Momentum dependence and nodes of the superconducting gap in iron-pnictides

A. V. Chubukov\textsuperscript{1}, M. G. Vavilov\textsuperscript{1}, and A. B. Vorontsov\textsuperscript{2}

\textsuperscript{1} Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA
\textsuperscript{2} Department of Physics, Montana State University, Bozeman, MT, 59717, USA

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We discuss the structure of the superconducting gap in iron pnictides. In the itinerant electron picture, gaps with or without nodes have the extended $s$--wave ($s^+$) symmetry and emerge within the same pairing mechanism, determined by the interplay between intra-pocket repulsion and interband pair hopping. If the pair hopping is stronger, the system develops an $s^+$ gap without nodes. In the opposite case the superconductivity is governed by one of the momentum-dependent part of the pair-hopping, and an $s^+$ gap shows nodes on electron Fermi surfaces. We argue that the gap without/with nodes emerges in systems with a stronger/weaker tendency towards a spin order.

Introduction. The structure of the superconducting (SC) gap is one of the most controversial topics in the rapidly growing field of iron-based pnictide superconductors. Electronic band configuration of the pnictides assumes two hole pockets centered at the $\Gamma$ point $q = (0,0)$ and two electron pockets centered at $(0,\pi)$ and $(\pi, 0)$ in the unfolded Brillouin zone (BZ) to which we will refer in this paper, Fig. 1a. Multiple Fermi surfaces (FSs) create a number of different possibilities for the gap structures.

Majority of theoretical works predict gaps of one sign on the hole FSs, and of another sign, on average, on the electron FSs\textsuperscript{3,4,7,8,9}. We will refer to such gap structure as an extended $s^+$ state. There is no consensus, however, on whether the $s^+$ order parameter has nodes on electronic FS. Gaps without nodes have been found in the 2-band and 5-band itinerant models\textsuperscript{3,4,7,8,9} and in the localized spin models. On the other hand Graser et al found\textsuperscript{10} an $s^+$ state with nodes in the 5-orbital Hubbard model.

Previous results for the gap structure have been obtained numerically, and there is a call for a simple analytical analysis of the pairing mechanisms and the gap. In this paper, we show that different results for the gap structure are not fundamentally conflicting, and that both nodal and node-less $s^+$ gaps may emerge in the same pairing scenario.

Electron-phonon interaction is weak in Fe-pnictides\textsuperscript{10} and the pairing likely has an electronic origin. In the weak-coupling approach, the most natural candidate for a pairing glue is the hopping of electron pairs between hole and electron pockets ($u_3$ term in Fig. 1b). For small pockets, a repulsive pair hopping gives rise to an $s^+$ state with the sign change of the gap between hole and electron FSs, but without nodes, due to small, in parameter $E_F/W$, angular variations of the gaps along the FSs, where $W$ is the fermionic bandwidth. This simple scenario is, however, incomplete as there also exists a repulsive interaction within each pocket ($u_4$ in Fig. 1b). This interaction does not cancel out from the equation for the $s^+$ gap, and we show the $s^+$ state without nodes is only possible when at low energies (smaller than $E_F$) the pair-hopping term exceeds the intra-pocket repulsion.

The restriction to energies smaller than $E_F$ is essential here because bare intra-pocket repulsion is very likely larger than the pair hopping term, and the latter may win only if the two interactions are renormalized by high-energy fermions and flow from their bare values at energies of order $W$ to new values at energies $\sim E_F$, Fig. 1b. Because of near-nesting between at least one hole and one electron FSs the renormalizations in particle-particle and particle-hole channels are equally important in between $E_F$ and $W$, and the analysis of the appropriate parquet renormalization group (RG) shows\textsuperscript{11} that the couplings' flow is controlled by a density-density inter-pocket interaction which determines the system’s tendency towards a spin density wave (SDW) order. When this tendency is strong, pair-hopping coupling gets pushed up. The intra-pocket repulsion meanwhile decreases under RG as one should expect for a repulsive pairing interaction. As a result, when the system has a strong tendency towards a SDW order, the pair-hopping term becomes larger than the intra-pocket repulsion somewhere between $W$ and $E_F$, and the system develops an $s^+$ gap without nodes.

We discuss here what happens for weaker renomal-
ization of the coupling constants, when the pair-hopping interaction remains smaller than the intra-pocket repulsion at energies of order $E_F$. Our key message is that, despite strong repulsion, the system still develops a pairing instability due to momentum-dependent part of the pair-hopping term. This instability leads to the $s^+$ gap with nodes on the two electron FS and occurs in the clean limit at an arbitrary weak pair-hopping. The reason why the pairing occurs despite strong repulsion is quite generic and is related to the fact that the gap that oscillates along the electron FS is insensitive to the intra-pocket repulsion. The gap at the hole FS is still affected by the intra-pocket repulsion, but it turns out that the elimination of the repulsion from just the electron FS is a sufficient condition for the SC instability, still driven by the pair-hopping term between electron and hole FSs.

