Symmetry of superconducting order parameter in minimal model of iron-based HTSC: variational cluster approximation

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Abstract. Two-orbital model describing iron-based high-temperature superconductors is studied within the limits of variational cluster approximation. It is found that in the undoped regime the stripe antiferromagnetic ordering is realized, while in doped regime antiferromagnetism and superconductivity coexist. In the superconducting state, two types of symmetry are found: extended inter-orbit s-wave and intra-orbit d-wave, in agreement with known experimental results.

1. Introduction
Iron-based superconductors are known since 2006, when the presence of superconductivity was reported below $T_c = 3.5$ K in LiOFeAs [1] and $T_c = 4.5$ K in LaONiP [2]. This discovery was not given much importance due to low values of the critical temperatures. The situation changed drastically in 2008, when the superconductivity was discovered in LiO$_{1-x}$F$_x$FeAs with $T_c = 26$ K [3]. This value of the critical temperature made it possible to classify this compound as a high-temperature superconductor (HTSC). After this finding, the whole family of FeAs-based compounds (named pnictides) were synthesized with critical temperatures up to $T_c = 55$ K in SmO$_{1-x}$F$_x$FeAs [4].

The properties of iron-based HTSCs in many aspects resemble the properties of cuprate HTSCs: they have similar phase diagrams [5]; parent compounds in both cases are antiferromagnets. Also, in both cases there is a quasi-two-dimensional structure, that is, these compounds are layered: cuprates are based on CuO$_2$ layers, while in pnictides there are Fe- and As- planes. Due to the strong anisotropy of the crystal structure, the electronic structure of iron-based HTSCs has pronounced quasi-two-dimensional properties.

Calculations of electron-phonon coupling in LiO$_{1-x}$F$_x$FeAs showed [6] that the standard electron-phonon pairing mechanism cannot provide the observed high value of the critical temperature. This issue raised the question of the role of electron correlations in iron-based compounds in the formation of the superconducting state. Despite the common features, there are also fundamental differences between cuprate and iron-based HTSCs. First, undoped cuprates are Mott insulators, while iron-based HTSCs are bad metals. Second, the form factors of the magnetic ordering are different: "chess" ordering in cuprates and "stripes" in pnictides. It means that the modes of electron correlations are different. Until now, the degree of electron correlations in iron-based HTSCs is not established. However, there are several experimental results that testify the presence of strong correlations such as the temperature reorganization of the band structure measured with the help of angle-resolved photoelectron spectroscopy (ARPES) [7].
Since iron-based HTSCs are correlated electronic systems, corresponding techniques are required for their investigation. The main modern methods of studying the electronic structure of correlated electron systems are the following:

1. Density functional theory (DFT) is the main technique of studying electronic systems since it is based on first-principles calculations. However, DFT is not capable to account for both dynamic and nonlocal correlations, which have a significant importance when considering the electronic subsystem of iron-based HTSCs and are manifested themselves in the presence of superconductivity and antiferromagnetic ordering. Also, DFT is widely used as the starting point for all methods described below.

2. Mean field theory (MFT), although capable of taking into account nonlocal correlations, has the same serious drawback as DFT, namely, the lack of the ability to calculate the dynamic response of the system.

3. Dynamical mean-field theory (DMFT) enhances DFT with regard to taking into account dynamical correlations, but nonlocal electron correlations are also absent in DMFT.

4. Lattice Quantum Monte-Carlo algorithms (QMC) have in principle the ability to calculate both long-range nonlocal, as well as dynamical electron correlations, but suffer from the sign problem that does not allow calculations at low temperatures, in which the superconducting state of the system emerges.

5. Variational cluster approximation (VCA) takes into account dynamical and short-range nonlocal correlations and does not have the sign problem.

The most relevant pros and cons of the abovementioned methods are summarized in Table 1. It seems that VCA is the most suitable method for studying electron correlations in iron-based HTSCs.

