Time-Dependent Density-Matrix Renormalization Group: A Systematic Method for the Study of Quantum Many-Body Out-of-Equilibrium Systems

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The density-matrix renormalization-group algorithm is extended to treat time-dependent problems. The method provides a systematic and robust tool to explore out-of-equilibrium phenomena in quantum many-body systems. We illustrate the method by showing that attractive interactions enhance the tunneling current between two Luttinger liquids, whereas repulsive interactions suppress it, in qualitative agreement with analytical predictions. Enhancement of the transport current through a quantum dot in the Kondo regime is also exhibited.

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The study of out-of-equilibrium phenomena in quantum many-body systems has mainly focused on steady state properties, such as the conductance of quantum dot systems [1,2] and of point contacts between two Luttinger liquids [3,4]. More recently, attention has been paid to time-dependent phenomena in these systems [5–14]. One goal of the work has been to identify the hierarchy of time scales which arise when quantum many-body systems are driven out of equilibrium by a variety of time-dependent perturbations. This information is relevant for experiments involving potentially important technological applications of quantum dots and junctions built from carbon nanotubes, and quantum wires which behave as Luttinger liquids (LL) [4,15]. However, many studies have employed either uncontrolled approximations, or exact solutions at special values of the model parameters which are rather remote from experimentally accessible systems.

By contrast, the density-matrix renormalization-group (DMRG) algorithm [16,17] has been successfully employed to calculate many static and frequency-dependent properties of quasi-one-dimensional quantum many-body systems [17]. The numerical method does not depend on whether the system is integrable or not, and in many cases it provides essentially exact results as errors induced by truncating the Hilbert space are controlled in a systematic way.

We employ the so-called infinite-size DMRG [16,17] as it treats the center of the chain, the region where we focus our attention, most accurately. Our starting point is a quantum Hamiltonian representing a chain of L sites. If we denote by D the dimension of the Hilbert space on each site, then the dimension of the Hilbert space $\mathcal{H}$ is D^L. The DMRG algorithm organizes the Hilbert space into blocks, $\mathrm{B_L}\bullet\bullet\mathrm{B_R}$, where $\bullet\bullet$ represents the Hilbert space of the two central sites (of dimension D) and $\mathrm{B_L}$, $\mathrm{B_R}$ are, respectively, the blocks representing the Hilbert space of the remaining left and right sites, each of dimension $D^{L/2-1}$. An initial small chain of $L = 4$ sites is first enlarged to six sites by cutting it in half and inserting two sites at the center. As this process is repeated, the Hilbert space grows exponentially and eventually exceeds a limit, $(D * M)^2$, beyond which it is truncated. As the calculation may be systematically improved by increasing the size of the retained block Hilbert space, M, up to limits imposed by computer memory and speed, it is straightforward to check for convergence in the observables. The end result of the algorithm is an approximation to the exact many-body ground state $|\Psi_{\mathrm{o}}^{\mathrm{trunc}}\rangle$, the ground state energy E_0, and a truncated representation of the Hamiltonian, H_{trunc}.

The extension to time-dependent problems, which we call time-dependent DMRG (TdDMRG), takes the infinite-size DMRG algorithm described above as its starting point. After the penultimate iteration, when the chain has $L - 2$ total sites, either a quantum dot paired with an ordinary site or two sites linked by a tunneling junction (depending on the choice of problem to be studied) are inserted at the center of the chain, yielding a chain with a total of L sites. Finally, a time-dependent perturbation, $H'(t)$, is added to H_{trunc}, and the resulting time-dependent Schrödinger equation is then integrated forward in time:

$$i\hbar\,\frac{\partial}{\partial t}\,|\Psi(t)\rangle = [(H_{\mathrm{trunc}} - E_0) + H'(t)]\,|\Psi(t)\rangle. \quad (1)$$

The initial state is chosen to be the ground state of the unperturbed truncated Hamiltonian, $|\Psi(t=0)\rangle = |\Psi_{\mathrm{o}}^{\mathrm{trunc}}\rangle$.

