Ground-state pairing correlations in the $S_4$ symmetric microscopic model for iron-based superconductors

YANG Wu$^1$, GUANGKUN Liu$^1$ and TIANXING Ma$^{1,2(a)}$

$^1$ Department of Physics, Beijing Normal University - Beijing 100875, China
$^2$ Beijing Computational Science Research Center - Beijing 100084, China

received 10 July 2013; accepted in final form 19 October 2013
published online 22 November 2013

PACS 74.20.Mn – Nonconventional mechanisms
PACS 71.10.Fd – Lattice fermion models (Hubbard model, etc.)

Abstract – We present the ground-state pairing correlations in the $S_4$ symmetric microscopic model for iron-based superconductors, computed with the constrained-path Monte Carlo method. For various electron fillings and interaction strengths, we find that the $s_{xy}$ pairing dominates over other pairing correlations and is positive when the pair separation exceeds several lattice constants, both for iron-pnictides and iron-chalcogenides. These ground-state properties, especially the long-range part pairing correlations reconfirm the previous finite-temperature results published in Phys. Rev. Lett., 110 (2013) 107002. We further our study by including the nearest-neighbour interaction $V$ and it is found that the $s_{xy}$ pairing correlation is slightly suppressed by increasing $V$.

Copyright © EPLA, 2013

Introduction. – Iron-based superconductors are the major field in superconductivity now [1–4]. One of today’s major challenges in the study of iron-based superconductors is how to obtain a unified microscopic understanding of the different families of these materials, in particular, iron-pnictides and iron-chalcogenides, which distinguish from each other with distinct Fermi surface topologies [5–7]. Theoretical studies based on models with complicated multi-$d$ orbital band structures [8–18], lack of a support from more fundamental microscopic electronic physics [19–27]. Recently, it has been shown that the underlining electronic structure in iron-based superconductors, which is responsible for superconductivity at low energy, is essentially governed by a two-orbital model with an $S_4$ symmetry. The two-orbital model includes two nearly degenerated single-orbital parts that can be mapped to each other under the $S_4$ transformation. This electronic structure stems from the fact that the dynamics of the $d_{xz}$ and $d_{yz}$ orbitals are divided into two groups that are separately coupled to the top and bottom As(Se) planes in a single Fe-(As)Se trilayer structure. The two groups can thus be treated as an $S_4$ iso-spin. The dressing of other orbitals in the $d_{xz}$ and $d_{yz}$ orbitals cannot alter the symmetry characters. Despite the simplicity of this description, the model not only gives very good quantitative agreement with the band structure but also supplies a uniform model to mimic different iron-based material classes, especially for the iron-pnictides and iron-chalcogenides [28].

Some of us have performed a finite-temperature determinant quantum Monte Carlo (DQMC) study of the pairing correlation in the $S_4$ symmetric microscopic model on lattices mainly with $8^2$ sites. It is found that the pairing with an extensive $s$-wave symmetry robustly dominates over other pairings at low temperature in a reasonable parameter region regardless of the change of Fermi surface topologies. The pairing susceptibility, the effective pairing interaction and the $(\pi, 0)$ antiferromagnetic correlation strongly increase as the on-site Coulomb interaction increases, and these non-biased numerical results provide a possible unified understanding of the superconducting mechanism in iron-pnictides and iron-chalcogenides [29].