**Table 1.** Characteristic features of modern methods studying correlated electron systems. Benefits and drawbacks of each method are highlighted with green and red, correspondingly.

| Method   | Dynamical correlations | Non-local correlation | Finite temperature calculations | Sign problem | Completeness of system description |
|----------|------------------------|-----------------------|---------------------------------|--------------|------------------------------------|
| DFT      | No                     | No                    | No                              | No           | Ab initio                          |
| MFT      | No                     | Yes                   | No                              | No           | Model; no size restrictions         |
| DMFT     | Yes                    | No                    | Yes                             | Yes/No       | Monoatomic model; strong size restrictions |
| QMC      | Yes                    | Yes                   | Yes                             | Yes          | Model; no size restrictions         |
| VCA      | Yes                    | Yes                   | Yes/No                          | No           | Model; strong size restrictions     |

2. Method

The basis of the variational cluster approximation is cluster-perturbation theory (CPT), first introduced in [8, 9]. The main principle of CPT is dividing the lattice into clusters of the same shape; consequently, the Hamiltonian of the system may be represented as the sum of inter- and intra-cluster terms (Figure 1),

\[ H = H_0 + V, \]  

(1)

where \( H_0 \) is the intra-cluster part, and \( V \) describes inter-cluster interactions and consists of one-particle terms only.

The size of the clusters is selected in such a way that it is possible to calculate the Green's function of an individual cluster, e.g., using the method of exact diagonalization:
Here and below, the prime denotes values related to an individual cluster; \(i, j\) are the indices of cluster sites; \(|0\rangle\) is the ground state of the cluster; \(|n\rangle\) are excited states of the cluster; \(E_0\) and \(E_n\) are the energy of the ground and excited states, respectively. The perturbation matrix \(V\) of the inter-cluster one-particle part of the Hamiltonian is represented in the mixed basis of the cluster indices and the vectors of the reciprocal super-lattice of clusters:

\[
G_{ij\sigma}(\omega) = \sum_n \left( \frac{\langle 0 | c_{i\sigma}^+ | n \rangle \langle n | c_{j\sigma} | 0 \rangle}{\omega + i\eta + E_n - E_0} + \frac{\langle 0 | c_{i\sigma} | n \rangle \langle n | c_{j\sigma}^+ | 0 \rangle}{\omega + i\eta + E_0 - E_n} \right).
\]  

(2)

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{The scheme for dividing a square lattice into clusters.}
\end{figure}

\[
V_{ij}(K) = \sum_n t_{ij}^{(n)} e^{iK\cdot r_n}.
\]  

(3)

One of the main drawbacks of the CPT is its inability to describe spontaneous symmetry breaking. Therefore, CPT is not suitable for studying systems which undergo a phase transition. However, CPT can be expanded with the help of the self-energy theory (SFT) [10], which together give VCA. The energy of the ground state of the system can be calculated using the Potthoff functional:

\[
\Omega = \Omega - \int_0^\infty \frac{d\omega}{\pi} \int_{BZ} \ln|\text{det}\left(1 + V(K)G'(i\omega)\right)|.
\]  

(6)

The physical states of the system correspond to the stationary points of the functional determined from the condition \(\partial \Omega / \partial V = 0\). To determine the presence or absence of a particular physical state of the system, a one-particle term \(W\) (Weiss field) is added to the Hamiltonian in the following way:

\[
H = (H_0 - W) + (V + W).
\]  

(7)

3. Results
The most useful model of iron-based HTSCs in the context of numeric calculations is the two-orbital model which describes the physics of two iron orbitals \(d_{xz}, d_{yz}\) giving the main contribution to the
Fermi surface obtained from ab-initio calculations [12]. The model contains four types of hoppings and has the following Hamiltonian:

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

where operator \( a_{i,(x,y),\sigma} \) creates (annihilates) an electron with spin \( \sigma \) on site \( i \) and orbital \( x(y) \); \( t_i, \ i = 1, \ldots, 4 \) are the hopping amplitudes between \( d_{x^2} \) and \( d_{y^2} \) orbitals defined as \( x \) and \( y \), respectively. In addition to \( H_{\text{kin}} \), it is required to include the local Slater-Kanamori Hamiltonian, which takes into account the Coulomb inter- and intra-orbital interaction, as well as the Hund's exchange inter-orbital interaction:

\[
H_{\text{int}} = U \sum_{l,a} n_{l,a,\uparrow} n_{l,a,\downarrow} + V \sum_{l} n_{l,x} n_{l,y} - \mu \sum_{l} n_l - J \sum_{l} (n_{l,x,\uparrow} n_{l,x,\downarrow} + n_{l,y,\uparrow} n_{l,y,\downarrow}) - J \sum_{l} (a_{l,x,\downarrow}^+ a_{l,y,\downarrow,\uparrow}) a_{l,x,\downarrow} a_{l,y,\uparrow,\downarrow} + a_{l,y,\uparrow}^+ a_{l,x,\uparrow,\downarrow} a_{l,y,\downarrow,\uparrow} + a_{l,y,\downarrow}^+ a_{l,x,\downarrow,\uparrow} a_{l,y,\uparrow,\downarrow} + a_{l,x,\downarrow}^+ a_{l,y,\downarrow,\uparrow} a_{l,x,\uparrow,\downarrow},
\]

