Interplay between nematic fluctuation and superconductivity in a two-orbital Hubbard model: a quantum Monte Carlo study

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Received 24 July 2018, revised 30 August 2018
Accepted for publication 19 September 2018
Published 12 October 2018

Abstract
To understand the interplay between nematic fluctuation and superconductivity in iron-based superconductors, we performed a systematic study of the realistic two-orbital Hubbard model at intermediate correlation regimes by using the constrained-path quantum Monte Carlo method. Our numerical results showed that the on-site nematic interaction induces a strong enhancement of nematic fluctuations at various momentums, especially at \((\pi, \pi)\). Simultaneously, it was found that the on-site nematic interaction suppresses the \((\pi, 0)/(0, \pi)\) antiferromagnetic order and long-range electron pairing correlations for dominant pairing channels. Our findings suggest that on-site nematic fluctuation seems to compete with superconductivity in iron-based superconductors.

Keywords: nematicity, superconductivity, two-orbital Hubbard model

(Some figures may appear in colour only in the online journal)

1. Introduction

Iron-based superconductors (FeSCs) continue to attract the interests of the condensed matter community [1, 2, 3, 4]. One common strategy to understand the superconducting phase in FeSCs is to study the normal states where superconductivity arises. For most FeSCs, superconductivity is found in proximity to a nematic state, in which the systems spontaneously break the rotational symmetry and preserve time-reversal symmetry below certain temperatures [5–10]. Debating about the origin of nematicity still exists among spin-nematic [11, 20, 21], ferro-orbital order [4, 24–26] and other scenarios [22, 23]. Much experimental evidence indicates that nematicity and superconductivity have a common microscopic origin. For instance, angular-dependent magnetoresistance and static magnetization measurement on FeSe samples showed that the onset temperature \(T_n\) of nematic order has a universal linear relationship with the superconducting transition temperature \(T_c\) [17]. Therefore, it is essential to understand the nematic state as it may play an important role to understand superconductivity.

Regarding the relationship between nematicity and superconductivity, it is still under debate [12, 18]. Some experimental and theoretical researches seem to support the coexisting scenario between nematicity and superconductivity. For instance, McQueen et al [13] reported the low temperature structural properties of FeSe by high resolution synchrotron x-ray power diffraction, transmission electron microscopy, and electron diffraction. Their results indicated a coexistence of superconductivity and nematic order. Lederer et al [18] considered a low \(T_c\) metallic superconductor weakly coupled to the soft fluctuations associated with proximity to a nematic quantum critical point (NQCP) and found an enhancement of superconductivity near the NQCP. Zhang et al [19] performed a numerically-exact sign-problem-free quantum Monte Carlo simulations to study the spin fluctuation and...
nematic fluctuation mediated electron pairing and concluded a pairing enhancement by nematic fluctuations. On the other hand, many researchers also found evidence for the competition between superconductivity and nematicity. For example, Kim et al. [14] studied the evolution of the temperature dependence of the in-plane London penetration depth, $\Delta\lambda(T)$ in high-quality single crystals of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ and found a power law behavior of $\Delta\lambda(T)$ in the under doped region, indicating a competition between nematicity and superconductivity. Besides, Cai et al. [15] studied the doping dependence of quasiparticle interference (QPI) in NaFe$_{1-x}$Co$_x$ and the QPI pattern at optimal doping is still fourfold symmetric, which suggests that nematic fluctuation is not a prerequisite for electron pairing. Moon et al. [16] presented a general theory of competition between superconductivity and nematic order, in which the concomitant instabilities of both orders are produced by the underlying Fermi surface.

In this work, we will not focus on the origin of nematic state, instead, by introducing nematic fluctuation to the realistic two-orbital Hubbard model through an on-site nematic interaction, we are trying to explore the important issue concerning the relationship between nematicity and superconductivity. Our motivation comes from recent quantum Monte Carlo (QMC) and random phase approximation studies on a simple two-orbital model [27, 28], which only considered the electron hopping and on-site nematic interaction terms. The model offers a new way to analyze the effect of nematicity, however, the coupling of electron correlation and nematicity in FeSCs calls for inclusion of electron Coulomb interactions in the microscopic level. By introducing both nematic and electron Coulomb interactions, our simulation results based on the constrained-path quantum Monte Carlo method (CPQMC) [36, 37] show that the introduced on-site nematic interaction would induce a strong enhancement of orbital fluctuations in the intermediate $U$ regime. Such fluctuations decrease the ($\pi, 0$)/($0, \pi$) magnetic order and also suppress the possible long-range electron pairings. Our findings suggest that there exists a competition between nematic fluctuation and superconductivity at the intermediate correlation strength.

