Self-restraint effect of superconductivity from spin fluctuations

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Abstract

We study the superconducting instability mediated by spin fluctuations in the Eliashberg theory for a minimal two-band model of iron-based superconductors. While antiferromagnetic spin fluctuations can drive superconductivity (SC) as is well established, we find that spin fluctuations necessarily contain a contribution to suppress SC even though SC can eventually occur at lower temperatures. This self-restraint effect stems from a general feature of the spin-fluctuation mechanism, namely the repulsive pairing interaction, which leads to phase frustration of the pairing gap and consequently the suppression of SC.

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Iron-based superconductors (FeSC) provide a platform to explore a mechanism of high-temperature (high-$T_c$) superconductivity (SC) \[1\]. Since SC is realized close to a spin-density-wave (SDW) phase, the importance of spin fluctuations is widely recognized as a possible mechanism of SC \[2–4\]. A close look at the phase diagram of FeSC reveals the presence of an electronic nematic phase, which is also close to the SC phase. While the origin of the nematic phase is still controversial \[5\], it was shown that orbital nematic fluctuations lead to strong coupling SC with an onset temperature comparable to the observation \[6, 7\]. The electronic structure of FeSC is characterized by multibands originating from five $3d$ orbitals of Fe ions \[3\]. Hence the orbital fluctuations are also explored as a possible mechanism of SC \[8–10\]. While electron-phonon coupling is present in real materials and is expected to lead to SC, the transition temperature ($T_c$) is believed to be too low compared to the observation \[11\].

The distinction between different SC mechanisms is a key issue of FeSC. Typically spin fluctuations lead to the so-called $s_{\pm}$-wave symmetry \[2–4\] whereas nematic \[6, 7, 12\] and orbital \[8, 9\] fluctuations yield $s_{++}$-wave symmetry. Obviously this symmetry difference is crucial, but it is not easy to resolve the phase of SC order in experiments. Furthermore, an $s_{\pm}$-wave pairing gap was found to be stabilized even for nematic fluctuations when a partial contribution from spin fluctuations is considered in Ref. \[13\], suggesting that the gap symmetry itself cannot be decisive in identifying the SC mechanism.

The momentum dependence of the pairing gap is expected to depend on the underlying SC mechanism. However, it turned out \[7\] that nematic fluctuations lead to a pairing gap similar to that from spin fluctuations, except for the sign of the pairing gap. Considering simplifications involved in many theoretical studies, it is not easy to extract a robust and key difference of the gap structure, which can distinguish between the different SC mechanisms.

Irrespective of the underlying SC mechanism in FeSC, it is tacitly assumed that spin, orbital, and nematic fluctuations work positively on driving SC. However, in this paper, we find that spin fluctuations tend to suppress the SC instability even though spin fluctuations can eventually lead to SC at lower temperatures. This self-restraint effect is a general feature originating from a repulsive pairing interaction, which yields a sign change of the pairing gap on the Fermi surfaces (FSs) connected by a momentum transfer of the spin fluctuations.
A minimal model for the band structure of FeSC may read as \[ H_0 = \sum_{\mathbf{k}, \sigma, \alpha, \beta} \epsilon_{\alpha \beta}^{\mathbf{k}} c_{\mathbf{k} \alpha \sigma}^{\dagger} c_{\mathbf{k} \beta \sigma} \]

on a square lattice, where the unit cell contains one iron and $\alpha = 1$ and 2 refer to the $d_{xz}$ and $d_{yz}$ orbital, respectively; $c_{\mathbf{k} \alpha \sigma}^{\dagger}$ and $c_{\mathbf{k} \sigma}$ are the creation and annihilation operators for electrons with momentum $\mathbf{k}$, orbital $\alpha$, and spin orientation $\sigma$; intraorbital dispersions are given by $\epsilon_{11}^{\mathbf{k}} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y - \mu$ and $\epsilon_{22}^{\mathbf{k}} = -2t_2 \cos k_x - 2t_1 \cos k_y - 4t_3 \cos k_x \cos k_y - \mu$, whereas the interorbital dispersion is $\epsilon_{12}^{\mathbf{k}} = -4t_4 \sin k_x \sin k_y$; $\mu$ is the chemical potential. The typical FSs observed in FeSC are well captured by choosing the parameters as $t = -t_1$, $t_2/t = 1.5$, $t_3/t = -1.2$, $t_4/t = -0.95$, and $\mu/t = 0.6$.

