Nonadiabatic Dynamics of Ultracold Fermions in Optical Superlattices

Atsushi YAMAMOTO,†1 Makoto YAMASHITA,‡3 and Norio KAWAKAMI§

1Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan
2NTT Basic Research Laboratories, NTT Corporation, Atsugi, Kanagawa 243-0198, Japan
3Japan Science and Technology Agency, CREST, Chiyoda-ku, Tokyo 102-0075, Japan
§Department of Physics, Kyoto University, Kyoto 606-8502, Japan

We study the time-dependent dynamical properties of two-component ultracold fermions in a one-dimensional optical superlattice by applying the adaptive time-dependent density matrix renormalization group to a repulsive Hubbard model with an alternating superlattice potential. We clarify how the time evolution of local quantities occurs when the superlattice potential is suddenly changed to a normal one. For a Mott-type insulating state at quarter filling, the time evolution exhibits a profile similar to that expected for bosonic atoms, where correlation effects are less important. On the other hand, for a band-type insulating state at half filling, the strong repulsive interaction induces an unusual pairing of fermions, resulting in some striking properties in time evolution, such as a paired fermion co-tunneling process and the suppression of local spin moments. We further address the effect of a confining potential, which causes spatial confinement of the paired fermions.

KEYWORDS: optical lattice, ultracold atoms, quantum dynamics, density matrix renormalization group

Ultracold atoms in optical lattices offer unprecedented potential for exploring many-body effects. This system is considered to be an ideal realization of the Hubbard model that has been intensively studied for many years in condensed matter physics. Recent successful demonstrations of the Mott-insulator phase transitionprove that we can obtain a comprehensive understanding of complicated many-body effects from a quantitative comparison of experiments and theories.

High controllability of experimental parameters is one of the outstanding features of ultracold atoms. In optical lattices, this allows us to study the nonadiabatic dynamics of ultracold atoms by measuring the time evolution of atomic states after a quick modification of the lattice potentials or a sudden change in inter-atomic interactions via Feshbach resonance. Experiments are carried out in an ultrahigh vacuum so that energy is conserved and the quantum dynamics can remain coherent during the time evolution. Various intriguing properties have already been reported: the collapse and revival of a Bose-Einstein condensate, the quantum version of Newton’s cradle, the co-tunneling of bound atom pairs, spin dynamics mediated by exchange interactions, and second-order atom tunneling. These experimental observations have stimulated theoretical investigations. Several numerical approaches have been applied to the Bose-Hubbard model and the Fermi-Hubbard model to reveal the nonequilibrium dynamics of many-body states that is largely unavailable in traditional condensed matter systems. However, most theoretical investigations have focused on bosonic systems owing to the current experimental situation. This naturally motivates us to study the nonadiabatic dynamics of fermions with strong correlations.

In this paper, we investigate the nonadiabatic dynamical properties of two types of insulating states in a one-dimensional (1D) optical superlattice with two-site periodic potential,

\[ H = -J \sum_{i=1}^{L} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + H.c. \right) + U \sum_{i=1}^{L} n_{i,\uparrow} n_{i,\downarrow} \]

\[ -V_d \sum_{i=odd,\sigma} n_i + V_c \sum_{i=1}^{L} \left( i - \frac{L+1}{2} \right)^2 n_i, \]

where \( c_{i,\sigma}^\dagger (c_{i,\sigma}) \) is a creation (annihilation) operator of a fermion at the \( i \)-th site with spin \( \sigma (=\uparrow, \downarrow) \). Here \( J \) is the nearest-neighbor hopping integral, \( L \) the total number of lattice sites, \( U (> 0) \) is the on-site repulsive interaction and \( V_d \) is the strength of the two-site periodic superlattice potential. \( V_c \) is the curvature of a harmonic confining potential, which will be dealt with later in this paper. The ground state properties of the system without a confining potential were clarified in connection with quasi-1D organic molecules and the effect of confinement was addressed in the context of cold fermions. Among several intriguing phases caused by the superlattice structure, here we consider two types of insulating states as an initial state of time evolution: Mott-type and band-type insulating states, which are respectively realized at quarter- and half-filling with a large potential.
difference, $V_d \gg J$.

In the following, we deal with the dynamics of the above fermionic superlattice at quarter- and half-filling (we temporarily set $V_i = 0$). To realize nonadiabatic control of our system, we suddenly change the lattice potential from $V_d/J = 20(t = 0)$ to $V_d = 0(t > 0)$ as shown in Fig. 1. We make use of the adaptive time-dependent density matrix renormalization group (adaptive t-DMRG) method which is an extended version of the original DMRG supplemented by the time-evolving block decimation algorithm. The adaptive t-DMRG method can deal with the real-time dynamics of strongly correlated systems. We thus calculate the time-dependence of the density profile $\langle n_i \rangle$, the variance of local spins $\Delta S_i^z = \langle S_i^z \rangle^2 - \langle S_i^z \rangle^2$ and the double occupancy of fermions $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$. We check the accuracy of t-DMRG by comparing the results with the time-dependent exact diagonalization for small systems. In the following, we adopt $J$ as units of energy and time is measured in the unit of $1/h$.

