Variational Monte Carlo study for superconductivity in multi-orbital systems

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Abstract. To understand the mechanism of superconductivity in iron-based superconductors in a minimal model, we have studied the two-orbital Hubbard model in a two-dimensional square lattice with variational Monte Carlo method. We have found that the \(s_{+}^{-}\)-wave symmetry, where the gap function changes its sign between hole and electron pockets, is favored among the various pairing symmetries. We have also discussed the mechanism of the \(s_{+}^{-}\)-wave superconductivity.

1. Introduction

Recently, the roles of orbital degrees of freedom in strongly correlated electron systems have attracted much attention. The multi-orbital effect is considered to be important for many superconducting (SC) materials including \(\text{Sr}_2\text{RuO}_4\), heavy-fermion superconductors, and iron-based superconductors [1]. Among them, the iron-based superconductors have been extensively studied because of their rather high transition temperature \(T_c\)'s. For this class of superconductors, even the details of the SC symmetry have not been settled: some theoretical studies propose the \(s_{+}^{-}\)-wave symmetry with sign changes between electron and hole pockets [2, 3, 4, 5, 6], and others propose the \(s_{+}^{+}\)-wave symmetry without any sign changes [7, 8]. Understanding the mechanism of superconductivity in multi-orbital systems is important for searching a novel superconductor with a higher \(T_c\).

Our present study is intended to understand the mechanism of superconductivity in iron-based superconductors. Although we have to consider all five \(d\) orbitals of Fe atoms for precise quantitative discussion, it certainly takes a huge amount of calculation cost to treat the effect of electron correlation in the five-orbital model. In this study, we use the Hubbard model considering only the \(yz\) and \(zx\) orbitals [9, 10, 11], which have large density of states on the Fermi surface, and attempt to treat the electron correlation correctly within these two orbitals. The variational Monte Carlo method (VMC) is used to study the ground state properties of the two-orbital Hubbard model.

2. Model and method

We study the following two-orbital Hubbard model in a two-dimensional square lattice,
$$H = \sum_{\mathbf{k},\alpha,\beta,\sigma} \varepsilon_{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}\alpha\sigma}^\dagger c_{\mathbf{k}\beta\sigma} + U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + (U' - J/2) \sum_{i} n_{i\alpha\uparrow} n_{i\alpha\downarrow} - 2J \sum_{i} S_{ix} \cdot S_{iy} + J' \sum_{i} (c_{ix\alpha\uparrow}^\dagger c_{iy\beta\downarrow} + \text{H.c.}).$$  \hspace{1cm} (1)$$

The indices $\alpha$ and $\beta$ represent the orbital degrees of freedom and $\alpha, \beta = x(y)$ represents $d_{xz}(d_{yz})$ orbital. The first term is the kinetic energy, $\varepsilon_{xx} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y$, $\varepsilon_{yy} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y$, and $\varepsilon_{xy} = -4t_4 \sin k_x \sin k_y$. These parameters are set to be $t_1 = -1.0, t_2 = 1.3, t_3 = -0.85$, and $t_4 = -0.85$, following the previous study for the two-orbital model \cite{9, 10}. The rest are the Coulomb interaction terms: $U, U', J$, and $J'$ denote the coupling constants for intraorbital Coulomb, interorbital Coulomb, exchange (Hund’s coupling), and pair-hopping interactions. The constraint of $U = U' + J + J'$ and $J = J'$ for rotational symmetry is assumed in the following.

We consider the following trial wave function for the present VMC study,

$$|\Psi\rangle = P_{\chi} P_{G} |\Phi\rangle.$$  \hspace{1cm} (2)

Here, $|\Phi\rangle$ is the one-body part and obtained by diagonalizing the following Hamiltonian,

$$H_{\text{MF}} = \sum_{\mathbf{k}\sigma} \left( \varepsilon_{xx}^{\mathbf{k},\alpha} c_{\mathbf{k}x\alpha\uparrow}^\dagger c_{\mathbf{k}y\beta\downarrow}^\dagger c_{-\mathbf{k}y\gamma\uparrow} c_{-\mathbf{k}x\delta\downarrow} \right) \left( \begin{array}{cccc} \xi_{xx} & \xi_{xy} & \Delta_{xx} & \Delta_{xy} \\ \xi_{xy} & \xi_{yy} & \Delta_{xy} & \Delta_{yy} \\ \Delta_{xx} & \Delta_{xy} & -\xi_{xx} & -\xi_{xy} \\ \Delta_{xy} & \Delta_{yy} & -\xi_{xy} & -\xi_{yy} \end{array} \right) \left( \begin{array}{c} c_{\mathbf{k}x\alpha\uparrow} \\ c_{\mathbf{k}y\beta\downarrow} \\ c_{-\mathbf{k}x\gamma\uparrow} \\ c_{-\mathbf{k}y\delta\downarrow} \end{array} \right).$$  \hspace{1cm} (3)

where

$$\begin{align*}
\xi_{xx} &= -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y - \bar{\mu} \\
\xi_{yy} &= -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y - \bar{\mu} \\
\xi_{xy} &= -4t_4 \sin k_x \sin k_y
\end{align*}$$  \hspace{1cm} (4)

The deformation of the original Fermi surface is considered by the renormalization of the hopping integrals, $t_i \rightarrow \tilde{t}_i$ ($t_1$ is fixed as one). $\bar{\mu}$ is an effective chemical potential. $\Delta_{\alpha\beta}$ is a pairing form factor between $\alpha$ and $\beta$ orbitals. We consider the various pairing forms and find the lowest energy states. Here, $\tilde{t}_i, \bar{\mu}$, and $\Delta_{\alpha\beta}$ are all variational parameters.

