Magnetism, superconductivity, and pairing symmetry in Fe-based superconductors

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We analyze antiferromagnetism and superconductivity in novel Fe-based superconductors within the itinerant model of small electron and hole pockets near (0,0) and (\(\pi, \pi\)). We argue that the effective interactions in both channels logarithmically flow towards the same values at low energies, \textit{i.e.}, antiferromagnetism and superconductivity must be treated on equal footings. The magnetic instability comes first for equal sizes of the two pockets, but loses superconductivity upon doping. The superconducting gap has no nodes, but changes sign between the two Fermi surfaces (extended \(s\)-wave symmetry). We argue that the \(T\) dependencies of the spin susceptibility and NMR relaxation rate for such state are exponential only at very low \(T\), and can be well fitted by power-laws over a wide \(T\) range below \(T_c\).

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\section*{INTRODUCTION}

Recent discovery of superconductivity in the iron-based layered pnictides with \(T_c\) ranging between 26 and 52K generated enormous interest in the physics of these materials \textsuperscript{1,2,3,4}. The superconductivity has been discovered in oxygen containing RFeAsO (R=La, Nd, Sm) as well as in oxygen free AFe\(_2\)As\(_2\) (A=Ba, Sr, Ca). Like the cuprates, the pnictides are highly twodimensional, their parent material shows antiferromagnetic long-range order below 150K \textsuperscript{5,6,7,8,9}, and superconductivity occurs upon doping of either electrons \textsuperscript{1,2,3,4,5} or holes \textsuperscript{6} into the FeAs layers.

The close proximity of antiferromagnetism and superconductivity fueled early speculations that the physics of the pnictides is similar to the cuprates, and involves insulating behavior\textsuperscript{10,11,12}. However, there is a growing consensus among researchers that Mott physics does not play a significant role for the iron pnictides, which remain itinerant for all doping levels, including parent compounds, in which magnetic order is of spin-density-wave (SDW) type rather than Heisenberg antiferromagnetism of localized spins\textsuperscript{13,14}. This is evidenced by, \textit{e.g.}, a relatively small value of the observed magnetic moment per Fe atom, which is around 12 – 16\% of \(2\mu_B\) \textsuperscript{2,3}. In another distinction to the cuprates, electronic structure proposed by band structure calculations\textsuperscript{15,16,17,18,19} and supported by ARPES \textsuperscript{20,21} consists of two small hole pockets centered around \(\Gamma\) point \((p=(0,0))\) and two small electron pockets centered around \(M\) point \((p=Q=(\pi,\pi))\) in the \textit{folded} Brillouin zone (BZ) (two Fe atoms in the unit cell, we set interatomic spacing \(a=1\)).

In this paper, we address three issues for the pnictides: (i) what interactions cause SDW order and superconductivity, (ii) what is the gap symmetry, and (iii) what are the implications of the gap symmetry for the experiments in the superconducting (SC) state. We argue that both magnetic and pairing instabilities are determined by the same interband pair hopping which transforms two fermions near the hole Fermi surface into two fermions near the electron Fermi surface (and vice versa). This interaction may be weak at high energies (of order bandwidth), but it flows under renorm-group (RG) and...
ultimately determines the couplings in both SDW and Cooper channels at low-energies. When electron and hole pockets are nearly identical, SDW instability occurs at a higher $T_c$. When the near-identity is broken by either hole or electron dopings, the Cooper instability comes first. This pairing interaction sets the gaps in hole and electron pockets to be of equal magnitude $\Delta$, but of opposite signs (an extended $s-\text{wave}$ symmetry, $s^+$. The ratio $2\Delta/T_c = 3.53$ is, however, the same as in BCS theory, as there is no angular variations of the gap along the FS.

A fingerprint of $s^+$ gap symmetry and near-equal electron and hole pockets is the existence of a magnetic collective mode inside the gap for momenta near $Q$ (a spin resonance), whose dispersion $(\Omega^2_0 + (v_F^2/2)(q - Q)^2)^{1/2}$, where $v_F$ is the Fermi velocity, closely resembles Anderson-Bogolubov mode in uncharged superconductors. Another fingerprint is a strong reduction of the nuclear magnetic resonance (NMR) relaxation rate $1/T_1$ in the clean limit, due to vanishing of the coherence factor for $\chi''(q,\omega)/\omega$ for $q = Q$. We argue that in this situation, $1/T_1$ is predominantly due to impurities, which are partly pair-breaking even when non-magnetic. We show that, in the presence of impurity scattering, $1/T_1$ is exponential in $T$ only for very low temperatures, and over a wide range of $T < T_c$ is well described by $1/T_1 \propto T^3$, as if the gap had nodes. Over the same range of $T$, the uniform susceptibility is near-linear in $T$.

Our results partly agree and partly disagree with some earlier works on Fe-pnictides. Mazin et al. [18] and Gorkov and Barzykin [22] conjectured that the pairing symmetry should be $s^+$. Our results agree with theirs and also with Ermin and Korshunov [23], who analyzed numerically the magnetic response at $Q$ within RPA for an $s^+$ superconductor and found the resonance peak below $2\Delta$. Cvetkovic and Tesanovic [24] noticed that for identical electron and hole pockets, Cooper and particle-hole channels become undistinguishable and should be treated equally— the notion we share. Wang et al. [25, 26] performed numerical RG study of the pairing symmetry and found an $s^+$ gap symmetry for two-band model and a conventional $s-\text{wave}$ symmetry for five-band model. We can only compare the results for the two-band model, for which we also found an attraction in in $s^+$ channel. There is, however, an important difference between our results and those of Wang et al. In our case, the bare interaction in $s^+$ channel is repulsive, and attraction emerges only below some energy scale, due to RG flow of the coupling. In their analysis, the bare interaction is zero, and attraction emerges already after an infinitesimal RG transformation. Lorenziana et al. [27] used unrestricted Hartree-Fock approximation and studied possible phases that may compete with superconductivity in FeAs layers. We found that SDW is the main competitor, but CDW with complex order parameter is close second.

