Three-component Repulsive Fermionic Atoms in Optical Lattices at finite temperatures

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Abstract. We investigate finite-temperature properties of three-component (color) repulsive fermionic atoms in optical lattices at half filling using a self-energy functional approach. For a certain anisotropy of the interactions, we find a color density-wave (DW) state at low temperatures. In the weakly interacting region, the second-order phase transition from the color DW state to the Fermi-liquid state occurs with increasing temperature. In the strongly interacting region, by contrast, the first-order transition from the color DW state to a color selective Mott transition (CSMT) state or a Mott insulating state occurs. As the interaction increases above the critical temperatures, we observe a crossover from the CSMT state to the Mott insulating state.

1. Introduction
Recent significant progress in cold fermionic atoms trapped in optical lattices provides us with a way to investigate the fascinating aspects of quantum many-body effects. For example, the Mott transition was successfully demonstrated in $^{40}$K fermionic atoms [1, 2]. Quite recently, the Mott insulating states of six-component $^{173}$Yb fermionic atoms in an optical lattice were observed [3]. The $^{173}$Yb system can be a candidate for realizing three-component repulsive lattice fermionic atoms. The three-component system attracts much interest of both theorists and experimentalists. It was shown theoretically that its ground state for the isotropic interactions is a color density-wave (DW) state [4], and that the Mott transition for the isotropic interactions occurs at commensurate 1/3 and 2/3 fillings but never occur at incommensurate half filling [5].

In a recent study, we investigated the ground state of three-component repulsive fermionic atoms in optical lattices at zero temperature [6]. We showed that, depending on the anisotropy of the interactions, two kinds of ordered states appear at half filling and that both states obey a first-order quantum phase transition at the isotropic interaction point. When fluctuation effects are taken into account, a color-selective Mott transition (CSMT) state appears, where two different-color atoms are localized at the different sites and the third color atoms are itinerant throughout the system. In the strongly interacting region, a Mott insulating state appears. Both states have slightly higher energies than those of the ordered ground states. By analogy with strongly correlated electron systems [7, 8], the CSMT state and the Mott insulating state are considered to extend at finite temperatures, and thus they are expected to be observed in experiments. These motivate us to investigate the ordered states and the Mott transition states...
at finite temperatures. In this paper, we investigate three-component repulsive fermionic atoms in optical lattices at zero and finite temperatures using a self-energy functional approach (SFA) [9, 10, 11].

2. Model and method
In accordance with the conventional model for cold atoms in optical lattices [12], we set the nearest-neighbor hopping and the on-site interaction between the atoms with different colors. Low-energy properties can be described by the repulsive three-component Hubbard model,

\[ \mathcal{H} = - \sum_{\langle i,j \rangle}^{3} t_{ij}(c_{\alpha}^\dagger_{i}c_{\alpha}_{j}) + \frac{1}{2} \sum_{\alpha \neq \beta} U_{\alpha \beta} n_{\alpha} n_{\beta}, \]

where \( c_{\alpha}^\dagger \) (\( c_{\alpha} \)) is the fermionic creation (annihilation) operator for the state with color \( \alpha = 1, 2, 3 \) in the \( i \)th site and \( n_{\alpha} = c_{\alpha}^\dagger c_{\alpha} \). Here, \( t \) denotes the nearest-neighbor hopping integral, \( \mu_{\alpha} \) is the chemical potential for the atom with color \( \alpha \), and \( U_{\alpha \beta} (> 0) \) is the on-site repulsive interaction between two atoms with colors \( \alpha \) and \( \beta \). The condition \( \mu_{\alpha} = (1/2)(U_{\alpha \beta} + U_{\alpha \gamma}) \) is imposed to maintain a half-filled system with a balanced population of three-component atoms. We assume a homogeneous optical lattice and neglect the confinement potential for a first approximation.

