can involve hundreds of runs.

An alternative approach to dynamics with DMRG is via a real-time simulation. Cazalilla and Marston introduced a real-time DMRG and used it to calculate the time evolution of one-dimensional systems under an applied bias [5]. In their approach, DMRG is used only to calculate the ground state, and the time evolution is obtained by integrating the time-dependent Schrödinger equation in a fixed basis. Consequently, one expects it to lose accuracy when the wave function starts to differ significantly from the ground state. In the systems studied by Cazalilla and Marston, the time evolution could be carried out for a reasonable length of time before this happened. Luo, Xiang, and Wang [6] showed how to construct a basis which applies to a time-evolving wave function over a whole range of times simultaneously. This approach was shown to be more accurate than that of Cazalilla and Marston, but it is not very efficient—the basis must be quite large to apply to a long interval of time, and the whole evolution is performed at every DMRG step.

Recently, Vidal developed a novel time-dependent simulation method for near-neighbor one-dimensional systems which overlaps strongly with DMRG [7]. The crucial new idea of the method is to use the Suzuki-Trotter decomposition for a small time evolution operator $\exp(-i\tau H)$. The second order Suzuki-Trotter breakup is

$$e^{-i\tau H} \approx e^{-i\tau H_A/2} e^{-i\tau H_B} e^{-i\tau H_A/2}, \tag{1}$$

where $H_A$ contains the terms of the Hamiltonian for the even links, and $H_B$ for the odd. The individual link terms $\exp(-i\tau H_j)$ (coupling sites $j$ and $j+1$) within $H_A$ or $H_B$ commute. Writing the wave function in matrix product form (which underlies the DMRG block form [8]), Vidal showed that one can apply each link term directly to the wave function, exactly and efficiently. After each such application, a Schmidt decomposition, equivalent to diagonalizing the DMRG density matrix, is performed to return the wave function to the matrix product form. One applies all the $H_A$ terms, and then all the $H_B$ terms, etc.

Although this method seems very efficient, a number of aspects are novel for DMRG users, stemming from the fact that one does not ordinarily deal with the matrix product representation directly. Implementing this idea into a DMRG algorithm may be time consuming and may require a very substantial rewriting of one's program.

In this Letter we take the key idea of the Suzuki-Trotter decomposition, but we modify it and apply it in a more natural way within the context of DMRG. The result is a surprisingly simple yet very powerful modification of the algorithm for real-time dynamics which we believe can be incorporated into a typical program in only a day or two of programming. We illustrate the approach with real-time simulations which set a new paradigm for the size and accuracy obtainable.

The standard DMRG representation of the wave function at a particular step $j$ during a finite-system sweep is

$$|\psi\rangle = \sum_{l\alpha\beta r} \psi_{l\alpha_j\alpha_{j+1}r} |l\rangle|\alpha_j\rangle|\alpha_{j+1}\rangle|r\rangle. \tag{2}$$

Here we have a left block containing many sites (with states $l$), two center sites (with states $\alpha_j$, $\alpha_{j+1}$), and a right block (states $r$). The states $l$ and $r$ are formed as eigenvectors of a density matrix, and represent a highly truncated but extremely efficient basis for representing the ground state, plus any other targeted states which have been included in the density matrix. Now suppose we have an arbitrary operator $A$ acting only on sites $j$ and $j+1$. This operator can be applied to $|\psi\rangle$ exactly, and reexpressed in terms of the same optimal bases, with

$$[A\psi]_{l\alpha_j\alpha_{j+1}r} = \sum_{\alpha'_j\alpha'_{j+1}} A_{\alpha_j\alpha_{j+1};\alpha'_j\alpha'_{j+1}} \psi_{l\alpha'_j\alpha'_{j+1}r}. \tag{3}$$

  

If $A$ included terms for other sites, we could not write this simple exact relation; new bases would need to be adapted to describe both $|\psi\rangle$ and $A|\psi\rangle$, requiring perhaps several finite-system sweeps through the lattice.

