Electronic instabilities in iron-based superconductors: A variational Monte Carlo study

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The variational approach has a glorious history in condensed matter physics. Examples of successful wave functions include the BCS wave function, Laughlin wave function, Jastrow wave function, etc. In the study of the cuprate superconductivity, Anderson’s projected BCS wave function has been shown to capture many important aspects of the cuprates. Despite the successes, all variational approaches have the drawback of being biased; i.e., they are based on the assumption that the few variational parameters built into the variational ansatz enable it to capture the essence of the true ground state wave function. Understanding the pairing mechanism and possible electronic instabilities in iron-based superconductors has been a focus of interests in the past few years. This is not only for their high $T_c$, but also for many similarities they share with the cuprates. Presently most of the works attribute the superconducting (SC) gap function to the antiferromagnetic fluctuations, and it is widely believed that the superconducting (SC) gap function takes pairing to the antiferromagnetic fluctuations, and it is widely the cuprates. Presently most of the works attribute the electron pairings of the SC gap function takes opposite signs on the electron and hole Fermi surfaces. This is believed that the superconducting (SC) gap function takes pairing to the antiferromagnetic fluctuations, and it is widely believed in the cuprates. Despite the successes, all variational approaches have the drawback of being biased; i.e., they are based on the assumption that the few variational parameters built into the variational ansatz enable it to capture the essence of the true ground state wave function.

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The band structure we use is that of Kuroki et al. We model the electronic correlations by the Hubbard and Hund's rules. The Hamiltonian is given as

$$H = H_{\text{band}} + U_1 \sum_{\mu \nu} n_{i \mu \uparrow} n_{i \mu \downarrow} + U_2 \sum_{i, \mu < \nu} n_{i \mu \nu} + J_H \left[ \sum_{ \mu < \nu \sigma' \sigma} C_{\mu \sigma'} C_{\mu \sigma} C_{\nu \sigma'} C_{\nu \sigma} + C_{\mu \uparrow} C_{\mu \downarrow} C_{\nu \downarrow} C_{\nu \uparrow} + H.c. \right].$$

(1)

where $H_{\text{band}}$ and its parameters can be found in Ref. 15 and its Table I. In most of the paper we shall use $(U_1, U_2, J_H) = (4.2, 0.7)$ eV. While these parameters are compatible with Ref. 22 it is larger than what is reported in Ref. 21. The additional reasons for doing so are (1) similar large correlation parameters are concluded from LDA + DMFT calculations although with controversy, (2) smaller interaction parameters will make the energy gain associated with the superconducting and orbital order too small for our VMC accuracy. As the energy reduction due to normal state FS distortion is relatively larger, smaller interaction parameters, e.g., $(U_1, U_2, J_H) \sim (2.1, 0.35)$ eV, were also used.

We use the following partially projected variational wave functions:

$$|\psi \rangle = g_1 \hat{N}_1 g_2 \hat{P}_N |\psi_{MF}\rangle,$$

(2)

where

$$\hat{N}_1 = \sum_{i, \mu} \hat{n}_{i \mu \uparrow} \hat{n}_{i \mu \downarrow}, \quad \hat{N}_2 = \sum_{i, \mu < \nu} \hat{n}_{i \mu \nu}.$$

(3)

$\hat{P}_N$ fixes the total number of electron to $N_e$, and $0 \leq g_1, g_2 \leq 1$ suppress configurations according to the number of electrons residing in the same and different on-site orbitals. The mean-field wave function $|\psi_{MF}\rangle$ depends on the type of electronic order we are studying, and it will be discussed in detail later.
The VMC was carried out on \( L^2 = 10 \times 10 \) and \( 18 \times 18 \) lattices with periodic boundary condition. In choosing the doping level, we were careful to avoid degeneracy in the band energy between different Slater determinants. A standard Markovian chain Monte Carlo approach was used with the Metropolis update algorithm. After an initial “equilibration” using 10\(^5\) Monte Carlo steps, about 10\(^5\), 10\(^6\), and 10\(^7\) samples were used in the study of Fermi surface distortion, orbital order and SC pairing, respectively. The adjacent samples are separated by 5\(L^2\) Monte Carlo steps with each showing an acceptance ratio of about 0.23, which is enough to eliminate autocorrelation and thus guarantee an efficient sampling. Due to the higher demand of accuracy when studying SC pairing, we have applied the “reweighting” scheme. The error bars are estimated by calculating the variance of the band energy between different Slater determinants. A standard form factor at 13% hole doping.