The gap equation. We label fermions near different FSs as $f$ (hole) and $c$ (electron). For simplicity, we consider the case when the gaps $\Delta_h(q)$ are equal on the two hole FSs, and the gaps $\Delta_c(q)$ along the two electron FSs transform into each other under rotations by $\pi/2$, and reflections in all symmetry planes. The extension to the case of non-equal gaps on two hole FSs is straightforward. For a model of itinerant electrons, we consider the interactions within each pocket $u_4(q - q')/(c_q c_{-q'} f_{q'} f_q + f_q f_{-q'} c_{-q'} c_q)$, and between the pockets $u_3(q - q') c_q c_{-q'} f_{q'} f_q + h.c.$ (we borrowed the notation from Ref. 8). Functions $u_3(q - q')$ and $u_4(q - q')$ have projections onto one-dimensional $A_{1g}$ ($s$-wave) and $B_{1g}$ ($d$-wave) and two-representations of the crystal symmetry. We focus on the $A_{1g}$ component $u_3^{A_{1g}}(q, q') \propto Y_{A_{1g}}(q) Y_{A_{1g}}(q')$ with $Y_{A_{1g}}(q) = 1 + b \cos q_x + c \cos q_y$ ($b$ is a constant).

For small hole and electron pockets, $Y_{A_{1g}}(q) \approx 1 + 2b$ on the hole FSs and $Y_{A_{1g}}(q) = 1 - (b k_F^2)/2 \cos 2\varphi$ on the electron FSs, see Fig. 1b. Then $u_4(q - q') \approx u_4$ and $u_3^{A_{1g}}(q, q') \approx u_3 + \sqrt{2} u_3 \cos 2\varphi$ ($\varphi$ corresponds to the pair $q$ or $q'$, whichever is on the electron FS). We also studied a $B_{1g}$ gap, but found that it emerges at a lower $T_c$.

We assume that the couplings $u_3$, $u_3^*$ and $u_4$ are already renormalized by fermions with energies between $W$ and $E_F$, see Fig. 1b, and consider the system behavior below $E_F$, when the pairing channel is decoupled from the SDW channel, and the SC instability problem can be treated within the BCS approximation. The set of the coupled BCS equations for $\Delta_h(q)$ and $\Delta_e(q)$ is obtained in the standard manner. On the hole FSs $\Delta_h(q)$ is approximately a constant $\Delta_h$, while on electron FSs $\Delta_e(q) = \Delta_e + \Delta_e \cos q_x + c \cos q_y$ $\approx \Delta_e + \Delta_e \sqrt{2} \cos 2\varphi$ with $\Delta_e = -k_F^2 \Delta_e/2\sqrt{2}$. The coupled linearized equations for three gaps $\Delta_h$, $\Delta_e$, and $\tilde{\Delta}_e$ are (we take all FSs as cylindrical)

$$\Delta_h = -u_4 L \Delta_h - u_3 L \Delta_e - \tilde{u}_3 L \tilde{\Delta}_e; \quad (1a)$$
$$\Delta_e = -u_4 L \Delta_e - u_3 L \Delta_h; \quad (1b)$$
$$\tilde{\Delta}_e = -\tilde{u}_3 L \Delta_h; \quad (1c)$$

where $L = \ln(1.13 \Lambda/T_c)$, $\Lambda \sim E_F$ is the upper energy cutoff. From Eqs. 1 we obtain the equation for the critical temperature $T_c$ in the form

$$(1 + u_4 L)^2 - u_3^2 L^2 = \tilde{u}_3^2 (1 + u_4 L)^2. \quad (2)$$

It is invariant with respect to sign change of $\tilde{u}_3$ and $u_3$.

The gap that emerges at $T_c$ has generally nonzero $\Delta_h$, $\Delta_e$, and $\Delta_e$. Their ratios are

$$\frac{\Delta_h}{\Delta_e} = \frac{u_3}{u_3} (1 + u_4 L); \quad \frac{\Delta_e}{\Delta_h} = -\frac{u_3 L}{(1 + u_4 L)}, \quad (3)$$

where $L$ is a solution of Eq. 2. Note that $\Delta_e$ and $\Delta_h$ have opposite signs if $u_3 > 0$. When the ratio $\Delta_e/\Delta_c < 1/\sqrt{2}$, the $s^+$ state has no nodes, otherwise there are nodes on the electron FSs.

