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Anomalous non-equilibrium electron transport in one-dimensional quantum nano wire at half-filling: time dependent density renormalization group study

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Abstract. We study non-equilibrium properties of one-dimensional Hubbard model by the density-matrix renormalization-group method. First, we demonstrate stability of “doublon”, which characterized by double occupation on a site due to the integrability of the model. Next, we present a kind of anomalous transport caused by the doublons created under strong non-equilibrium conditions in an optical lattice system regarded as an ideal testbed to investigate fundamental properties of the Hubbard model. Finally, we give a result on development of the pair correlation function in a strong non-equilibrium condition. This can be understood as a development of coherence among many excited doublons.

1. Introduction

Recently, photoinduced insulator-metal transition has attracted a lot of attention since the experimental observation of the surprisingly ultrafast non-equilibrium phase-transition \cite{1,2,3}. Several theoretical studies has been made to understand the mechanism of the ultrafast dynamics during the phase transition. However, all properties of the phase transition have been not fully resolved \cite{4}. On the other hand, optical lattice system is a new fascinating avenue toward “quantum simulator” \cite{5,6}. This system gives us an almost pure Hubbard model because of its perfectly clean feature. Thus, one can easily observe dynamical properties of the Hubbard model in various non-equilibrium conditions. Namely, one can systematically examine unsolved non-equilibrium properties of the Hubbard model.

The theoretical description of non-equilibrium phenomena is one of the most challenging problems in many-body physics. In weak non-equilibrium cases, we have a very powerful tool to evaluate physical quantities, i.e., the linear response theory \cite{7}. But, the theory is limited to “weak” non-equilibrium (near equilibrium) system. Thus, “strong” non-equilibrium system is still a frontier in many-body Physics. Recently, non-equilibrium phenomena in one-dimensional (1D) system attract much interest of theorists, because some kinds of 1D systems show curious behaviors, i.e., no relaxation to thermal equilibrium if the system’s Hamiltonian is almost integrable. This was demonstrated by not only numerical simulations \cite{8} but also
surprisingly cold atom experiments [9]. The experiments also indicate that the cold atom system is an ideal testbed for 1D non-equilibrium phenomena. For example, the doublon tunneling was indeed observed in both the bosonic optical well [10] and the center of mass motion of attractive interacting fermions in an optical lattice [11], while the doublon decay was found out in 3D fermionic optical lattice [12] as our expectation.

In this paper, we present non-equilibrium dynamics of 1D Hubbard model obtained by using time-dependent density-matrix renormalization group (TDDMRG) method [13, 14, 15] which enables us to access “strong” non-equilibrium condition in addition to strong correlation. This method is an extension of the density-matrix renormalization method, [16, 17, 15] which is a very powerful tool for investigation of static and dynamical properties of 1D Hubbard model.

2. Model and Method
Let us start with introducing the model employed throughout this paper. The main part of the model is the 1D Hubbard model, which is the most fundamental model describing strongly correlated fermions. The Hamiltonian is given

\[ H_H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \]  

where \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}, \sigma = \uparrow, \downarrow \), and \( \langle i,j \rangle \) represents summation with nearest neighbor sites. \( t \) is the hopping parameter and \( U \) is the on-site interaction strength.

In the rest of the paper, we add time-dependent perturbations to this Hamiltonian to observe non-equilibrium behaviors. In order to study the time evolution of the 1D Hubbard model, we use TDDMRG method [16, 17, 15].

3. Stability of Doublon
First, we examine the doublon creation and its stability. We study the following two conditions, one of which is the half-filling 1D Hubbard chain lying inside a flat 1D space with open boundary condition described by \( H_1 \) and another of which is 1D Hubbard chain confined by a harmonic well potential \( H_2 \).

\[ H_1 = H_H + H_{\delta t(\tau)}, \]  
\[ H_2 = H_H + H_V + H_{\delta t(\tau)}, \]  
\[ H_{\delta t(\tau)} = \delta t \sin(\omega \tau) \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma}, \]  
\[ H_V = \sum_{i,\sigma} V(x_i - x_c)^2 n_{i\sigma}, \]

where \( \delta t \) is the modulation strength of the hopping parameter, \( \omega \) is the modulation angular frequency, \( \tau \) is the normalized time by \( 1/t \), \( x_i = ai \) is the position of the \( i \)-th site, where \( a \) is the lattice constant, and \( x_c \) is the position of the trap center. In both cases, we use the following parameters, the system size \( U/t = 8, \omega/t = 8 \), and \( \delta t/t = 0.1 \). The total system size \( L = 40 \) for the flat potential case and \( L = 60 \) for the trapped potential case. In the latter case, we choose the trap strength \( V a^2/t = 0.01 \). The initial states in these Hamiltonians \( H_1 \) and \( H_2 \) are shown in Figs. 1 and 2, respectively. In both cases, the perturbation \( H_{\delta t(\tau)} \) is switched on at \( \tau = 0 \) and off at \( \tau = 20 \), and the number of the doublons \( N_d = \sum_i (n_{i\uparrow} n_{i\downarrow}) \) is measured.