First, we investigate the nonadiabatic time evolution of a Mott insulating state at quarter-filling. Fermionic atoms are initially located at every other site because of the large potential difference $V_d = 20$ between even and odd sites, which may be described by a sequence of empty and singly occupied sites $0, 1, 0, 1, \ldots$ In the following, we show the time evolution of $\langle n_i \rangle$ at $V_i = 0$. The variance of local spins $\Delta S_i^z$ shows somewhat complicated behavior in the intermediate $U$ region, since it is given by $\frac{1}{4}(\langle n_i \rangle - 2\langle n_{i,\uparrow} n_{i,\downarrow} \rangle)$. With a large $U$ limit, however, $\Delta S_i^z$ is simply proportional to the local density $\langle n_i \rangle$, since the double occupancy tends to be zero.

We next investigate the time evolution of a band insulating state realized at half filling. Owing to the two-site periodic superlattice structure, the atoms are initially distributed with a spatial configuration of $0, 2, 0, 2, \ldots$ since $V_d = 20$ is very large. This drives the system to a kind of band insulating state. To elucidate the dynamical properties of the band insulating state at half filling, we study the time evolution of the physical quantities mentioned above. In Fig. 3, we present results computed for several different choices of $U$. Let us first focus on the local density $\langle n_i \rangle$ for even and odd lattice sites as shown in Fig. 3(a) and (b). The local density at even and odd sites clearly exhibits the particle-hole symmetry. It is seen that the oscillation period decreases as $U$ increases. The short time region shows the $t^2$-dependence and its coefficient does not depend on $U$, which is also the case for quarter filling. On the other hand, the oscillation period in $\langle n_i \rangle$ is strongly affected by the on-site interaction, in contrast to the quarter filling case. The period is approximately estimated in the limit of $V_d \gg U \gg J$, where the local density can be expressed as $\frac{4J}{\pi}(1 - \cos(Ut))$ based on time-dependent perturbation theory. This implies that the oscillation period decreases as $U$ increases. The short time region shows the $t^2$-dependence and its coefficient does not depend on $U$, which is also the case for quarter filling. On the other hand, the oscillation period in $\langle n_i \rangle$ is strongly affected by the on-site interaction, in contrast to the quarter filling case. The period is approximately estimated in the limit of $V_d \gg U \gg J$, where the local density can be expressed as $\frac{4J}{\pi}(1 - \cos(Ut))$ based on time-dependent perturbation theory. This implies that the oscillation period decreases as $U$ increases.

![Fig. 1](image1.png)  
Fig. 1. (Color online) Schematic diagrams of nonadiabatic control of one-dimensional optical superlattice: (a) an initial two-site periodic superlattice with a large potential difference $V_d$ and (b) a normal lattice after a sudden disappearance of $V_d$ for $t > 0$.

![Fig. 2](image2.png)  
Fig. 2. (Color online) Time dependence of the local quantities for several choices of on-site interaction for the system at quarter filling with $L = 36$ and $N = 18$. Plots of local density $\langle n_i \rangle$, variance of local spins $\Delta S_i^z$, and double occupancy $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$ from top to bottom. The on-site interaction is chosen as $U = 1$ (solid line), 5 (dashed line), and 9 (dotted line) at (a) $i = 18$ and (b) $i = 19$. 

sites, which thus reduces its probability and shortens the oscillation period (see discussions below for the oscillation period). For odd sites, as seen in Fig. 2(b), the amplitude of $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$ is smaller than that for even sites, since doubly occupied states at odd sites may be dominated by higher order hopping processes. The variance of local spin fluctuations $\Delta S_i^z$ shows somewhat complicated behavior in the intermediate $U$ region, since it is given by $\frac{1}{4}(\langle n_i \rangle - 2\langle n_{i,\uparrow} n_{i,\downarrow} \rangle)$. With a large $U$ limit, however, $\Delta S_i^z$ is simply proportional to the local density $\langle n_i \rangle$, since the double occupancy tends to be zero.
occillation period is changed as $1/U$, which is indeed in accordance with the numerical results. The double occupancy $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$ shows similar properties to the local density as regards its oscillating properties, although the former exhibits $t^*$-dependence in the short time region. The variance of local spin fluctuations is given by $\Delta S_i^z = \frac{1}{4}(\langle n_i \rangle - 2\langle n_{i,\uparrow} n_{i,\downarrow} \rangle)$, and therefore it exhibits the same oscillation periodicity as for the local density and the double occupancy. Note that $\Delta S_i^z$ exhibits similar profiles for even and odd sites, owing to the particle-hole symmetry.