As shown in Fig. 1 (a), the Hamiltonian (1) yields two hole FSs around $\mathbf{k} = (0, 0)$ and $(\pi, \pi)$, and two electron FSs around $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, which we refer to as FS1, FS2, FS3, and FS4, respectively. FS1 and FS2 originate from both $d_{xz}$ and $d_{yz}$ orbitals whereas FS3 consists of $d_{yz}$ orbital and FS4 $d_{xz}$ orbital. These FSs capture the orbital components obtained in a more realistic 5-band model [16].

To clarify the effect of spin fluctuations on SC, we consider a system where electrons interact with each other via the spin exchange,

$$ H_I = \frac{1}{2} \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}), \tag{2} $$

where the spin operator is $\mathbf{S}(\mathbf{q}) = \frac{1}{2} \sum_{\mathbf{k}, \alpha, \sigma, \sigma'} c_{\mathbf{k} \alpha \sigma}^{\dagger} \sigma_{\sigma \sigma'} c_{\mathbf{k} + \mathbf{q} \sigma'}$ and $\sigma$ are Pauli matrices. This interaction term is viewed as a low-energy effective interaction generated by, for example, the repulsive Hubbard interaction by decreasing the energy scale in a functional renormalization group scheme [17]. The form of $J(\mathbf{q})$ depends on details of high-energy fluctuations. To keep a connection with FeSC, we assume that $J(\mathbf{q})$ shows a peak at $\mathbf{q} = (\pm \pi, 0)$ and $(0, \pm \pi)$ with a negative sign so that the stripe-type antiferromagnetic order typically observed in FeSC [18] is captured. We consider the so-called $J_1$-$J_2$-type interaction $J(\mathbf{q}) = 2J_1(\cos q_x + \cos q_y) + 4J_2 \cos q_x \cos q_y$ with $J_2 > J_1/2 > 0$. In this case, the sizable interaction extends up to the second nearest-neighbor sites in real space. Thus the systems may be regarded as being close to the limit of the localized spins even though the system remains metallic. As the itinerant limit, we may consider the Lorentz-type $J(\mathbf{q})$, but our major conclusions do not change; see Supplemental Material for explicit results.
For the interaction described by Eq. (2), the spin fluctuation propagator is computed from a bubble summation, namely

\[
\tilde{J}(q, iq_m) = J(q) - \frac{J(q)\chi_0(q, iq_m)J(q)}{1 + J(q)\chi_0(q, iq_m)}
\]

and \(\chi_0(q, iq_m) = -\frac{T}{2N} \sum_{k,\sigma,n} \text{Tr} G_0(k, ik_n)G_0(k + q, ik_n + iq_m)\). Here \(G_0\) is a 2 \(\times\) 2 matrix of the noninteracting Green function defined for Eq. (1), \(ik_n\) fermionic Matsubara frequency, \(T\) temperature, and \(N\) the total number of the lattice sites. The first term in Eq. (3) does not depend on frequency and describes the instantaneous interaction, whereas the second term accounts for the retardation effect on the pairing. A role of the instantaneous interaction for SC would be analyzed appropriately by including the Coulomb repulsion \cite{19}. In this work, we are interested in SC mediated by dynamical spin fluctuations and thus we focus on the second term.

The Eliashberg gap equations involve two coupled nonlinear equations for the pairing gap \(\Delta(k, ik_n)\) and the renormalization function \(Z(k, ik_n)\). In many interesting cases, it is highly demanding to solve the Eliashberg equations numerically. Hence \(Z(k, ik_n)\) would be set to unity and yet computation would be limited to a temperature region much higher than \(T_c\). To overcome these technological issues, we recall that SC instability is a phenomenon close to the FS and project the momentum on the FSs. We divide the FSs into many patches and define the Fermi momentum \(k_F\) on each patch. Thus \(k_F\) is a discrete quantity in this work. This idea allows us to achieve stable computations down to very low temperature with including the renormalization function \cite{6} as well as a fine momentum resolution \cite{7}.

