



What makes the T_c of monolayer FeSe on SrTiO₃ so high: a sign-problem-free quantum Monte Carlo study

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Abstract Monolayer FeSe films grown on SrTiO₃ (STO) substrate show superconducting gap-opening temperatures (T_c) which are almost an order of magnitude higher than those of the bulk FeSe and are highest among all known Fe-based superconductors. Angle-resolved photoemission spectroscopy observed “replica bands” suggesting the importance of the interaction between FeSe electrons and STO phonons. These facts rejuvenated the quest for T_c enhancement mechanisms in iron-based, especially iron-chalcogenide, superconductors. Here, we perform the first numerically-exact sign-problem-free quantum Monte Carlo simulations to iron-based superconductors. We (1) study the electronic pairing mechanism intrinsic to heavily

electron doped FeSe films, and (2) examine the effects of electron–phonon interaction between FeSe and STO as well as nematic fluctuations on T_c . Armed with these results, we return to the question “what makes the T_c of monolayer FeSe on SrTiO₃ so high?” in the conclusion and discussions.

Keywords High temperature superconductivity · Pairing mechanism · Iron-based superconductivity · FeSe/STO · Sign-problem-free quantum Monte-Carlo simulation

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1 Introduction

The strong Cooper pairing in monolayer FeSe film on SrTiO₃ substrate ((FeSe)₁/STO) [1] continues to attract a great deal of attentions (e.g. Refs. [2–17]). Recent developments in the study of FeSe-based high temperature superconductors clearly indicate there are at least two factors that are important to the enhancement of T_c from 8.9 K (bulk FeSe) to about 75 K in FeSe/BaTiO₃/SrTiO₃ [5]. These factors are (1) heavy electron doping [9–14] and (2) the effects of the substrate [15, 16].

The first factor, namely heavy electron doping, shapes the fermiology into that best for the intrinsic electron pairing mechanism to act [17]. Concerning the intrinsic pairing mechanism there are two main candidates: the spin [18–23] and orbital [24] fluctuations mediated pairing. However, these proposals are based on approximations that are often not controlled in the presence of strong correlations. By now there are mounting experimental [25–27] and theoretical [28–30] evidences that iron-based superconductors, in particular the iron-chalcogenide superconductors, are strongly correlated. Thus, a theoretical method free of uncontrolled

approximations suitable for handling such situation is in high demand.

An experiment that sheds lots of light on the second factor, i.e., the effects of substrate, is the ARPES result of Ref. [15], which shows “replica bands” approximately 100 meV away from all low binding energy bands. Such phenomenon is explained in terms of “phonon shake off”, and the phonons are identified with the longitudinal optical phonon branch of STO [15, 16]. This result suggests there is a strong coupling between the FeSe electrons and STO phonons. Moreover, it is conjectured that such coupling can substantially enhance the T_c intrinsic to heavily electron doped FeSe [15, 16].

In the rest of the paper, we perform large-scale projector quantum Monte Carlo (QMC) [31–33] simulation (details are discussed in Ref. [34]). It turns out that the fermiology, namely the existence of two separate electron Fermi pockets, of $(\text{FeSe})_1/\text{STO}$ allows the simulation to be free of the fermion minus sign problem. This enables us to perform approximation-free unbiased study of the intrinsic electronic pairing mechanisms, namely, the antiferromagnetic (AFM) and antiferro-orbital (AFO) fluctuation mediated pairing. It also allows us to study the effects of electron–phonon interaction between FeSe and STO [16] and nematic fluctuations [35, 36] on T_c .

A summary of our results is as follows. For the intrinsic pairing mechanisms we have studied two types of spin fluctuations and one type of orbital fluctuations. A commonality between these fluctuations is that they all scatter electrons from one Fermi pocket to the other. (1) For spin fluctuations mimicking the nearest-neighbor AFM exchange interaction (the “ J_1 -type” spin fluctuation) the ground state exhibits *nodeless* d -wave superconducting (SC) long range order. (2) For spin fluctuations mimicking the next-nearest-neighbor AFM exchange interaction (the “ J_2 -type” spin fluctuation) the ground state exhibits s -wave SC long range order. (3) The AFO fluctuations trigger s -wave pairing. For the enhancement mechanisms we have studied the small momentum transfer electron–phonon interactions and the nematic fluctuations. Our results clearly show (4) the small momentum transfer electron–phonon interaction significantly strengthens the Cooper pairing triggered by both spin and orbital fluctuations. (5) Similar to the electron–phonon interaction nematic fluctuations also strengthen the Cooper pairing triggered by all three intrinsic mechanisms discussed above. A highlight of some of the main results is shown in Fig. 1.