To illustrate the method, we apply the TdDMRG algorithm to two kinds of systems: quantum dots and tunneling junctions between two chains of one-dimensional interacting fermions. We first consider the easier problem of spinless fermions (with small on-site Hilbert space dimension $D = 2$) before turning to a more realistic model involving electrons with spin.

Spinless fermions.—We turn first to the problem of a quantum dot coupled to two leads. A similar problem

has been studied by Wingreen *et al.* [5] in the thermodynamic $L \to \infty$ limit. In terms of the fermion creation and annihilation operators $c_j^\dagger, c_j$, and the number operators $n_j \equiv c_j^\dagger c_j$, the time-independent part of the Hamiltonian for the quantum dot system reads

$$H_{\text{qdot}} = -\frac{w}{2} \sum_{j \neq q-1,q} [c_{j+1}^\dagger c_j + \text{H.c.}] + \varepsilon_q n_q - t_q [c_q^\dagger c_{q-1} + c_{q+1}^\dagger c_q + \text{H.c.}]. \quad (2)$$

In this equation q denotes the location of the right central site where the quantum dot is located, $q = L/2 + 1$. Here t_q is the hopping amplitude between the dot and either lead, and $w > 0$ is the half bandwidth of the leads, which are half filled. The local chemical potential at the quantum dot site, ε_q, is generally nonzero. It may be viewed as the energy of a localized level.

The time-dependent perturbation is a differential bias applied between the left and the right leads:

$$H'(t) = -\delta\mu_R(t) N_{\text{R}} - \delta\mu_L(t) N_{\text{L}}. \quad (3)$$

We typically set $\delta\mu_L(t) = -\delta\mu_R(t) = \delta\mu_{\text{o}}\theta(t - t_{\text{o}})$, where $\theta(t)$ is a smoothed step function with rise time t_s: $\theta(t) = 1/[\exp(-t/t_s) + 1]$. Operators $N_{\text{R}} = \sum_{j=q+1}^{L} n_j$ and N_{L} (which has a similar expression) count the number of fermions in the right and the left leads.

It is convenient to gauge transform the bias into a local, but time-dependent, hopping amplitude by means of the transformation $|\bar{\Psi}(t)\rangle = e^{i\Phi(t)[N_{\text{R}} - N_{\text{L}}]/\hbar} |\Psi(t)\rangle$, where $\Phi(t) = \int_{-\infty}^{t} \delta\mu_L(t')\, dt'$. Thus, the real-valued hopping amplitude t_q is replaced by a complex-valued one: $\bar{t}_q(t) = t_q e^{i\Phi(t)/\hbar}$, and the differential bias, which acts on all the sites in the blocks, is absorbed into an operator that acts only locally on the central region of the chain where the infinite-size DMRG is most accurate.

The expectation values of the currents along the central links may be evaluated during the course of the wave function's time evolution [18] by calculating:

$$J_{q,q-1}(t) = -\frac{2e}{\hbar} \text{Re}\{i\bar{t}_q(t) \langle \bar{\Psi}(t) | c_q^\dagger c_{q-1} | \bar{\Psi}(t) \rangle\}. \quad (4)$$

Following Refs. [5] and [9], we introduce an average transport current defined as $J(t) = \frac{1}{2}[J_{q,q-1}(t) + J_{q+1,q}(t)]$. The results of our calculation are shown in Fig. 1. The exact solution for noninteracting systems is obtained by integrating the equations of motion for the quantities $\gamma_{ij} = \langle c_i^\dagger(t) c_j(t) \rangle$ forward in time for systems of the same finite size L; therefore the results can be compared directly with the TdDMRG calculations.

