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Magnetic phase diagram of an extended Hubbard model at half filling: Possible application for strongly correlated iron pnictides

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ABSTRACT

We study the magnetic phase diagram within an extended half-filled Hubbard model, focusing on the roles of the next-nearest-neighbor (NNN) and the next-next-nearest-neighbor (3rd NN) hoppings in the magnetic configurations. We find that due to the spin frustration from the long range hopping and the competition between long-range hopping and Coulomb correlation, the striped antiferromagnetic (AFM) phase is stable when the NNN hopping is dominant, while the bicollinear AFM phase is robust when the 3rd NN hopping is considerably large. The triple points are found in various magnetic phase diagrams. Possible applications of the present theory on intermediately correlated LaFeAsO and strongly correlated FeTe are discussed.

1. Introduction

In a half-filled Hubbard model with only nearest-neighbor (NN) hopping on a two-dimensional square lattice, the system transits from paramagnetic (PM) metal to Néel antiferromagnetic (AFM) insulating ground state when the electron correlation exceeds a critical value [1–4]. The long range hopping may lead to spin frustration in the correlated regime, as shown in recent studies [5–8]: the increasing NNN hopping may drive the system to transit from the Néel AFM insulator to the PM metal, or to a striped AFM insulating state [9–11]. Such a theory was applied to explain the striped AFM metallic ground state in LaFeAsO [5,8]. However, it has been shown [12–15] that LaFeAsO compound is a correlated electron system. Whether the striped AFM metallic phase found in the mean field approximation in Ref. [5] exists or not is questionable. And their theory is not self-consistent for intermediate correlation regime. On the other hand, the ground state of FeTe compound is found to be bicollinear AFM [16]. How to understand these properties in the correlated electron scenario is still a challenge.

In order to understand the effect of electron correlation on the ground state magnetic properties of iron pnictides, especially the role of the spin frustration from the long range hoppings, we use the Kotliar–Ruckenstein slave-boson [17] (KRSB) mean-field theory to study the magnetic phase diagram of an extended Hubbard model at half filling at zero temperature. We find that the NNN hopping favors a striped AFM state and the 3rd NN hopping favors the bicollinear AFM state, showing that the magnetic phase diagram is more complex than expected, and the different magnetic ground states of iron pnictides could be understood in the present theory. The rest of the paper is organized as follows: in Section 2, we present the model and the KRSB mean-field method. In Section 3, we show our numerical results of the zero temperature phase diagram. Finally, we summarize our results in Section 4.

2. Model Hamiltonian and methods

At present it is widely believed that the band structures and the Fermi surface of iron pnictides should be multi-orbital character [12]. Meanwhile the five orbitals are involved into the low-energy physical process [18], suggesting that orbital symmetry in iron pnictides is not seriously broken. In iron pnictides, six electrons occupy five d-orbitals per iron, so the single orbital model at half-filling is a good approximation. Under the frustration picture, as the first step to understand the properties of the FeAs superconductivity, we start with the extended single-orbital Hubbard model, which is given by

$$H=-t_1\sum_{\langle i,j\rangle\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+t_2\sum_{\langle i,j\rangle\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+t_3\sum_{\langle i,j\rangle\sigma}c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}, \qquad (1)$$

where t_1,t_2,t_3 are the NN, NNN and 3rd NN hopping terms defined by overlap integral, respectively, $c^{\dagger}_{i\sigma}$ is the creation operator for an electron on site i with spin σ, $c_{i\sigma}$ is the annihilation operator for an electron on site i with spin σ, $n_{i\sigma}$ is the number operator, and U is the on-site repulsion interactions.

