Dielectric Breakdown in the 1-D Hubbard Model

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Abstract. Nonequilibrium transport in the one dimensional Hubbard model at half-filling is studied by the time-dependent density matrix renormalization group method. It is clearly demonstrated that dielectric breakdown of the Mott insulating phase to a nonequilibrium steady state occurs when an external voltage is larger than the charge gap. From the numerically obtained current-voltage characteristics we find that the current is suppressed by the correlation effect when compared with that of a band insulator and that the current is scaled only by the charge gap for small voltages compared to the band width.

1. Introduction
The Hubbard model has been extensively studied by variety of methods as one of the most simplified model that captures important features of interacting electrons. Especially in one dimension various analytical and numerical approaches have been developed[1]. When the band is half-filled and the Coulomb energy is sufficiently strong, a finite energy $\Delta_c$ is required to make a charge excitation and this is a manifestation of the Mott insulating ground state. The insulating state can be broken by applying a bias voltage larger than $\Delta_c$[2]. This process, dielectric breakdown of a Mott insulator, may be called as a nonequilibrium metal-insulator transition.

From a theoretical point of view, in order to formulate a proper theory of the dielectric breakdown of the Mott insulator it is required to treat electron correlation rigorously in a nonequilibrium situation beyond the linear response theory. This difficulty have prevented us to make significant progress in theoretical understanding of the phenomenon.

Recently the density matrix renormalization group (DMRG) method[3] was extended to time-dependent problems[4]. This new algorithm (TdDMRG) has been successfully applied to nonequilibrium problems in one spatial dimension with strong correlation, such as single quantum dot system under finite bias voltages[5] and the interacting resonant level model[6].

Oka and Aoki studied the breakdown of the Mott insulating phase of the 1-D Hubbard model caused by an external electric field[7] using the TdDMRG method. They showed that the phenomenological Landau-Zener formula for the transition probability is consistent with the $U$ dependence of the threshold electric field if one replaces the band gap in the formula by the many-body charge gap $\Delta_c$. However they only discussed the threshold field of the breakdown and it is necessary to investigate current-voltage (I-V) characteristics beyond the breakdown to elucidate nature of nonequilibrium steady states of the 1-D Hubbard model.

In this paper the 1-D Hubbard model with a finite bias voltage is studied by the TdDMRG method. We determine the I-V characteristics for the repulsive 1-D Hubbard model at half-filling, and show that nonzero steady current appears when the bias voltage exceeds $\Delta_c$. We
find that by increasing the voltage beyond $\Delta_c$, the steady current is scaled only by $\Delta_c$ if the voltage is small compared to the band width and the Coulomb energy $U$.

2. Model and Numerical Method

We consider the 1-D Hubbard model at half-filling and at $T = 0$ with an applied DC voltage. In order to study nonequilibrium steady states numerically we first calculate the ground state of the system without the voltage term by the usual DMRG method. Then the time evolution of the ground state wave function, which is governed by the Hamiltonian with the voltage term, is simulated by the TdDMRG algorithm. The desired nonequilibrium steady state is expected to appear after some transient behaviors. The model Hamiltonian to be considered is therefore written as follows:

$$H(\tau) = H_L + H_R - t' \sum_{\sigma} (c_{i\sigma}^\dagger c_{r\sigma} + h.c.) + \frac{eV}{2} \theta(\tau) (N_L - N_R), \quad (1)$$

$$H_\alpha = -t \sum_{i,i+1 \in \alpha,\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + U \sum_{i \in L} c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_{i\downarrow} c_{i\uparrow} \quad (\alpha = L, R), \quad (2)$$

where $L(R)$ represents the left (right) half of the system, $N_\alpha = \sum_{i \in \alpha,\sigma} c_{i\sigma}^\dagger c_{i\sigma}$. $\tau$ is the time variable, $t$ the hopping amplitude, $U$ the Coulomb energy, $V$ the bias voltage. $c_{i\sigma}$ annihilates an electron with spin $\sigma$ at $i$th site. $l(r)$ is the index of rightmost (leftmost) site in $L(R)$ and $t'$ is the hopping between the $l$th and $r$th sites. Here we consider only $t' = t$ case for simplicity. The time dependence of the voltage term is set as the smoothed step function $\theta(\tau) \equiv (1 + \exp [(\tau_0 - \tau)/\tau_1])^{-1}$, in order to mimic adiabatic switching-on. We fix $\tau_0 = 4\hbar/t$ and $\tau_1 = \hbar/t$ throughout this paper. The nonequilibrium steady states realized using the above model Eq.(1) are equivalent to the ones realized in the case of switching-on of the hopping $t'$ instead of $eV$.