Another problem of recent interest is transport through a point contact or junction between two Luttinger liquids. As the DMRG algorithm works equally well for interacting leads, we may turn on nearest-neighbor interactions $V n_j n_{j+1}$ between the spinless fermions (again

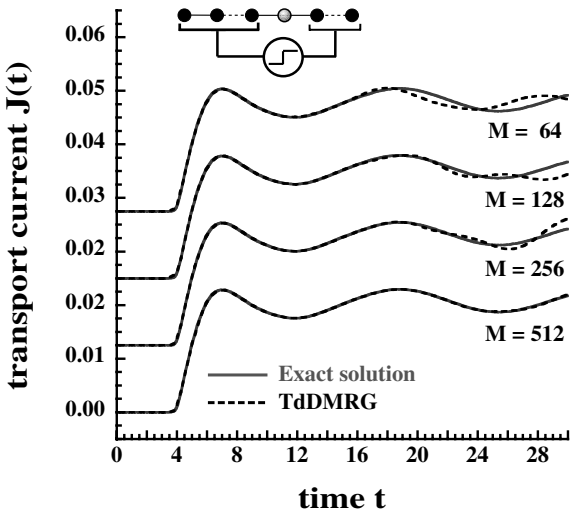

FIG. 1. Transport current $J(t)$ for the spinless quantum dot system defined by Eq. (2). The plots (which are offset in the vertical direction for clarity) illustrate systematic convergence towards the exact independent-particle solution with increasing block dimension M. Time is measured in units of $\tau_w \equiv \hbar/w$ and $J(t)$ is expressed in units of e/τ_w. The parameters are $t_q = 0.15w$, $\varepsilon_q = -0.25w$, and $L = 64$ sites. At time $t_{\text{o}} = 4\tau_w$, the chemical potential of the leads is shifted by a bias of $\delta\mu_{\text{o}} = -0.25w$ within a rise time of $t_s = 0.1\tau_w$. The period of the ringing oscillations is given by the expression reported in Ref. [5]: $\Delta t_R = 2\pi\hbar/|\delta\mu_R - \varepsilon_q| = 4\pi\tau_w$.

$q = L/2 + 1$):

$$H_{\text{junct}} = -\frac{w}{2} \sum_{j \neq q-1} [c_{j+1}^\dagger c_j + \text{H.c.}] + V \sum_{j \neq q-1} \left(n_{j+1} - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) - t_q [c_q^\dagger c_{q-1} + \text{H.c.}]. \quad (5)$$

At half filling the leads are metallic for $|V| < w$ and exhibit LL behavior [19]; otherwise a charge-density wave (CDW) forms and an insulating gap opens up. Kane and Fisher [3] studied this model in the continuum limit for $|V| < w$. Within perturbative RG and bosonization they concluded that intralead interactions strongly affect the transmittance of the junction. For attractive interactions ($V < 0$), the transmittance is enhanced, whereas for repulsive potentials ($V > 0$) it is suppressed.

Results for the two systems of spinless fermions are shown in Figs. 1 and 2. In both cases the short-time behavior of the current compares well with the available exact independent-particle results, even for rather small block Hilbert space dimension M (see also Fig. 3 below). This may seem surprising, as only the ground state was targeted in the DMRG portion of the algorithm. However, it is important to note that the DMRG algorithm is not a true renormalization-group method as the reduced density matrix, rather than energetics, determines which states are projected out of the Hilbert space. Over short times, the perturbation can create only a limited number of