After linearizing the Eliashberg equations with respect to \(\Delta(k, ik_n)\), we obtain

\[
\Delta(k_F, ik_n)Z(k_F, ik_n) = -\pi T \sum_{k_F', n'} N_{k_F'} \frac{\Gamma_{k_F'k_F'}(ik_n, ik_n')}{|k_n'|} \Delta(k_F', ik_n'),
\]

\[
Z(k_F, ik_n) = 1 - \pi T \sum_{k_F', n'} N_{k_F'} \frac{k_n' \Gamma_{k_F'k_F'}(ik_n, ik_n')}{|k_n'|}.
\]

Here \(N_{k_F}\) is a momentum-resolved density of states on each FS patch and \(\Gamma_{k_F'k_F'}(ik_n, ik_n')\) is the averaged pairing interaction over the FS patches specified by \(k_F\) and \(k_F'\):

\[
\Gamma_{k_F'k_F'}(ik_n, ik_n') = -\frac{1}{4} (W_{ab}(k, k')^2 \times \left( \tilde{J}(k - k', ik_n - ik_n') + 2\tilde{J}(k + k', ik_n + ik_n') \right))_{k_F'k_F'},
\]
where $\tilde{J}(\mathbf{k} - \mathbf{k}', ik_n - ik'_n)$ comes from longitudinal spin fluctuations and $\tilde{J}(\mathbf{k} + \mathbf{k}', ik_n + ik'_n)$ transverse ones. The vertex part $W_{ab}(\mathbf{k}, \mathbf{k}') = (U^\dagger(\mathbf{k})U(\mathbf{k}'))_{ab}$ comes from the $2 \times 2$ unitary matrix diagonalizing the kinetic term Eq. (1), and $a$ and $b$ denote band indices. Since each band forms FSs, the indices $a$ and $b$ can be absorbed into the FS indices $\mathbf{k}_F$ and $\mathbf{k}'_F$. Similarly, we can compute $\Gamma_{Z_{k_F k'_F}}(ik_n, ik'_n)$ in Eq. (5) as

$$
\Gamma_{Z_{k_F k'_F}}(ik_n, ik'_n) = \frac{1}{4} \langle W_{ab}(\mathbf{k}, \mathbf{k}')^2 \times \left( 3\tilde{J}(\mathbf{k} - \mathbf{k}', ik_n - ik'_n) - 2J(\mathbf{k} - \mathbf{k}') \right) \rangle_{k_F k'_F}.
$$

(7)

$Z(\mathbf{k}_F, ik_n)$ is directly obtained from Eq. (5). It is then straightforward to solve the eigenvalue equation Eq. (4) numerically. When the eigenvalue $\lambda$ exceeds unity, SC instability occurs.

Since the SC instability is expected near the antiferromagnetic phase, we choose $J_2 = 1.7t$ where the stripe-type SDW order occurs below $T = 0.030t$. Our conclusions, however, do not depend on a precise choice of $J_2$. In the following, all quantities with the dimension of energy are measured in units of $t$.

The solid line in Fig. 1(b) shows the temperature dependence of the eigenvalue of Eq. (4). With decreasing temperature, the eigenvalue is enhanced and reaches as large as 0.6 at $T \approx 0.03$. If the temperature is decreased further, SDW instability would preempt SC instability. While the SC instability therefore does not occur in a strict sense, the eigenvalue less than unity is frequently obtained in many theoretical studies for FeSC and consistent with the literature [20–22]. Note that the eigenvalue can exceed unity if we neglect the self-energy effect (see Fig. 3).

