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Ground-state properties of fermions in double-well optical lattices

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Abstract. We investigate the ground-state properties of fermions trapped in a one-dimensional double-well optical lattice by means of the density-matrix renormalization group method. A weak harmonic confinement potential inherent in real experiments, which makes the system inhomogeneous, is also considered. Under certain conditions for interactions, we find that two kinds of insulating regions coexist at half-filling and three-quarters filling due to the double-well structure and the system inhomogeneity. We further study the dynamical properties of the system by employing the adaptive time-dependent density-matrix renormalization group method. When the double-well lattice is suddenly changed into a normal single-well lattice, the two insulating regions gradually disappear under time evolution, which is accompanied by oscillating behavior of the local density characteristic of many-body fermionic systems.

Recent remarkable progress in atom manipulation techniques has realized unprecedented experiments with ultracold neutral atoms\cite{1, 2, 3}. An optical lattice, formed by a standing wave of laser light, is a typical example which provides the ideal stages for an experimental investigation of many-body problems in condensed matter physics via ultracold atomic gases. It is well known that the quantum phase transition from a superfluid (SF) to a Mott-insulator (MI) was observed by loading Bose-Einstein condensed atoms into a three-dimensional cubic optical lattice. The metal-insulator transition was also successfully demonstrated quite recently using fermionic $^{40}$K atoms\cite{3}.

On the other hand, the optical lattices consisting of double-well structures, i.e., double-well optical lattices\cite{4, 5, 6, 7, 8} have been realized in the recent reports. This system allows us to experimentally study a broad range of physics: quantum phase transition in condensed matter physics, atomic interferometer, quantum dynamics of atom tunneling, and quantum information processing. Theoretical investigations of double-well optical lattices, though focused on a bosonic system so far, have clarified the interesting reentrant phase transition (MI-SF-MI)\cite{9}.

In this paper, we numerically analyze the ground state properties of ultracold fermions trapped in a double-well optical lattice, and clarify the coexistence of two insulating regions caused by the double-well structure of lattice potentials and the system inhomogeneity. We then develop our calculations to study the quantum dynamics of the system, which are used to elucidate the time-evolution after the double-well lattice is suddenly changed into a normal single-well lattice.

A one-dimensional double-well optical lattice system is well captured by the following...
dimerized Hubbard model[10] with harmonic confinement:

$$\mathcal{H} = -J \sum_{i=even,\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + H.c. \right) - J' \sum_{i=odd,\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + H.c. \right) + U \sum_{i=1}^{L} n_{i,\uparrow} n_{i,\downarrow} + V_c \sum_{i,\sigma} \left( i - \frac{L + 1}{2} \right)^2 n_{i,\sigma},$$  \tag{1}

where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) a fermion at the $i$-th site with spin $\sigma$. Here $J$ and $J'$ are the hopping integral parameters at the even and odd sites respectively. $U$ is the one-site repulsive interaction, $n_i = c_{i,\sigma}^\dagger c_{i,\sigma}$ is the atom number operator, $L$ is the total number of lattice sites, and $V_c$ is the curvature of week harmonic trapping potential.

**Figure 1.** Profiles of local density (solid circle), variance of local density (solid triangle) and variance of local spin density (open square): (a) normal single-well lattice with $J'/J = 1.0$ and (b) double-well lattice with $J'/J = 0.2$. The other parameters are fixed as $L = 120$, $N_f = 70$, $U/J = 3.0$, and $V_c/J = 0.005$.

We first study the ground state of the 1D double-well lattice system by the density matrix renormalization group method[11]. Note here that the present model naturally includes a normal lattice system, i.e., $J'/J = 1.0$ in Eq. (1). For comparison, we first show the results computed for the normal single-well lattice in Fig.1(a) by choosing the parameters as $J'/J = 1.0$, $L = 120$, $U/J = 3.0$, $V_c/J = 0.005$, and the total number of fermions $N_f = 70$. The profile of local density $\langle n_i \rangle = \langle \sum_\sigma n_{i,\sigma} \rangle$ (solid circle) shows a convex structure reflecting the existence of weak harmonic confinement in our model. Both variance of local density $\Delta n_i = \langle n_i^2 \rangle - \langle n_i \rangle^2$ (solid triangle) and that of local spins $\Delta S_i^z = \langle S_i^z \rangle^2$ (open square) are smooth functions as expected from the profile of local density. From Fig.1(a) and the results on local compressibility[12, 13], we see that the system is metallic for the normal lattice.