Numerical approaches like DQMC, however, have their own difficulties, typically being limited to small sizes, high temperatures, and they experience the infamous fermion sign problem, which causes exponential growth in the variance of the computed results and hence an exponential growth in computer time as the lattice size is increased and the temperature is lowered [30,31]. In general, to determine which pairing symmetry is dominant by numerical calculation for finite-size models, we have to look at the long-range part of the pair-correlation function at zero...
temperature, and it seems to be dangerous to extrapolate the long-range behavior of the pair-correlation function from a lattice with \(8^2\) sites. In order to shed light on this critical issue, it is important to discuss the results obtained from the constrained-path Monte Carlo (CPMC) [32] on a larger lattice. In a variety of benchmarking calculations, the CPMC method has yielded very accurate results of the ground-state energy and many other ground-state observables for large systems [32]. In the CPMC method, the ground-state wave function \(|\Psi_0\rangle\) is projected from an initial wave function \(|\Psi_T\rangle\) by a branching random walk in an overcomplete space of constrained Slater determinants \(|\phi\rangle\), which have positive overlaps with a known trial wave function. In such a space, we can write \(|\Psi_0\rangle = \Sigma \phi(\phi)|\phi\rangle\), where \(\chi(\phi) > 0\). The random walk produces an ensemble of \(|\phi\rangle\), called random walkers, which represent \(|\Psi_0\rangle\) in the sense that their distribution is a Monte Carlo sampling of \(\chi(\phi)\). The resulting method is free of any decay of the signal-to-noise ratio. For more technique details we refer to refs. [32,33].

In this paper, we report the ground-state results in the \(S_4\) symmetric microscopic model for various electron fillings and the interaction strength by using the CPMC method. The simulations were mainly performed on a \(12^2\) lattice, and compared to the pairing correlation on an \(8^2\), a \(16^2\) and a \(20^2\) lattice. All the lattices are with periodic boundary conditions. Our unbiased numerical calculation shows that the ground-state \(s_{xy}\) pairing dominates over other pairing correlations. The \(s_{xy}\) pairing correlation is positive when the pair separation exceeds several lattice constants, both for iron-pnictides and iron-chalcogenides. These ground-state properties, especially the long-range pair pairing correlations reconfirm our previous finite-temperature results with the DQMC method [29]. We further our study by including the nearest-neighbor interaction \(V\). It is found that the \(s_{xy}\) pairing correlation is slightly suppressed by increasing \(V\).

**Model and results.** — The minimum extended Hubbard model for a single \(S_1\) iso-spin component in the iron-square lattice is described by [28,29]

\[
H = t_1 \sum_{lk\sigma} (a_{l\sigma}^\dagger b_{l+\delta_k\sigma} + h.c.)
+ t_2 \left[ \sum_{l\sigma} a_{l\sigma} a_{l+1\bar{\delta}_k\sigma} + \sum_{l\sigma} b_{l\sigma} b_{l+1\bar{\delta}_k\sigma} \right]
+ t'_2 \left[ \sum_{l\sigma} a_{l\sigma} a_{l+1\delta_k\sigma} + \sum_{l\sigma} b_{l\sigma} b_{l+1\delta_k\sigma} \right]
+ U \sum_{l\sigma} (n_{l\uparrow} n_{l\downarrow} + n_{l\downarrow} n_{l\uparrow})
+ V \sum_{lk\sigma} (a_{l\sigma}^\dagger b_{l+\delta_k\sigma} + h.c.)
+ \mu \sum_{l\sigma} (n_{l\sigma} + n_{l\bar{\sigma}}).
\]

(1)

Here, \(a_{l\sigma}\) \((a_{l\sigma}^\dagger)\) annihilates \(c\) (creates) electrons at the site \(R_i\) with spin \(\sigma\) \((\sigma = \uparrow, \downarrow)\) on sublattice \(\Lambda\), \(b_{l\sigma}\) \((b_{l\sigma}^\dagger)\) annihilates (creates) electrons at the site \(R_i\) with spin \(\sigma\) \((\sigma = \uparrow, \downarrow)\) on sublattice \(\Lambda\). The pairing correlation function we computed is

\[
C_{\alpha}(r = R_i - R_j) = \langle \Delta_{\alpha}^\dagger(i) \Delta_{\alpha}(j) \rangle,
\]

(2)

where \(\alpha\) stands for the pairing symmetry. And the corresponding order parameter \(\Delta_{\alpha}^\dagger(i)\) is defined as

\[
\Delta_{\alpha}^\dagger(i) = \sum_{l} f_{\alpha}(\delta_i) (a_{l\uparrow} b_{l+\delta_i\downarrow} - a_{l\downarrow} b_{l+\delta_i\uparrow})^\dagger,
\]