For the FSs typical to FeSC, there are three different low-energy scattering processes "intra", "($\pi, 0$)" and "($\pi, \pi$)" as shown in Fig. 1(a). To identify the dominant scattering process leading to the SC, we also compute the eigenvalue of the Eliashberg equation Eq. (4) by choosing particular scattering processes. Since spin fluctuations are characterized by momenta ($\pi, 0$) and $(0, \pi)$, it is reasonable that the eigenvalue for "($\pi, 0$)" scattering processes becomes much larger than the other two. Our finding here is the substantial suppression of the eigenvalue from "($\pi, 0$)" by including the intrapocket scattering processes; see the line of "intra + ($\pi, 0$)" in Fig. 1(b). Intrapocket scattering processes are characterized by small momentum transfers and correspond to a tail of spin fluctuations with a peak around $(\pi, 0)$ and $(0, \pi)$. In fact, "intra" scattering processes alone yield the eigenvalue less than 0.1. Therefore the contribution from "intra" scattering processes seems irrelevant to SC,
FIG. 1: (Color online) (a) Hole Fermi pockets (1 and 2) around $\Gamma$ and $M$ points and electron pockets (3 and 4) around $X$ and $Y$ in the normal state. ”intra”, ”$(\pi,0)$”, and ”$(\pi,\pi)$” denote scattering processes inside each pocket, between the hole and electron pockets, and between the two hole (or electron) pockets, respectively. (b) Temperature dependence of the eigenvalues $\lambda$ (solid line). The eigenvalues are also computed by focusing on particular scattering processes as denoted by ”intra”, ”$(\pi,\pi)$”, and ”$(\pi,0)$”. Below $T = 0.030$, SDW order occurs before SC instability.

but Fig. 1 (b) reveals that it plays a vital role to suppress the SC tendency, which is the major finding of this work.

This self-restraint effect can be understood in terms of phase frustration of pairing gap. As is well known [23], spin fluctuations give rise to a repulsive pairing interaction and in fact $\Gamma_{k'i'k_k} (i\k_n, i\k'_n)$ in Eq. (6) is positive. In this case, pairing gap tends to have the opposite sign between the hole and electron pockets connected by ”$(\pi,0)$” scattering processes. The resulting gap has the same sign inside each pocket. On the other hand, spin fluctuations necessarily contain ”intra” scattering processes as a tail of the major antiferromagnetic fluctuations. These processes also yield a repulsive pairing interaction and thus tend to drive the sign change of pairing gap inside each pocket. Therefore there occurs frustration of the phase of pairing gap from ”$(\pi,0)$” and ”intra” scattering processes. The numerical
finding in Fig. 1 (b) implies that this phase frustration effect is crucially important to the suppression of the eigenvalue of the Eliashberg equations even though the "intra" scattering processes alone are not effective to the SC instability itself. This self-restraint effect can be a general feature because the phase frustration is necessarily involved in the spin-fluctuation mechanism as long as it yields repulsive pairing interaction.

While "intra" scattering processes are the major source of the self-restraint effect, "(π, π)" scattering processes also lead to the phase frustration of the SC gap. This is because they wish to have the opposite sign between the hole (electron) pockets whereas the major "(π, 0)" scattering processes eventually lead to the same sign between the hole (electron) pockets. Quantitatively, however, such a phase frustration effect is not effective compared to the "intra" processes as shown in Fig. 1 (b). In fact, the eigenvalue of the Eliashberg equations is almost reproduced by considering only "intra" and "(π, 0)" scattering processes. That is, "intra" processes are much more destructive to the SC than "(π, π)" ones. See Supplemental Material for the case of the Lorentz-type interaction where the contribution from "(π, π)" scattering processes suppresses SC more than Fig. 1 (b), but still "intra" scattering processes play a major role of the self-restraint effect.

The "intra" scattering processes should not be confused with ferromagnetic fluctuations. The self-restraint effect cannot be understood in terms of the competition of, for example, singlet and triplet pairings. In fact, the static magnetic susceptibility does not show any peak around (0, 0). Moreover, we checked that the eigenvector obtained from the "intra" pocket scattering processes alone is not triplet pairing.