On experimental side, ARPES [28, 29, 30] and Andreev spectroscopy [31] measurements have been interpreted as evidence for a nodeless gap, while NMR data were argued to follow $1/T_1 \propto T^3$ and were interpreted as evidence for a $d-\text{wave}$ gap [32, 33] or multiple gaps [34]. Our results show that the $T$ dependence of $1/T_1$ in a dirty $s^+$ superconductor mimics $T^3$ over a wide range of $T$ and become exponential only at very low temperatures.

### THE MODEL

We model iron pnictides by an itinerant electron system with two electronic orbitals, and we assume that the hybridization between the orbitals leads to small hole and electron pockets located near $(0, 0)$ and $(\pi, \pi)$, respectively in the folded BZ (two $Fe$ atoms per unit cell) (Fig.1). The extension to a more realistic case of four (or even five) orbitals and two hole and two electron pockets is straightforward, and does not lead to new physics except for a magnetically ordered state, where four-pocket structure is essential for proper identification of relative magnetic ordering of spins of the two $Fe$ atoms from the unit cell in folded BZ [26, 32, 33].

We assume that electron-electron interaction is short-range (Hubbard-like) and involves two couplings — between fermionic densities from the same orbital and from different orbitals [37]. The Hamiltonian has the form $H = H_2 + H_4$, where

\[
\begin{align*}
\mathcal{H}_2 &= \sum_{p,\sigma} \epsilon_{1,p} \psi_{1,p,\sigma}^\dagger \psi_{1,p,\sigma} + \epsilon_{2,p} \psi_{2,p,\sigma}^\dagger \psi_{2,p,\sigma} + \Gamma_p \left( \psi_{1,p,\sigma}^\dagger \psi_{2,p,\sigma} + \psi_{2,p,\sigma}^\dagger \psi_{1,p,\sigma} \right), \\
\mathcal{H}_4 &= \frac{U_{11}}{2} \sum_{p_1,\sigma \neq \sigma'} \left[ \psi_{1,p_1,\sigma}^\dagger \psi_{2,p_2,\sigma} \psi_{2,p_1,\sigma'}^\dagger \psi_{1,p_2,\sigma'} + \psi_{2,p_1,\sigma} \psi_{2,p_2,\sigma'} \psi_{1,p_1,\sigma'}^\dagger \psi_{1,p_2,\sigma} \right] + U_{12} \sum_{p_1,\sigma,\sigma'} \psi_{1,p_1,\sigma} \psi_{2,p_2,\sigma} \psi_{2,p_1,\sigma'}^\dagger \psi_{2,p_2,\sigma'},
\end{align*}
\]

where $p_1 + p_2 = p_3 + p_4$, and $U_{11}$ is intra-orbital, and $U_{12}$ inter-orbital interactions which we approximate
by momentum-independent (on-site) values.

The quadratic form can be easily diagonalized by

\[ \psi_{1,p,s} = \cos \theta_p c_{p,s} + \sin \theta_p f_{p,s} \]
\[ \psi_{2,p,s} = \cos \theta_p f_{p,s} - \sin \theta_p c_{p,s} \]  
(2)

with \( \tan 2\theta_p = 2\Gamma_p/(\epsilon_{2,p} - \epsilon_{1,p}) \). This yields

\[ \mathcal{H}_2 = \sum_{p,s} \epsilon_p^{c,f} c_{p,s}^\dagger c_{p,s} + \epsilon_{f,p,s} f_{p,s}^\dagger f_{p,s} , \]
(3)

where \( \epsilon_c^{p,f} = \frac{\epsilon_1 + \epsilon_2 + 1}{2} + \frac{1}{2} \sqrt{\epsilon_1 - \epsilon_2} + \frac{1}{2} \Gamma_p^2 \)
(4)

Under some conditions on the original dispersions \( \epsilon_1, \epsilon_2 \) and \( \Gamma_p \), and on the hybridization term \( \Gamma_p \), the two bands of fermionic excitations form small hole and electron pockets near \( (0,0) \) and \( Q = (\pi, \pi) \), with roughly equal size, as in the iron pnictides. This happens if, e.g., \( \epsilon_1, \epsilon_2 \) and \( \Gamma_p \) change sign under \( p \rightarrow p + Q, \epsilon_1, \epsilon_2, \Gamma_p \rightarrow -\epsilon_1, \epsilon_2, \Gamma_p \).

Under these conditions, \( \epsilon_p^c = -\epsilon_p^{f+Q} \), and \( \epsilon_p^c \) describes a hole band with the maximum of energy at \( (0,0) \), while \( \epsilon_p^f \) describes an equivalent electron band with the minimum of energy at \( Q \). Upon doping, chemical potential shifts, one Fermi surface gets larger while the other gets smaller, see Fig.1.

In itinerant systems, the interactions are expected to be small compared to the fermionic bandwidth, and the physics is dominated by fermions near the Fermi surface (FS). The projection of the Hubbard interaction term \( \mathcal{H}_2 \) onto \( c \) and \( f \) fermions leads to five different interactions:

where the momenta of \( c \)- fermions are near \((0,0)\), the momenta of \( f \)-fermions are near \((\pi, \pi)\), and the momentum conservation is assumed. We present these interactions graphically in Fig.2.

We label the couplings with subindex ”0” to emphasize that these are the bare couplings. The terms with \( U^0_4 \) and \( U^0_5 \) are intraband interactions, the terms with \( U^0_1 \) and \( U^0_2 \) are interband interactions with momentum transfer \( 0 \) and \( Q \), respectively, and the term with \( U^0_3 \) is interband pair hopping.