(3)

with \(f_{\alpha}(\delta_i)\) being the form factor of the pairing function, and the vectors \(\delta_i\) \((\delta_j)\) denote the nearest-neighbour inter-sublattice connections (the next-nearest-neighbour inner sublattice connections), where \(l = 1, 2, 3, 4\) denoting the four different directions. As shown in ref. [29], we focus on four kinds of pairing form, where

\[
\begin{align*}
\text{d}_{x^2-y^2}-\text{wave:} & \quad d_{d_{x^2-y^2}}(\delta_i) = 1 \{ \delta_i = (\pm x, 0) \} \\
& \quad \text{and} \quad d_{d_{x^2-y^2}}(\delta_i) = -1 \{ \delta_i = (0, \pm y) \}, \\
\text{d}_{xy}-\text{wave:} & \quad d_{d_{xy}}(\delta_i') = 1 \{ \delta_i' = (\pm x, \pm y) \} \\
& \quad \text{and} \quad d_{d_{xy}}(\delta_i') = -1 \{ \delta_i' = (\pm x, \mp y) \}, \\
\text{s}_{x^2+y^2}-\text{wave:} & \quad f_{s_{x^2+y^2}}(\delta_i) = 1, \quad l = 1, 2, 3, 4, \\
\text{s}_{xy}-\text{wave:} & \quad f_{s_{xy}}(\delta_i') = 1, \quad l = 1, 2, 3, 4.
\end{align*}
\]

(4)

To facilitate the contact with prior simulations, we also examined the vertex contributions to the correlations defined by

\[
V_{\alpha}(r) = C_{\alpha}(r) - \overline{C_{\alpha}(r)},
\]

(5)

where \(\overline{C_{\alpha}(r)}\) is the shorthand notation for the uncorrelated pairing correlation. For each term in \(C_{\alpha}(r)\) like \(\langle a_{l\uparrow} a_{l\downarrow} a_{l'\uparrow} a_{l'\downarrow} \rangle\), it has a term like \(\langle a_{l\uparrow} a_{l\downarrow} \rangle \langle a_{l'\uparrow} a_{l'\downarrow} \rangle\).

In fig. 1(a), we compare the long-range part of pairing correlations with different pairing symmetries on the \(12^2\) lattice at \(t_1 = 0.3, t_2 = 1.4, t'_2 = -0.6\), which is a typical case for iron-pnictides [34–38]. Here, the electron filling is \(n = 1.0\), which corresponds to a closed-shell case with \(N_0 = N_\uparrow = 72\). The simulations are performed at \(U = 3.0\). One can readily see that \(C_{s_{xy}}(r)\) (solid red line) is larger than pairing correlations with any other pairing symmetry for almost all long-range distances between electron pairs. With the same set of parameters as that of fig. 1(a), fig. 1(b) shows the vertex contribution defined in eq. (5). Obviously, the vertex contribution of the \(s_{xy}\) (dashed red...
Ground-state pairing correlations in the $S_4$ symmetric microscopic model for iron-based superconductors

Fig. 1: (Color online) (a) Pairing correlation $C_\alpha$ as a function of distance for different pairing symmetries on the 12$^2$ lattice with $t_1 = 0.3, t_2 = 1.4, t_2' = -0.6$ (a typical case for iron-pnictides [34–38]). (b) The vertex contribution $V_\alpha$ with the same parameters.

Fig. 2: (Color online) (a) Pairing correlation $C_\alpha$ as a function of distance for different pairing symmetries on the 12$^2$ lattice with $t_1 = 0.3, t_2 = 1.2, t_2' = -0.8$. (b) The vertex contribution $V_\alpha$ with the same parameters.

line) pairing symmetry dominates that of any other pairing forms. The vertex contribution of the $s_{xy}$ pairing symmetry is a finite value over the long-range part, while the vertex contributions of $d_{xy}$, $s_{x^2+y^2}$ and $d_{x^2-y^2}$ are simply fluctuating around zero. In the numerical results, the ratio of the statistical error to the pairing correlation $C_\alpha$ is no more than 0.5 percent, and most of the error bars are almost within the symbols. The ratio of the statistical error to the vertex contribution $V_\alpha$ is no more than 3 percent. This remark applies to all the following figures.