First, let us study the model \( H_1 \). We find that the doublons are created by the perturbation \( H_{\delta t} \) until it is switched off (Fig. 3, upper blue line). After switching off (\( \tau > 20 \)), the number of the doublons does not change at all (see Fig. 4, upper blue line). This reflects the absence of
Figure 1. An initial state in the $H_1$ model. The horizontal and vertical axes represent the site number and both the density of the fermions and the spin polarization.

Figure 2. An initial state in the $H_2$ model. The horizontal and vertical axes represent the site number and both the density of the fermions and the spin polarization.

Figure 3. The time evolution of the number of doublons in the $H_1$ (the upper blue line) and $H_2$ (the lower red line) models. The horizontal and vertical axes represent the normalized time and the number of doublons, respectively.

Figure 4. The enlarged figure of the time evolution of the number of doublons in $H_1$ (the upper blue line) and $H_2$ (the lower red line) models. The horizontal and vertical axes represent the normalized time and the number of doublons, respectively.

thermal equilibrium due to the integrability. Then, the doublon is a stable excited particle in the 1D Hubbard model if it is once created.

On the other hand, in the model $H_2$ (Fig. 3, the lower red line), the number of doublons $N_d$ slightly decreases. This is because that the integrability is partly broken by the confinement harmonic potential $H_V$ in $H_2$. However, the decay speed is not so fast (see Fig. 4, lower red line). Then, the doublon can be regarded as a quasi-stable particle. These strong doublon stability is clearly contrast to the experimental results in 3D optical lattice [12]. This difference is reasonable because the spatial dimension plays a crucial role in the non-equilibrium process as mentioned above.

In this section, we have shown that the doublon is a (quasi-)stable particle in 1D Hubbard chain if it is once created. We have demonstrated that the created doublons play an important
role in transport in the following sections.

4. Anomalous Center of Mass Motion in Optical Lattice System
In this section, we examine the center of mass (CoM) motion of fermionic atoms loaded on 1D optical lattice system in order to study transport properties of 1D Hubbard model. The reason why we pay attention to such a specific CoM motion is that the confinement potential is an inevitable setup in the optical lattice systems. However, we would like to note that the optical lattice is perfectly pure without any impurities. Such a system is quite excellent for studies of the transport (non-equilibrium) physics intrinsic to the Hubbard model.

The CoM motion is caused by a sudden shift of the confining potential (see Fig. 5). Then, the target Hamiltonian is given by

$$H_3 = H_H + H_{V(\tau)},$$

(6)

$$H_{V(\tau)} = \sum_{i,\sigma} V (x_i - x_c + d\theta(\tau))^2 n_{i\sigma},$$

(7)

where $d$ is a shift distance of the trap center (Fig. 5), and $\theta(\tau)$ is the step function. In this study, we choose the system size $L = 40$, the number of particles $N = N_1 = 12$, the trap strength $Va^2/t = 2.63 \times 10^{-3}$, the trap center $x_c/a = 20.5$, and the shift distance $d/a = 3$. We prepare four initial states with $U/t = 1, 2, 3,$ and $4$ respectively (Fig. 6), where one finds that the phases are metallic for all $U$’s. We define CoM as $X = \sum_i i n_i / N$ and we also define $X = X - x_c + d$ for convenience.

![Figure 5](image-url)  
**Figure 5.** A cartoon picture of the way to drive the center of mass motion in optical lattice system.

![Figure 6](image-url)  
**Figure 6.** Initial states with $U/t = 1, 2, 3,$ and $4$ in the $H_3$ model. The horizontal and vertical axes represent the site number and the density of the fermions, respectively.

We display the time evolution of $X$ (Fig. 7) and the number of doublons $N_d$ (Fig. 8). One finds damped oscillating behaviors when $U/t = 1$ and $2$ (Fig. 7). In addition, one also finds the damped oscillation of $N_d$ (Fig. 8). From these doublon behaviors, we can interpret that the CoM motion is mainly governed by single fermion tunneling, because the number of doublons vary during the single fermion tunneling (Fig. 9). On the other hand, one finds the over-damped motion when $U/t = 3$ and $4$ (Fig. 7). In these cases, $N_d$ does not change oscillatory (Fig. 8). This implies that the over-damped motion is caused by the doublon tunneling, because this process does not effectively change $N_d$ (Fig. 10). From these consideration, we expect that the
doublon causes the over-damped motion. In fact, such a motion was also observed in attractive interaction cases, where the doublons are obviously stable due to the interaction. This scenario can be easily confirmed by a comparison between experiments and simulations in the attractive cases.