The SFA allows us to deal efficiently with zero- and finite-temperature properties concerning the phase transition driven by correlation effects [9, 10]. This method is based on the Luttinger-Ward variational method. The framework of this variational approach enables us to introduce a proper reference system which has to include the same interaction term as that of the original Hamiltonian (1). Other parameters, \( t \), of the reference system correspond to variational parameters, where \( t \) is the parameter matrix of the noninteracting part of the reference Hamiltonian. In the SFA [9, 10], we calculate the grand potential \( \Omega \) as a function of the self-energy of the reference system \( \Sigma_{t} \). Then, from the condition \( \partial \Omega / \partial t = (\partial \Sigma_{t} / \partial t)(\partial \Omega / \partial \Sigma_{t}) = 0 \), we obtain the reference self-energy \( \Sigma_{t} \) which properly describes the original correlated system. Here, we apply the two-site Anderson impurity model as the reference system. This approximation is in some sense regarded as a finite-temperature extension of the two-site DMFT [13, 6]. To examine the staggered ordered state, we divide the bipartite lattice into two sublattices [7, 14]. We then calculate the order parameter of the staggered state \( M_{\alpha} \), which is defined by the difference in the atom numbers \( (n_{A(B), \alpha}), M_{\alpha} = n_{A, \alpha} - n_{B, \alpha} \), between the sublattices \( A \) and \( B \) with color \( \alpha \) per site. We use a semicircular density of states for an infinite dimensional Bethe lattice, which is independent of \( \alpha \).

We investigate the anisotropically interacting system. For this purpose, we set \( U_{12} = U \), \( U_{13} = U' \), and \( U_{23} = U'' \), and then set \( U'/U = 0.6 \) and \( U''/U = 2 \). In the following, the hopping integral \( t \) is used in units of energy.

3. Numerical results
In Fig. 1(a), we show \( M_{\alpha} \) for \( T = 0 \). As \( U/t \) increases, \( M_{1} \) and \( M_{2} \) increase towards unity, and \( M_{2} \) decrease towards minus unity. The results indicate that sites doubly occupied by color-1 and 3 atoms and sites solely occupied by color-2 atoms appear alternately. This state is a color DW state. In this case, color-2 and 3 atoms are localized at the different sites rigidly, while color-1 atoms occupy the site more flexibly. In fact, \( M_{1} \) approaches unity slowly compared with \( M_{3} \). From this result, it is expected that color-1 atoms may become itinerant at the lower critical temperature than the critical temperature above which color-2 and 3 atoms become itinerant. In this case, a CSAF state emerges between these two critical temperatures. In Fig. 1(b), we show \( M_{\alpha} \) for the weak interaction \( U/t = 0.8 \) as a function of \( T/t \). We find that \( M_{\alpha} \) approach
zero continuously at the same critical temperature $T/t = 0.11$. The results indicate that in this weakly interacting region the CSAF state does not appear and the direct second-order phase transition from the color DW state to the Fermi liquid state occurs.

We investigate the phase transition from the color DW state for the stronger $U/t$. It is considered that, as temperature is increased, the ordered state disappears because of thermal fluctuations and Mott transition states are expected to appear. In Fig. 2, we show the grand potentials. From the analysis by the SFA, we find that the grand potential with the right-aro...
the itinerant atoms and the second term stem from the localized two-color atoms which are distributed randomly. Therefore, in \( T/t > 0.18 \), color-2 and 3 atoms with the strongest \( U'' \) are localized at the different sites randomly as a result of the Mott transition, while color-1 atoms are itinerant throughout the system. This state is a CSMT state.

For \( U/t = 12.0 \), both grand potentials cross at \( T/t = 0.13 \). In \( 0.13 < T/t < 0.4 \), the lower grand potential obeys the temperature dependence \( \Omega/t \sim -\ln(T/t) \), leading to \( S \sim \ln 2 \). This state is the Mott insulating state, where color-1 and 3 atoms are localized at the same sites and the color-1 atoms are localized solely at the different sites. The stronger repulsions \( U \) and \( U'' \) push the color -1 and 3 atoms with the weakest \( U' \) localized at the same sites. The paired sites and solely localized sites appear randomly. In \( T/t > 0.4 \), the lower grand potential obeys \( \Omega/t \sim -b(T/t)^2 - (\ln 2)T/t \) with a positive constant \( b \) and thus \( S \sim 2bT/t + \ln 2 \). This state is the CSMT state as mentioned above. From the numerical results, we find that at \( T/t \sim 0.13 \) the first-order phase transition occurs from the color DW state to the Mott insulating state with increasing temperature. When temperature is further increased, a crossover occurs from the Mott insulating state to the CSMT state around \( T/t \sim 0.4 \).

4. Summary

We have investigated finite-temperature properties of three-component repulsive fermionic atoms in optical lattices at half filling using the SFA. In the present anisotropy of the interactions, we have shown that the color density-wave state survives in the low temperature region. In the high temperature region, the Fermi liquid state, the color-selective Mott transition state, and the Mott insulating state appear. These high temperature states are considered to be observed in experiments. Finding a way to detect these three states is our important future issue.

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