where parameters \( U \) and \( V \) describe the Coulomb interaction within and between orbitals, respectively; \( J \) is the exchange integral; \( \mu \) is the chemical potential. Recently, this model was intensively studied by mean-field methods [17], exact diagonalization of small clusters [13], and quantum Monte-Carlo algorithms [18]. The parameters of the Hamiltonian were taken from [13]:

\[
t_1 = -0.25; \quad t_2 = 0.375; \quad t_3 = -0.3; \quad t_4 = -0.2375; \quad U = 2.0; \quad V = 1.0; \quad J = 0.5.
\]

It is known that in the case of zero doping iron-based HTSCs have an antiferromagnet ordering. To establish the form-factor \( Q \) of the corresponding SDW phase, the following Weiss field was added to the Hamiltonian:

\[
W_{\text{AFM}} = M \sum_{l} e^{iQr_l} (n_{l\uparrow} - n_{l\downarrow}).
\]

It was found that only for \( Q = (\pi, 0) \) the functional has a stationary point (minimum in this case); this corresponds to stripe magnetic ordering, which was observed experimentally [14]. The corresponding band structure and the momentum distribution are shown in Figure 2. Clearly visible flat bands correspond to the AFM ordering. The system is in the state of the Mott insulator; in addition, there is a breaking of \( C_4 \) symmetry, that is, a manifestation of nematicity.

\[\text{Figure 2. Band structure for zero doping (left) and the momentum distribution (right).}\]

For the case of the two-orbital model, there is a plenty of possibilities of realization of superconducting (SC) ordering in the doped regime. Symmetry types of superconducting pairing are
listed in Table 2, and their schematic images are shown in Figure 3. The Weiss field in this case should be chosen in the following form:

\[ W_{SC} = D \sum_{ij} (\Delta_{ij} c_i^\dagger c_j + h.c.), \]  

where \( \Delta_{ij} \) is the superconducting order parameter.

### Table 2. Possible types of superconducting pairing for two-orbital model.

| Symmetry type | Inter-orbit s-wave | Intra-orbit s-wave | Inter-orbit extended s-wave | Intra-orbit extended s-wave | Inter-orbit d-wave | Intra-orbit d-wave |
|---------------|--------------------|--------------------|-----------------------------|-----------------------------|--------------------|--------------------|
| Coordination number | 0 | 0 | 1 | 1 | 1 | 1 |
| Amplitude of SC pairing | s-wave | s-wave | extended s-wave | extended s-wave | d-wave | d-wave |
| Inter-orbital pairing | Yes | No | Yes | No | Yes | No |

**Figure 3.** Symmetry types of superconducting pairing in the two-orbital model; for the description see Table 2.

All these types of symmetry were checked within the limits of VCA; the resulting graph is presented in Figure 4. As can be seen, for two types of symmetry of superconducting order parameter the functional as a function of the amplitude of the Weiss field has a stationary point, namely for extended s-wave inter-orbit and d-wave intra-orbit pairings. The superconducting gap can be seen at the band structure picture shown in Figure 5.

We, therefore, can conclude that in the doped regime of the two-orbital model these two types of SC pairing coexist. This conclusion is well agreed with experimental results clearly indicating multiple contributions of various symmetries to the superconducting gap [15,16].
Figure 4. Potthoff functional as a function of the amplitude of SC Weiss field for various types of symmetry of SC pairing; doping $\delta = 0.1$.

Figure 5. Superconducting gap in the two-orbital model at electron doping $\delta = 0.1$. $U = 2$; $J = 0.5$, $\mu = -2.6$.

4. Conclusions
The two-orbital model describing iron-based high-temperature superconductors was studied with the help of variational cluster approximation. All the findings are in a good agreement with experimentally observed results: stripe antiferromagnetic ordering in normal phase, manifestation of the nematicity in the Mott insulator state, the presence of two types of symmetry in the superconducting state: extended inter-orbit s-wave and intra-orbit d-wave. These results count in favor of VCA in studying the full phase diagram of iron-based HTSCs.

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