The organization of this paper is as follows: the two-orbital Hubbard model with on-site nematic interaction and CPQMC method are briefly described in section 2. Section 3 contains our numerical results, and finally in section 4 we present our conclusions.

### 2. Model and method

We will focus on the two-orbital Hubbard model for FeSCs, together with an on-site nematic interaction which was originally introduced in [27, 28], on square lattices. Briefly, the model is composed of the tight-binding contribution $H_t$, the on-site Coulomb interactions $H_{\text{Coul}}$, and the on-site nematic interaction $H_{\text{nem}}$. The full Hamiltonian can be expressed as $H = H_t + H_{\text{Coul}} + H_{\text{nem}}$.

The tight-binding component is described as

$$H_t = -t_1 \sum_{i,\sigma} (d_{i,\sigma}^\dagger d_{i+\hat{x},\sigma} + d_{i+\hat{x},\sigma}^\dagger d_{i,\sigma} + \text{h.c.}) - t_2 \sum_{i,\sigma} (d_{i,\sigma}^\dagger d_{i+\hat{y},\sigma} + d_{i+\hat{y},\sigma}^\dagger d_{i,\sigma} + \text{h.c.}) - t_3 \sum_{i,\sigma,\mu,\nu} (d_{i,\sigma}^\dagger d_{i+\hat{\mu}+\hat{\nu},\sigma} + d_{i+\hat{\mu}+\hat{\nu},\sigma}^\dagger d_{i,\sigma} + \text{h.c.}) + t_4 \sum_{i,\sigma} (d_{i,\sigma}^\dagger d_{i+\hat{\gamma},\sigma} + d_{i+\hat{\gamma},\sigma}^\dagger d_{i,\sigma} + \text{h.c.}) - t_4 \sum_{i,\sigma} (d_{i,\sigma}^\dagger d_{i+\hat{\gamma},\sigma} + d_{i+\hat{\gamma},\sigma}^\dagger d_{i,\sigma} + \text{h.c.}),$$

where $x$ and $y$ denote the $d_{xz}$ and $d_{yz}$ orbitals, respectively. The operator $d_{\alpha \sigma}^\dagger$ ($d_{\alpha \sigma}$) creates (annihilates) an electron on orbital $\alpha$ in Fe site $i$ with spin $\sigma$, and the index $\mu(\nu) = \hat{x}$ or $\hat{y}$ denotes a unit vector linking the nearest-neighbor (NN) sites. As shown in figure 1, $t_1$ ($t_2$) is corresponding to the intraorbital NN hopping amplitude; $t_3$ represents the intraorbital next-nearest-neighbor (NNN) hopping; and $t_4$ represents the interorbital NNN hopping amplitude. In order to gain a full understanding of FeSCs, we adopt two sets of hopping parameters [28, 29]: one is taken as $t_1 = -1.0$, $t_2 = 1.3$ and $t_3 = t_4 = -0.85$, which we marked as Raghu hopping parameters, and the other is set as $t_1 = -1.0$, $t_2 = 1.5$, $t_3 = -1.2$, and $t_4 = -0.95$, which we marked as Dumitrescu hopping parameters. Raghu hopping parameters and Dumitrescu hopping parameters are corresponding to iron pnictides and iron selenides, respectively.
The Coulombic interaction $H_{\text{Coul}}$ is defined as
\[ H_{\text{Coul}} = U \sum_{i} n_i \delta_i n_{i\sigma} + (U' - J/2) \sum_{i} n_i \delta_i n_{i\sigma} - 2J \sum_{i} S_{i\sigma}^x S_{i\sigma}^y, \]
(2)
where $n_{i\alpha} = n_i \delta_i + n_{i\sigma}$ is the electron density operator at orbital $\alpha$ ($\alpha = xz, yz$) on site $i$. The $z$-component of spin operator is defined as $S_{i\alpha}^z = \frac{1}{2} (n_{i\alpha} - n_{i\alpha})$. We also keep $U' = U - 2J$ and $J = U/4$ as in previous literature, which are believed to be the realistic regimes for iron-based superconductors [30, 32, 33]. Note that we simplified Hund’s coupling term, $\sum_i S_{i\sigma}^x S_{i\sigma}^y$, to its Ising contribution, and also ignored the pair-hopping items. These simplifications are based on two observations [30, 31]: (1) previous QMC studies have shown that the Ising contribution of the Hund’s interaction could capture the main physics and (2) QMC simulations could produce higher numerical accuracy after these simplifications.