Note that in our Fermi-liquid description, all vertices in Eq. 4 are \( \delta \)-functions in spin indices, i.e., all interactions are in the charge channel \( c\bar{c} \), and there are no direct spin-spin interaction terms with spin matrices in the vertices. However, if the original Hubbard interaction is on-site, one can use another, equivalent, description in which Pauli principle is built into the Hamiltonian, and the intra-orbital terms with equal spin projections are eliminated from the Hamiltonian. In this description, \( U^0_1 \), \( U^0_4 \), and \( U^0_5 \) terms appear as effective Hubbard interactions, while \( U^0_2 \) and \( U^0_3 \) appear as a magnetic, Hund term \( \frac{\Gamma_p}{2} \).

In explicit form, \( U^0_i \) are

\[ U^0_1 = \frac{1}{2} [(U_{11} + U_{12}) - \cos 2\theta_0 \cos 2\theta_Q (U_{11} - U_{12})] \]
\[ U^0_{2,3} = U^0_{11} + U_{12} + U_{11} - U_{12} \cos 2\theta_Q \]
\[ U^0_4 = U^0_{11} + U^0_{12} + \frac{1}{2} \vec{U}_{11} - U_{12} \cos 2\theta_Q , \]
\[ U^0_5 = U^0_{11} + U^0_{12} + \frac{1}{2} \vec{U}_{11} - U_{12} \cos 2\theta_Q , \]  
(6)

For the case that we considered above (\( \epsilon_1, \epsilon_2 \), and \( \Gamma_p \) have the same sign), we have

\[ U^0_1 = U^0_4 = U^0_5 = U^0_{11} + U^0_{12} + \frac{1}{2} U_{11} - U_{12} \cos 2\theta_Q , \]
\[ U^0_2 = U^0_3 = U^0_{11} + U^0_{12} + \frac{1}{2} U_{11} - U_{12} \cos 2\theta_Q , \]  
(7)
We assume that the intra and inter-orbital Hubbard-type interactions \( U_{11} \) and \( U_{12} \) are positive (repulsive). We see from (7) that density-density couplings \( U_1^{(0)}, U_4^{(0)}, \) and \( U_5^{(0)} \) are positive and the largest. The couplings \( U_2^{(0)} \) and \( U_3^{(0)} \) are smaller for the case when the hybridization term is even under \( \mathbf{p} \rightarrow \mathbf{p} + \mathbf{Q} \), i.e., \( \Gamma_{\mathbf{p}} = \Gamma_{\mathbf{p} + \mathbf{Q}} \), and are the same as \( U_1^{(0)}, U_4^{(0)}, \) and \( U_5^{(0)} \) when \( \Gamma_{\mathbf{p}} = \Gamma_{\mathbf{p} + \mathbf{Q}} \). The first case corresponds to on-site hybridization and is more realistic that the second one, which requires hybridization to involve predominantly nearest neighbors. Below we will consider only the first case \( \Gamma_{\mathbf{p}} = \Gamma_{\mathbf{p} + \mathbf{Q}} \). Note that in this situation, the sign of \( U_2^{(0)} = U_3^{(0)} \) depends on \( \theta_0 \) and on the relative strength of the intra-orbital and inter-orbital Hubbard terms. If \( U_{11} > U_{12} \sin^2 2\theta_0/(1 + \cos^2 2\theta_0) \), these couplings are positive, if \( U_{11} < U_{12} \sin^2 2\theta_0/(1 + \cos^2 2\theta_0) \), they are negative. A more likely situation is when the intra-orbital Hubbard term \( U_{11} \) is larger than inter-orbital \( U_{12} \), in which case \( U_2^{(0)} \) and \( U_3^{(0)} \) are positive.

For convenience, below we will be using dimensionless interactions

\[
u_i = U_i N_0
\]

where \( N_0 \) is the fermionic density of states (DOS) which we approximate by a constant. For itinerant systems, \( |\nu_i| < 1 \) and can be treated within Fermi liquid theory. We will also count the momenta of f—fermions as deviations from \( \mathbf{Q} \) (\( f_{\mathbf{p}} \rightarrow f_{\mathbf{p} + \mathbf{Q}} \)) in which case all running momenta in the vertices are small.

**Density wave and pairing instabilities**

We searched for possible density-wave and Cooper-pairing instabilities for our model, and found that the ones which may potentially occur are spin density wave (SDW) and charge density wave (CDW) instabilities with momentum \( \mathbf{Q} \) and with either real or imaginary order parameter, and superconducting (SC) instability either in pure s channel (the gaps \( \Delta_s \) and \( \Delta_f \) have the same sign), or in \( s^+ \) channel (the gaps \( \Delta_s \) and \( \Delta_f \) have opposite sign). Density-wave instabilities with \( \mathbf{q} = 0 \) and pairing instabilities with \( \mathbf{q} = \mathbf{Q} \) do not occur within our model because the corresponding kernels vanish for a constant DOS. The instabilities with momentum-dependent order parameter, like a nematic instability also do not occur simply because we set all interactions to be momentum-independent and weak, and will neglect regular (non-logarithmic) corrections which give rise to the momentum dependence of the scattering amplitude in a Fermi liquid.

The temperatures of potential density-wave and pairing instabilities are obtained by conventional means, by introducing infinitesimal couplings

\[
\begin{align*}
\Delta_{sdw} & = \sum_k c_k^\dagger \sigma_{\alpha\beta} f_{k+\mathbf{Q},\beta}, \\
\Delta_{cdw} & = \sum_k c_k^\dagger \delta_{\alpha\beta} f_{k+\mathbf{Q},\beta}, \\
\Delta_{sc} & = \sum_k c_k^\dagger \sigma_{\alpha\beta} c_{-k,\beta} + \Delta_{s} \sum_k f_{k+\mathbf{Q},\alpha} \sigma_{\alpha\beta} \bar{f}_{-k-\mathbf{Q},\beta}
\end{align*}
\]

with complex \( \Delta_{sdw}, \Delta_{cdw}, \) and real \( \Delta_{sc}^{\dagger} \), and analyzing when the response functions diverge. We label the corresponding instability temperatures as \( T_{sdw}^{(r,i)} \), \( T_{cdw}^{(r,i)} \), and \( T_{sc}^{(s,s^+)} \), where \( r,i \) mean real or imaginary density-wave order parameter, and \( s, s^+ \) mean s—wave or extended s—wave, respectively. The linearized equations for the order parameters are presented graphically in Fig. They have non-zero solutions when

