Superconductivity and Ferromagnetism in Charge-Ordered Metallic Phases of Extended Hubbard Models

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Abstract. We analyze the Fermi-surface instability of charge carriers in the charge-ordered metallic phases of a triangular-lattice extended Hubbard model at quarter filling and an extended Hubbard ladder near half filling. We derive and analyze strong-coupling effective Hamiltonians for the charge carriers, and then, we find $f$-wave superconductivity in the triangular-lattice model and ferromagnetism in the ladder model. The origin of these orderings can be associated with the following terms in the effective Hamiltonians: $f$-wave superconductivity is stabilized by the inter-site attraction and correlated hopping, and ferromagnetism results from positive second-neighbor hopping and an infinitely large on-site repulsion.

1. Introduction

The extended Hubbard model with nearest-neighbor repulsions, i.e., $H = -t \sum_{\langle i,j \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j$ with the standard notation, is a minimal model for describing charge-ordered (CO) phenomena. Motivated by experimental observation of COs in $\theta$-type organic conductors [1] and ladder compound Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ [2], extensive theoretical studies have been conducted on a triangular-lattice extended Hubbard model at quarter filling [3] and an extended Hubbard ladder near half filling [4].

In this study, we analyze the CO metallic phases of the above mentioned two models in the strong coupling region $t \ll U, V$. (For the stability of COs, it is assumed that $V > V_c \simeq U/3$.) As shown in Fig. 1, the triangular-lattice model has a three-fold CO insulating ground state at electron density $n = 2/3$, and the ladder model has a checkerboard-type CO insulating state at $n = 1$. These CO insulators are our starting points, and hole doping into these insulators leads to CO metallic phases. If we completely neglect the bare hopping term in $H$, then we have the ground-state degeneracy depending on the manner in which the doped holes are arranged. The introduction of the bare hopping term resolves this degeneracy and is expected to induce an ordering of the doped holes. In order to study this additional ordering, we derive a second-order effective Hamiltonian for doped holes, within the two-particle approximation [5].

Here, we comment on the rigidity of CO with hole doping. In the case of the ladder model, Vojta et al. used the density matrix renormalization group (DMRG) method to analyze the stability of the checkerboard-type CO in the ground state; it was found that this type of CO is stable down to $n = 1/2$ [6]. In the case of the triangular-lattice model, we use the quantum Monte Carlo (QMC) method to check whether the three-fold CO is stable against a rather high
Second-order perturbation processes make doped holes be itinerant within the A-sublattice, as shown by the gray arrows.

Figure 1. Schematic representations of (a) triangular-lattice and (b) ladder models. We define the A-sublattice to be a lattice made from doubly occupied sites. CO metallic phases are obtained by hole doping into the insulating states at \( n = 2/3 \) in (a) and \( n = 1 \) in (b). Second-order perturbation processes make doped holes be itinerant within the A-sublattice, as shown by the gray arrows.

Figure 2. Scaling plots of the order parameter for charge ordering at (a) \( n = 2/3 \) and (b) \( n = 1/2 \), where the 3D Ising universality class is assumed.

doping rate of \( \delta = (2/3 - 1/2)/(2/3) = 0.25 \). The model parameters are chosen as \( t = 1, U = 4, V = 3 \), and \( n = 2/3 \) and \( 1/2 \). Our maximum system size is \( N = 12 \times 12 \) (\( L = 12 \)). We calculate the charge correlation function, i.e., \( Q_c = N^{-1} \sum_{i,j} \langle c^{(2\pi/3,2\pi/3; (r_i-r_j))} \rangle \). In Fig. 2, we show the scaling plot of the order parameter, i.e., \( \Delta_{co} = \sqrt{Q_c/N} \); from this figure, it can be noted that the order parameter exhibits a good scaling behavior. The estimated CO transition temperatures \( T_{co}(n = 2/3) = 1.9 \) and \( T_{co}(n = 1/2) = 1.3 \) indicate that the CO survives even for \( \delta = 0.25 \).

2. Superconductivity in the Triangular-Lattice Extended Hubbard Model

We turn to the study of dynamics of doped holes in the three-fold CO back ground. In order to write down the effective Hamiltonian for doped holes, it is convenient to carry out particle-hole transformation for the A-sublattice according to \( c_{\ell\sigma} = a_{\ell\sigma}^\dagger \), where \( a_{\ell\sigma}^\dagger \) are the creation operators of the A-sublattice holes. Then, the second-order effective Hamiltonian can be expressed as

\[
H_{\text{eff}} = T_1 \sum_{\langle \ell, \ell' \rangle} h_{\ell, \ell'}^a + V_0 \sum_{\ell} n_{\ell}^a n_{\ell}^a + V_1 \sum_{\langle \ell, \ell' \rangle} n_{\ell}^a n_{\ell'}^a + \bar{T}_1 \sum_{\ell} \sum_{\ell' \in T_{\ell, \ell'}} n_{\ell'}^a h_{\ell, \ell'}^a, \tag{1}
\]

where \( \ell \) is an A-sublattice site; \( \langle \ell, \ell' \rangle \), a nearest-neighbor pair of A-sublattice sites; \( T_{\ell, \ell'} \), a set of A-sublattice sites that form regular triangles together with the lattice points \( \ell \) and \( \ell' \); \( h_{\ell, \ell'}^a = \sum_{\sigma} (a_{\ell\sigma}^a a_{\ell'\sigma} + \text{h.c.}) \); and \( n_{\ell}^a = \sum_{\sigma} n_{\ell\sigma}^a = \sum_{\sigma} a_{\ell\sigma}^a a_{\ell\sigma} \). In this effective Hamiltonian, \( V_0 \sim U \) and \( V_1, \bar{T}_1 \sim O(t^2/V) \). (Explicit expressions of matrix elements are given in Ref. 7.) The
intersite interaction $V_1$ is attractive and the correlated hopping $\tilde{T}_1$ is positive, which provide driving forces of superconductivity in the present system.