This implies that we can apply the link time evolution operator $\exp(-i\tau H_j)$ exactly on DMRG step $j$. Accordingly, we adapt the Suzuki-Trotter decomposition to match the DMRG finite-system sweeps. We decompose the time propagator as

$$e^{-i\tau H} \approx e^{-i\tau H_1/2} e^{-i\tau H_2/2} \ldots e^{-i\tau H_2/2} e^{-i\tau H_1/2}. \quad (4)$$

This decomposition is good to the same order (errors of order $\tau^3$) as the usual odd/even link decomposition, and gives a reversible time evolution. When applied $1/\tau$ times to evolve one unit of time, the errors are $\tau^2$. The main idea is then to apply $\exp(-i\tau H_1/2)$ at DMRG step 1, then $\exp(-i\tau H_2/2)$ at step 2, etc., forming the usual left-to-right sweep, then reverse, applying all the reverse order terms in the right-to-left sweep.

This procedure requires one to use the step-to-step wave function transformation first developed to provide a good guess for the Lanczos or Davidson diagonalization [9]. It transforms the wave function from the basis of step $j \pm 1$ to that of step $j$. Assuming this transformation is present, the real-time algorithm introduces only a very minor modification: at step $j$, instead of using the Davidson method, one evolves the transformed wave function by applying $\exp(-i\tau H_j/2)$. Before the time evolution starts, we typically use ordinary DMRG to find the ground state. Next, we either (i) change the Hamiltonian, or (ii) apply an operator to the ground state to study a new wave function which is a combination of excited states.

As a first test case, of type (i), we study the models of Eqs. (2) and (5) in Ref. [5] corresponding to a quantum dot connected to two noninteracting leads, and a junction between two Luttinger liquids, respectively, driven out of equilibrium by a voltage bias. In these cases at $t = 0$ a bias in the chemical potential is turned on as a smoothed step function, making the new Hamiltonian time-dependent. At each time step, the expectation value of the current operator [defined by Eq. (4) of Ref. [5]] is calculated. In Fig. 1 we show the results for a chain of length $L = 64$ and the same set of parameters used in Ref. [5], keeping only $m = 128$ states and using a time step $\tau = 0.2$. It should be compared to Figs. 1 and 2 in Ref. [5] and Figs. 1 and 2 in Ref. [6]. Our results exceed the accuracy obtained by the previous methods, with fewer states. For the noninteracting problem, the agreement with the exact results is excellent up to times $t \sim 70$. We obtain higher accuracy for fixed $m$ compared to Ref. [6] because at any step we only need to target one state at one instant of time. Note that the ground state DMRG gives essentially exact results keeping only ~64 states, roughly half as many as the time-dependent one.

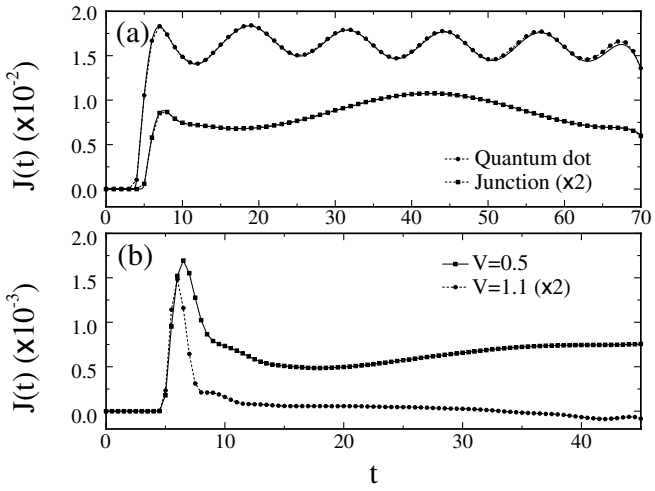


FIG. 1. (a) Tunneling current through a noninteracting quantum dot and a junction as defined in Eqs. (2) and (5) in Ref. [5], respectively. The full lines correspond to exact results. (b) Tunneling current through an interacting junction, with $V = 0.5$ and $V = 1.1$. All the DMRG results where obtained with $M = 128$ and a time step $\tau = 0.2$.