To understand the electronic correlation in iron pnictides, the many-body Gutzwiller variational approach, slave spin/rotor method and the dynamical mean-field approach have been applied to various modified Hubbard models [19,20]. However, to explain the complex

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magnetic ground states of iron pnictides with variable correlation strength and electron doping concentration, the KRSB method is a proper technique, in addition to the Gutzwiller variational method. The slave-boson or auxiliary-boson formulation is first proposed by Barnes [21] and rediscovered and extended by Coleman [22], Read and Newns [23] in their work on the mixed-valence problem. It has so far been mainly used to treat the infinite correlation case through replacing the infinite correlations by a local constraint which is then treated by the standard field-theoretical methods. Later, Kotliar and Ruckenstein extended such a collective boson approach to any value of the correlation U, hence it is suitable for handling various magnetic configurations, magnetic phase transitions and the metal–insulator transitions (MIT). Next, we use KRSB mean-field method to deal with the Hubbard model and calculate the ground state energy of the magnetic structure.

The wavefunctions of $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ consist of a set of complete orthonormalized basis for each site. Within the KRSB approach, the collective bosons $e_i^\dagger$, $p_{i\sigma}^\dagger(\sigma=\uparrow,\downarrow)$, $d_i^\dagger$ act as projection operators onto the empty, singly occupied with spin up and spin down, and doubly occupied electronic states at each site, respectively. At the meantime, making use of the completeness condition, we can obtain

$$\sum_\sigma p_{i\sigma}^\dagger p_{i\sigma}+e_i^\dagger e_i+d_i^\dagger d_i=1 \tag{2}$$

Particle conservation condition is given by

$$n_{i\sigma}=f_{i\sigma}^\dagger f_{i\sigma}=p_{i\sigma}^\dagger p_{i\sigma}+d_i^\dagger d_i \tag{3}$$

We can obtain the chemical potential from the particle conservation conditions,

$$(1/N)\sum_{k\sigma}\langle f_{k\sigma}^\dagger f_{k\sigma}\rangle=1+x \tag{4}$$

where x is the doping density, here we let $x=0$ be the half-filling case. We can transform the particle representation to the occupation representation using slave-boson method

$$c_{i\sigma}^\dagger\to f_{i\sigma}^\dagger z_{i\sigma}^\dagger, c_{i\sigma}\to z_{i\sigma}f_{i\sigma} \tag{5}$$

with

$$z_{i\sigma}=(1-d_i^\dagger d_i-p_{i\sigma}^\dagger p_{i\sigma})^{-1/2}(e_i^\dagger p_{i\sigma}+p_{i\bar\sigma}^\dagger d_i)(1-e_i^\dagger e_i-p_{i\bar\sigma}^\dagger p_{i\bar\sigma})^{-1/2} \tag{6}$$

So the effective Hamiltonian is

$$H=-t_1\sum_{\langle i,j\rangle\sigma}z_{i\sigma}^\dagger z_{j\sigma}f_{i\sigma}^\dagger f_{j\sigma}+t_2\sum_{\langle i,j\rangle\sigma}z_{i\sigma}^\dagger z_{j\sigma}f_{i\sigma}^\dagger f_{j\sigma} +t_3\sum_{\langle i,j\rangle\sigma}z_{i\sigma}^\dagger z_{j\sigma}f_{i\sigma}^\dagger f_{j\sigma}+U\sum_i d_i^\dagger d_i \tag{7}$$

In the mean-field approximation, we have the boson probabilities

$$\langle p_{i\sigma}^\dagger\rangle=\langle p_{i\sigma}\rangle=p_1,\quad \langle p_{i\bar\sigma}^\dagger\rangle=\langle p_{i\bar\sigma}\rangle=p_2$$
$$\langle e_i^\dagger\rangle=\langle e_i\rangle=e_0,\quad \langle d_i^\dagger\rangle=\langle d_i\rangle=d_0 \tag{8}$$

and the magnetic moment is defined as

$$m=n_\uparrow-n_\downarrow \tag{9}$$

Within this approximation, we can calculate the groundstate energy to find the lowest magnetic ordered phase, and obtain the magnetic moment, density of states, etc.