In addition to the characteristic oscillating properties, we encounter some striking behavior at half filling. As seen in Fig.3, the variance of spin fluctuations $\Delta S_i^z$ at $i = 18$ and $i = 19$ is suppressed as $U$ increases, in contrast to the naive expectation that the local spin develops with increasing $U$. Also, all the quantities cease to oscillate as $U$ increases. To clarify the origin of this behavior, we plot the double occupancy summed in the unit cell $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle_{\text{sum}} = \langle n_{i=\text{odd},\uparrow} n_{i=\text{odd},\downarrow} \rangle + \langle n_{i=\text{even},\uparrow} n_{i=\text{even},\downarrow} \rangle$ in Fig.4. It is notable that $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle_{\text{sum}} \approx 0.9$ is hardly changed with time evolution for a large $U$, while it shows rather a strong time dependence for a small $U$. With a sudden change in $V_d$, two atoms occupying an odd site try to move apart from each other, but this process is not allowed for $U \gg J$, since the large potential energy $U$ cannot be transferred to the kinetic energy. This leads to an unusual pairing of fermions induced by a repulsive interaction. The resulting bound pairs can hop around lattice sites via a higher tunneling process called the co-tunneling process. For bosons, similar bound states and the associated co-tunneling process were proposed and observed experimentally.7 The bound pairs induced by the repulsive interaction are stable during time evolution and suppress the development of local spins, thus reducing $\Delta S_i^z$ for a large $U$. This naturally explains the unusual suppression of $\Delta S_i^z$ found in Fig.3, which is also confirmed by the fact that the local density profile is roughly given by twice the double occupancy $\langle n_{i,\uparrow} n_{i,\downarrow} \rangle$ for a larger $U$, as seen in Fig.3.

Finally, to make the model more accessible to experiments, we consider the effect of the harmonic confining potential given by the last term in Eq.(1). Figure 5 shows the time evolution of the physical quantities discussed above. The initial ground state ($t=0$) is assumed to be in a coexisting phase including two different insulating regions that roughly satisfy the conditions of half- and quarter-filling. We have confirmed that all the quantities in each insulating region exhibit the characteristic time dependence discussed above: the two-site alternating profiles are gradually smeared after the superlattice potential $V_d$ is turned off. According to the local density averaged in a unit cell $\langle n_i \rangle_{\text{ave}} = \frac{1}{2}(\langle n_{i=\text{odd}} \rangle + \langle n_{i=\text{even}} \rangle)$ shown in Fig.5, we can see that the plateau structure is quite stable around the center (half-filling), while it gradually collapses around the quarter-filling regions since they are close to the edges of the system. Although the spatial extent of the half-filling region ($\langle n_i \rangle_{\text{ave}} = 1$) is little changed with time evolution, its insulating characteristic gradually disappears. After the sudden potential change, the fermions form bound pairs and the resulting hard-core bosons can move via a co-tunneling process by keeping the number of doubly occupied sites unchanged. Correspondingly, the spin is not developed even in the long-time region, although the system is in a good condition $\langle n_i \rangle_{\text{ave}} = 1$ to realize an ordinary Mott insulator for $t > 0$. On the other hand, the quarter filling regions are dominated by unpaired fermions with strong repulsion, which are characterized by large spin fluctuations and vanishing double occupancy, as seen in Fig.5.

It should be stressed here that the half-filling region specified by $\langle n_i \rangle_{\text{ave}} = 1$, which is rather robust during time evolution, is spatially confined around the center, because hard-core bosons (paired fermions) created around the center experience the high pressure imposed by strongly correlated unpaired fermions from outside. This causes a unique confinement phenomenon as regards
striking features emerge: the strong repulsive interaction between fermions. On the other hand, in the half-filling case, more complex phenomena are observed. For a homogeneous system at quarter-filling, the time dependence exhibits a similar process to the paired fermions due to the strong repulsive interaction.

In summary, by using adaptive t-DMRG simulations, we have uncovered several intriguing dynamical features of repulsive fermions in a 1D optical superlattice. We have clarified how the correlated fermions evolve in time when a two-site periodic superlattice is suddenly changed. For a homogeneous system at quarter-filling, the time dependence exhibits a similar process to the paired fermions due to the strong repulsive interaction. When a two-site periodic superlattice is suddenly changed, the paired fermions due to the strong repulsive interaction are suppressed, and the time dependence exhibits a similar process.

**Fig. 5.** (Color online) Spatial distribution of the local fermion density \( \langle n_i \rangle \), the average fermion density \( \langle n_i \rangle_{ave} \), the variance of local spins \( \Delta S_j^z \), and the double occupancy \( \langle n_{i\uparrow} n_{i\downarrow} \rangle \) for (a) \( t = 0 \), (b) \( t = 1 \), (c) \( t = 2 \), and (d) \( t = 3 \). The system parameters are taken as \( U = 5.0 \), \( V_c = 0.025 \), \( L = 72 \) and \( N = 32 \). The initial state is in a coexisting phase including quarter- and half-filling insulating regions. Characteristic saw-toothed profiles are gradually smeared with time evolution.

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