In method (ii), we apply the operator $A$ to the ground state $|\phi\rangle$ at $t = 0$, to obtain $|\psi(t = 0)\rangle$, and evolve in time. To calculate time-dependent correlation functions, we time evolve both $|\phi(t)\rangle$ and $|\psi(t)\rangle$, including both as target states for the DMRG density matrix. Although the time dependence $\exp(-iE_G t)$ of $|\phi(t)\rangle$ is known ($E_G$ is the ground state energy), by evolving it we keep its representation in the current basis. In addition, we expect some cancellation in the errors due to the Suzuki-Trotter decomposition in constructing the correlation functions. A typical correlation function is calculated as

$$\langle\phi|B(t)A(0)|\phi\rangle = \langle\phi(t)|B|\psi(t)\rangle, \quad (5)$$

We use a complete half-sweep to apply $A$ to $|\phi\rangle$. In particular, if $A$ is a sum of terms $A_j$ over a number of sites, then we apply an $A_j$ only when $j$ is one of the two central, untruncated sites. During this buildup of $A$ at step $j$ we target both the ground state $|\phi\rangle$ and $\sum_{j'=1}^{j} A_{j'}|\phi\rangle$.

As an example, we consider the spin-1 Heisenberg chain, with Hamiltonian

$$H = \sum_j \vec{S}_j \vec{S}_{j+1}, \quad (6)$$

where we have set the exchange coupling $J$ to unity. This system has a gap (the "Haldane gap") of $\Delta_H = 0.4105$ to the lowest excitations, which are spin-1 magnons at momentum $\pi$, and a finite correlation length of $\xi = 6.03$ [10]. (Note that the models of Fig. 1 are gapless.) The single-magnon dispersion relation has been calculated with excellent accuracy [3]. However, determination of the full magnon line is quite tedious with existing DMRG

methods. Here we show how to calculate the entire magnon spectrum with only one time-dependent DMRG run.

We take $A = S^+(j)$ for a single site $j$ in the center of a long chain. This operator constructs a localized wave packet consisting of all wave vectors, which then spreads out. The different components move at different speeds, given by the group velocity, determined as the slope of the dispersion curve at $k$. In Fig. 2 we show the local magnetization $\langle\psi(t)|S^z|\psi(t)\rangle$ for a chain of length $L = 200$, with time step $\tau = 0.1$. At $t = 0$, the wave packet has a finite extent, with size given by the spin-spin correlation length $\xi$. At later times, the different speeds of the different components give the irregular oscillations in the center of the packet. We kept $m = 150$ states per block, giving a truncation error of about $6 \times 10^{-6}$.

From this type of simulation we can construct the Green's function

$$G(x, t) = -i\langle\phi|T[S_x^-(t)S_0^+(0)]|\phi\rangle \qquad (7)$$

as $G(x, t) = -i\langle\phi(|t|)|S_x^-|\psi(|t|)\rangle$. Here $x$ is measured from the site $j$ where $S^+$ is applied. We make one measurement of $G(x, t)$ for each left-to-right DMRG step, namely, for step $x$. For efficiency we measure as we evolve in time, rather than, say, devoting every other sweep to measurements without time evolving. This may worsen the Suzuki-Trotter error somewhat, but we have found the results quite satisfactory. Since $G(x, t)$ is even in $x$ and $t$, the Fourier transform is

$$G(k, \omega) = 2\int_0^\infty dt \cos\omega t \sum_x \cos kx G(x, t). \qquad (8)$$