\[
\begin{align*}
1 & = -T_{sdw}^{(r,i)} \sum_{\omega_m} \Gamma_{sdw}^{(r,i)} \int d\epsilon_k G_{k\omega_m}^{\dagger} G_{k+\mathbf{Q},\omega_m} \\
1 & = -T_{cdw}^{(r,i)} \sum_{\omega_m} \Gamma_{cdw}^{(r,i)} \int d\epsilon_k G_{k\omega_m}^{\dagger} G_{k+\mathbf{Q},\omega_m} \\
1 & = -T_{sc}^{(s,s^+)} \sum_{\omega_m} \Gamma_{sc}^{(s,s^+)} \int d\epsilon_k G_{k\omega_m}^{\dagger} G_{-k,-\omega_m}
\end{align*}
\]

Here

\[
\begin{align*}
\Gamma_{sdw}^{(r,i)} & = u_1 \pm u_3, \quad \Gamma_{cdw}^{(r,i)} = u_1 \mp u_3 - 2u_2, \\
\Gamma_{sc}^{(s)} & = u_4 + u_3, \quad \Gamma_{sc}^{(s^+)} = u_4 - u_3
\end{align*}
\]
are the full interactions in the SDW, CDW, and SC channels. Eq. (10) is only valid for the largest instability temperature. Below such $T$, the ordering in one channel affects susceptibilities in the other channels.

For the bare parameters as in (1)

\[
\begin{align*}
\Gamma_{sdw}^{(r)} &= u_1^0 + u_3^0 \approx u_{11}(1 + \cos^2 \theta_0), \\
\Gamma_{sdw}^{(i)} &= u_1^0 - u_3^0 \approx u_{12} \sin^2 \theta_0, \\
\Gamma_{cdw}^{(r)} &= u_1^0 - u_3^0 - 2u_2^0 \approx 2u_{12} \sin^2 \theta_0 - u_{11}(1 + \cos^2 \theta_0), \\
\Gamma_{cdw}^{(i)} &= u_1^0 + u_3^0 - 2u_2^0 \approx u_{12} \sin^2 \theta_0, \\
\Gamma_{sc}^{(s)} &= u_4^0 + u_3^0 \approx u_{11}(1 + \cos^2 \theta_0), \\
\Gamma_{sc}^{(s^+)} &= u_4^0 - u_3^0 \approx u_{12} \sin^2 \theta_0.
\end{align*}
\] (12)

where $u_{11} = U_1 N_0$, $u_{12} = U_2 N_0$ are dimensionless intra-orbital and inter-orbital Hubbard couplings. The Stoner-like SDW and CDW instabilities require $\Gamma_{sdw} > 0$. At the bare level, $\Gamma_{sdw}^{(r)}$ is the largest positive interaction when $u_{11}(1 + \cos^2 \theta_0) > u_{12} \sin^2 \theta_0$ and $\Gamma_{cdw}^{(r)}$ is the largest positive interaction when $u_{11}(1 + \cos^2 \theta_0) < u_{12} \sin^2 \theta_0$, i.e., the system undergoes a conventional SDW or CDW instability. The SC instabilities requires an attraction (a negative $\Gamma_{sc}^{(s)}$ and $\Gamma_{sc}^{(s^+)}$) and do not occur at this level because both $\Gamma_{sc}^{(s)}$ and $\Gamma_{sc}^{(s^+)}$ are positive.

**RG FLOW**

Beyond mean-field, the potential SDW and SC instabilities are determined by $u_i$ at energies below the Fermi energy $E_F$, and generally differ from bare $u_i^0$ defined at energies comparable to the bandwidth, $W$. For small size of the FS, $W >> E_F$, and the intermediate range is quite large. At $u_i^0 < 1$ the renormalization can be considered in one-loop approximation. The one-loop diagrams, shown in Fig (a) contain particle-particle and particle-hole bubbles. The external momenta in these diagrams are of order running $E \geq E_F$, while internal momenta are generally of order $W$, i.e., much larger. In this situation, the dependence on the directions of the external momenta is lost, i.e., a SC vertex with zero total momentum and an SDW vertex with transferred momentum $Q$ are renormalized in the same way. The crucial element of our analysis is the observation that, for $\epsilon_F^p = -\epsilon_{p+q}^f$, particle-hole channel is indistinguishable from particle-particle channel, such that the renormalization in both channels are logarithmic and interfere with each other. The presence of the logarithms in both channels implies that the one-loop perturbation theory must be extended to one loop RG analysis for the running $u_i$ (in the diagrammatic language, one needs to sum up series of logarithmically divergent parquet diagrams). The derivation of the RG equations is straightforward (see Fig. (b)). Collecting combinatoric pre-factors for the diagrams, we obtain

\[
\begin{align*}
\dot{u}_1 &= u_1^2 + u_3^2, \\
\dot{u}_2 &= 2u_2(u_1 - u_2), \\
\dot{u}_3 &= 2u_3(2u_1 - u_2 - u_3), \\
\dot{u}_4 &= -u_4^2 - u_3^2.
\end{align*}
\] (13)

where the derivatives are with respect to $\log W/E$, and $E$ is the running energy scale. Similar, though not identical equations have been obtained in the weak-coupling studies of the cuprates with the “t–only” dispersion (39).