Finally, in order to study the effect of nematic correlation, the on-site nematic interaction $H_{\text{hem}}$ is added to the Hamiltonian, which is defined as [27, 28]
\[ H_{\text{hem}} = -\frac{g}{2} \sum_i (n_{i\sigma} - n_{i\pi})^2. \]
(3)

$H_{\text{hem}}$ breaks the orbital symmetry and directly induces nematic correlation without any prior orbital order.

For the magnetic and nematic properties, we examine the spin structure factor and nematic structure factor as follows,
\[ S(q) = 1/N \sum_q e^{iq \cdot (r_i - r_j)} \langle (n_i^\uparrow - n_i^\downarrow)(n_j^\uparrow - n_j^\downarrow) \rangle, \]
\[ N(q) = 1/N \sum_q e^{iq \cdot (r_i - r_j)} \langle (n_{i\sigma} - n_{i\pi})(n_{j\sigma} - n_{j\pi}) \rangle, \]
where $q$ and $r$ are the momentum and coordinate points, respectively, $N$ counts the number of $r_i$ and $r_j$ pairs.

For the superconducting property, the classification of possible NN pairing symmetries in [34] is followed. The pairing operator can be defined as [31, 35]
\[ \Delta_{\alpha}(q) = \frac{1}{\sqrt{2}} f(q)(\tau_1)_{\alpha,\beta}(d_{q,\alpha,\pi}^+ d_{-q,\beta,\downarrow} - d_{q,\alpha,\downarrow}^+ d_{-q,\beta,\pi}), \]
(6)
where $d_{q,\alpha,\sigma}^\dagger$ creates an electron in orbital $\alpha$ with momentum $q$ and spin $\sigma$, and $f(q)$ is the form factor and $\tau_1$’s are the Pauli matrices ($i = 1, 2, 3$) or identity matrix ($i = 0$).

Using the Fourier transformation, we can get the pairing operator in coordinate space $\Delta(i)$, and the corresponding pairing correlation function is defined as $P(r = |i - j|) = \langle \Delta(i) \Delta(j) \rangle$. We also calculated averaged pairing correlations through all distances $P_{\text{all}}$ and long-range distances $P_{\text{long}}$ as $P_{\text{all}} = \frac{M}{M'} \sum_r P(r)$ and $P_{\text{long}} = \frac{M}{M'} \sum_{r > \bar{r}} P(r)$, with $M$ and $M'$ representing the numbers of $P(r)$.

We study the Hamiltonian by using the CPQMC method, which is a sign-problem-free auxiliary-field quantum Monte Carlo method. It projects out the ground state from a trial state by random walks in the Slater determinant space. A constrained-path approximation is adopted in the CPQMC algorithm to prevent the sign problem [36, 37]. For more applications of CPQMC, we refer the readers to [30, 31, 40]. In a typical large-scale CPQMC simulation, we set the average number of random walkers to be 4800 and the time step $\Delta \tau = 0.04$. 2000 Monte Carlo steps were sampled before measurements, and 10 blocks of 480 Monte Carlo steps each were used to ensure statistical independence during the measurements. Closed-shell fillings were chosen in the simulations. To judge the accuracy of the CPQMC method, we compared the CPQMC energies against those employing the Lanczos method on a small systems: the maximum energy difference is within 1% up to $U = 4.0$ eV.