The spectral function is $-1/\pi \mathrm{Im} G(k, \omega)$. We inevitably have some cutoff in time $T$ for the available data. The maximum usable value of $T$ depends on the length of the chain: when the leading edge of the wave front hits the ends of the chain, the data no longer describe an infinite chain. However, before that point the data do describe an infinite chain with boundary effects dying off exponentially from the edges. This allows us to precisely specify the momentum $k$, for times $t < T$. To perform the time integration we multiply $G(x, t)$ by a windowing function $W(t)$ which goes smoothly to zero as $t \to T$. We have chosen a Gaussian, $\exp[-4(t/T)^2]$, which has the advantage of having a non-negative Fourier transform, yielding a non-negative spectral function [except for possible terms of size $\exp(-4)$]. Note that if the true spectral function has an isolated delta function peak, the windowed spectrum will have a Gaussian peak centered precisely at the same frequency. Thus it is possible to locate the single-magnon line with an accuracy much better than $1/T$. If a continuum is also present nearby, the peak is less well determined. In the case of the $S = 1$ chain, for $k$ near $\pi$ the peak is isolated, but at some point near $k = 0.3\pi$ the peak enters the two magnon continuum and develops a finite width. Note that from our single simulation we determine the spectral function for a continuum of values of $k$ and $\omega$.

In Fig. 3 we summarize the results for the single-magnon peak, determined automatically as the maximum of the spectrum. To gauge the errors we present several runs with various parameters. The values are very close; the largest errors are due to a finite $\tau$, with the $\tau = 0.4$ run

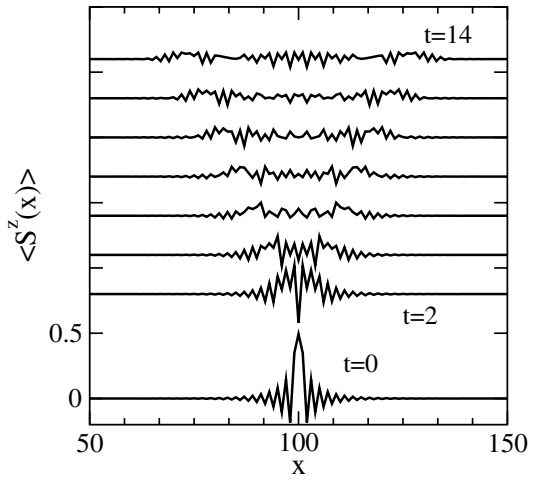


FIG. 2. Time evolution of the local magnetization $\langle S^z(x)\rangle$ of a 200 site spin-1 Heisenberg chain after $S^+(100)$ is applied.

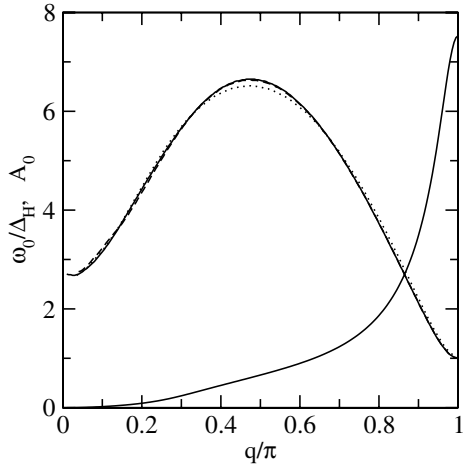


FIG. 3. The single-magnon line of the spin-1 Heisenberg antiferromagnetic chain. The entire spectrum is obtained from one DMRG run, by Fourier transforming the time and position dependent correlation function $\langle S_l^-(t)S_0^+(0)\rangle$. The broad solid curve shows the location of the maximum in the spectra for a particular $q$, in units of the Haldane gap, 0.41050(2), for a system of $L = 600$ sites, using a time step $\tau = 0.02$, running for $T = 27.3$, and keeping $m = 200$ states. For comparison, results from two other runs are shown: $L = 400$, $\tau = 0.1$, $T = 60$, and $m = 150$ (dashed curve); and. $L = 400$, $\tau = 0.4$, $T = 72$, and $m = 200$ (dotted curve). The solid curve peaked at $q = \pi$, shown only for the first run, is the weight $A_0$ in this quasiparticle peak, i.e., $S(\omega) \approx A_0\delta(\omega - \omega_0)$.