Let us observe how the double-well structure of lattice affects the ground state properties. In Fig.1(b), we show the results for the double-well lattice system calculated with the same parameters except $J'/J = 0.2$. The profile of local density forms the plateaus at half-filling ($\langle n_i \rangle \sim 1.0$) and three-quarters filling ($\langle n_i \rangle \sim 1.5$) respectively, indicating that two different insulating regions coexist. In the plateau regions at half-filling, $\Delta n_i$ is rather large and $\Delta S_i^z$ is smaller than the value corresponding to the formation of local spin moment, i.e., $\Delta S_i^z < 0.25$. We find that the state in the half-filling regions is not a conventional Mott-insulator but a spontaneously dimerized insulator (SDI)[14, 15]. Further calculations on the spin correlation function have clarified that spin-singlet state is formed within the unit-cell of double-well lattice in the half-filling regions, which is closely related to the spin-Peierls phase in the uniform system[16]. In the plateau region at three-quarters filling, on the other hand, we can expect
another insulating state with large dimerization [10, 17], which is accompanied by doubling of the unit cell having three electrons in average. This leads to larger $\Delta n_i$ and smaller $\Delta S^z_i$ values as compared with those in the half-filling SDI regions (Fig. 1(b)).

We now turn to the time evolution of the present system [18] by suddenly changing the $J'$ value from $J'/J = 0.2$ to $J'/J = 1.0$ at the initial time $t = 0$. This corresponds to a sudden deformation of the lattice structure from the double-well lattice to a normal single-well lattice. We describe the time-evolution of the many-body states by means of the adaptive time-dependent density matrix renormalization group method [19]. Note that we consider a smaller-size lattice in this case, compared with the one used in Fig. 1, in order to carry out the computation more efficiently within restricted resources.

![Figure 2](image_url)

**Figure 2.** Time evolution of local density (solid circle) and variance of local density (solid triangle) after a sudden change of $J'$ value at $t = 0$ (from $J'/J = 0.2$ to $J'/J = 1.0$): (a) $t = 0.0$, (b) $t = 3.0$, (c) $t = 5.0$, and (d) $t = 7.0$. The other parameters are fixed as $L = 36$, $N_f = 20$, $U/J = 3.0$, and $V_c/J = 0.005$.

In Fig. 2, we show the results of the local density profile (solid circle) and its variance (solid triangle) at $t = 0.0$, 3.0, 5.0, and 7.0. As mentioned above, initially at $t = 0$, there are two kinds of insulating regions characterized by half-filling and three-quarters filling. It is seen that these two kinds of insulating regions gradually disappear after the double-well structure is switched off at $t = 0$, driving the system towards a metallic phase. Let us first focus on the region of three-quarters filling located around the center of the system. We find a dramatic change in time evolution of the local-density profile. After a sudden change in $J'$, a dip structure immediately emerges, giving rise to a two-peak structure in the density profile, as seen in Fig. 2(b) ($t = 3.0$). At $t = 5.0$, however, the dip disappears again and is replaced by a rather sharp peak structure, which is then smeared at $t = 7.0$. In this way, the density profile around the three-quarters filling is gradually smeared with characteristic oscillating behavior. We find that the behavior in time evolution appears quite differently around half-filling regions; the plateau like structure is rather robust under time evolution. In the ground state of double-well lattice at $t = 0$, the half filling regions are characterized by the spontaneously dimerized insulating state, while the corresponding ground state in long-time limit (normal single-well lattice) should realize a Mott-insulating state around there. Since the ground state in both limits has the insulating nature, the plateau structure is rather robust compared with the three-quarter region, although it is
indeed smeared due to non-adiabatic effects.

The above characteristic features stand in total contrast to those for free bosons, where the density profile is uniformly smeared. The striking time-dependence found here indeed originates from Fermi statistics and/or the strong repulsion between atoms: fermions have various momenta up to the Fermi momentum at $t = 0$, and this triggers high-energy fermions to move rapidly from the high to low density regions, giving rise to characteristic time dependence. Therefore, we can say that characteristic time evolution of the local density profile found here characterizes a many-body feature of interacting fermionic systems.

Summarizing, we have studied the ground state properties of ultracold fermions trapped in one-dimensional double-well optical lattices. It has been shown that two different insulating states can coexist under certain conditions. We have further investigated time-dependent phenomena by suddenly changing the double-well structure to the normal one. Some striking properties have been found for time evolution of the density profile around the two insulating regions. Characteristic oscillating behavior found here around three-quarters filling region is especially interesting. It remains an important issue to elucidate the nature of the oscillating behavior in detail, e.g. what really determines the period of oscillation, which is now under investigation.

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