Multiband effects on fermionic atoms in optical lattices

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Abstract. The superfluid-insulator transition of two-band fermionic atom systems in optical lattices is investigated by the two-site dynamical mean-field theory. Because of the spin-flip and pair-hopping interactions, orbital fluctuations are enhanced, leading to the suppression of the Mott insulating state. The numerical results are discussed in comparison with the effective boson model.

1. Introduction
Recent experiments have revealed fascinating aspects of ultracold atomic Fermi gases [1, 2, 3, 4, 5, 6]. The tunable interaction by Feshbach resonances [7] has made it possible to observe a crossover between the BCS superfluid for the weak attractive interaction and the Bose-Einstein condensate of bound fermion pairs for the strong attractive interaction. Furthermore, by loading fermionic $^{40}$K atoms into optical lattices, the topological change in the Fermi surface was observed by increasing the band-filling [8]. In this experiment, a band insulator was also observed by controlling the interaction. By increasing the depth of the optical lattice potential near the Feshbach resonance, a transition from a superfluid state to an insulating state was observed for fermionic $^{6}$Li atoms [9]. In this experiment, the possibility of the Mott insulator was discussed.

Stimulated by these experiments, various theoretical studies have been carried out concerning the superfluid-insulator transition [10, 11, 12, 13, 14]. In these experiments, it was argued that the usual single-band model was no longer applicable, because the strength of the on-site interaction exceeded the gap between the lowest and the next-lowest bands. To consider the superfluid-insulator transition for the fermionic atoms in optical lattices, therefore, both the correlation effects and the multiband effects have to be taken into account precisely.

In this study, we investigate the superfluid-insulator transition of interacting fermionic atoms in optical lattices, taking the two-band effects into account. For this purpose, we make use of a dynamical mean-field theory (DMFT) [15]. This method enables us to treat local correlation effects precisely and retains nontrivial local quantum fluctuations missing in conventional mean-field theories.

2. Model and method
Let us consider fermionic atoms in a periodic optical lattice potential: $V(r) = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz)$. In the low-tunneling limit, each lattice potential is regarded as a harmonic
one [16, 17]. In this case, the lowest orbital is nondegenerate, while the next-lowest orbital is three-fold degenerate. To introduce the effects of the lowest and next-lowest orbitals, we approximately neglect the degeneracy of the next-lowest orbital for simplicity. The hopping integrals between the lowest orbitals ($t_1$) and between the next-lowest orbitals ($t_2$) satisfy the relation $t_1 \sim \sqrt{V_0/E_r} t_0$, where $E_r = \hbar^2 k^2/2m$ is the recoil energy. Since $V_0/E_r < 10$ in the experiments [8, 9], we approximately set that $t_1 = t_2 \equiv t$. The system is assumed to involve the same number of fermionic atoms in two different hyperfine states, which are described as the pseudospins. The thus-modeled Hamiltonian reads

$$
\mathcal{H} = \sum_{<i,j>\sigma} (t - \mu \delta_{i,j}) c_{i\alpha \sigma}^{\dagger} c_{j\alpha \sigma} + \frac{D}{2} \sum_{\sigma} (n_{i2\sigma} - n_{i1\sigma}) + U \sum_{i\alpha} n_{i\alpha \uparrow} n_{i\alpha \downarrow} + \sum_{\sigma \sigma'} (U' - J \delta_{\sigma,\sigma'}) n_{i1\sigma} n_{i2\sigma'} - J' \sum_{i\alpha} c_{i1\sigma}^{\dagger} c_{i1\sigma} c_{i2\sigma}^{\dagger} c_{i2\sigma} - J'' \sum_{i} (c_{i1\uparrow}^{\dagger} c_{i1\downarrow}^{\dagger} c_{i2\uparrow} c_{i2\downarrow} + H.c.),
$$

where $c_{i\alpha \sigma}$ is the fermionic annihilation operator for the state with pseudospin $\sigma (\uparrow, \downarrow)$ on orbital $\alpha = (1, 2)$ in the $i$th lattice site and $n_{i\alpha \sigma} = c_{i\alpha \sigma}^{\dagger} c_{i\alpha \sigma}$ is the number operator. $t$ represents the hopping integral, $\mu$ the chemical potential, $D$ the splitting between the two orbitals. The third and fourth terms represent the intraorbital attractive on-site interaction between fermionic atoms and the interorbital ones, respectively. The last two terms are the interorbital ‘spin-flip’ and pair-hopping interactions, respectively, which may play an important role in fermionic optical lattice systems. For the lowest and the next-lowest orbitals, the coupling constants satisfy the relation $U' = J = J' = U/2(<0)$. We assume that the intraorbital attractive interaction induces an $s$-wave superfluid state.

In DMFT, the lattice model is mapped onto a single impurity model connected dynamically to a heat bath. We solve it self-consistently, applying the two-site DMFT method [18]. This method allows us to study the Mott transitions of orbitally degenerate lattice fermions qualitatively [19, 20]. To study the superfluid of lattice fermions, we extend this method to the case when the superfluid order exists [13]. A semicircular density of states (DOS) $\rho(\omega) = 4/(\pi W) \sqrt{1 - (\omega/W)^2}$ is used, where $W$ is the band width. Since the hopping integrals are assumed to be independent of $\alpha$, $W = 4t$ and the DOS are the same for both bands. The chemical potential is set $\mu = U/2 + U' - J/2$ so that particle-hole symmetry can be satisfied in both bands. In this case, the system is half filling. In the following, the hopping integral $t$ is used in units of energy.