Fig. 3: (Color online) (a) Pairing correlation $C_\alpha$ as a function of distance on the 12$^2$ lattice with $t_1 = 0.3, t_2 = 1.4, t_2' = -0.6$ for $\langle n \rangle = 1.00$, $\langle n \rangle = 0.89$ and $\langle n \rangle = 0.83$. (b) Pairing correlation $C_\alpha$ as a function of distance on the 12$^2$ lattice with $t_1 = 0.3, t_2 = 1.2, t_2' = -0.8$ for $\langle n \rangle = 1.00$, $\langle n \rangle = 1.13$ and $\langle n \rangle = 1.18$.

Fig. 4: (Color online) (a) Pairing correlation $C_\alpha$ as a function of the distance at the nearest-neighbour interaction $V = 0.3, 0.5$ and 1.0 on the 12$^2$ lattice with $t_1 = 0.3, t_2 = 1.4, t_2' = -0.6$. (b) The same as (a) but at $t_1 = 0.3, t_2 = 1.2, t_2' = -0.8$. 

27013-p3
Figure 2 shows the long-range part of pairing correlations with different pairing symmetries on the 122 lattice at \(t_1 = 0.3, t_2 = 1.2, t'_2 = -0.8\). With this set of parameters, the system shows no hole packet \([29]\). Again we see that both the long-range part pairing correlation and the vertex contribution indicate that the \(s_{xy}\) type dominates over that of other pairing forms. Thus, the behavior of the long-range part pairing correlation re-enforces our findings on pairing susceptibility of an 82 lattice in ref. [29].

In fig. 3, we address the question of what happens to those “long-range” correlations if the system is doped away from half-filling. In fig. 3(a), for a closed-shell case with electron filling \(\langle n \rangle = 0.83\) \((N_t = N_{\downarrow} = 60)\), \(\langle n \rangle = 0.89\) \((N_t = N_{\downarrow} = 64)\) and \(\langle n \rangle = 1.00\) \((N_t = N_{\downarrow} = 72)\), we show the CPMC results of the \(s_{xy}\) pairing correlation for \(U = 3.0\) and \(t_1 = 0.3, t_2 = 1.4, t'_2 = -0.6\). Figure 3(b) shows results of the \(s_{xy}\) pairing correlation for \(t_1 = 0.3, t_2 = 1.2, t'_2 = -0.8\) at \(\langle n \rangle = 1.00\), \(\langle n \rangle = 1.13\) \((N_t = N_{\downarrow} = 81)\) and \(\langle n \rangle = 1.18\) \((N_t = N_{\downarrow} = 85)\). We notice that for both systems with and without hole packet, the pairing correlations decrease as the system is doped away from the half-filled case.

We have also studied the effect of the nearest-neighbour interaction on the pairing correlation at a fixed \(U = 3.0\). In fig. 4, the pairing correlations for \(s_{xy}\) pairing symmetries are displayed as a function of the distance on the 122 lattice with different nearest-neighbour interactions \(V\)’s. For both systems with and without hole packet, we notice that the \(s_{xy}\) pairing correlation is suppressed by the repulsive nearest-neighbour interaction \(V\).

Finally, we compare the pairing correlation on an 82 (green down triangle), a 122 (red circle), and a 162 (pink up triangle) lattices in fig. 5 to exclude the size effect. Figure 5(a) shows the pairing correlation with \(s_{xy}\) symmetry for \(t_1 = 0.3, t_2 = 1.4, t'_2 = -0.6\), and fig. 5(b) shows the pairing correlation with \(s_{xy}\) symmetry for \(t_1 = 0.3, t_2 = 1.2, t'_2 = -0.8\). In the inset of fig. 5, we examine the evolution of \(C_\alpha\) with increasing the lattice size up to 202. The average of the long-range pairing correlation, \(\overline{C_\alpha} = \frac{1}{N^2} \sum_{r \geq 3} C_\alpha(r)\), where \(N'\) is the number of electron pairs with \(r \geq 3\), is plotted as a function of \(N\) at half-filling. It is clear to see that \(\overline{C_\alpha}\) (red circle) is larger than the average of the long-range pairing correlations with any other pairing symmetry for whichever lattice size we investigate.