To see how the self-restraint effect affects the momentum dependence of the pairing gap, we plot $k_F$ dependence of the pairing gap in Fig. 2. The pairing gap has the same sign in each pocket and the opposite sign between the hole (FS1 and FS2) and electron pockets (FS3 and FS4). The so-called $s_{±}$-wave symmetry is realized as expected [2, 3]. The pairing gap exhibits a large $k_F$ dependence on FS1, FS3, and FS4. While the gap has a fourfold symmetry on FS1 and FS2, it has a two-fold symmetry on FS3 and FS4, because the FS has a two-fold symmetry around $k = (π, 0)$ and $(0, π)$, respectively. All these features are consistent with the literature [24]. The point here is that those gaps suffer from the self-restraint effect. The pairing gap without the self-restraint effect is obtained by considering "(π, 0)" scattering processes alone and the obtained results are shown in Fig. 2 (b). A comparison with Fig. 2 (a) demonstrates that the self-restraint effect causes the large $k_F$
dependence of the pairing gap on FS1, FS3, and FS4 to minimize the phase frustration effect of the pairing gap although the $s_{\pm}$ symmetry does not change.

FIG. 2: (Color online) Momentum dependence of the pairing gap $\Delta$ on each Fermi pocket at the lowest temperature $T = 0.03$ from "all" scattering processes (a) and "($\pi,0$)" scattering processes alone (b). The polar angle $\theta$ is measured from the horizontal axis on each pocket as shown in Fig. 1 (a).

The self-restraint effect is different from the self-energy effect. We compute the eigenvalue of the Eliashberg equations by neglecting the self-energy effect, namely by putting $Z = 1$. The result is shown in Fig. 3 in the same fashion as Fig. 1 (b) and essentially the same results are obtained except for the absolute value of $\lambda$. The "($\pi,0$)" scattering processes yield the SC instability at $T = 0.042$, which is then reduced to $T = 0.034$ by adding "intra" scattering processes; the resulting eigenvalue then reproduces the eigenvalue for "all" scattering processes. The self-restraint effect reduces $T_c$ by $(0.042 - 0.034)/0.042 = 19\%$. At $T = 0.042$, we have obtained $\lambda = 0.65$ in Fig. 1 (b) for "($\pi,0$)" scattering processes. Hence the self-energy effect suppresses the SC tendency by $(1 - 0.65)/1 = 35\%$. That is, the suppression of the SC instability due to the self-restraint effect is comparable to that due to the self-energy effect.

Antiferromagnetic spin fluctuations are widely discussed as a possible high-$T_c$ mechanism. While there is no doubt that spin fluctuations can drive the SC, this mechanism needs to overcome the self-restraint effect to achieve high-$T_c$. In this sense, a favorable condition is required to realize high-$T_c$ from spin fluctuations. To reduce the self-restraint effect substantially, we would invoke an interaction term $J(q)$, whose magnitude becomes very small for a small momentum transfer so that the contribution from "intra" scattering processes is substantially weakened.

On the other hand, orbital fluctuations with a large momentum transfer [8, 9] and nematic fluctuations [6, 7] are also proposed as a possible high-$T_c$ mechanism in FeSC. These
FIG. 3: (Color online) Temperature dependence of the eigenvalues \( \lambda \) (solid line denoted by "all"). The eigenvalues are also computed by focusing on particular scattering processes as denoted by "intra", "(\( \pi, \pi \))", and "(\( \pi, 0 \))". The self-energy effect is discarded by assuming \( Z = 1 \).

fluctuations yield an attractive pairing interaction and thus tend to have the same sign of the paring gap on all FSs as far as we neglect the effect of spin fluctuations \[13, 25\]. Hence the self-restraint effect does not occur and all "intra", "(\( \pi, \pi \))", and "(\( \pi, 0 \))" scattering processes work positively for the SC instability. In this sense, it seems easier to achieve high-\( T_c \) if those fluctuations are dominant. While the electron-phonon coupling is believed to be too small to explain \( T_c \) of FeSC \[11\], it is also free from the self-restraint effect as long as it yields an attractive pairing interaction.

In summary, it is tacitly assumed that antiferromagnetic spin fluctuations work positively for a SC instability. However, the present work finds that spin fluctuations have a contribution to suppress the SC tendency. This self-restraint effect comes from scattering processes inside the Fermi pockets with a small momentum transfer, which corresponds to a tail of the major antiferromagnetic spin fluctuations. We have shown that such a seemingly negligible contribution plays a remarkably important role to suppress the SC instability (Figs. 1 and 3). This effect is comparable to the suppression of SC by the self-energy effect.