Equation 2 is a cubic equation in $L$ and can be analyzed for arbitrary $\delta = \tilde{u}_3/u_3$ and $\gamma = u_3/u_3$. For $\delta = 0$, it gives $L = L_0 = 1/(u_3 - u_4) = 1/(u_3(1 - \gamma))$, and a solution for finite $T_c$ exists only when $\gamma < 1$. The gap satisfies $\Delta_e = -\Delta_h$ and $\Delta_e = 0$.

Consider now $\delta \neq 0$. A naive expectation would be a smooth monotonic evolution of the gap with increasing $\delta$. One indeed finds a smooth evolution, but only for $\gamma < 1$, when superconductivity exists even at $\delta = 0$. For such $\gamma$, $L$ gradually decreases with $\delta$, and the oscillating component $\tilde{\Delta}_c$ continuously increases. The nodes on the electron FS appear above some critical $\delta_c(\gamma)$, see Fig. 2. We find $\delta_c(\gamma \ll 1) \approx 1/\sqrt{2} - \gamma/\sqrt{3}$ and $\delta_c(\gamma) \approx \sqrt{8}/11$ for $\gamma < 1$.

For $\gamma \geq 1$, we found a new behavior: the superconductivity develops for any $\delta \neq 0$. Indeed, the r.h.s of Eq. 2 scales as $u_3^2(\gamma^2 - 1)L^2$ at $L \gg 1$, while the l.h.s. scales as $u_3^3 L^3$. Comparing the two, we find $L = (\gamma^2 - 1)/(u_3^3 \delta^2)$, i.e. $T_c$ remains finite (but exponentially small for $\delta \rightarrow 0$):

$$T_c = 1.13 \Lambda \exp \left( -\frac{\gamma^2 - 1}{u_3^3 \delta^2} \right). \quad (4)$$

The oscillating component of the gap $\tilde{\Delta}_c$ now dominates and exceeds both $\Delta_h$ and $\Delta_e$ by $1/\delta$. The reason why $T_c$ is non-zero even when the intra-pocket repulsion is stronger than the pair hopping (i.e., when $\gamma > 1$) is the absence of the $u_4 \tilde{\Delta}_e$ term in Eq. 1c because the angular integral of $\tilde{\Delta}_c(\varphi)$ vanishes along the electron FS. In other words, oscillations of the gap along the electron FS allow a system to avoid strong intra-pocket repulsion and develop SC order.

We see that there is a qualitative change in the system behavior near $\gamma \approx 1$ and at $\delta \ll 1$. In this region $\Delta_e/\Delta_h = (\sqrt{2} + (1 - \gamma)^2 + (\gamma - 1))/\delta$ is nearly discontinuous, evolving from $O(\delta)$ at $\gamma < 1$ to $\sqrt{2} \gamma$ at $\gamma = 1$, and to $O(1/\delta)$ at $\gamma > 1$. The ratio $\Delta_e/\Delta_h \approx -1/\delta$ at $\delta \ll 1$ and $\gamma \leq 1$, and decreases as $\Delta_e/\Delta_h \approx -1/\gamma$ for $\gamma \gg 1$.

On a more careful look, we find two sub-regimes for $\gamma > 1$, when the gap has nodes. One is the regime of small
\(\delta\), where the gap is fully adjusted to minimize the effect of repulsive \(u_4\). In this regime, \(\Delta_e \gg \Delta_c, \Delta_h\), i.e., the gap is essentially \(\cos 2\phi\) on electron FS and much smaller in magnitude on the hole FS. The other is the regime of large \(\delta\), where the ratio \(\Delta_e/\Delta_c\) is again large, but not because the system tends to avoid \(u_4\) but rather because the momentum-dependent part of the effective pair-hopping becomes the dominant interaction. In between, \(\Delta_e/\Delta_c\) passes through minimum, at \(\delta = \delta_{\text{min}}(\gamma)\). Near \(\gamma = 1\), \(\delta_{\text{min}}(\gamma) \approx \sqrt{\gamma - 1}\), while for large \(\gamma\), \(\delta_{\text{min}}(\gamma) \approx (\sqrt{3}/2)\gamma\). The ratio \(\Delta_e/\Delta_h\) monotonically decreases with increasing \(\delta\) and is not affected by the change of the physics upon crossing of \(\delta_{\text{min}}(\gamma)\).