We see from Eq. (10) that the pair hopping term $u_3$ is not generated by other interactions, i.e., $u_3 = 0$ if $u_3^0 = 0$. In the absence of $u_3$, $\Gamma_{sdw}$ and $\Gamma_{sc}^{r,s^+} = \Gamma_{sdw} = u_{11}$ increases and drives $T_{sdw}$ up, while $\Gamma_{sc}^{r,s^+} = u_4$ logarithmically decreases, as it is expected for a repulsive interaction (40). However, once $u_3^0$ is finite, the system moves into the basin of attraction of another fixed point, at

![Diagram](image-url)
which

\[ u_3 \propto u \frac{u}{1 - |u| \ln \frac{W}{E}} \quad u_1 = -u_4 = \frac{|u_3|}{\sqrt{5}} \quad u_2 \propto |u_3|^{1/3} \quad (14) \]

where \( u \) depends on the bare values of the couplings. In Figs. 6a and b we show the RG flow obtained by the numerical solution of Eq. (13).

The two key features of the new fixed point are (i) \( |u_3| \) rapidly increases and eventually becomes larger than \( u_1 \) by a factor \( \sqrt{5} \), and (ii) \( u_4 \) decreases, passes through zero, changes sign, and then increases by magnitude and approaches \(-|u_3|/\sqrt{5}\) (see Fig. 5).

For positive \( u_0^3 \approx u_0^2 \), these results imply that \( \Gamma_{\text{sdw}}^{s} = u_1 + u_3 \) remains positive and the largest out of density-wave vertices i.e., the highest density-wave instability is a conventional SDW instability (see Fig. 6a). Note, however, that \( \Gamma_{\text{sdw}}^{(i)} \) is close second as it only differs by \( u_2 \) which under renormalization becomes relatively small compared to \( u_1 \) and \( u_3 \) \((u_2 \propto (u_3)^{1/3})\). The interaction in the \( s^+ \) SC channel, \( \Gamma_{\text{sc}}^{(s)} = u_4 - u_3 \), becomes negative (attractive) below some scale (Fig. 6b), while \( \Gamma_{\text{sc}}^{(s)} \) remains repulsive. We emphasize that the density-density vertex \( u_4 \) changes sign under renormalization, becomes attractive (attractive), and also supports SC. Moreover, the interactions in the SDW and the \( s^+ \) SC channel \( \Gamma_{\text{sdw}}^{(r)} = u_1 + u_3 \) and \( \Gamma_{\text{sc}}^{(s)} = u_3 - u_4 \), become comparable to each other and eventually flow to the same value \( u_3(1+1/\sqrt{5}) \). The implication is that the SDW order and \( s^+ \) superconductivity are competing orders, determined by effective interactions of comparable strength.

For negative \( u_0^3, u_0^2 \), \( \Gamma_{\text{cdw}}^{(r)} = u_1 + |u_3| + 2|u_2| \) is the strongest, positive, density-wave vertex, and \( \Gamma_{\text{sdw}}^{(s)} = u_1 + |u_3| \) is a close second (see Fig. 6b). \( \Gamma_{\text{sc}}^{(s)} = u_4 + |u_3| \) is now positive (repulsive), but \( \Gamma_{\text{sc}}^{(s)} = u_4 - |u_3| \), changes sign under the renormalization and becomes negative (attractive), see Fig. 6b). This implies that CDW now competes with a conventional \( s^- \) wave SC. Near the fixed point, the interaction in the \( s^- \) channel \( \Gamma_{\text{sc}}^{(s)} \approx -|u_3|(1 + 1/\sqrt{5}) \) is now larger than \( \Gamma_{\text{cdw}}^{(r)} \approx |u_3|(1 - 1/\sqrt{5}) \) which implies that in this case \( s^- \) wave SC likely wins over CDW.

The generalization of this analysis to 4-band model (or even five) is straightforward and yields qualitatively similar behavior.

**Competing orders**

We next analyze in more detail Eqs. (10) for \( u_0^3 > 0 \). By construction, the upper limit of the integration over internal energies there is \( O(E_F) \) as the contributions from
higher energies are already absorbed into the renormalized verti
ces. When hole and electron Fermi surfaces are near-identical, i.e., $\epsilon_{k}^c = -\epsilon_{k+Q}^f$ holds down to the lowest
ergies, both SDW and SC susceptibilities are logarithmic in $T$
\[-T \sum_\omega \int d\epsilon_k G^c_{k,\omega m} G^f_{k+Q,\omega m} = T \sum_\omega \int d\epsilon_k G^c_{k,\omega m} G^c_{-k,\omega m}
\]
= \int_0^{E_F} \tan\left(\frac{\omega}{2T}\right) \frac{d\omega}{\omega} = \log \frac{E_F}{T}
\]
and from (10) the largest instability temperature is either
$T_{sdw}^{(r)} \sim E_F e^{-\Gamma_{sdw}^{(r)}},$ or $T_{sc}^{(s)} \sim E_F e^{-\Gamma_{sc}^{(s)} / T}$. (16)

As $\Gamma_{sdw}^{(r)}$ is still larger than $\Gamma_{sc}^{(s)}$, the SDW instability
comes first. This is what, we believe, happens at zero
doping. Whether SC emerges as an extra order at a
smaller $T$ requires a separate analysis as the pairing sus
ceptibility changes in the presence of the SDW order. At
a finite doping, all evidence is that the two FS become
unequal, i.e., the condition $\epsilon_{k}^c = -\epsilon_{k+Q}^f$ breaks down. In this
situation, the log $1/T$ behavior of the SDW polarization
is cut, and $T_{sdw}^{(r)}$ decreases and eventually becomes
smaller than $T_c^{(s)}$. At larger dopings, $T_c^{(s)}$ remains
roughly doping independent, while magnetic correlations
decrease.

A remark about the SDW state. In the coordinate frame associated with folded BZ, Fe ions are located at
$\mathbf{r}_1 = (n_x, n_y)$, where $n_x, n_y$ are integers (we recall that we set interatomic spacing to one), but also at $\mathbf{r}_2 = (n_x + 1/2, n_y + 1/2)$. SDW instability with $Q = (\pi, \pi)$ order antiferromagnetically spins within the sublattice where $\mathbf{r} = \mathbf{r}_1$, and within the sublattice where $\mathbf{r} = \mathbf{r}_2$, but do not fix relative orienta
tion between the spins in the two sublattices. To obtain full spin structure, we would need to analyze spin ordering within full four-band structure (two electron and and two hole orbitals), or go back into unfolded Brillouin zone. For localized spins, this type of order is described by $J_1 - J_2$ model for $J_2 > 0.5J_1$. In the classical model, the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$ sublattices is arbitrary, but quantum fluctuations select $(0, \pi)$ or $(\pi, 0)$ state [41, 42]. There is then an extra Ising degree of freedom, which was argued [32, 42] to remain broken even at $T > T_{sdw}$, when $SU(2)$ spin symmetry is restored.