3. Results

3.1. Nematic and spin correlations

Firstly we check the effect of on-site nematic correlation in the doped systems. By using Dumitrescu hopping parameters [28], figure 2(a) illustrates the nematic structure factor along the high symmetric momentum-space points in the Brillouin zone. Increasing the on-site nematic correlation $g$ enhances all the nematic structure factors, especially for the $(\pi, \pi)$ point. We also examined the real space nematic correlation versus distance $r$ as $N(r = |i - j|) = \sum_{\alpha,\sigma} \langle (n_{i\alpha} - n_{i\pi})(n_{j\alpha} - n_{j\pi}) \rangle$. The real-space correlations rapidly decay to zero, which indicates a possible signal that there are no obvious long-range
nematic orders in the studied system. Hence, we conclude that the enhanced nematic correlation mainly comes from short-range nematic fluctuations.

Secondly we investigate the responses of magnetic order on the onset of nematic fluctuation. For most FeSCs, the antiferromagnetic (AFM) orders usually locate near nematic and superconducting regimes in the phase diagram. Previous QMC studies on the two-orbital Hubbard models suggest a robust \((\pi,0)\) or \((0,\pi)\) AFM order upon increasing the on-site Hubbard \(U\) [31]. As shown in figure 2(b), the on-site nematic interaction \(g\) clearly suppresses \((\pi,0)\) magnetic order, which is reasonable since the on-site nematic interaction in equation (2) effectively reduces the strength of Hubbard \(U\).

In figure 3 we present the nematic and spin structure factors by using Raghu hopping parameters, which give a good description for iron pnictides. Figure 3(a) demonstrates a similar but much more clear \((\pi,\pi)\) nematic fluctuation upon increasing the on-site nematic interaction strength \(g\). Figure 3(b) shows that the spin structure factor is depressed by the on-site nematic interaction, especially for the \((0,0)\) point. Based on the results from figures 2 and 3, we conclude that the on-site nematic interaction acts to enhance nematic fluctuations and suppress AFM spin fluctuations in FeSCs.

3.2. Pairing correlations

In this section, we will discuss another important issue about the influence of the on-site nematic interaction on electron pairings. We first briefly discuss the pairing operators for multi-orbital models. As shown in equation (6), the pairing operators in the two-orbital model consist of not only the spatial- but also the orbital- distributions, in which the factor \(f(q)\) is the spatial part and \(\tau\) stands for the orbital distribution. In general, there will be dozens of pairing candidates in the two-orbital model.

In figure 4(a), we show \(P_{\text{all}}\) for four typical pairings, wave2, wave3, wave6, and \(s_{\pm}\), whose definitions could be reached in table 1 and equation (5). Pairing wave2 with \(A_{1g}\) symmetry is one of pairings with large pairing amplitude [31]. Pairing \(s_{\pm}\) also has large amplitude and is one of the possible pairing candidates in FeSCs. Pairing wave3 was studied in the simple two-orbital model [28]. One can see that \(P_{\text{all}}\) for wave2 and \(s_{\pm}\) is decreased with increasing the on-site nematic interaction \(g\), whereas wave3 and wave6 exhibit an opposite behavior. Note that the enhancement of \(P_{\text{all}}\) for wave3 is in agreement
with previous finding in the simple two-orbital model [28], in which Coulombic interactions were neglected.

Since the short-ranged pairing correlations contain the contributions from local spin and/or charge components [38, 39], in certain cases they may mislead our understanding on the intrinsic superconducting property. To exclude the effect of short-ranged pairing correlations, we show the long-distance averaged pairing correlation \( P_{\text{all}} \) in figure 4(a). There are two significant differences compared with \( P_{\text{all}} \) in figure 4(a): (1) the dominant pairing seems to be \( s^{\pm} \)-wave, instead of wave2; (2) all pairing channels respond negatively to the on-site nematic interaction \( g \). We found that all the pairing channels, including other ones not presented here, are suppressed by \( g \). In particular, pairing wave3 and wave6 show different behaviors with increasing \( g \) for all-distance and long-distance averaged pairing correlations. These differences are induced by short-ranged contribution of wave3 and wave6, which usually has much larger amplitude than the long-distance counterpart.

