Superfluid-insulator transition of two-band fermionic atom systems in optical lattices

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Abstract. We study the multiband effects on ultracold fermionic atoms in optical lattices by two-site dynamical mean-field theory. We find that the density wave state becomes stable for a small orbital splitting region. As the orbital splitting is increased, the transition from the density wave state to the superfluid state occurs. By systematically changing the orbital splitting and the attractive interaction, we obtain the phase diagram at half-filling.

Since the superfluid state was observed for ultracold fermionic atoms in optical lattices [1], intensive studies have been done for lattice fermion systems. In experimental studies, Feshbach resonances provide the means for controlling both the strength of the interaction between fermionic atoms and its sign [2]. Furthermore, by loading fermionic atoms into optical lattices, diverse interaction configurations can be introduced. The combination of these experimental techniques offers experimental descriptions of various intriguing quantum many-body phenomena.

In the ETH experiment, the topological change in the Fermi surface was observed by increasing the band-filling [3]. They produced a band insulator in the lowest band and then observed the partially populated higher bands. In the MIT experiment, a superfluidity of fermionic atom pairs was observed [1]. By increasing the depth of the lattice potential near the Feshbach resonance, a superfluid-insulator transition was observed. In these experiments, it was argued that the usual single-band model was no longer applicable, because the strength of the on-site interaction exceeded the gap between the lowest and the next-lowest bands. Accordingly, the effects of the higher bands have to be taken into account for detailed investigations. For the optical lattice systems, it was pointed out that the supersolid state was stabilized in the presence of an confining potential [4]. From the analysis of the single-band model in homogeneous systems, it was shown that the density wave (DW) state and superfluid state are degenerate at half-filling [5, 6, 7]. However, it is not clear whether both states are also degenerate or not in the multiband systems.

In this study, we investigate the ground state of ultracold 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) [8], which enables us to treat local correlation effects precisely. We show that the DW state is stable for a small orbital splitting region and that the transition to the superfluid state takes place with increasing the orbital splitting.

Let us consider the fermionic atoms in a three-dimensional optical lattice potential. In the low-tunneling limit, each lattice potential is regarded as a harmonic one [9, 10]. In this case, the lowest orbital is nondegenerate, while the next-lowest orbital is three-fold degenerate. To
investigate 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 same orbitals of the nearest neighbor sites are assumed to take the same value for both orbitals. We set that the system involves the same number of fermionic atoms in two different hyperfine states, which are described as the pseudospins. The model Hamiltonian we consider here reads

\[ H = \sum_{\langle i,j >\alpha} (t - \mu \delta_{i,j}) c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma} + \frac{D}{2} \sum_{i\sigma} (n_{i\sigma} - n_{i\bar{\sigma}}) + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \sum_{i\sigma\sigma'} (U' - J \delta_{\sigma,\sigma'}) n_{i1\sigma} n_{i2\sigma'}, \tag{1} \]

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 \( n_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma} \). \( t \) represents the hopping integral, \( \mu \) the chemical potential, and \( D \) 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. For the lowest and the next-lowest orbitals, the coupling constants satisfy the relation \( U' = J = U/2(<0) \). 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. This retains nontrivial local quantum fluctuations missing in conventional mean-field theories. We apply here the two-site DMFT method [11], which allows us to study the Mott transitions of orbitally degenerate lattice fermions qualitatively [12, 13]. To study the superfluid of lattice fermions, we extend this method to the case when the superfluid order exists [14].

In order to consider the DW state, we further divide the bipartite lattice into \( A \) and \( B \) sublattices [8]. In this case, the local Green’s function have the following form:

\[ \hat{G}^{-1}_{\text{loc},\alpha}(\omega) = \int dz \rho(z) \hat{G}^{-1}_{\alpha}(z, \omega), \tag{2} \]

\[ \hat{G}^{-1}_{\alpha}(z, \omega) = \begin{pmatrix} \omega + \mu - (-1)^{n_{i\alpha\uparrow}} \frac{D}{2} & -\frac{z}{2} \\ -\frac{z}{2} & \omega + \mu - (-1)^{n_{i\alpha\downarrow}} \frac{D}{2} - \Sigma_{A,\alpha}(\omega) \end{pmatrix}, \tag{3} \]

where \( \rho(z) \) is the density of states (DOS). \( \Sigma_{A(B),\alpha}(\omega) \) is the self-energy on orbital \( \alpha \) for \( A(B) \) sublattice, which can be obtained by solving two effective impurity models. We use a semicircular DOS, \( \rho(\omega) = 4/(\pi W) \sqrt{1 - (\omega/W)^2} \), where \( W \) is the band width. Since the hopping integral is 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.