Results shown in this paper are obtained by the TdDMRG calculations for $L = 120$ system keeping $m = 1200$ states and using the 2nd order Suzuki-Trotter decomposition with time step $\Delta \tau = 0.05\hbar/t$. Examples of the truncation error and the Trotter error are shown in Fig.1 for $U/t = 3$ and $eV/t = 1$ and the errors are sufficiently small.

3. Results of Current as a Function of Time

Expectation values of the current operator after the switching-on of the bias voltage

$$J(\tau) = e \langle \psi(\tau) | \hat{N}_R | \psi(\tau) \rangle \quad (3)$$

is shown in Fig.1. In each case the current shows a steady-like behavior (in some cases with an oscillation) after relaxation. After a certain time the steady-like behavior collapses. We refer to the state in the time interval where the current stays at a constant value as a quasi-steady state.

The setup of the system inevitably involves reflection of the current at the edge[5, 8, 9]. The reflected excitations eventually arrive at the center of the chain and disturb the steady current. This effect forces one to take sufficiently long system size to simulate completely relaxed steady states before the disturbances. As a by-product one can estimate velocity of the excitations carrying the transient current from the the time the quasi-steady behavior ends. For $U = 0$ excitations of the system are the particle-hole excitations in the $-2t \cos k$ band, and the reflected waves moving with the Fermi velocity, which is 2 in the units of Fig.1, appears at the time $L/2$. The velocity slightly increases from 2 by increasing $U$, reflecting the fact that the velocity of the charge excitations of the ground state is an increasing function of $U$[1].
The steady currents are calculated by averaging $J(\tau)$ inside an interval $[30, 50]$ and shown in Fig.2. For comparison we also plot exact nonlinear currents in a (noninteracting) band insulator with the same magnitude of the charge gap. The Hamiltonian for the band insulator we used is obtained by replacing the interaction term in Eq.(2) by an alternating potential $(\Delta_b/2) \sum_{j\sigma} (-1)^j n_{j\sigma}$. The dispersion relation of the model has a band gap $\Delta_b$. From Fig.2 it is obvious that the current for $eV < \Delta$ is zero while for $eV > \Delta$ the current has a finite value, where $\Delta$ is $\Delta_c$ for the Mott insulator and $\Delta_b$ for the band insulator. One can see that the dielectric breakdown is successfully reproduced in our simulation. Comparison of the currents for both models shows that the correlation effect suppresses the current not only in the Mott insulating phase but also beyond the breakdown.

In Fig.2 we also show the I-V characteristics scaled by the gap $\Delta$. For each model data points of $J(V)$ for different values of $\Delta$ sit in a single curve when the voltage is small compared with the band width $D \simeq 4t$. When $eV$ becomes comparable to $D$ the energy dependence of the density of states of the band is not negligible, and therefore $J(V)$ deviates from the scaling curve. Likewise when $eV$ is comparable to $U$, excitations which are not influenced by the correlation effect can
Figure 2. (left) Current-voltage characteristics of the Mott insulator and the band insulator. The values of $\Delta_c$ obtained from the exact expression[1] are $\Delta_c(U = 1) = 0.005$, $\Delta_c(U = 2) = 0.173$, $\Delta_c(U = 2.5) = 0.371$ and $\Delta_c(U = 3) = 0.631$ in units of $t$. The band gap $\Delta_b$ are chosen to be the same as $\Delta_c$. (right) Current-voltage characteristics rescaled by the gap $\Delta_c$ or $\Delta_b$.

contribute to the current. Therefore the scaling behavior appears for $eV \ll \min(D, U)$.

5. Conclusions
We have studied nonequilibrium transport in the 1-D Hubbard model at half-filling with a finite bias voltage using the TdDMRG method. We have successfully reproduced the behavior of the dielectric breakdown in the I-V characteristics and found that the correlation effect suppresses the current compared to the noninteracting band insulator. Moreover we found that the current in the region $eV \ll \min(D, U)$ shows a universal behavior. We believe that these newly discovered nonequilibrium properties stimulate future studies of the dielectric breakdown. At the same time these reliable results demonstrate that various nonequilibrium problems in strongly correlated 1-D systems can be accurately investigated by the TdDMRG method.

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