2 Sign-problem-free quantum Monte Carlo

The effective actions we consider are given in the Electronic Supplementary Materials I–IV (online). These

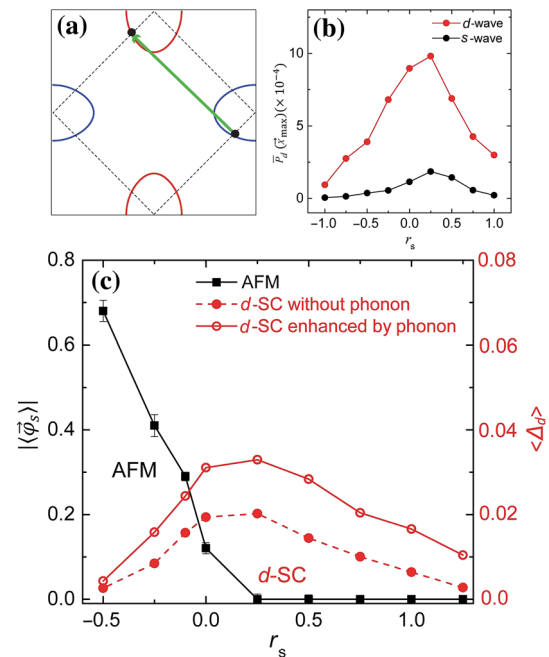


Fig. 1 **a** The Fermi surfaces of the bandstructure used in our simulations. The J_1 -type AFM fluctuations can cause the inter-pocket scattering (green arrow). **b** The SC correlation in s - and d -wave pairing channels as a function of the parameter that controls the J_1 -type spin fluctuations (the size $L = 18$). **c** The phase diagram for the J_1 -type spin fluctuations where the d -wave SC is substantially enhanced by the electron–phonon coupling (solid red curve) compared to the one without electron–phonon couplings (dashed red curve). Here we use the ground state expectation value of the AFM and SC order parameters as a measure of their ordering temperatures

actions consist of three parts: (1) the bandstructure of electrons, (2) various fluctuating Bose fields, and (3) the “Yukawa” coupling between the Bose fields and electrons. The bandstructure is chosen to mimic the Fermi surfaces of $(\text{FeSe})_1/\text{STO}$ as shown in Fig. 1a. We use the one-iron Brillouin zone because it has been shown experimentally that when folded to the corners of the two-iron Brillouin zone the electron pockets show negligible hybridization at their crossings [37].

For intrinsic pairing mechanisms the Bose fields we studied include $\vec{\varphi}_s$ and φ_o associated with the spin and orbital fluctuations respectively. These fields scatter electrons between the Fermi pockets as shown by the green arrow in Fig. 1a. For the pairing enhancement mechanisms, we studied STO phonons and nematic fluctuations. The Bose fields associated with them are φ_{ph} and φ_n , they cause small momentum transfer (i.e. intra-pocket) scattering of the FeSe electrons. The reason we only consider small momentum phonon scattering is due to the forward-focusing nature of the electron–phonon interaction deduced from Ref. [15]. In Eqs. (S2), (S5) and (S9) (online), the parameters $r_{s,o,n}$ tune $\vec{\varphi}_s$, φ_o , φ_n across their respective

quantum phase transitions. Large negative values correspond to strongly ordered phase and large positive values correspond to the strongly disordered phase. The parameter r_{ph} in Eq. (S7) (online) controls the optical phonon frequency at $\vec{q} = 0$. Remarkably, in all cases our QMC calculation has no minus sign problem [38–40] (see the Electronic Supplementary Material VI online). The QMC simulation is carried out on a square lattice with $N = L \times L$ sites using periodic boundary conditions. In the following we present the simulation results.

3 The spin fluctuation mediated pairing

3.1 The J_1 -type spin fluctuation

The effective action is given by Eqs. (S1)–(S3) (online). The reason we refer to it as the J_1 -type spin fluctuation is because integrating out $\vec{\varphi}_s$ generates an AFM exchange interaction whose momentum space coupling constant has the same sign as that of the nearest-neighbor (J_1) AFM exchange interaction. From the Binder cumulant [41] of the AFM order parameter (not shown), we estimate the AFM quantum critical point $r_{s,c}$ to lie in the range of (0, 0.25). To study superconductivity we compute the equal-time pair–pair correlation function $\bar{P}_{s/d}(\vec{x}_{max})$ (see Eqs. (S11)–(S13) online). Here s/d denotes s -wave (same sign on the two electron pockets) and (nodeless) d -wave (opposite sign on the two electron pockets) pairing, respectively. $\vec{x}_{max} = (L/2, L/2)$ is the maximum separation between the two pair fields in a system of size L . In Fig. 1b, we plot $\bar{P}_{s/d}(L/2, L/2)$ for $L = 18$ as a function of r_s . Clearly superconductivity is enhanced near the magnetic quantum critical point. Moreover, the d -wave pairing is favored over the s -wave [42].