Normal state FS distortion. FRG predicts two leading FS distortions: one preserves the 90\(^\circ\) rotation symmetry and the other breaks it. The former shrinks both the electron and hole pockets and produces a relative energy shift of the electron and the hole bands. The latter is the band version of orbital ordering, and is suggested to be stabilized by the AFM. The mean-field state \( |\psi_{MF}\rangle \) for the two types of FS distortion are the ground state of the following quadratic Hamiltonian:

\[
H_{MF} = \sum_{k,\sigma} [E_{k}^0 + \chi(k)] n_{k\sigma} + G_{\mu\nu} M_{\mu\nu} + \sum_i \epsilon_i c_i^\dagger c_i,
\]

where \( E_{k}^0 \) is the bare band dispersion, \( n_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma} \) and \( \chi(k) \) can be \( \chi_0 \cos k_x \cos k_y \) (90\(^\circ\) preserving) or \( \chi_0 \cos k_x - \cos k_y \) (90\(^\circ\) breaking).

In the absence of AFM order, the results for 0.6% hole-doping on a \( 18 \times 18 \) lattice using \( (U_1, U_2, J_H) = (4, 2, 0.7) \) eV are shown in the main panel of Fig. 1. The black and red symbols represent \( \chi_0 \cos k_x \cos k_y \) and \( \chi_0 \cos k_x - \cos k_y \) at their optimal values. The size of points represents the error bar and the dotted lines are a guide to the eyes. The main panel is for \( U_1 = 2, U_2 = 1, J_H = 0.35 \) eV and \( \cos k_x \cdot \cos k_y \) form factor is shown.

Orbital order in the AFM state. The \( |\psi_{MF}\rangle \) for the AFM ordered state is the ground state of the following mean-field Hamiltonian:

\[
H_{MF} = H_0 + \sum_{i,\mu\nu} \epsilon_i c_i^\dagger c_i M_{\mu\nu} e^{\dagger Q} R_i + \sum_{\mu\nu} M_{\mu\nu} M_{\mu\nu},
\]

where \( H_0 \) is given by either Eq. (4) or Eq. (6). Here \( Q = (\pi, 0) \) is the AFM ordering wave vector. As for \( M_{\mu\nu} \) we used the mean-field result of Ref. 30 where the nonzero \( M_{\mu\nu} \) are \( M_{01}, \ldots, 5, \ldots, 5, M_{15}, M_{15} = 0.5 \). The variational study is performed by keeping the ratio between the optimal mean-field parameters, \( M_{22}, M_{55}, M_{44}, M_{55}, M_{15} / M_{11} = (0.95, 1.03, 1.1, 0.76, -0.96) \), while allowing \( M_{11} \) to vary.

For \( (U_1, U_2, J_H) = (4, 2, 0.7) \) eV at 0.6% hole-doping (on \( 18 \times 18 \) lattice) we found \( \epsilon_i = (0.49, 0.76) \), \( M_{11} = 1.4 \) eV, with a total energy reduction of about 3.0 eV per site, with nearly 2\(\mu_B\) ordering moment. This value is significantly larger than the measured ones for the stoichiometric compounds. The discrepancy can be due to the omission of the fluctuations in the orientation of magnetic moments and the

FIG. 1. (Color online) Energy gain per site as functions of \( \chi_0 \) for the normal state FS distortion, and the band and real space version of orbital ordering. The results were obtained on a \( 18 \times 18 \) lattice under periodic boundary condition. The parameters \( g_1, g_2 \) are fixed at their optimal values. The size of points represents the error bar and the dotted lines are a guide to the eyes. The main panel is for \( U_1 = 2, U_2 = 1, J_H = 0.35 \) eV and \( \cos k_x \cdot \cos k_y \) form factor is shown.

FIG. 2. The Fermi surfaces at 0.6% hole doping. (a) In the absence of FS distortion. (b) The distorted Fermi surfaces associated with \( \chi(k) = \chi_0 \cos k_x \cos k_y \).

\[
\chi(k) = \chi_0 \cos k_x \cos k_y
\]
FIG. 3. (Color online) The energy gain per site in the AFM state as function of $\chi_0$ for the three types of electronic orders studied in Fig. 1(a). The same lattice size and interaction parameters were used. The doping is 0.6%-electron doping. The variational parameters $g_1, g_2, M_\mu$, are fixed at their optimized values. The size of points represents the error bar. The dotted lines are just guides to the eyes.

