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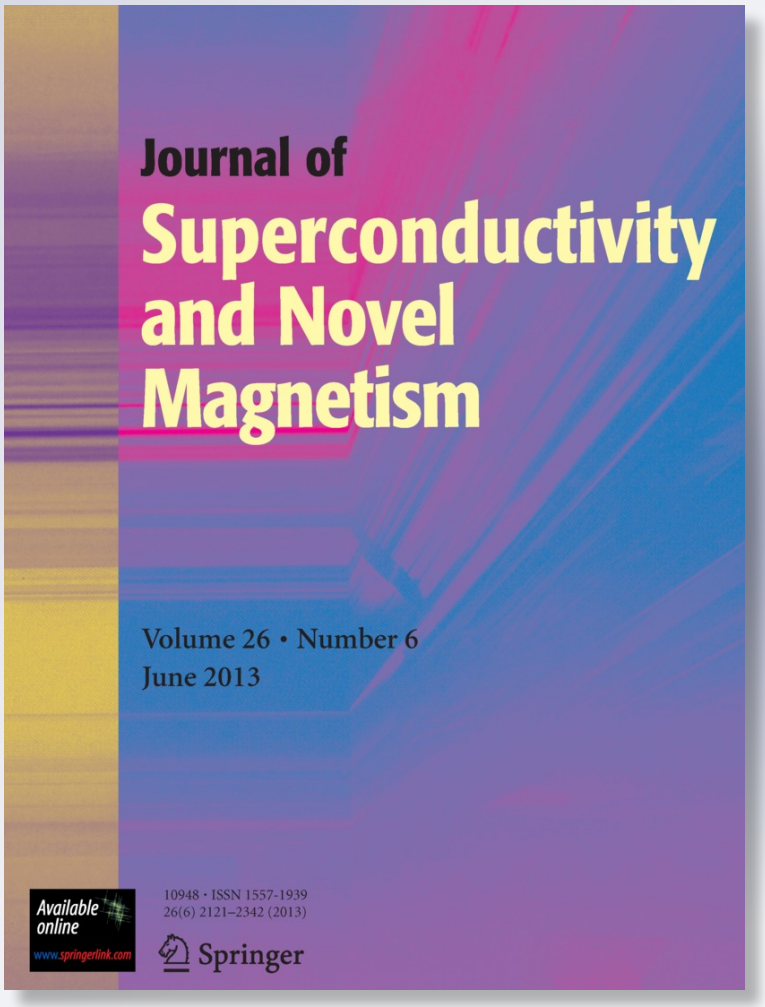

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ORIGINAL PAPER

Charge Excitations in Two-Leg Ladders: A tDMRG Approach

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Abstract We study the dynamics of holon–doublon pairs in two-leg Hubbard ladders with the time-dependent Density Matrix Renormalization-Group approach. Benchmark results show that the Krylov algorithm is well suited to calculate the time dependence of observables in these systems. Furthermore, we show that the dynamics of the holon–doublon depend strongly on the coupling asymmetry within the ladder, indicating that the ladder geometry plays a role in the decay of these elementary charge excitations.

Keywords DMRG · Hubbard model · Two-leg ladders · Excitations

1 Introduction

Photo-excited charge excitations in strongly correlated electron systems (SCES) offers interesting possibilities for energy harvesting in oxide-based solar cells. Experiments indirectly suggest that many highly correlated oxides could become technologically useful for light-to-energy conversion. For example, photo-catalytic processes are not quenched in manganite composites. A crucial question is whether charge excitations in the metal-insulator will be able to properly transfer the charge into the metallic contacts, thus establishing a steady-state photocurrent.

Theoretical studies of one-dimensional Mott insulators indicate that the mechanism for the decay of electron–hole excitations (i.e., a holon–doublon pair) into magnetic excitations is inefficient, making the holon–doublon pair is long lived [1, 2]. However, experimental realizations of SCES are seldom strictly one-dimensional. To control the values of their potentially useful intrinsic gaps, transition metal oxides are grown in complex layered superlattices. Therefore, this real-time study of the excitation propagation on ladders and other layered structures—as was done on one-dimensional chains—helps clarify the exciton decay and bound state formation.