We also calculated the all-distance and long-distance averaged pairing correlations by using Raghu hopping parameters, and the obtained results are shown in figures 5(a) and (b). Similar suppression of \( P_{\text{long}} \) by the on-site nematic interaction is clearly observed. One difference from Dumitrescu hopping parameters is that wave2 with \( A_{1g} \) symmetry seems to be the dominant pairing channel from both all-distance

**Figure 5.** (a) Averaged pairing correlation function through all pairing distances, \( P_{\text{all}} \), and (b) the long-range-averaged pairing correlations, \( P_{\text{long}} \), for selected pairing channels with hole doping density \( \rho = 0.125 \) and \( U = 2 \text{eV} \) on an \( 8 \times 8 \) square lattice. Different symbols represent different pairing channels, and the detailed definitions of the pairings see table 1 and equation (5). Periodic boundary conditions and close-shell filling are used during the simulations. The results are obtained by using Raghu hopping parameters.

and long-distance averaged pairing correlations. In addition, \( P_{\text{all}} \) for wave3 and wave6 is no longer enhanced by \( g \). The universal suppression of long-range pairing correlations by \( g \) suggests that the main effect of the on-site nematic interaction is to suppress superconductivity in the studied model.

Note that all-distance averaged pairing correlation \( P_{\text{all}} \) of wave3 and wave6 behaves differently on the two sets of hopping parameters, as shown in up panels of figures 4 and 5. However, the trend of long-distance \( P_{\text{long}} \) for all pairing channels are consistent. As we pointed out previous, \( P_{\text{all}} \) is more easily affected by local spin/charge fluctuations, differences of local fluctuations on different hopping parameters leads to \( P_{\text{all}} \) of wave3 and wave6 behaved differently. \( P_{\text{long}} \), on the contrary, concerns more on long-range contributions and are less affected by local fluctuations.

In order to clearly demonstrate the long-range pairing behavior on \( g \), we pick the dominant pairing wave2 as an example and investigate the pairing distance dependence of long-range pairing correlation of wave2. Figures 6(a) and (b) show the long-range pairing correlation \( P_{2}(r) \) as a function of \( r \) by using Dumitrescu hopping parameters on the \( 8 \times 8 \) and \( 10 \times 10 \) square lattices under various nematic interaction strengths, respectively. One can readily see a suppression of \( P_{2}(r) \) at different distances as \( g \) is increased. Similar results by using Raghu hopping parameters are shown in figures 7 (a) and (b). Obviously, the on-site nematic interaction \( g \) still acts to suppress \( P_{2}(r) \) at different distances.

Why are the long-range pairing correlations suppressed by the on-site nematic interaction \( g \) in our model? Since the model contains both electron–electron and nematic interactions, such
suppression may mainly come from decreases of spin fluctuations around $(\pi, 0)/(0, \pi)$ as shown in figures 2(b) and 3(b), which may lead to strong reductions of pairing amplitude for several dominant pairing channels [41], although the contribution of enhanced nematic fluctuations may still strengthen electron pairing [27, 28].

4. Conclusions

We studied the nematic, magnetic, and pairing properties of the two-orbital Hubbard model that consists of Coulombic interactions and on-site nematic interaction at intermediate correlation strength. The main advantage of our model is that we could completely study the impact of nematic interaction on electron pairings by taking electronic correlations into account.

Our results based on the CPQMC simulations indicate that the on-site nematic interaction seems to prompt antiferro-orbital nematic fluctuations and suppress the $(\pi, 0)/(0, \pi)$ AFM order. Most importantly, the universal suppression of $P_{\text{long}}$ for several dominant pairing channels by $g$ suggests that the enhancement of nematic fluctuation plays a negative role on superconductivity at intermediate correlations. Our finding is useful for understanding the interplay of nematic fluctuation and superconductivity in FeSCs.

Acknowledgments

GL thanks Yan Zhang and Yong-Jun Wang for insightful discussions. This work was supported by the National Natural Science Foundation of China under grant No. 11674087.

Figure 7. Long-range correlation function of wave2 versus pairing distance $r$ by using Raghu hopping parameters. (a) Hole doping density $\rho = 0.125$ and $U = 2\text{eV}$ on an $8 \times 8$ square lattice; (b) hole doping density $\rho = 0.08$ and $U = 2\text{eV}$ on a $10 \times 10$ square lattice.

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