$P_{G} = \prod_{i,\gamma} \left[ 1 - (1 - g_{\gamma}) |\gamma\rangle \langle \gamma| \right]$ is a Gutzwiller factor extended for the two-orbital system. $i$ is a site index and $\gamma$ runs over all possible spin configurations at each site. In the two-orbital system, the total number of the spin configuration at each site is $4^2 = 16$. We control the weight of each spin configuration by varying $g_{\gamma}$ from 0 to 1. The set of $\{g_{\gamma}\}$ is a variational parameter to be optimized. In this study, we classify the possible 16 patterns into 10 groups by Coulomb interaction and symmetry and therefore the number of variational parameter is 10.

$P_{\chi} = \exp \left[ -\sum_{ij} v_{ij} n_{i\alpha\uparrow} n_{j\beta\downarrow} \right]$ is a charge Jastrow factor that controls the long-range charge correlation. The long-range charge correlation is known to be important for describing strongly-correlated electron systems. In this study, we assume that $v_{ij}$ depends only on the distance between charges, $v_{ij} = v(|r_i - r_j|)$. Since $i$ and $j$ run over all lattice sites, the number of variational parameter increases with the system size. For $10 \times 10$ square lattice, we consider up to 19th-neighbor correlation and therefore the number of variational parameter is 19.

The ground state energy is calculated with the VMC method. The variational parameters mentioned above are simultaneously optimized by using the stochastic reconfiguration method \cite{12}. This method makes it possible to optimize many parameters efficiently and stably. Once the trial wave function is determined, we can easily calculate physical quantities.
Figure 1. (a) Band dispersion of the present two-orbital model. Dotted line represents the Fermi energy. (b) Electron occupation in \( k \)-space. Black, white, and gray circles show that 0, 1, and 2 electrons occupy the \( k \) points, respectively. Dotted lines represent the nodes in the \( s^\pm \)-wave symmetry.

3. Numerical results

The calculation is performed on the \( 10 \times 10 \) lattice with a periodic-antiperiodic boundary condition. The parameters are set to be \( U/|t_1| = 8.0, U'/|t_1| = 4.0, J/|t_1| = 2.0 \), and \( n = 188/100 = 1.88 \) (12\% hole doping). First, we show the band dispersion and electron occupation in \( k \)-space used in the calculation in Fig. 1. The unfolded Brillouin zone scheme \([3]\), where the unit cell contains one Fe atoms in the real space, is used.

We show the energy comparison between the normal and various SC states in Fig. 2(a). \( \tau_0 \) and \( \tau_1 \) denote intraorbital and interorbital pairing, respectively. Among them, the form factor with next-nearest-neighbor (nnn) and intraorbital pairing, namely \( \Delta_{\alpha\beta} = \Delta_0 (\cos k_x \cos k_y) \tau_0 \), shows a reasonable condensation energy within error bars. It corresponds to the \( s^\pm \)-wave symmetry where the gap function changes its sign between hole and electron pockets.

Then we consider the mechanism of the appearance of the \( s^\pm \)-wave symmetry. Figure 2(b) shows the \( \Delta_0 \) dependence of the expectation values of each term in Eq. (1). One can see that as \( \Delta_0 \) increases, the system has energy loss on \( E_{\text{kin}} \) and \( E_U \) and energy gain on \( E_{U'} \), \( E_J \) and \( E_{J'} \). When the nnn pairing is formed, the parallel spin configuration is favored since it leads to the superexchange energy gain through the nnn interorbital hopping \( t_4 \). As a result, the system has energy gain mainly on the Hund’s coupling (\( E_J \) term) and the \( s^\pm \)-wave SC state is stabilized, although we cannot determine the precise optimal value of \( \Delta_0 \) within the accuracy of this calculation. In the real space representation, the Cooper pair is formed by the electrons on nnn sites, which is suitable for the \( (\pi, 0) \)-type stripe AF order observed in the mother materials of iron-based superconductors. The nodes originated from the form factor (\( \propto \cos k_x \cos k_y \)) are locating at \( k_x, k_y = \pm \pi/2 \) and do not cross the Fermi surface as shown in Fig. 1(b). This fact is also advantageous for the appearance of the \( s^\pm \)-wave symmetry.

Finally, we discuss the validity of using the two-orbital model. A lot of theoretical studies for the five-orbital model have proposed the \( s^\pm \)-wave symmetry, where the gap function changes its sign between hole and electron pockets [2, 3, 4, 5, 6]. Indeed, the detailed shape of the gap function differs from one another and cannot be represented by a simple form like \( \cos k_x \cos k_y \). However, our two-orbital model captures the essence of the gap structure that naturally arises near the \( (\pi, 0) \)-type stripe AF order. Of course, we have to take care of the effect of neglecting other orbitals. Indeed, there are some discussion that the two-orbital model favors a \( p \)-wave symmetry with particular nodal structure, which may be an artifact of neglecting other orbitals. The study for full five-orbital model is left for our future problem.

Recently, the \( s^{+++} \)-wave symmetry without any sign changes in the gap function has also
proposed [7, 8]. This symmetry is induced by the electron-phonon interaction and orbital fluctuation, different from the spin-fluctuation mechanism of $s_{+-}$-wave symmetry. It is an interesting future problem to study the effect of the electron-phonon interaction and the resulting SC states within our calculation.

4. Summary

We have studied the two-orbital Hubbard model in a two-dimensional square lattice with hole and electron pockets that mimics the electronic structure of iron-based superconductors. The VMC method is used for the calculation of the ground state energy. We have found that the $s_{+-}$-wave symmetry, where the gap function changes its sign between hole and electron pockets, is favored among the various pairing symmetries. This symmetry naturally arises near the $(\pi, 0)$-type stripe AF order and is considered to be suitable for the iron-based superconductors.

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