**SUPERCONDUCTING STATE**

The SC $s^+$ state that we found has two features similar
to a conventional isotropic $s$-wave state. First, the
superconducting gaps on the hole and electron FS are op
posite in sign, but equal in magnitude. They, however,
become unequal when $E_F$ on the two FS become is different,
which happens once the doping increases (or when
intraband density-density interactions $u_4$ and $u_5$ become unequal). Second, solving the non-linear gap equation, we immediately find that the gap $\Delta$ obeys the same BCS relation $2\Delta = 3.53T_c$ as for an isotropic $s-$wave state simply because the pairing kernel contains either two $c-$fermions or two $d-$fermions, but no $cf$ pairs.

The $s^+$ and $s$ SC states, however, differ qualitatively
in the presence of non-magnetic impurities. For $s-$state,
non-magnetic impurities do not affect $T_c$ and non-linear
gap equation [43]. For $s^+$ state, the impurity potential $U_i(q)$ has intra and interband components $U_i(0) and $U_i(\pi)$, respectively. The $U_i(\pi)$ components scatter fermions with $+\Delta$ and $-\Delta$ and acts as a “magnetic impurity” [44, 45]. Specifically, for the $s^+$ state, normal and anomalous Greens functions in the presence of impurities are

$$G^c_{k,\omega m} = \frac{Z_{\omega m}\omega_m \pm \epsilon_k}{Z^2_{\omega m}(\omega_m^2 + \Delta^2_{\omega m}) + \epsilon_k^2},$$

and the fermionic $Z = 1 + \Sigma(\omega_m)$, and the renormalized gap $\Delta_{\omega m}$ in the Born approximation are given by

$$Z = 1 + U_i(0) + U_i(\pi) \sqrt{\Delta^2 + \omega_m^2},$$

$$\frac{\Delta_{\omega m}}{\Delta} - 1 = -\frac{b_T\Delta_{\omega m}}{\sqrt{\Delta^2 + \omega_m^2}},$$

where $\Delta = \Delta(T) is the frequency-independent order parameter, and $b_T = 2U_i(\pi)/\Delta(T)$. Below we use $b_T = b$ as a measure of the strength of impurity scattering. Note that $b$ is a complex function of the impurity strength as the order parameter is also affected by impurities (see below).

For $U_i(\pi) = 0$, $\Delta \sim \Delta$, i.e., superconductivity is not
influenced by impurities. For $U_i(\pi) \neq 0$, $\Delta_{\omega m}$ becomes frequency dependent, as if the impurities were magnetic.
At $T = 0$, and $b > 1$, the system displays gapless superconductivity [46]; in real frequencies $\Delta_{\omega m} \propto -i\omega$ at small $\omega$, and the DOS at zero energy acquires a finite
value $N(\omega = 0) = (1 -(1/b)^2)^{1/2}$. Superconductivity at $T = 0$ eventually disappears when $\Delta$ vanishes, i.e., when $b$ tends to infinity.

The parameter $\Delta$ can be re-expressed in terms of $\Delta_0(T)$, which is the BCS gap in the absence of impurities,
and $b_0 = 2U_i(\pi)/\Delta_0(T)$, which linearly depends on the impurity strength. The relation between $\delta = \Delta/\Delta_0$ and $b_0$ (and between $b = b_0/\delta$ and $b_0$) is obtained from the self-consistent condition on the order parameter

$$\Delta = u_{eff} \int^{\omega_{max}}_0 \frac{\Delta_{\omega m}}{\sqrt{\Delta^2_{\omega m} + \omega_{m}^2}}$$

The dynamical spin susceptibility of a superconductor is given by an RPA-type formula

$$\chi_s(q, \Omega) = \frac{\chi^0_s(q, \Omega)}{1 - \Gamma^{(r)}_{sdw} \chi^0_s(q, \Omega)},$$

where $\chi^0_s(q, \Omega)$ is the (dimensionless) susceptibility of an ideal $s^+$ SC (the sum of $GG$ and $FF$ terms with spin matrices in the vertices). In our case, when $\epsilon^c_k \approx -\epsilon^f_{k+Q}$, and the gap changes sign between hole and electron FS, one can easily verify that $\chi^0_s(q, \Omega \approx Q, \Omega) \approx 0$ only weakly (logarithmically) depends on frequency. This could be verified in INS experiments.

1. In the normal state, $\chi^0_s(q, \Omega) = \log E_F/(-\Omega)$, that is $\Im \chi_s(q, \Omega)$ only weakly (logarithmically) depends on frequency. This is only valid if $\Omega \ll \Delta$, otherwise the dispersion becomes more complex.

2. In a superconducting state, $\chi_s(q, \Omega)$ has a resonance below $2\Delta$. Indeed, at $T = 0$, in the clean limit and at small $\Omega$, we have

$$\chi^0_s(q, \Omega) = \frac{E_F}{E_0} + \frac{1}{4\Delta^2}(\Omega^2 - \nu^2(q - Q)^2)$$

where $\nu = v_F/\sqrt{2}$ is the velocity of the Anderson-Bogolyubov mode in two dimensions (2D), and $E_0$ is the largest of $\Delta$ and the cutoff energy associated with non-equivalence of the two FS. Substituting this into $\chi_s(q, \Omega)$, and assuming $\Gamma^{(r)}_{sdw} \log E_F/E_0 < 1$, i.e., no SDW instability, we find the resonance at $\Omega = \sqrt{(\nu^2(q - Q)^2 + \Omega_0^2)}$, where $\Omega_0 = 2\Delta(1/\Gamma^{(r)}_{sdw} - \log E_F/E_0)^{1/2}$. This resonance has been earlier obtained in the numerical analysis in Refs. [23, 47].