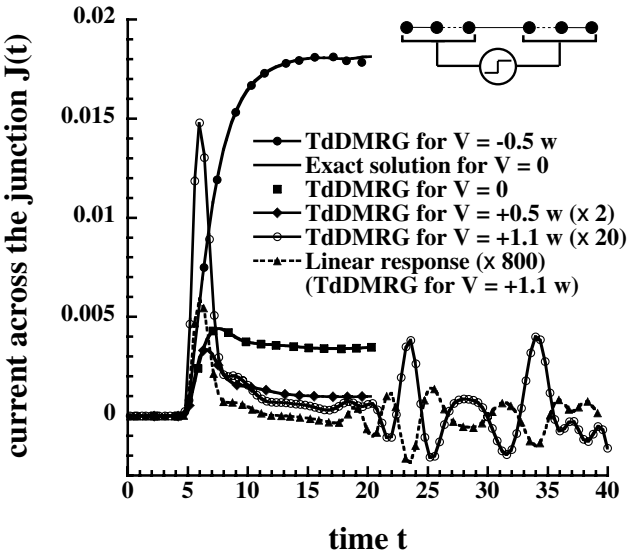

FIG. 2. Current across a junction between two systems of one-dimensional interacting electrons in response to a step bias applied between the two leads. Interactions strongly affect the currents, in qualitative agreement with the predictions of Ref. [3]. The junction consists of a weakened link with $t_q = 0.125w$ lying at the center of a chain of $L = 64$ sites. At time $t_o = 5\tau_w$, the bias is shifted by $\delta\mu_o = 0.0625w$ in a rise time of $t_s = 0.1\tau_w$. The label "linear response" refers to the application of a much smaller bias $\delta\mu_o = 6.25 \times 10^{-4}w$. Lines are for the more accurate $M = 512$ truncation (or, in the noninteracting $V = 0$ case, depict the exact solution), while data points are for $M = 256$. For clarity, currents have been multiplied by factors of 2, 20, and 800 as indicated. Note the good convergence with increasing blocksize M, and with the exact result in the noninteracting case. The units of current and time are the same as in Fig. 1. The reflection time $t_{refl} = 64\tau_w$ is longer than the time period shown.

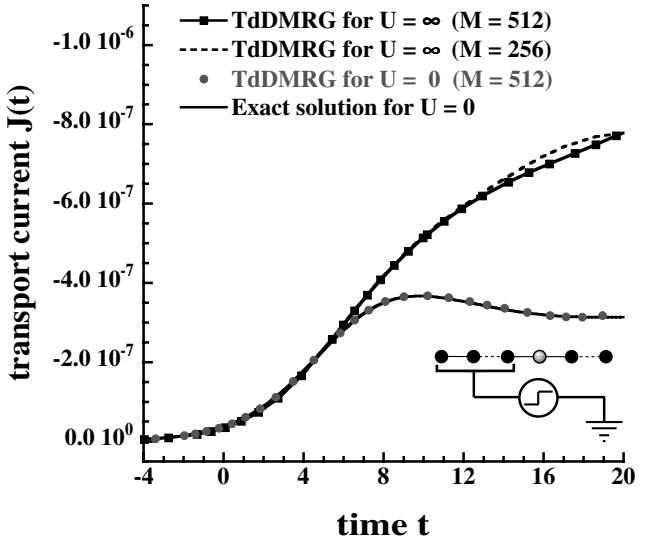

FIG. 3. Transport current $J(t)$ for a quantum dot in the Kondo regime driven out of equilibrium by a step bias applied to the left lead. $J(t)$ is enhanced compared to the noninteracting $U = 0$ case. The parameters used in the calculation are $L = 100$, $t_q = w/(4\sqrt{2})$, $\varepsilon_q = -0.25w$, and $U = \infty$, with a corresponding Kondo energy scale of order $k_B T_K = 0.003w$. The step in the bias is turned on at time $t_o = 4\tau_w$ within a rise time of $t_s = 2\tau_w$. The bias reduces the chemical potential of the left lead by a small amount, $\delta\mu_o = -5 \times 10^{-6}w$. As the time advances, small discrepancies show up between the more accurate $M = 512$ truncation (continuous curve with filled squares) and the $M = 256$ truncation (dotted curve). The units of current and time are the same as in Fig. 1.

excitations about the ground state, so the time-evolved state remains closely connected with the ground state and can be accurately represented with a superblock of relatively small Hilbert space dimension. Figure 1 also illustrates the systematic convergence with increasing blocksize M. By retaining more Hilbert space, we are able to extend the accurate solution forward in time. Nevertheless, even short-time behavior often suffices to reveal interesting physics. For example, the initial behavior of the junction current depicted in Fig. 2 is consistent with the prediction of Kane and Fisher [3]: An attractive interaction enhances the current $J(t)$, whereas a repulsive interaction suppresses it. It is interesting to observe that in the insulating CDW regime $V > w$ current oscillations develop after the initial transient. We emphasize that the TdDMRG method enables us to access short-time out-of-equilibrium phenomena in an accurate way, and thus goes well beyond bosonization.

