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[6, 7] and of point contacts between two Luttinger liquids[4, 15]. More recently, attention has been paid to time-dependent phenomena in these systems[6, 7, 11, 12, 13, 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, 13]. 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[14]. 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, \( B_L \), where \( B_L \) represents the Hilbert space of the two central sites (of dimension \( D \)) and \( B_L \), \( B_R \) 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 6 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 \( |\Psi_o^{\text{trunc}}\rangle \), the ground state energy \( E_0 \), and a truncated representation of the Hamiltonian, \( H^{\text{trunc}} \).

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 \( H^{\text{trunc}} \), and the resulting time-dependent Schrödinger equation is then integrated forward in time:

\[
\frac{d}{dt} |\Psi(t)\rangle = \left[(H^{\text{trunc}} - E_0) + H'(t)\right] |\Psi(t)\rangle. \tag{1}
\]

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

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 di-
mension $D = 2$) before turning to a more realistic model involving electrons with spin.

1. 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.\cite{Wingreen} 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:

$$H_{\text{qd}} = -\frac{w}{2} \sum_{j \neq q-1, q} \left[ c_{j+1}^\dagger c_j + \text{H.c.} \right] + \varepsilon_q n_q$$

$$- t_q \left[ c_q^\dagger c_{q-1} + c_{q+1}^\dagger c_q + \text{H.c.} \right]. \quad (2)$$

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-band width of the leads, which are half-filled. The local chemical potential at the quantum dot site, $\varepsilon_q$, 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 right leads:

$$H'(t) = -\delta \mu_R(t) N_R - \delta \mu_L(t) N_L.$$  \quad (3)

We typically set $\delta \mu_L(t) = -\delta \mu_R(t) = \delta \mu_0 \theta(t-t_0)$, where $\theta(t)$ is a smooth step function with rise time $t_s$: $\theta(t) = 1/[\exp(-t/t_s) + 1]$. Operators $N_R = \sum_{j=q+1}^L n_j$ and $N_L$ (which has a similar expression) count the number of fermions in the right and left leads.

It is convenient to gauge-transform the bias into a local, but time-dependent, hopping amplitude by means of the transformation $\hat{\Psi}(t) = e^{i \Phi(t)/\hbar} |\Psi(t)\rangle$, where $\Phi(t) = \int_{-\infty}^t \delta \mu(t') dt'$. Thus the real-valued hopping amplitude $t_q$ is replaced by a complex-valued one: $i \tilde{t}_q(t) = t_q e^{i \Phi(t)/\hbar}$, 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 wavefunction’s time-evolution\cite{Fisher} by calculating:

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

Following Refs.\cite{Fisher} and\cite{Wingreen} 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.\cite{Wingreen}. The exact solution for non-interacting 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 $q = L/2 + 1$):

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

At half-filling the leads are metallic for $|V| < w$ and exhibit LL behavior\cite{Kane}; otherwise a charge-density wave (CDW) forms and an insulating gap opens up. Kane and Fisher\cite{Fisher} 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.\cite{Fisher} and\cite{Wingreen}. 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.\cite{Fisher} below).
in the insulating CDW regime
interaction suppresses it. It is interesting to observe that
M the non-interacting
interaction enhances the current
the junction current depicted in Fig. 2 is consistent with
interesting physics. For example the initial behavior of
to extend the accurate solution forward in time. Never-
size
relatively small Hilbert space dimension. Fig. 1 also illus-
and can be accurately represented with a superblock of
of excitations about the ground state, so the time-evolved
states are projected-out of the Hilbert space. Over short
time, the current oscillations
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 nec-
essarily 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 $t_{\text{rel}} = L_0/v_F$, where $v_F = w/\hbar$
is the Fermi velocity and $a$ 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 $t_{\text{rel}}$. There is no limit on the size
of the applied bias: large biases can be applied, driv-
ing the system far outside of the linear-response regime,
though we find that larger biases generally require larger
block sizes $M$ to maintain the accuracy of the solution.
Sizeable biases were applied in the above two model prob-
lems, Figs. 1 and 2. The non-linear effects of the bias are
illustrated by the response in the $V > w$ regime shown
in Fig. 3, as the form of the oscillations depends strongly
on the size of the applied bias.

2. 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:

$$H_{\text{qdot}} = -\frac{w}{2} \sum_{\sigma \neq q-1, q} \left[ c_{j+1}^{\dagger} c_{j\sigma} + H.c. \right]$$

$$- \varepsilon_q n_q + U n_{q\uparrow} n_{q\downarrow}$$

$$- t_q \sum_{\sigma} \left[ c_{q\sigma}^{\dagger} c_{q-1\sigma} + c_{q+1\sigma} c_{q\sigma} + H.c. \right].$$

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 de-
scribe a quantum dot with spinning electrons coupled
to leads. The model also arises in studies of strongly
correlated electrons systems in the limit of infinite spa-
tial 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,
$H'(t) = -\delta H_L(t) N_L$, 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 esti-
ated to be of order $k_B T_K = 0.003w$ [22]. For comparison
we also plot the current in the non-interacting $U = 0$
limit, calculated both exactly within the independent-
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