It bears both similarities and differences with the spin resonance in $d_{x^2-y^2}$ SC. On one hand, both are excitonic resonances, and both occur because the gap changes sign between the FS points $k$ and $Q$. On the other hand, the resonance frequency in a $d_{x^2-y^2}$ SC disperses downwards because of the nodes, while for a nodeless $s^+$ SC, the resonance disperses upwards, with large velocity. Indeed, this is only valid if $\Omega \ll \Delta$, otherwise the dispersion becomes more complex.

In passing that, because the two gaps have opposite signs, there should also exist a resonance in the momentum $k = Q$, similar to the Leggett mode in a two-band superconductor [48].

3. An $s^+$ superconductor has a rather peculiar low-frequency behavior of $\Im \chi_s(q \approx Q, \Omega \rightarrow 0)$. In the clean limit,

$$\Im \chi^0_s(q, \Omega) \bigg|_{\Omega \rightarrow 0} \propto \sum_k C_{k,q} \frac{\partial n_F(E_k)}{\partial E_k},$$

where $E_k = \sqrt{\Delta^2 + \epsilon^c_k}$, $n_F(E)$ is Fermi function, and $C_{k,q} = 1 + (\epsilon^c_k + \Delta + \Delta^* / E_k)^{-1}(E_k E_{k+q})$ is the coherence factor. We see that the coherence factor vanishes identically for $q = Q$ such that $\Im \chi^0_s(q, \Omega) \big|_{\Omega \rightarrow 0} \propto (q - Q)^2$. 

The vanishing of superconductivity at $T = 0$ when $b_0$ approaches 1/2 also follows from the generic dependence of $T_c$ on the impurity strength. The calculation parallels the one for an $s$-wave superconductor with magnetic impurities [47] and yields

$$\ln \frac{T_0}{T_c} = \delta \left( \frac{1}{2} + \frac{3.53 b_0 T_0^2}{4\pi} \right) - \psi \left( \frac{1}{2} \right)$$

where $\psi(z)$ is the diGamma function. One can easily check that $T_c$ vanishes when $b_0$ approaches 1/2. We plot $T_c(b)$ and $T_c(b_0)$ in Fig. 7(a).

![FIG. 7: $T_c$ vs $b$ and $b_0 = 2U_i(\pi)/\Delta_0$ (b) as functions of $b = 2U_i(\pi)/\Delta$, where $\Delta$ is the order parameter, and $\Delta_0$ is the gap in the absence of impurities. The inset in (a) shows the dependence of $T_c$ on $b_0$.](image)

The dynamical spin susceptibility of a superconductor

1. In the normal state, $\chi^0_s(q, \Omega) = \log E_F/(-\Omega)$, that is $\Im \chi_s(q, \Omega)$ only weakly (logarithmically) depends on frequency. This could be verified in INS experiments.

2. In a superconducting state, $\chi_s(q, \Omega)$ has a resonance below $2\Delta$. Indeed, at $T = 0$, in the clean limit and at small $\Omega$ and $q \approx Q$, $\chi^0_s(q, \Omega) = \frac{E_F}{E_0} + \frac{1}{4\Delta^2}(\Omega^2 - \nu^2(q - Q)^2)$

3. An $s^+$ superconductor has a rather peculiar low-frequency behavior of $\Im \chi_s(q \approx Q, \Omega \rightarrow 0)$. In the clean limit,

$$\Im \chi^0_s(q, \Omega) \bigg|_{\Omega \rightarrow 0} \propto \sum_k C_{k,q} \frac{\partial n_F(E_k)}{\partial E_k},$$

where $E_k = \sqrt{\Delta^2 + \epsilon^c_k}$, $n_F(E)$ is Fermi function, and $C_{k,q} = 1 + (\epsilon^c_k + \Delta + \Delta^* / E_k)^{-1}(E_k E_{k+q})$ is the coherence factor. We see that the coherence factor vanishes identically for $q = Q$ such that $\Im \chi^0_s(q, \Omega) \big|_{\Omega \rightarrow 0} \propto (q - Q)^2$. 

The vanishing of superconductivity at $T = 0$ when $b_0$ approaches 1/2 also follows from the generic dependence of $T_c$ on the impurity strength. The calculation parallels the one for an $s$-wave superconductor with magnetic impurities [47] and yields

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where $\psi(z)$ is the diGamma function. One can easily check that $T_c$ vanishes when $b_0$ approaches 1/2. We plot $T_c(b)$ and $T_c(b_0)$ in Fig. 7(a).
The spin-lattice relaxation rate measured by nuclear magnetic resonance (NMR) is given by

\[
\frac{1}{T_1} \propto T \sum_q \frac{\text{Im} \chi_s(q, \Omega)}{\Omega} \bigg|_{\Omega=0} \propto T \sum_q \chi_s^2(q, 0) \left[ \frac{\text{Im} \chi_s^0(q, \Omega)}{\Omega} \right]_{\Omega=0}. \tag{25}
\]

Because \(\chi_s(q, \Omega = 0)\) is enhanced near \(Q\), this region contributes most to the momentum sum. The smallness of \(\text{Im} \chi_s^0(q, \Omega)/\Omega|_{\Omega=0}\) for \(q \sim Q\) then implies that \(1/T_1\) has extra smallness in a clean \(s^+\) SC [by the same reason, there is no Hebel-Slichter peak in \(1/T_1\) near \(T_c\)].