\[ U/t = 1, 2, 3, 4 \]

\[ X = a \]

**Figure 7.** The time evolution of the CoM for the \( H_2 \) model with \( U/t = 1, 2, 3, \) and \( 4. \) The horizontal and vertical axes represent the normalized time and \( X \) defined in the text, respectively.

\[ N_d \]

**Figure 8.** The time evolution of the number of the doublons for the \( H_2 \) model with \( U/t = 1, 2, 3, \) and \( 4. \) The horizontal and vertical axes represent the normalized time and the number of the doublons defined in the text, respectively.

**Figure 9.** A cartoon picture of the single tunneling.

**Figure 10.** A cartoon picture of the doublon tunneling.

5. Time Evolution of Pair Correlation

In the previous section, the doublon, i.e., a bosonic excitation plays a crucial role in non-equilibrium physics in 1D fermionic Hubbard model. However, we have not examined "coherence" among many doublons yet. Then, we investigate the coherence of the doublons in this section. In order to study the time evolution of the coherence of doublons created by some strong disturbance, we examine the following Hamiltonian with AC field.

\[ H_4 = H_H + H_W(\tau), \]

\[ H_W(\tau) = \sum_{i,\sigma} W i \theta(\tau) \sin(\omega \tau) n_{i\sigma}, \]

where \( W \) is the amplitude of the AC field and \( \omega \) is the angular frequency of the AC field (Fig. 11). In this study, we choose the following parameters, the system size \( L = 10, \) the number of particles \( N_1 = N_1 = 5, \) the interaction strength \( U/t = 8, \) the angular frequency \( \omega/t^{-1} = 8, \)
and the AC field strength $W/t = 1$. In such a system, we evaluate the time evolution of the magnetic (spin) and superconductivity (pair) correlation functions defined by

$$\Delta(r) = \frac{\sum_{|i-j|=r}[\Delta_i^\dagger \Delta_j]}{\sum_{|i-j|=r}},$$  

$$S(r) = \frac{\sum_{|i-j|=r}(S_i \cdot S_j)}{\sum_{|i-j|=r}},$$

where

$$\Delta_i = c_i^\dagger c_i,$$

$$S_i = \begin{pmatrix} c_i^\dagger \\ c_i \end{pmatrix} \sigma \begin{pmatrix} c_i^\dagger \\ c_i \end{pmatrix}.$$

Here, $\sigma$ is the vector representation of the Pauli matrix. The following is the simulated situation. Firstly, we prepare the ground state of half-filled 1D Hubbard model $H_H$ with $L=10$, $U/t=8$, which is the Mott insulating state. Secondly, we add the AC field from $\tau = 0$ to create carriers, i.e., doublons as well as holons (Fig. 11). In this paper, we choose just a resonant AC field frequency ($\omega/t = U/t = 8$). The doublons and holons are not created, if we take off-resonant frequency (not shown in this paper). During the carrier creation process, the number of the doublons increases as shown in Fig. 12. This implies that the system is finally excited far from the ground state by the AC field. Then, it is expected that the correlation in the excited state is considerably different from the ground state. Indeed, one finds that the pair correlation drastically develops (Fig. 13) in the far non-equilibrium-state while the spin-spin correlation does not vary significantly during the addition of the AC field (Fig. 12). This result indicates that the created doublons gains a coherence in non-equilibrium excited states. This non-trivial result can be obtained by the TDDMRG method allowing us to trace the time evolution of strongly correlated systems.

6. Summary

In this paper, we clarified some fundamental properties of 1D Hubbard model in non-equilibrium conditions. First, we demonstrated that the doublon is a (quasi-)stable particle when it is created once by pumping externally. Second, we exhibited that the doublon plays a crucial role in CoM motion of strongly correlated fermions in trapped optical lattices. Indeed, the doublon tunneling (co-tunneling) causes the overdamped motion of CoM. Finally, we presented that the created doublons gains coherence in non-equilibrium situations. Some of these results are detectable in the future optical lattice experiments. We believe that non-equilibrium condition in strongly correlated matters is a quite promising frontier of advanced physics.
Figure 12. The time evolution of the number of the doublon by the irradiation of AC field. The horizontal and vertical axes show the normalized time and the number of doublons, respectively.

Figure 13. The magnetic (spin) (the upper blue line) and the superconductivity (pair) (the lower red line) correlation functions at \( \tau = 100 \). The horizontal and vertical axes show the distance \( r \) and the absolute value of the correlation functions, respectively. The value of these correlation functions at \( \tau = 0 \) are shown as green lines for comparison.

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