The equilibrium properties of ladder systems have been previously studied in the literature with different techniques: nonperturbative methods to solve extended Hubbard models include [3] (i) quantum Monte Carlo methods, (ii) "diagonalization" methods, such as Lanczos algorithms and the density matrix renormalization-group (DMRG) method [4, 5]. These two paths to solve the problem are more or less complementary. Quantum Monte Carlo methods, being formulated in Matsubara frequency, have difficulty obtaining real frequency properties of the model (such as the density-of-states), and sometimes suffer from the so-called "sign problem" [6].

The DMRG method is a numerical variational technique to study quantum many body Hamiltonians and thus could be classified as a diagonalization method. For one-dimensional and quasi one-dimensional systems, the DMRG

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algorithm is able to truncate, with bounded errors and in a general and efficient way, the underlying Hilbert space to a constant size. Recently, a time-dependent version of the DMRG technique (tDMRG) has been introduced [7, 8], allowing for calculations of the dynamics of observables when time-dependent perturbations are applied to the equilibrium state.

In this contribution, we address this issue by studying the time evolution of charge excitations in two-leg ladders with tDMRG using the DMRG++ code [9, 10]. The model is introduced in Sect. 2. In Sect. 3, we present the results: We first establish benchmarks for the time evolution by comparing tDMRG calculations for the noninteracting case with exact results and also the chain and a disconnected ladder. We then present results for interacting ladders, showing a strong dependence of the holon–doublon decay with the relative coupling between the ladder legs. Finally, we present our closing remarks in Sect. 4.

2 Model and Methods

We consider the total Hubbard-like Hamiltonian

$$\hat{H} = \sum_{i,j} t_{ij} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma} + U \sum_{i} \hat{n}_{i\uparrow} n_{i\downarrow} + \sum_{i,j} V_{i,j} \hat{n}_i \hat{n}_j, \tag{1}$$

where the notation is similar to that of [1]. The hopping matrix t, however, now corresponds to that of a 2-leg ladder, such that $t_{ij} = t_x$ if i and j are nearest neighbors in the x direction, $t_{ij} = t_y$ if i and j are nearest neighbors in the y direction, and 0 (zero) otherwise. The same is true for V_{ij}, which is equal to V_x if i and j are nearest neighbors in the x direction, to V_y if i and j are nearest neighbors in the y direction, and 0 (zero) otherwise.

We define the holon and doublon operators, respectively, as $h^{\dagger}_i = \sum_{\sigma} \hat{c}_{i\sigma}(1 - \hat{n}_{i\bar{\sigma}})$, and $d^{\dagger}_i = \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{n}_{i\bar{\sigma}}$, where $\bar{\uparrow} = \downarrow$ and $\bar{\bar{\sigma}} = \sigma$.

As in [1, 2], we model the electron and hole created by light absorption with the excited state at time $\tau = 0$ $|\Psi_e(0)\rangle = h^{\dagger}_i d^{\dagger}_j |\Psi_0\rangle$, where $|\Psi_0\rangle$ is the ground state of the system before the excitation, and i and j are chosen fixed sites where the excitation occurs. In [1], these sites were situated in the center of the chain. In our case, we will also locate the interaction in the center, but since we are using a 2-leg ladder, we use the configuration depicted in Fig. 1.

2.1 Time Evolution with the Krylov Method for the DMRG Algorithm

The next step is to calculate the time evolution of observables $\langle \hat{O} \rangle(\tau) = \langle \Psi_e(\tau) | \hat{O} | \Psi_e(\tau) \rangle$ where $|\Psi_e(\tau)\rangle = e^{-i\hat{H}\tau} |\Psi_e(0)\rangle$ with tDMRG. Many methods for the calculation of dynamic observables with DMRG have been proposed. For a review, see [11]. Here, we will use the time-step-targeting Krylov method, as described in [12]. The main reason for this choice instead of, let us say, the Trotter–Suzuki decomposition method is that the latter depends on the form of the Hamiltonian, whereas the Krylov method is more generic and more suitable for the treatment of ladders.