In the presence of impurities, \(\text{Im} \chi_s^0(q, \Omega)/\Omega|_{\Omega=0}\) remains nonzero, and \(1/T_1 \approx T\text{Im} \chi_s(q, \Omega)/\Omega|_{\Omega=0} = \int d^2q \chi^2_s(q, \Omega = 0)\). The full expression for \(1/T_1\) is rather involved as one has to include the full \(G\) and \(F\), and the full vertex. It simplifies considerably if we neglect vertex corrections and assume that intraband scattering \(U_i(0)\) (harmless for superconductivity) well exceeds \(\Delta\). In this case, we obtained analytically, at a finite \(T\),

\[
\frac{1}{T_1} = \frac{1}{T_1} \bigg|_{T_c} \times \int_0^\infty dx \frac{4 \cosh^2 \frac{x}{2T}}{2x} \left( 1 - \frac{\tilde{\Delta}^2 - x^2}{\sqrt{(\tilde{\Delta}^2 - x^2)^2 + 4x^2(\Delta^2)^2}} \right), \tag{26}
\]

where \(\tilde{\Delta}\) is given by Eq. \([18]\) with BCS \(T\)-dependent \(\Delta(T)\). We verified numerically that lowest order vertex corrections do not change the result in any significant way.

In Fig. 8 we plot the normalized temperature dependence of \(1/T_1(T)\) for several values of \(b = 2U_i(\pi)/\Delta(T = 0)\). Stronger impurity scattering corresponds to larger \(b\) [it doesn’t make a difference whether to parametrize the impurity strength in terms of \(b\), which depends on impurity strength in a complex way, or \(b_0\), which scales linearly with the impurity strength, because of one-to-one correspondence between \(b\) and \(b_0\); see Eq. \([20]\)].

For \(b < 1\), the low-\(T\) behavior is exponential, as is expected for a superconductor without nodes. However, we see that for \(b \geq 0.3\), there is a wide intermediate \(T\) range where the behavior of \(1/T_1\) closely resembles a power-law \(T^\alpha\). The exponent \(\alpha\) decreases as \(b\) increases from \(\alpha \approx 3\) for \(b = 0.3\) to \(\alpha \approx 2\) for \(b = 0.9\). The \(T^3\) behavior was suggested based on experimental fits and was presented as evidence for \(d\)-wave superconductivity in Fe-pnictides. Our results show that \(1/T_1(T)\) in a dirty \(s^+\) superconductor mimics a power-law over a wide \(T\) range even when the DOS still vanishes at \(\omega = 0\), and \(T_c\) is only slightly affected by impurities. Furthermore, we argue, based on Fig. 8(a) that the experimental \(T\) dependence of \(1/T_1\) can only approximately be fitted by a particular power of \(T\). We believe that the reported power-law form reflects intermediate asymptotics of a complex \(T\) behavior of \(1/T_1\), and one should reduce temperature further to be able to distinguish between a true power-law and exponential behavior \([49]\).

Note in passing that the theoretical behavior is exponential at the lowest \(T\) only if \(b < 1\). For \(b = 1\), which is the critical \(b\) for a gapless \(s^+\) SC, \(1/T_1 \propto T^{5/3}\) at the lowest \(T\), and for larger \(b\), \(1/T_1(T) \propto T\).
The uniform susceptibility for various values of $b$ where

\[ \chi_s(T) = \chi_s(T_c) \left[ 1 - \int_0^\infty \frac{x}{2T} \tanh \frac{x}{2T} \left( \frac{\Delta^2}{\Delta(T)} - \frac{1}{\Delta(T)} \right) \frac{\Delta^2}{(\Delta^2 - x^2)^{3/2} - 2U_i(\pi)x^2} \right] \]

Finally, we also computed uniform spin susceptibility $\chi_s(T) \approx \chi_s^0(q = \Omega = 0)$, measured by Knight shift. It is obtained by standard means [51] and for a superconductor with $s^+$ gap symmetry is given by

\[ \chi_s^0(T) = \chi_s^0(T_0) \left[ 1 - \int_0^\infty \frac{x}{2T} \tanh \frac{x}{2T} \left( \frac{\Delta^2}{\Delta(T)} - \frac{1}{\Delta(T)} \right) \frac{\Delta^2}{(\Delta^2 - x^2)^{3/2} - 2U_i(\pi)x^2} \right] \]

CONCLUSIONS

To conclude, in this paper we presented Fermi liquid analysis of SDW magnetism and superconductivity in $Fe\text{--}pnictides$. We considered a two-band model with small hole and electron pockets located near (0,0) and $Q = (\pi, \pi)$ in the folded BZ. We argued that for such geometry, particle-hole and particle-particle channels are nearly identical, and the interactions logarithmically increase at low energies. We found that the interactions in the SDW and extended $s$--wave channels ($\Delta_{\pi} = -\Delta_{\pi+Q}$) become comparable in strength due to the increase of the intraband pair hopping term and the reduction of the Hubbard-type intraband repulsive interaction. We argued that at zero doping, SDW instability comes first, but at a finite doping, $s^+$ superconducting instability occurs at a higher $T$.

This $s^+$ pairing bears similarity to magnetically mediated $d_{x^2-y^2}$ pairing in systems with large FS with hot spots in the sense that in both cases the pairing comes from repulsive interaction, peaked at $Q$, and requires the gap to change its sign under $k \rightarrow k + Q$. The difference is that for small pockets, the gap changes sign away from the FS and remains constant along the FS.

We analyzed spin response of a clean and dirty $s^+$ superconductor and found that (i) it possess a resonance mode which disperses with the same velocity as Anderson-Bogolyubov mode, (ii) intraband scattering by non-magnetic impurities is harmless, but interband scat-
tering affects the system in the same way as magnetic impurities in an s-wave SC, (iii) $1/T_1$ has an extra smallness in the clean limit due to vanishing of the coherence factor, (iv) in the presence of impurities, there exists a wide range of $T$ where the $T$-dependencies of $1/T_1$ and the uniform susceptibility for an $s^+$ SC resemble the ones for a SC with nodes.

Note added While completing this work we became aware that similar results for spin-lattice relaxation rate, $1/T_1$, in the superconducting state have been obtained in Ref. [31].

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model to describe SDW and superconductivity.

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