The self-restraint effect can be understood in terms of phase frustration of the paring gap caused by a repulsive pairing interaction inherent in antiferromagnetic spin fluctuations. To compromise with the frustration, the system tends to have a larger \( k_F \) dependence of the pairing gap (Fig. 2). The self-restraint effect is expected also in other models of SC mediated by antiferromagnetic fluctuations, but its quantitative aspect may depend on details of the models. As a possible connection with cuprate high-\( T_c \) superconductors, it is interesting to explore how strong the self-restraint effect is in a typical one-band model.
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SUPPLEMENTAL MATERIAL

LORENTZ-TYPE INTERACTION

We have considered the $J_1$-$J_2$-type interaction in the main text, which may be appropriate to a system close to the localized limit even though the system remains metallic. To the opposite limit, we may consider the Lorentz-type interaction,

$$J_L(q) = -2J \sum_{l=1}^{2} \sum_{n,m} \frac{\Gamma}{(q - Q_{lm}^n)^2 + \Gamma^2},$$

(8)

where $Q_{lm}^n = (\pi + 2n\pi, 2m\pi)$, $Q_{lm}^{nm} = (2m\pi, \pi + 2n\pi)$, and $n$ and $m$ are integers. $\Gamma$ determines the peak width and $J$ the magnitude. In real space $J_L(q)$ describes an exponential-like decay of exchange interaction. In this sense, $J_L(q)$ may be appropriate in the itinerant limit.

We perform the same calculations as Fig. 1 (b), but employing the interaction term Eq. (8). We take the parameters as $n = 0, \pm 1, \pm 2, \pm 3, -4$, $m = 0, \pm 1, \pm 2, \pm 3$, $\Gamma = 1$, and $J = 2.1$ for which the system has a SDW long range order below $T = 0.032$. Obtained results are shown in Fig. 4, which is essentially the same as Fig. 1 (b). First, the eigenvalue of the Eliashberg equations is determined essentially by the scattering processes "intra+$(\pi, 0)$". Second, the SC tendency from "$(\pi, 0)$" scattering processes is substantially suppressed by "intra" scattering processes. This self-restraint effect is weaker than Fig. 1 (b). This can be easily understood by observing in Fig. 4 that "intra" scattering processes alone yield eigenvalues smaller than those in Fig. 1 (b) and thus the effect of "intra" scattering processes should become weaker.

On the other hand, the "$(\pi, \pi)$" scattering processes alone give eigenvalues larger than those in Fig. 1 (b). However, the eigenvalue of the Eliashberg equations is almost reproduced by considering the "intra+$(\pi, 0)$" scattering processes only. In this sense, "intra" scattering processes are much more destructive to the SC than "$(\pi, \pi)$" scattering processes.

MOMENTUM DEPENDENCE OF RENORMALIZATION FUNCTION

We show in Fig. 5 the momentum dependence of the renormalization function $Z$ along the FSs at the lowest temperature; the corresponding results of $\lambda$ and $\Delta$ are shown in Figs. 1 (b) and 2 (a), respectively. While a value of $Z$ on FS2 stays in 1.2 - 1.8 and thus weak-coupling
FIG. 4: (Color online) Temperature dependence of the eigenvalues $\lambda$ (solid line denoted by "all") for the Lorentz-type magnetic interaction. The eigenvalues are also computed by focusing on particular scattering processes as denoted by "intra", "$(\pi, \pi)$", and "$(\pi, 0)$". Below $T = 0.032$, SDW order occurs before SC instability.

theory would work there, the value of $Z$ amounts to 5.6 on FS1 and 2.4 on FS3 and FS4, indicating the importance of the self-energy effect beyond the weak coupling theory.

FIG. 5: (Color online) Momentum dependence of the renormalization function $Z$ on each Fermi pockets at the lowest temperature $T = 0.03$. The polar angle $\theta$ is measured from the horizontal axis on each pocket as shown in Fig. 1 (a).