ordering wave vectors, and/or the large values of the interaction parameters. In view of the strong atomic-like ordering moments in the AFM state obtained above, when studying the orbital ordering in the magnetic state we also adopt a real space version of orbital ordering,28 where $|\psi_{MF}\rangle$ is the ground state of

$$H_{MF} = \sum_{k_{123}} \varepsilon^{0}_{k} n_{i,\sigma} - \chi_0 \sum_{i,\sigma} (n_{i,yz,\sigma} - n_{i,xz,\sigma}).$$  \hspace{1in} (6)

Here $n_{i\alpha\sigma} = \hat{c}_{\alpha\sigma}^\dagger \hat{c}_{i\alpha\sigma}$. We note that the orbital $d_{xz},d_{yz}$ we use are 45° rotated from the $d_{x^2-y^2},d_{y^2-x^2}$ orbitals in Ref. 15. From Fig. 3, we conclude that in the presence of AFM, the real-space $d_{xz}/d_{yz}$ orbital order is the most energetically favorable (we suspect this is due to the fact that the large, localized, ordering moment in the AFM state). It produces a total energy gain of about 4.6 meV per site. At the optimal $\chi_0$ the occupation-number difference between the $xz$ and $yz$ orbitals is $\tilde{n}_{d_{xz}} - \tilde{n}_{d_{yz}} = 0.20(1)$. This value is enhanced above the ~0.15 occupation difference already present in the pure AFM state. Our result agrees qualitatively with a recent photoemission result27 and a first principle Wannier function calculation.28 Comparing this result with the green symbols of Fig. 1(a), we conclude that this orbital order is stabilized by the AFM.

Superconducting pairing. The $|\psi_{MF}\rangle$ we use for studying the pairing is the ground state of the following mean-field Hamiltonian:

$$H_{MF} = \sum_{k_{123}} \varepsilon^{0}_{k} n_{i,\sigma} - \mu_c n_{i,\sigma} + \sum_{k_{123}} (\Delta_{k}^{u}\hat{c}_{\alpha,k}\hat{c}_{\alpha,k}^{+} + \text{H.c.}).$$ \hspace{1in} (7)

We have studied four different types of gap functions:

$$\Delta_{k}^{u} = \Delta_0 (\cos k_x + \cos k_y), \quad \Delta_{k}^{u} = \Delta_0 \cos k_x \cdot \cos k_y, \quad \Delta_{k}^{u} = \Delta_0 (\cos k_x - \cos k_y).$$ \hspace{1in} (8)

In addition we only allow pairing in bands that cross the Fermi energy. This is an excellent approximation because, as shown below, the gaps are quite small.

Our calculations for the SC state were carried out on a 10 × 10 lattice at 10% hole doping. The optimized $(g_1, g_2) \approx [0.31(1), 0.76(2)]$. Again, to an excellent approximation, the optimal values of $g_1, g_2$ and $\mu_c$ do not depend on $\Delta_0$. The results for $\tilde{E}(\Delta_0) - \tilde{E}(0)$ with $(g_1, g_2, \mu_c)$ fixed at their optimal values are shown in Fig. 4. The results suggest that while both conventional-$s$ and $d_{x^2-y^2}$ pairing raise the energy, $s_\pm$ and extended $s$ lower it.

Interestingly, our result suggests the extended $s$ form factor is slightly favored (by 0.1 ± 0.08 meV) over the $s_\pm$ one. On the surface this contradicts the predictions of $s_\pm$ pairing form factor. However it is important to realize that the $s_\pm$ gap function is not synonymous to $\cos k_x \cos k_y$. Indeed, the $s_\pm$ form factor obtained from several weak coupling approaches has a strong variation around the electron Fermi surfaces. We believe the near degeneracy of the extended-$s$ and the $\cos k_x \cos k_y$ form factors suggests the optimal pairing form factor is a linear combination of the two (hence is anisotropic on the electron pockets). However it is extremely computationally time consuming to verify this, and we have not been able to do it. In addition, we caution that the degree of the gap function variation on the electron pockets will depend on the values of the parameters. We cannot rule out that for other parameter sets the $\cos k_x \cos k_y$ can be the leading pairing form factor. Finally, the optimal gap amplitudes for the two symmetries are about 18 meV and 20 − 22 meV, respectively. Order-of-magnitude-wise these values are not far from the experimentally measured gap scales.

In conclusion, we have performed a variational Monte Carlo calculation to check the validity of our previous results based on a weak-coupling approximation. The results are qualitatively consistent. We caution that because of the time-consuming nature of the calculation we are only able to study two sets of interaction parameters. Clearly we cannot rule out the possibility that quantitative aspects of the above results will be sensitive to the precise values of the interaction parameters.

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