Antiferromagnetic and spectral properties of two-orbital model of iron-based HTSC

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Abstract. Two-orbital model describing iron-based high-temperature superconductors was studied within the limits of variational cluster approximation. The electron density of states for each orbital, as well as momentum distribution, were calculated; the magnetic ordering was determined. The results obtained are in a good agreement with known experimental data.

1. Introduction
The superconductivity was discovered more than a hundred years ago, but studies of this phenomenon continue to this day, and a unified microscopic theory of high-temperature superconductivity is still lacking. At present, most of the work in this area is focused on a new class of iron-based high-temperature superconductors (HTSCs) [1]. The rapid progress in the study of iron-based HTSCs was facilitated by techniques and ideas developed in the study of cuprate HTSCs. The properties of these two classes of superconductors turned out to be very similar. For example, the crystal structure of iron-based HTSCs is constructed by alternating FeAs or FeSe planes separated by LaO planes, just as alternating CuO$_2$ planes are separated by La or Y-Ba planes in cuprate HTSCs. Because of this layered structure, the electronic states in these compounds are quasi-two-dimensional.

One of the main differences between cuprate and iron HTSCs compounds is their magnetic ordering. A stripe magnetic ordering and a metallic phase are realized in iron HTSCs, while cuprate HTSCs have staggered magnetic ordering and Mott insulating phase. The main obstacle in the study of HTSCs is that they have a number of ordered phases, such as antiferromagnetic, superconducting, SDW phases, which compete with each other and sometimes coexist [2]. It is believed that the reason for this is the presence of strong or at least moderate electronic correlations. To answer the question of their role in HTSCs, it is necessary to investigate the density of electronic states and to determine the spectral properties of these materials. After correctly taking into account the electronic correlations, it will be possible to construct phase diagrams characterizing the presence of a particular phase in the system.

2. Two-orbital model
For a theoretical study based on analytical or numerical methods, a model of iron-based HTSCs is needed. When constructing a model, it is necessary to start from the crystalline structure of these compounds. Between the layers of As atoms forming a square lattice, a plane composed of a square lattice of Fe atoms is located; each Fe ion is surrounded by a tetrahedron of As atoms (Figure 1). An analysis of the band structure [3, 4] shows that Fe-3d atomic states dominate near the Fermi level, with
the largest contribution being made by $d_{xz}$ and $d_{yz}$ orbitals. Therefore, a minimal two-orbital model may be used to describe the electronic properties of iron-based HTSCs (Figure 2).

**Figure 1.** The crystal structure of FeAs layer; As atoms of the upper and the lower planes are shown in white and in black, respectively.

**Figure 2.** Two-orbital model of iron-based HTSCs; orbitals and hoppings are shown.

The Hamiltonian of the two-orbital model has the following form:

\[
H = H_{\text{int}} + H_{\text{kin}};
\]

\[
H_{\text{int}} = U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + V \sum_i n_{i\alpha\uparrow} n_{i\alpha\downarrow} - \mu \sum_i n_i - J \sum_i (n_{i\alpha\uparrow} n_{i\beta\uparrow} + n_{i\alpha\downarrow} n_{i\beta\downarrow}) - J \sum_i (a_{i\alpha\uparrow}^+ a_{i\beta\uparrow}^+ a_{i\beta\downarrow} + a_{i\beta\uparrow}^+ a_{i\beta\downarrow} a_{i\alpha\downarrow} + a_{i\alpha\downarrow}^+ a_{i\beta\downarrow} a_{i\alpha\uparrow} + a_{i\beta\downarrow}^+ a_{i\alpha\downarrow} a_{i\beta\uparrow});
\]

\[
H_{\text{kin}} = -t_1 \sum_{i\sigma} (a_{i\alpha\uparrow}^+ a_{i+1\downarrow,\sigma} + a_{i\sigma\uparrow} a_{i+1\downarrow,\sigma}) - t_2 \sum_{i\sigma} (a_{i\sigma\uparrow} a_{i+1\downarrow,\sigma} + a_{i\sigma\uparrow} a_{i+1\downarrow,\sigma}) - t_3 \sum_{i\sigma} (a_{i\uparrow,\sigma} a_{i+1\downarrow,\sigma} + a_{i\downarrow,\sigma} a_{i+1\downarrow,\sigma} + a_{i\uparrow,\sigma} a_{i+1\downarrow,\sigma} + a_{i\downarrow,\sigma} a_{i+1\downarrow,\sigma}) + t_4 \sum_{i\sigma} (a_{i\sigma\uparrow} a_{i+1\downarrow,\sigma} + a_{i\sigma\uparrow} a_{i+1\downarrow,\sigma} - a_{i\sigma\downarrow} a_{i+1\downarrow,\sigma} - a_{i\sigma\downarrow} a_{i+1\downarrow,\sigma}) + \text{h.c.}
\]

Here operator $a_{i\alpha(y)\sigma}^+(a_{i\alpha(y)\sigma})$ creates (annihilates) an electron with spin projection $\sigma$ on site $i$ and orbital $\chi(y)$; $t_i, i = 1, ..., 4$ are hopping amplitudes between orbitals $\chi(y)$; $U$, $V$, and $J$ are Coulomb interaction terms; $\mu$ is the chemical potential.

3. Variational cluster approximation

Variational Cluster Approximation (VCA) [5] is effectively used for strongly correlated systems and is able to take into account spatial correlations and nonlocality of the self-energy.