3. Results and discussion

We calculate the superfluid order parameter $\Phi = \langle c_{i\alpha \uparrow} c_{i\alpha \downarrow} \rangle$, the quasiparticle weight $Z$, and the filling of each band $n_1$, $n_2$ for $U' = J = J' = U/2$ in the attractive $U$. For half filling, $\Phi$ becomes independent of $i$ and $\alpha$ in the DMFT procedure. $Z$ represents the coherent spectral weight of the Bogoliubov quasiparticle [21].

In Fig. 1(a), we show $\Phi$, $Z$, $n_1$, and $n_2$ as functions of $D$ for three values of $U$. As $D$ increases, $\Phi$ decreases rapidly around $D = 3$ and asymptotically approaches zero. For $U = -1.0$ Z increases monotonously towards $Z = 1.0$, while for $U = -2.0$ and $-3.0$ $Z$ first decreases for small $D$ and then increases towards $Z = 1.0$. The results are consistent with those for $n_1$ and $n_2$. As $D$ increases, $n_1$ ($n_2$) decreases (increases) monotonously from unity and asymptotically approaches zero (two). These findings indicate that the superfluid state becomes unstable towards the band insulating state. Since $\Phi$, $Z$, $n_1$, and $n_2$ asymptotically approach the fixed values, it is difficult to determine the superfluid-band insulator transition point. Such asymptotic behavior is considered to be caused by the interorbital spin-flip and pair-hopping interactions. Owing to these interactions, orbital fluctuations are enhanced, leading to the asymptotic behavior of $\Phi$, $Z$, $n_1$, and $n_2$. 


Figure 1. (Color Online) The superfluid order parameter $\Phi$, the quasiparticle weight $Z$, and the filling of each band $n_1, n_2$ for $U' = J = J' = U/2$. The results are show as functions of $D$ (a) and $U$ (b). In (b), $n_1 < 1 < n_2$ for $D = 1.0$ and $2.0$, while $n_1 = n_2 = 1$ for $D = 0$.

To see the possibility for the Mott insulating state, we show the $U$ dependence of $\Phi$, $Z$, $n_1$, and $n_2$ in Fig. 1(b) for three values of $D$. Even for large $|U|$, $Z$ and $\Phi$ stay nonzero and $n_1 < 1 < n_2$ at $D \neq 0$. The results imply that the superfluid state is robust. These findings are in contrast with those for $J' = 0$, where the Mott insulating state emerges for adequate values of $U$ and $D$ [13]. Because of the interorbital spin-flip and pair-hopping interactions, the Mott insulating state is suppressed to come into existence. To realize the Mott insulator, larger on-site attractive interaction may be needed.

We now discuss the numerical results from a viewpoint of the effective boson model, which is derived from the Hamiltonian (1) in the strongly attractive $U$,

$$\mathcal{H}_{\text{Boson}} = t_{\text{eff}}^B \sum_{\langle i,j \rangle} b_i^\dagger b_j + U_{\text{eff}}^B \sum_i n_i(n_i - 1),$$

where $b_i$ and $n_i = b_i^\dagger b_i$ represent the annihilation operator and the number operator of a bosonic fermion pair on the $i$th lattice site, and $t_{\text{eff}}^B = -2t^2/U$ and $U_{\text{eff}}^B = -(J'/2)(D/J')^2$ denote the effective hopping integral and the effective on-site interaction between two bosonic fermion pairs. In deriving the effective boson model, we assume that $D$ is smaller than $|U|$. Since the original model has only two orbitals, at most two bosonic fermion pairs occupy the same lattice site in the effective boson model. Under the condition for the lowest two orbitals: $U' = J = J' = U/2(< 0)$, we obtain $U_{\text{eff}}^B > 0$. The repulsive $U_{\text{eff}}^B$ plays a part in stabilizing the superfluid state but is probably too small to drive the superfluid state into the Mott insulator. The results based on
the effective boson model are consistent with the numerical results. In fact, the order of the effective interaction $U_{\text{eff}}^{B} \sim O(D^2/U)$ is rather smaller than that for $J' = 0$: $U_{\text{eff}}^{B} \sim O(U)$ [13], where the superfluid-Mott insulator transition occurs.

Comparing our previous results [13], we find that the superfluid state remains stable up to fairly large $|U|$ owing to orbital fluctuations caused by the interorbital spin-flip and pair-hopping interactions. If the degeneracy of the next-nearest orbital is introduced, orbital fluctuations are enhanced, rendering the superfluid state more stable. Recently, we have found that for $J' = 0$ the density wave (DW) state is more stable than the Mott insulating state [22]. Since the DW state is considered to be hardly affected by orbital fluctuations, the DW state probably emerges in the appropriately small $D$ and large $|U|$ region of the present system. On the other hand, the DW state may become unstable by thermal fluctuations. It is an interesting issue to investigate the superfluid-insulator transition of two-band fermionic atoms in optical lattices at finite temperatures. Such studies are now in progress.

Acknowledgments
We thank A. Koga, A. Yamamoto, and M. Yamashita for useful comments and valuable discussions. Numerical computations were carried out at the Supercomputer Center, the Institute for Solid State Physics, University of Tokyo. K.I. was supported by the Japan Society for the Promotion of Science. This work was supported by a Grant-in-Aid (No. 20540390) for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology, Japan.

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