Several other aspects of the TdDMRG method are worth mentioning. First, as the numerical method necessarily addresses only systems of finite size, the current averaged over long times must always vanish, regardless of the bias. This is so because any current pulse created by the bias eventually reaches the open ends of the chain within a time of order $t_{refl} = La/v_F$, where $v_F = wa/\hbar$ is the Fermi velocity and a is the lattice spacing. At that point the pulse is reflected back, leading to oscillations in the current. To be useful, model parameters must be chosen such that the physics of interest occurs over time scales shorter than t_{refl}. There is no limit on the size of the applied bias: Large biases can be applied, driving the system far outside of the linear-response regime, though we find that larger biases generally require larger blocksizes M to maintain the accuracy of the solution. Sizable biases were applied in the above two model problems (Figs. 1 and 2). The nonlinear effects of the bias are illustrated by the response in the $V > w$ regime shown in Fig. 2, as the form of the oscillations depends strongly on the size of the applied bias.

Spinning electrons.—To illustrate the application of the TdDMRG method to a more realistic problem involving spinning electrons, we turn now to the study of the one-impurity Anderson model described by the Hamiltonian

$$H_{\mathrm{qdot}} = -\frac{w}{2}\sum_{\sigma j \neq q-1,q}[c_{j+1}^{\dagger\sigma}c_{j\sigma} + \mathrm{H.c.}] + \varepsilon_q n_q + U n_{q\uparrow} n_{q\downarrow} - t_q \sum_{\sigma}[c_q^{\dagger\sigma}c_{q-1\sigma} + c_{q+1}^{\dagger\sigma}c_{q\sigma} + \mathrm{H.c.}]. \quad (6)$$

Here $\sigma = \uparrow, \downarrow$ labels the spin and $n_q \equiv n_{q\uparrow} + n_{q\downarrow}$ is the total number of electrons at the dot site. The one-impurity Anderson model is a minimal model to describe a quantum dot with spinning electrons coupled to leads [1]. The model also arises in studies of strongly correlated electron systems in the limit of infinite spatial dimension, in particular, within dynamical mean field theory (DMFT) [20]. The method presented here can be adapted to the calculation of the imaginary-time Green's functions needed in the DMFT calculations [21].

In this case only the bias of the left lead is shifted, $H'(t) = -\delta\mu_L(t)N_{\rm L}$, but again this shift can be gauge transformed into a time-dependent hopping amplitude. Results for the initial transport current $J(t)$ are shown in Fig. 3. Here $\varepsilon_q = -0.25w$ and the width $\Delta = 0.125w$; thus in the large-U limit the quantum dot is in the Kondo regime. For these parameters, the Kondo scale is estimated to be of order $k_B T_K = 0.003w$ [22]. For comparison, we also plot the current in the noninteracting $U = 0$ limit, calculated both exactly within the independent-particle picture, and via TdDMRG. The current for $U = \infty$ shows the expected Kondo enhancement [1,9]. Upon decreasing the hopping amplitude between the dot and the leads to $t_q = 0.05w$, we find by contrast that the current at $U = \infty$ is less than at $U = 0$. We attribute this drop to the existence of a Coulomb blockade, which now overwhelms the vanishingly small Kondo resonance [$k_B T_K = O(10^{-19}w)$]. A more detailed discussion of our results, also in other settings, will be given elsewhere [21].

In conclusion, we have shown that the DMRG algorithm can be extended to treat time-dependent problems. The TdDMRG method is a systematic tool to study the transient behavior of quantum many-body systems. The method has been illustrated by applying it to three systems: spinless and spinful quantum dots and a junction between two Luttinger liquids. Our results agree with previous predictions but do not rely on uncontrolled approximations. Reliable results can be obtained, even for systems driven far out of equilibrium.

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