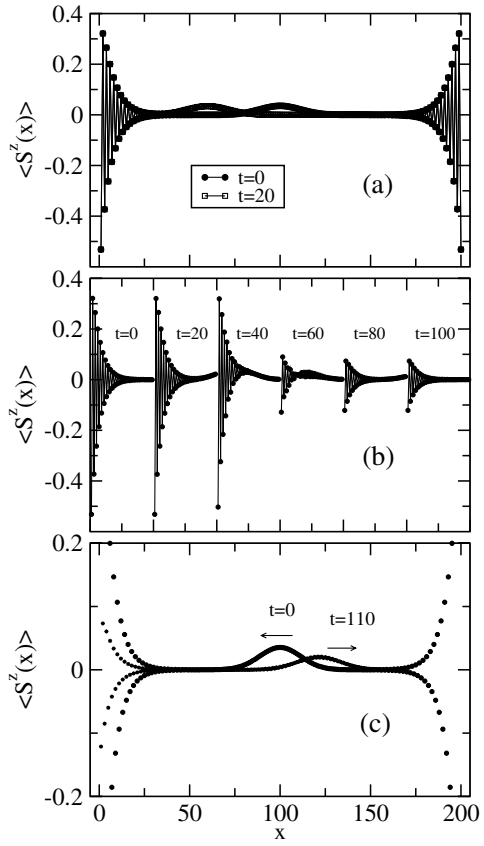


FIG. 4. A Gaussian magnon wave packet with momentum $k = 0.8\pi$, $S^z = 1$, and half-width 16 scattering off the left end of a 200 site spin-1 chain. The chain end states initially have $S^z = -1/2$. We measure $\langle S^z(x)\rangle$ at time $t$, and $\tau = 0.2$. In (a) we show $t = 0$ and $t = 20$. In (b), we show the leftmost 50 sites for a number of times. In (c), we show the whole chain for $t = 0$ and $t = 110$. After the scattering, the system is in a nonlocal superposition of spin-flip and non-spin-flip states.

showing some non-negligible errors. The results agree very well with accurate frequency-based DMRG results [3] and quantum Monte Carlo calculations [11].

With real-time dynamics, we can simulate processes which would be very difficult to understand via frequency dynamics. As an example, we consider a magnon wave packet scattering off the end of a spin-1 chain, shown in Fig. 4. The magnon is a triplet, with $S^z = 1$, and travels to the left with a speed of about 2.0. The open ends of a spin-1 chain have spin-1/2 degrees of freedom, which have received considerable attention [10,12]. An antiferromagnetic oscillation accompanies this state, decaying exponentially with the correlation length away from the edge. We choose the ground state with total spin $S^z = -1$, making the end states each have $S^z = -1/2$. When the wave packet hits the left end, it can scatter either with or without a spin flip occurring. If the spin flip occurs, the end spin changes to $S^z = 1/2$ and the wave packet to $S^z = 0$. We see from the figure that after the scattering, the end spin seems to have taken on an intermediate value of $S^z$, in particular $\langle S^z\rangle \approx -0.11$. Meanwhile, the wave packet seems to have a total spin of $\langle S^z\rangle \approx 0.61$. The intermediate values occur because we are observing a "macroscopic" quantum superposition of the state with and without the spin flip. Specifically, the scattering is described by the entangled state

$$|-\tfrac{1}{2}, 1\rangle \rightarrow a|-\tfrac{1}{2}, 1\rangle + b|\tfrac{1}{2}, 0\rangle, \tag{9}$$

where $a^2 \approx 0.61$, $b^2 \approx 0.39$. Note that the scattered $S^z = 0$ magnon does not show up when we measure $S^z_x$. A local description of the wave function, as $(\alpha|-\frac{1}{2}\rangle+\beta|\frac{1}{2}\rangle)\times(\gamma|1\rangle+\delta|0\rangle)$, is not possible; it does not conserve total $S^z$. Our measurement of $S^z_x$, $\langle\psi(t)|S^z_x|\psi(t)\rangle$, does not affect the state, but if one performed a real experiment and measured the spin of, say, the magnon after scattering one would obtain either $S^z = 1$ or $S^z = 0$. Our results raise the possibility of using such spin chains for experimental studies of quantum measurement and quantum computation.

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*Note added.*—After submission of this work, we became aware of closely related work by Daley, Kollath, Schollwoeck, and Vidal [13].

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