In Fig. 2a (red curve), we show the size-dependence of $\bar{P}_d(L/2, L/2)$ at $r_s = 0.25$ for $L = 12, 14, 16, 18, 20, 22$ (the red points). The red curve is the best fit using a second order polynomial in $1/L$. This allows us to extrapolate to $L \rightarrow \infty$ to obtain $\bar{P}_d(L \rightarrow \infty) = (4.3 \pm 1.1) \times 10^{-4}$. This establishes the fact that the ground state possesses nodeless d -wave SC long-range order!

3.2 The J_2 -type spin fluctuation

The effective action is given by Eqs. (S1), (S2) and (S4) (online). In this case, integrating out the spin boson $\vec{\varphi}_s$ generates an AFM exchange interaction whose momentum space coupling constant has the same sign as that of the next nearest neighbor (J_2) AFM exchange interaction. From the Binder cumulant (not shown here) we deduce the quantum critical point to be situated within $0.0 \leq r_{s,c} \leq 0.25$. In Fig. 3a, we plot $\bar{P}_{s/d}(L/2, L/2)$ for $L = 14$ as a function of r_s . Here s -wave superconductivity is enhanced near the magnetic quantum critical point.

In Fig. 2b (red curve), we study the size-dependence of $\bar{P}_d(L/2, L/2)$ at $r_s = 0.25$ for $L = 12, 14, 16, 18, 20, 22$ (the red points). The red curve is the best fit using a second order polynomial in $1/L$. This allows us to extrapolate to $L \rightarrow \infty$ to obtain $\bar{P}_d(L \rightarrow \infty) = (1.4 \pm 0.5) \times 10^{-4}$. This establishes the fact that the ground state possesses nodeless s -wave SC long-range order.

4 The AFO fluctuation mediated pairing

In this section, we study the effects of AFO fluctuation (φ_o) on superconductivity. The effective action is given by Eqs. (S1), (S5) and (S6) (online). Like the AFM fields the

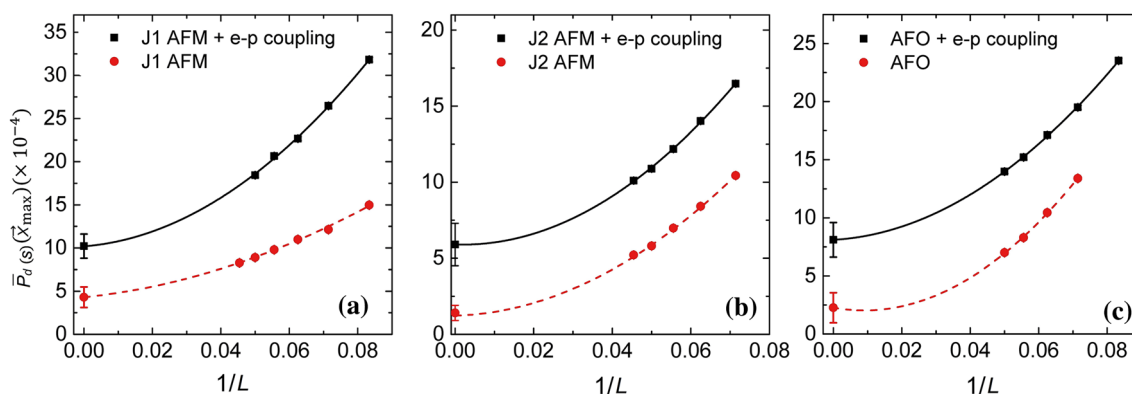


Fig. 2 The enhancement of SC correlation by the small momentum transfer electron–phonon interaction. In each panel the SC correlation in the dominant pairing channel, $\bar{P}_d(L/2, L/2)$, is plot as a function of $1/L$ with and without the electron–phonon interactions. **a–c** For J_1 -type spin (**a**), J_2 -type spin (**b**), and AFO (**c**) fluctuations, respectively