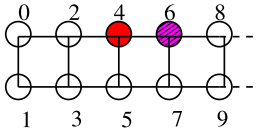

Fig. 1 Two-leg Hubbard ladder considered. The *filled circles* represent the sites where the holon and doublon excitations are created. The *numbers* are the site indexes

3 Results

3.1 Accuracy of the Krylov Method: $U = 0$ Benchmark

We started our computational runs for this project by first testing the Krylov method, and indirectly the convergence of the DMRG, for the noninteracting $U = 0$ system. There are two advantages to using the $U = 0$ system as a test case. First, we can compute all results exactly with polynomial complexity (code available at http://www.ornl.gov/~gz1/FreeFermions.), and second, the U term, being on-site, is not a major source of convergence problems for the DMRG algorithm.

The observable we test in this section is the local charge, defined as

$$n_{i,j,p}(\tau) = \sum_{\sigma=\uparrow,\downarrow} \langle \Psi_0 | d_j h_i e^{i\hat{H}\tau} n_{p\sigma} e^{-i\hat{H}\tau} h^{\dagger}_i d^{\dagger}_j | \Psi_0 \rangle, \tag{2}$$

calculated on the state $|\Psi_e(\tau)\rangle$. Results are shown in Fig. 2 for the holon–doublon pair created at sites $i = 10$ and $j = 11$ and the charge measured at site $p = 11$ (see Fig. 3 for site indexes). The agreement with exact results is excellent, indicating the time-evolution with the Krylov method works well.

3.2 Comparison Between the Chain and Disconnected Ladder

The remaining results will refer to the double occupation

$$N^d_{i,j,p}(\tau) = \langle \Psi_0 | d_j h_i e^{i\hat{H}\tau} n_{p\uparrow} n_{p\downarrow} e^{-i\hat{H}\tau} h^{\dagger}_i d^{\dagger}_j | \Psi_0 \rangle, \tag{3}$$

of the state $|\Psi_e\rangle(\tau)$.

In Fig. 3, we compare the time evolution of the total double occupation $N^d = \sum_p N^d_{i,j,p}$ with the WFT-Krylov

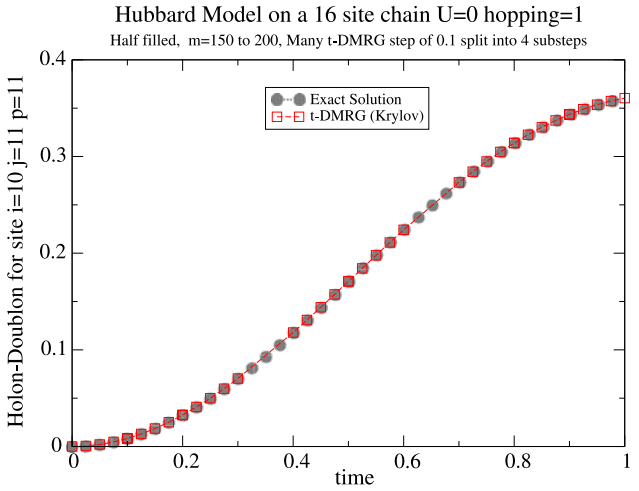

Fig. 2 Local charge at site $p = 11$ for a holon–doublon pair created at sites $i = 10$ and $j = 11$ with $U = 0$. The *filled circles* represent the exact solution

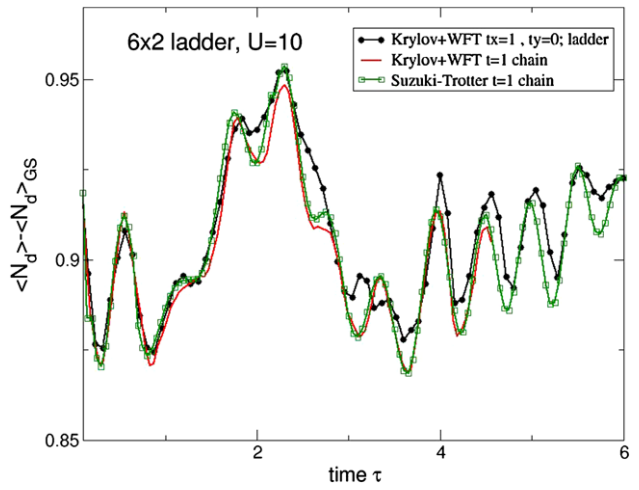

Fig. 3 Double occupation $N_d(\tau)$ vs. time for the chain and unconnected ladder cases with $U \neq 0$