It was shown [5] that a Green's function of a system $\mathcal{G}$ may be characterized by the Luttinger-Ward functional $\Phi[\mathcal{G}]$, and

\[
\frac{\delta \Phi[\mathcal{G}]}{\delta \mathcal{G}(i\omega_n)} = \frac{1}{\beta} \Sigma[G](i\omega_n).
\]
Using the Legendre transform, Potthoff showed [6] that the Hamiltonian \( H = T + V \), which includes the single-particle term \( T \) and the many-particle term \( V \), can be characterized by the following functional:

\[
\Omega_{T,V} [\Sigma] = F_V [\Sigma] - \text{Tr} \ln (G_0^{-1} - \Sigma),
\]

where \( F_V \) is a functional whose form depends only on the term \( V \).

If the self-energy \( \Sigma \) corresponds to the physical state of the system, then the Dyson equation \( \Sigma = G_0^{-1} - G^{-1} \) is satisfied, and the functional \( \Omega_{T,V} \) at this value of \( \Sigma \) is at a stationary point, which means that

\[
\frac{\delta \Omega}{\delta \Sigma} = 0.
\]

In addition, the functional \( \Omega_{T,V} \) at this point is the grand free energy of the system.

The use of the functional of the self-energy \( \Sigma \) instead of the functional of the Green's function \( G \) is related to the fact that \( \Sigma \) has a more local character than \( G \). This makes it possible to apply this functional in various cluster methods.

Let us now consider a set of reference systems, the Hamiltonian of which is \( H' = T' + V \), and differs from the original one only in the one-particle term. Since the form of the functional \( F_V \) depends only on the term \( V \), it can be expressed in terms of the functional of this set of systems \( \Omega_{T,V} \). We have:

\[
\Omega_{T,V} [\Sigma] = \Omega_{T,V'} [\Sigma] + \text{Tr} \ln (G_0'^{-1} - \Sigma) - \text{Tr} \ln (G_0^{-1} - \Sigma).
\]

It is important to note that the resulting expression (5) is exact while \( \Omega_{T,V'} \) depends on the same \( \Sigma \) as the initial functional. In variational cluster approximation, the value of the functional is calculated exactly, but on a restricted domain of the variational space \( \Sigma \). The problem is solved in the region of space where \( \Sigma \) is the self-energy \( \Sigma' \) of the selected set of reference systems. Therefore, the key points in choosing a set of reference systems are the following: on the one hand, their self-energy \( \Sigma' \) should be as close as possible to the self-energy of the initial system \( \Sigma \), and, on the other hand, it should be possible to solve numerically such a set of systems.

Denoting \( \Omega_{T,V'} [\Sigma'] \equiv \Omega' \), we obtain:

\[
\Omega_{T,V} [\Sigma'] = \Omega' + \text{Tr} \ln (G_0'^{-1} - \Sigma') - \text{Tr} \ln (G_0^{-1} - \Sigma').
\]

Since \( \Sigma' \) also satisfies the Dyson equation \( \Sigma' = G_0'^{-1} - G'^{-1} \), we have:

\[
\Omega_{T,V} [\Sigma'] = \Omega' + \text{Tr} \ln [1 + (G_0^{-1} - G'^{-1})G'].
\]

The obtained result makes it possible to find the grand free energy of the initial system.

4. Results

To apply the variational cluster approximation, the entire system was divided into clusters of size 2×2 with four iron atoms. The small reference system was exactly solved by exact diagonalization technique with the help of the band Lanczos algorithm.

The presence of a particular phase in the system which is characterized by long-range order effects, such as, for example, magnetic ordering or superconductivity, cannot be detected for the chosen reference system because of the smallness of the cluster. Therefore, a term \( W \) called Weiss field was added to the Hamiltonian of the reference system:

\[
W_{AFM} = M \sum_i e^{iQr_i(n_{i1} - n_{i1})},
\]

where \( Q \) is the form factor of magnetic ordering. The existence of a stationary point of the functional (7) for a nonzero value of the Weiss field amplitude \( M \) characterizes the presence of the AFM ordering in the system.

Figure 3 shows the dependence of the functional \( \Omega_{T,V} [\Sigma'] \) for various form-factors of AFM ordering. As can be seen, the stationary point corresponding to the nonzero amplitude of the Weiss
field exists only for $Q = (\pi, 0)$, which corresponds to the presence of antiferromagnetic stripe ordering, in agreement with experimental results [8].

**Figure 3.** The dependence of the functional $\Omega_{TV}[\Sigma']$ for various form-factors of AFM ordering. $U = 2, J = 0.5$. There is the stationary point only for $Q = (\pi, 0)$.

The spectral function describing the electronic density of states for each orbital, the momentum distribution, as well as the band structure were calculated for various values of the parameters $U$ and $J$ of the Hamiltonian (1). Figures 4 and 5 show the electron density of states for two cases, $U = 4; J = 0.7$ and $U = 2; J = 0.5$, when the system is in the Mott insulating or metallic phase, respectively. This result is in a good agreement with calculations of [7].

**Figure 4.** The electron density of states for each orbital; $U = 4; J = 0.7$. There is the gap at the Fermi level ($\omega = 0$).

**Figure 5.** The electron density of states for each orbital; $U = 2; J = 0.5$. The system is in the metallic state.
5. Conclusions
In this work, the variational cluster approximation was applied to study the magnetic properties of the two-orbital model describing iron-based high-temperature superconductors. It was shown, that the variational cluster approximation correctly reproduces the AFM ordering and spectral properties of the model. This approach can be deepened to study the superconducting properties of the model, such as the symmetry of the superconducting order parameter and the dependence of the amplitude of the superconducting order parameter on the doping.

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