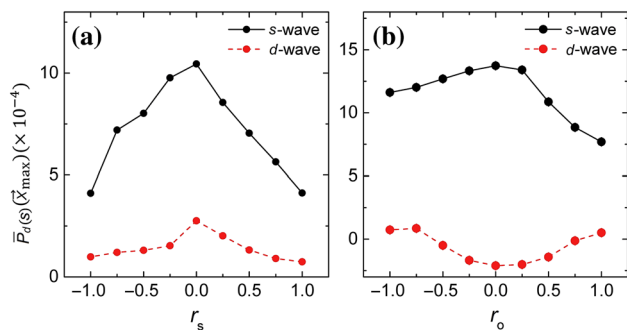


Fig. 3 The SC correlation, $\bar{P}(L/2, L/2)$, in the *s*- and *d*-wave pairing channels for $L = 14$ triggered by the **a** J_2 -type spin and **b** AFO fluctuations. For both cases, the *s*-wave pairing is favored over the *d*-wave

AFO field also scatters electrons between the two Fermi pockets (the green arrow in Fig. 1a).

From the Binder cumulant associated with the AFO order parameter (not shown here) we deduce the AFO quantum critical point to be situated within $0.0 \leq r_{o,c} \leq 0.25$. In Fig. 3b, we plot $\bar{P}_{s/d}(L/2, L/2)$ for $L = 14$ as a function of r_o . Clearly *s*-wave SC correlation is favored over the *d*-wave, and it is peaked near the AFO quantum critical point. In Fig. 2c (red curve) we study the size-dependence of $\bar{P}_d(L/2, L/2)$ at $r_o = 0.25$ for $L = 12, 14, 16, 18, 20, 22$ (the red points). The red curve is the best fit using a second order polynomial in $1/L$. This allows us to extrapolate to $L \rightarrow \infty$ to obtain $\bar{P}_s(L \rightarrow \infty) = (2.1 \pm 0.9) \times 10^{-4}$. This indicates that the ground state possesses *s*-wave SC long-range order.

5 The pairing enhancement due to STO phonons

Motivated by Ref. [15], here we study the effect of small momentum transfer electron–phonon coupling on the superconductivity triggered by pure AFM and AFO fluctuations. This is done by adding the coupling to φ_{ph} [see Eqs. (S7), (S8) online]. The parameter r_{ph} that controls the phonon frequency is fixed at 0.5. The strength of the electron–phonon coupling is controlled by λ_{ph} . The value of λ_{ph} is chosen so that the dimensionless strength of the phonon mediated attraction $\lambda = \frac{\lambda_{ph}^2}{r_{ph}W} = 0.6$. Here W is the electron band width. This value is similar to the estimate given in Ref. [15]. In the following we fix the parameter $r_{s,o}$ at 0.25. In Fig. 2 we compare the size dependence of the SC correlation function in the dominant pairing channels with (black curve) and without (red curve) phonons. Clearly the SC order is enhanced by the electron–phonon interaction regardless of the intrinsic pairing mechanisms.

The phase diagram in Fig. 1c is constructed from the extrapolated value of the AFM and SC order parameters

from finite-size analysis for each r_s . The plot is for the J_1 -type spin fluctuation, however we expect a similar plot holds for J_2 -type spin and AFO fluctuations as well. In the phase diagram, we use the ground state expectation value of the AFM and SC order parameters as a measure of their ordering temperatures. It is clear that the SC ordering temperature T_c is enhanced by the electron–phonon couplings for all value of r_s . Remarkably, the T_c enhancement by phonons is largest around the AFM quantum critical point.

In the Electronic Supplementary Material VII (online), we study the enhancement of the SC order parameter due to J_1 -type spin and AFO fluctuations as a function of the dimensionless phonon-mediated attraction strength λ . Apparently, the enhancement of superconductivity peaks at $\lambda = 1.5$ for the J_1 -type spin fluctuation triggered *d*-wave pairing. For the AFO induced *s*-wave pairing the pair–pair correlation increases monotonously with the electron–phonon coupling strength up to $\lambda = 2.2$.

6 The pairing enhancement by nematic fluctuations

In view of the possibility that nematic fluctuation can be substantial in heavily electron-doped FeSe films [17], here we study the effects of nematic fluctuations on superconductivity. The effective action is given by Eqs. (S1), (S9) and (S10) (online).

In Fig. 4, we compare the size dependence of the SC correlation function in the dominant pairing channels with (black curve) and without (red curve) nematic fluctuations. Like the electron–phonon interaction, the SC order is enhanced by the nematic fluctuations for all intrinsic pairing mechanisms considered.