Applying the BCS mean-field approximation with the triplet $f$- and singlet $d_{xy}$-wave symmetries to $H_{\text{eff}}$, we obtain the diagonalized mean-field Hamiltonian $H_{\text{mf}} = \sum_k E_k \alpha_k \alpha_k + \sum_k (\xi_k - E_k) + \gamma \Lambda^2$, where $\alpha_k \sigma$ is a quasi-particle annihilation operator and $E_k = (\xi_k^2 + \Delta^2 f_k^2)^{1/2}$ with $\xi_k = \epsilon_k - \mu$, $f_k = \frac{\mathcal{E}}{2} \sin \frac{k}{2} \left( \cos \frac{\sqrt{\mathcal{E}}}{2} - \cos \frac{\mathcal{E}}{2} \right)$ for $f$-wave and $f_k = \sin \frac{\mathcal{E}}{2} \sin \frac{k}{2}$ for $d_{xy}$-wave, and $\Delta = \gamma \Lambda$. The pairing interaction $\gamma$ is defined by $\gamma = 6(4\tilde{T}_1 - V_1) \equiv \gamma_f$ for $f$-wave and $\gamma = 4(2\tilde{T}_1 - V_1) \equiv \gamma_{d_{xy}}$ for $d_{xy}$-wave. The fact of $\gamma_f > \gamma_{d_{xy}}$ suggests the stability of $f$-wave pairing. The stability of the $f$-wave state is also shown by explicitly calculating the BCS mean-field equations.

We turn to the estimation of critical temperature $T_c$ for the $f$-wave state. To begin with, it should be noted that the value of $\gamma_f$ exceeds the band width $9T_1$ for $U/V \gtrsim 1.6$, as shown in Fig. 3(a). With regard to the BCS-BEC crossover, the relationship between critical temperature $T_c$ and the strength of pairing interaction was extensively studied on the basis of a 3D negative-U Hubbard model. The calculation of $T_c$ was carried out by using the QMC simulation [8]. The BCS result agrees with the QMC result only for $|U| \lesssim 2t$. On the other hand, if $|U|$ exceeds the band width, then the BEC formula $T_c \simeq t_B \times [\text{numerical constant} \sim 3]$, where $t_B = 2\mathcal{T}^2/|U|$ is the effective hopping amplitude of composite bosons, becomes a good approximation. Noting our pairing interaction $\gamma_f$ corresponds to $|U|$ in the attractive Hubbard model, we calculate $t_B = 2\mathcal{T}^2/\gamma_f$ as a measure of $T_c$. In Fig. 3(b), we show $t_B$ as a function of the on-site repulsion $U$ in the original Hamiltonian. This result suggests that $T_c = \mathcal{O}(0.01t)$.

3. Ferromagnetism in the Extended Hubbard Ladder

From the results of the DMRG study conducted by Vojta et al. on the doped extended Hubbard ladder, it was found that the total spin of the ground state is not zero, i.e., charge ordering coexisted with ferromagnetism. However, the origin of this ferromagnetism was not clarified. Therefore, it is interesting to apply the present strong coupling approach to this model.

We derive the effective Hamiltonian for doped holes and obtain the following result with the same notation as that used in the previous section:

$$
H_{\text{eff}} = T_1 \sum_{\ell} n_{\ell}^a n_{\ell+1}^a + T_2 \sum_{\ell} n_{\ell}^a n_{\ell+2}^a + V_0 \sum_{\ell} n_{\ell}^a n_{\ell}^a + V_1 \sum_{\ell} n_{\ell}^a n_{\ell+1}^a + V_2 \sum_{\ell} n_{\ell}^a n_{\ell+2}^a + T_1 \sum_{\ell} (n_{\ell-1}^a + n_{\ell+2}^a) h_{\ell+1} + T_2 \sum_{\ell} n_{\ell+1}^a h_{\ell+2},
$$

(2)
where $V_0 \simeq U$ and $T_1 = 2T_2 = \frac{V^2}{4-U/V} > 0$. (The other matrix elements are given in Ref. 9.)

If the intersite interactions and correlated hoppings (second line in eq. (2)) are neglected from $H_{\text{eff}}$, we obtain a railroad-trestle-lattice Hubbard model with a positive next-nearest neighbor hopping and an infinitely large on-site repulsion, which is known as a typical example exhibiting ferromagnetism [10,11]. On the basis of this fact, ferromagnetism in the lightly doped extended Hubbard ladder found by Vojta et al. can be explained, because intersite interactions and correlated hoppings are expected to be less important than the one-body hopping terms and the infinitely large on-site repulsion at low hole densities. In order to verify this fact, we numerically diagonalize $H_{\text{eff}}$ on finite size clusters up to 24 sites and calculate several lowest eigenvalues for $M = 0$ and 1, where $M$ is the total $S_z$. In Fig. 4, we show the obtained energy eigenvalues as a function of $U/V$, where energies are measured from the ground state. We find that the ground state is not a singlet state, which agrees with the DMRG result [6].

4. Summary

In summary, we have studied the coexistence state in a triangular-lattice extended Hubbard model at quarter filling and an extended Hubbard ladder near half filling. For the triangular-lattice model, we have found that the inter-site interaction between doped holes leads to superconductivity, and in the case of the ladder model, positive second-neighbor hopping of doped holes is crucial for ferromagnetism. Unfortunately, it has not been reported that a CO metallic phase is realized in real materials. In the near future we hope that the CO metallic phase is found experimentally, which will open new avenues for the physics of novel coexistence phases.

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