3. Numerical results

We use the KRSB mean-field theory to obtain the magnetic phase diagram of the extended Hubbard model at half filling at zero temperature. First, we consider the effect of the NN and the NNN hoppings so as to uncover the formation of striped AFM state. In the further study, we add the 3rd NN hopping to discuss the competition of different hoppings (t_1, t_2 and t_3) and the origin of bicollinear AFM state.

3.1. Striped antiferromagnetic phase

In the absence of the 3rd NN hopping, we find that at finite NNN hopping t_2, e.g. $t_2/t_1=0.76$, the energies of the striped and Néel AFM states are rather close. With the increase of the Coulomb interaction, the system transits from paramagnetic (PM) to striped AFM states at U_p, and then to Néel AFM state at U_n. Further increasing U leads the system to undergo from Néel to reenter the striped AFM phase at U_s, as seen from the energy comparison shown in Fig. 1.

The electronic correlation plays a crucial role in the magnetic moment and electronic states, as shown in Fig. 2. The correlation dependence of the sublattice magnetic moment in Fig. 2(a) has two transitions at $U_1/t_1=4.93$ and $U_2/t_1=6.3$. The former is a critical point for the PM-striped AFM phase transition in the metallic phase, and the latter corresponds to the metal–insulator transition. This can be seen from the density of states (DOS). In Fig. 2(b), the DOS show that there are plenty of electronic states at the Fermi surface for $U=4.0t_1<U_1$, the system is a PM metallic state. Around the first transition at $U=5.0t_1$, with plenty of electronic states at the Fermi surface, the system is a striped AFM metallic state; around the second transition at $U=8.0t_1>U_2$, with few electronic states near the Fermi surface, the system is in the striped AFM insulating state. Therefore, the first critical point corresponds to the magnetic transition and the second one to the MIT, and the magnetic transition does not coincide with the MIT.

By comparing the total energies of the PM, Néel AFM, striped AFM and bicollinear AFM states, we have obtained the slave-boson mean-field phase diagram of the extended Hubbard model at half filling in Fig. 3. In the strong coupling limit, $U\gg t_1$ and $U\gg t_2$, both the striped and the Néel AFM states are insulating since the lower Hubbard band is fully occupied and the upper Hubbard band is empty. In the opposite limit, $U\ll t_1$ and $U\ll t_2$, the ground state is a PM metallic state. When the NNN hopping is finite, the electronic spins are frustrated in the strongly correlated regime. It is well known that when there is only NN hopping, the ground state is the Néel AFM state. As t_2/t_1 increases, the magnetic configuration

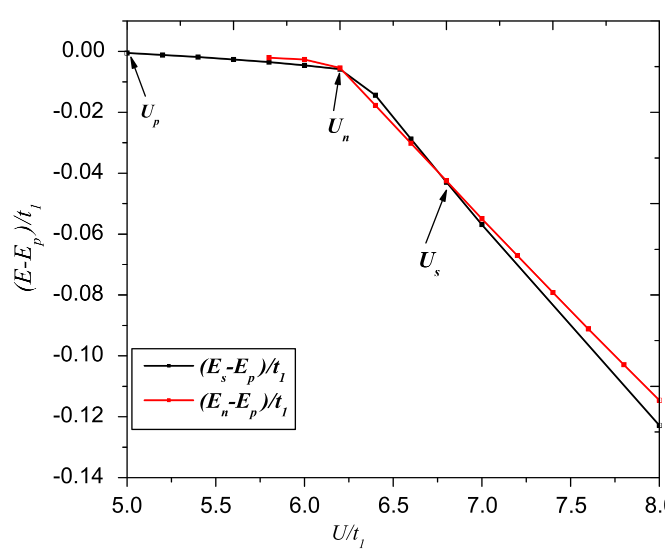

Fig. 1. Comparison of the total energies of PM, striped AFM and Néel AFM states at $t_2/t_1=0.76$ and $t_3/t_1=0$. E_s, E_n and E_p denote the total energies of striped AFM, Néel AFM, and PM states, respectively.