We consider three types of the possible states for \( D = 0 \): the superfluid state, the DW state, and the Mott insulating state. In Fig. 1(a), we show the results for the quasiparticle weight \( Z \) and the superfluid order parameter \( \Phi = \langle c_{i\alpha\uparrow} c_{i\alpha\downarrow} \rangle \). \( Z \) represents the coherent spectral weight of the Bogoliubov quasiparticle [7]. As \( |U| \) increases, \( Z \) decreases and jumps to 0 with vanishing \( \Phi \) simultaneously. The results indicate that the discontinuous quantum phase transition from the superfluid to the Mott insulator takes place [14]. Towards the transition point, the Bogoliubov quasiparticle is renormalized significantly. In Fig. 1(b), we show \( Z \) and the DW order parameter \( M = (1/4) \sum_{i\alpha\sigma} (\langle n_{iB\alpha\sigma} \rangle - \langle n_{iA\alpha\bar{\sigma}} \rangle) \), where \( n_{iB(A)\alpha\sigma} \) is the number operator of the \( B(A) \) sublattice. In this case, \( Z \) is nearly equal to 1 irrespective of \( U \) and \( M \) increases towards 1 with \( |U| \). The results indicate that for large \( |U| \) the typical DW state comes into existence, where the fully-occupied site by two bosonic fermion pairs and the empty site appear alternately. Comparing
Figure 1. (Color Online) Quasiparticle weight $Z$ and the order parameters of the two types of long range orders for $D = 0$. (a) The superfluid order parameter $\Phi$ and (b) the DW order parameter $M$.

Figure 2. (Color Online) The energies of the ordered states as a function of $D$ for $U = -1.0$.

the energies of these three ordered states, we confirm that the DW state is most stable for all $U$ at $D = 0$.

To see the behavior at finite $D$, we calculate the energy of the system as a function of $D$ for $U = -1.0$. The results are shown in Fig. 2. As $D$ increases, the energy of the superfluid state decreases steadily. Meanwhile, the energy of the DW state takes a constant value for at least $D \leq 0.5$. The energy of the Mott insulating state is slightly higher than that of the DW state. Therefore, we find that the DW state becomes unstable for a large $D$ region and the discontinuous transition to the superfluid state occurs. We note that the superfluid-insulator transition never occurs in the single-band attractive Hubbard model at half-filling [7, 15, 16]. Therefore, we can say that the DW state is caused by the two-band effects.

By changing $D$ and $U$ systematically, we investigate the ground state of the two-band attractive Hubbard model at half-filling. The results are summarized in the phase diagram shown in Fig. 3. In the large $D$ region, the band insulator appears. The transition line of the band insulator agrees well with the result obtained by conventional mean-field theory: $D = U/2 + 4$. In the small $D$ region, the DW state becomes stable and the transition point from the DW state to the superfluid state increases with $|U|$. For large $|U|$, orbital fluctuations are suppressed because of the formation of the robust DW state, which yields the direct transition to the band insulator with increasing $D$. 


In our recent research, the Mott insulating phase was shown to appear in the strong coupling region owing to the strong renormalization of the correlation effects [14]. In the present calculation, we have shown that the DW state is more stable than the Mott insulating state. However, the DW state may become unstable by frustrations or thermal fluctuations. Actually, the experiments have been performed in rather high temperature $T/T_F \sim O(10^{-1})$ with $T_F$ being the Fermi temperature [3]. Since the Mott insulator is robust against thermal fluctuations [8], competition between the Mott insulating state and the DW state at finite temperatures is expected. Detailed investigations for the ordered state including the effects of frustrations or thermal fluctuations are our future work.

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References
[1] Chin J K, Miller D E, Liu Y, Stan C, Setiawan W, Sanner C, Xu K and Ketterle W 2006 Nature 443 961.
[2] For a review, see Chen Q, Stajic J, Tan S, and Levin K, 2005 Phys. Rep. 412 1.
[3] Köhl M, Moritz H, Stöferle T, Günter K and Esslinger T 2005 Phys. Rev. Lett. 94 080403.
[4] Koga A, Higashiyama T, Inaba K, Suga S, Kawakami N 2008 J. Phys. Soc. Jpn. 77 073602.
[5] Scalettar R T, Loh E Y, Gubernatis J E, Moreo A, White S R, Scalapino D J, Sugar R L, and Dagotto E 1989 Phys. Rev. Lett. 62 1407.
[6] Capone M, Castellani C, and Grilli M 2002 Phys. Rev. Lett. 88, 126403.
[7] Garg A, Krishnamurthy H R, and Randeria M 2005 Phys. Rev. B 72 024517.
[8] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 Rev. Mod. Phys. 68 13.
[9] Zwerger W 2003 J. Opt. B 5 S9.
[10] Hofstetter W 2006 Phys. Rev. B 74 024501.