time evolution in two cases: (i) a 6×2 two-leg ladder with $t_x = 1$, $t_y = 0$ (uncoupled ladder legs), $U = 10$ and (ii) a 6-site Hubbard chain with $t = 1$ and $U = 10$. In the following, we have subtracted the (constant) ground-state contribution $N^d_{\mathrm{GS}} = \sum_p \langle \Psi_0 | n_{p\uparrow} n_{p\downarrow} | \Psi_0 \rangle$. We have also checked the Krylov method by comparing it with the case in which a Suzuki–Trotter decomposition is used for the chain.[1]

A comparison of the results show a good agreement, indicating that the Krylov time evolution for the ladder case yields the expected results in the limiting case when the ladder legs are disconnected. It should be noted that the two-leg ladder is numerically more demanding than the chain, causing the comparison not to be perfect. Nevertheless, the

[1]Suzuki–Trotter calculation done using a tDMRG code by Adrian Feiguin.

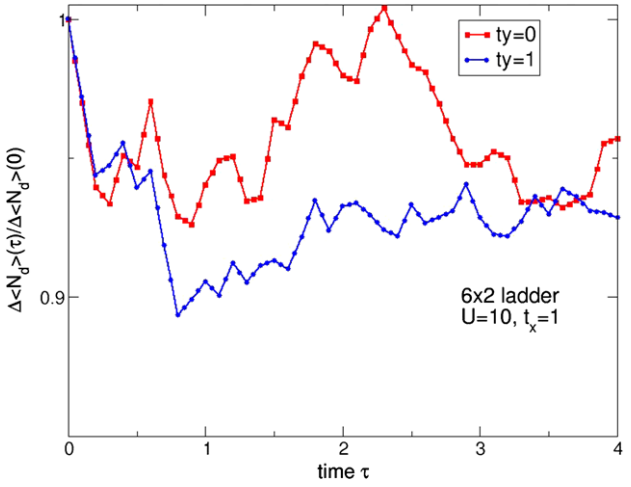

Fig. 4 Change in double occupation $\Delta N_d(\tau)$ (see text for details) vs. time for the two-leg ladder cases with $U = 10$, $t_x = 1$, and $t_y = 0, 1$

agreement in Fig. 3 shows that the errors accumulated during the Krylov time evolution do not imply significant deviations from the more amenable chain case.

3.3 Results for $U \neq 0$

Next, we have computed the total double occupation $N_d(\tau) = \sum_p N^d_{i,j,p}(\tau)$ for the case of a 6×2 ladder with $U = 10$ and horizontal hopping $t_x = 1$. Figure 4 shows $\Delta N_d(\tau) = N_d - N_d^{\mathrm{GS}}$ (where N_d^{GS} is the total double occupation of the ground state) for $t_y = 0, 1$. Due to the intense computational demand for this calculations, we present results for relatively small system sizes and short times. Even within those limitations, a distinctive difference in the decay of $\Delta N_d(\tau)$ is present, with a hint of a lower plateau in the $t_y = 1$ data. This might indicate that a more "2D-like" geometry affects the dynamics of the holon–doublon pair and the time evolution of the double occupation, possibly offering an additional decay channel that is not present in the strictly 1D case. Confirmation of this tendency can be obtained with calculations using larger system sizes and longer time scales, which will be reported elsewhere [13].

4 Conclusions

In this work, we have studied the time evolution of holon–doublon pairs in two-leg Hubbard ladders with the time-dependent DMRG method. Our benchmark results show that the Krylov algorithm is well suited to calculate the time dependence of observables in these systems. Furthermore, we find that the dynamics of the holon–doublon depend strongly on the coupling asymmetry within the ladder, indicating that the ladder geometry and dimensionality play an important role in the decay of these elementary charge excitations.

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