7 Conclusion and discussions

A definitive answer to “why T_c is so high in monolayer FeSe on SrTiO₃?” requires one to (1) determine the intrinsic pairing mechanisms which is primarily responsible to Cooper pairing in heavily electron doped FeSe-based high temperature superconductors, and (2) pin down the effects of substrate.

Regarding (2), our results show that small momentum transfer electron–phonon scattering enhances superconductivity regardless of whether it is triggered by the spin or orbital fluctuations, hence lend support to the phonon enhancement mechanism discussed in Refs. [15, 16]. However our result holds for all phonons that scatter the FeSe electron with small momentum transfer. It does not allow us to conclude that the particular branch of high frequency phonon which caused the replica bands in

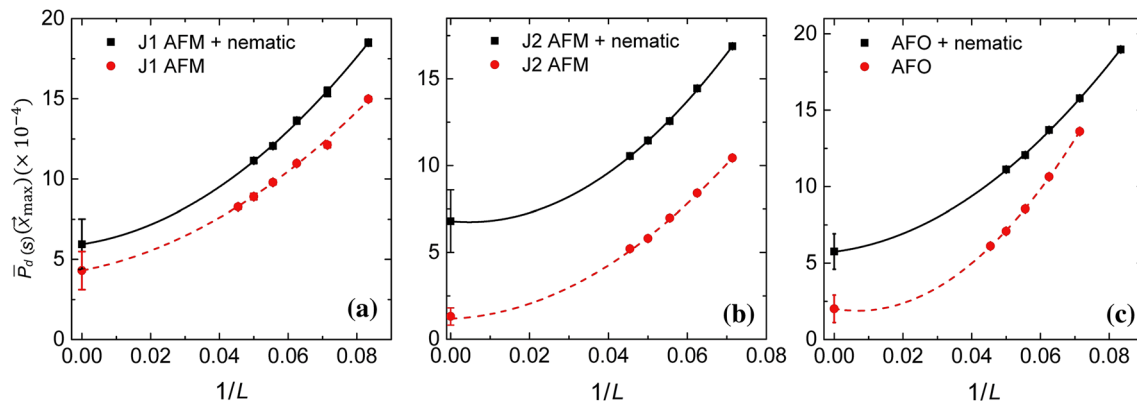


Fig. 4 The enhancement of SC correlation by nematic fluctuations. In each panel, the SC correlation in the dominant pairing channel, $\bar{P}_d(L/2, L/2)$, is plot as a function of $1/L$ with and without the electron phonon interaction. **a–c** For J_1 -type spin (a), J_2 -type spin (b) and AFO (c) fluctuations, respectively

Ref. [15] is *solely* responsible for the T_c enhancement. In particular it does not rule out the importance of other lower frequency polar phonons.

Regarding (1), our results do not allow us to answer whether spin or orbital fluctuation is main intrinsic pairing mechanism in heavily electron doped FeSe films. However we can confidently predict the pairing symmetry associated with each pairing mechanism. In particular if the pairing symmetry turns out to be s -wave it can come from several different mechanisms: J_2 -type spin fluctuation or anti-ferro orbital fluctuation, or the combination of them with nematic fluctuation. However if the pairing symmetry is d -wave our result uniquely pins down the J_1 -type spin fluctuation as the driving force.

Experimentally the pairing symmetry of $(\text{FeSe})_1/\text{STO}$ is still an open question. However we would like to list a number of circumstantial evidence that the pairing symmetry might be d -wave. The first is the existence of neutron resonance *below twice the SC gap* in materials with similar fermiology [43, 44], and the fact that the momentum locations of the resonance are consistent with inter-pocket scattering. The second is a recent high resolution ARPES study of the SC gap anisotropy of $(\text{FeSe})_1/\text{STO}$ [37]. It observes four minima in the SC gap at the momentum locations corresponding to the crossing of the two Fermi pockets (in the two iron Brillouin zone). This can be interpreted as the result due to weak inter-pocket hybridization on a *nodeless d*-wave gap [45]. Moreover the weakness of the inter-pocket hybridization is evidenced by the lack of splitting at the Fermi pocket crossings in the normal state.

Although there is no direct evidence of strong nematic fluctuation in $(\text{FeSe})_1/\text{STO}$ we can not rule out that it does play a partial role in the pairing of heavily electron doped FeSe films. By itself nematic fluctuation will not discriminate between s - and d -wave pairings. However when

coupled with the spin or orbital fluctuations it can significantly enhance the pairing strength favored by each of them.

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Note After our work was posted on arXiv.org, another sign-problem-free QMC on FeSe appeared [46]. However, the focus of Ref. [46] is quite different from ours.

Conflict of interest The authors declare that they have no conflict of interest.

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