Conclusions. – In summary, our unbiased numerical results show that the \(s_{xy}\) pairing dominates in the ground state of the \(S_4\) model, as we illustrated in our previous study. And such a domination is robust in a wide range of physical regions. We also find that the nearest-neighbour interaction slightly suppressed the pairing correlation. The consistent behaviour of our results on different clusters suggests that the \(S_4\) model captures the essence of iron-based superconductors.

This work is supported by NSFCs (Grant No. 11104014, No. 11374034 and No. 11334012), Research Fund for the Doctoral Program of Higher Education of China 20110003120007, SRF for ROCS (SEM).

REFERENCES

[1] Kamihara Y., Watanabe T., Hirano M. and Hosono H., J. Am. Chem. Soc., 130 (2008) 3296.
[2] Chen X. H., Wu T., Wu G., Liu R. H., Chen H. and Fang D. F., Nature, 453 (2008) 761.
[3] Chen G. F., Li Z., Wu D., Li G., Hu W. Z., Dong J., Zheng P., Luo J. L. and Wang N. L., Phys. Rev. Lett., 100 (2008) 247002.
[4] Guo J., Jin S., Wang G., Wang S., Zhi K., Zhou T., He M. and Chen X., Phys. Rev. B, 82 (2010) 180520.
[5] Wang X.-P., Qian T., Richard P., Zhang P., Dong J., Wang H.-D., Dong C.-H., Fang M.-H. and Ding H., EPL, 93 (2011) 57001.
[6] Zhang Y., Yang L. X., Xu M., Ye Z. R., Chen F., He C., Xu H. C., Jiang J., Xie B. P., Ying J. J. et al., Nat. Mater., 10 (2011) 273.
[7] Mou D., Liu S., Jia X., He J., Peng Y., Zhao L., Yu L., Liu G., He S., Dong X. et al., Phys. Rev. Lett., 106 (2011) 107001.
[8] Hirschfeld P. J., Korshunov M. M. and Mazin I. I., Rep. Prog. Phys., 74 (2011) 124508.
[9] Johnston D., Adv. Phys., 59 (2010) 803.
Ground-state pairing correlations in the $S_4$ symmetric microscopic model for iron-based superconductors

[10] Dong J., Zhang H. J., Xu G., Li Z., Li G., Hu W. Z., Wu D., Chen G. F., Dai X., Luo J. L. et al., *EPL*, 83 (2008) 27006.

[11] Mazin I. I., Singh D. J., Johannes M. D. and Du M. H., *Phys. Rev. Lett.*, 101 (2008) 057003.

[12] Kuroki K., Onari S., Arima R., Usui H., Tanaka Y., Kontani H. and Aoki H., *Phys. Rev. Lett.*, 101 (2008) 087004.

[13] Wang F., Zhai H., Ran Y., Vishwanath A. and Lee D.-H., *Phys. Rev. Lett.*, 101 (2008) 057003.

[14] Mazin I. I., Singh D. J., Johannes M. D. and Du M. H., *Phys. Rev. Lett.*, 101 (2008) 057003.

[15] Kuroki K., Onari S., Arima R., Usui H., Tanaka Y., Kontani H. and Aoki H., *Phys. Rev. Lett.*, 101 (2008) 087004.

[16] Wang F., Zhai H., Ran Y., Vishwanath A. and Lee D.-H., *Phys. Rev. Lett.*, 101 (2008) 057003.

[17] Kuroki K., Onari S., Arima R., Usui H., Tanaka Y., Kontani H. and Aoki H., *Phys. Rev. Lett.*, 101 (2008) 087004.

[18] Wang F., Zhai H., Ran Y., Vishwanath A. and Lee D.-H., *Phys. Rev. Lett.*, 101 (2008) 057003.