The generic phase diagram in the \((\gamma, \delta)\) plane is presented in Fig. 2. The bolder solid line is \(\delta_{\text{cr}}(\gamma)\) above which \(s^+\) gap acquires nodes, and the narrower solid line is \(\delta_{\text{min}}(\gamma)\), where the ratio \(\Delta_e/\Delta_c\) is at minimum.

**Role of spin fluctuations.** Above we considered only a direct four-fermion pairing interaction (terms to first order in \(u_{3,4}\)). The antisymmetrized pairing vertex created from this interaction has equal charge and spin components. Beyond first order, such vertex contain unequal spin and charge components, and the spin component describes the interaction mediated by collective spin fluctuations. Such interaction is enhanced near an SDW instability and, like \(u_{3,4}\), is attractive for a plus-minus \(s^+\) gap. Accordingly, it extends the boundary of an \(s^+\) state without nodes towards larger \(\gamma_{32}\). Still, unless the system is right at the SDW instability point, a SC with a plus-minus gap is not realized for sufficiently large \(u_4\), and, as before, one needs a momentum-dependent part of the pair-hopping (or of a spin-fluctuation exchange) to get \(T_c \neq 0\). This, in turn, gives rise to a gap with nodes on the electron FS.

**Role of impurities.** In the presence of potential impurities, the scattering of electrons results in mixing of electron states with different momenta. This mixing does not affect superconductors with isotropic order parameter. The plus-minus \(s^+\) SC state at \(\gamma < 1\) and \(\delta \ll 1\) is suppressed by inter-pocket impurity scattering \(\Gamma_\Delta\) but is not sensitive to a much stronger intra-pocket impurity scattering \(\Gamma_0\). We now show that \(\Gamma_0\) strongly reduces the critical temperature \(T_c(\Gamma_0)\) at \(\gamma \gtrsim 1\), when superconductivity develops through an anisotropic component of the order parameter on the electron Fermi surfaces. To evaluate the effect of \(\Gamma_0\) on \(T_c\), we derived the self-consistency equations within the Born approximation. We found that the linearized gap equations can be presented in the form of Eqs. (1), but with Eq. (1a) for the hole FS gap replaced by

\[
\Delta_h = -u_4 L \Delta_h - u_3 L \Delta_c - \tilde{u}_3 \mathcal{L}(\Gamma_0) \tilde{\Delta}_c,
\]

\[
\mathcal{L}(\Gamma_0) = \ln \frac{1.13A}{T_c(\Gamma_0)} + \psi \left(\frac{1}{2}\right) - \psi \left(\frac{1}{2} + \frac{\Gamma_0}{2\pi T_c(\Gamma_0)}\right),
\]

and \(\psi(x)\) is the digamma function. The equation for \(T_c(\Gamma_0)\) becomes

\[
(1 + u_4 L)^2 - u_3^2 L^2 = \tilde{u}_3^2 (1 + u_4 L) \mathcal{L}(\Gamma_0) .
\]

Both the l.h.s and the r.h.s of Eq. (5) now scale as \(L^2\) at \(T_c \to 0\) because \(\mathcal{L}(\Gamma_0)\) tends to a constant at \(T_c = 0\). As a result, the solution of Eq. (5) does not exist for sufficiently small values of \(\tilde{u}_3\), i.e., intra-pocket impurity scattering is pair-breaking for superconductivity driven by momentum-dependent pair hopping. For \(\gamma > 1\) and...
\( \delta \ll 1, T_c(\Gamma_0) \) vanishes when \( \Gamma_0 = T_c/1.13 \), where \( T_c \) is the transition temperature in clean samples.

**Application to the pnictides.** The electron and hole pockets in the pnictides are rather small in size, and it is likely that \( \delta \propto E_F/W \) is small.\(^6\) Our analysis shows that for small \( \delta \), two situations are possible. When the RG renormalizations of \( u_{3,4} \) are strong enough, due to a tendency to a nesting-driven SDW order, \( \gamma = u_4/u_3 \) is smaller than 1 at energies of order \( E_F \), and the system develops a plus-minus gap without nodes and near-equal magnitudes along nested hole and electron FS. In this situation, the leading instability of undoped system is towards an SDW order, so one should expect that it becomes a superconductor only after spin order is destroyed by a finite doping which acts against nesting.\(^7\) We believe this scenario should work for \( \text{FeAs} \) 1111 and 122 materials which do show an SDW order at small doping and superconductivity at larger dopings.

If the tendency towards SDW order is less strong and \( u_4 - u_3 \) remains positive down to \( E_F \) (i.e., \( \gamma > 1 \)), then the pairing is predominantly determined by the angle-dependent component of the pair-hopping term. In this situation, \( T_c \) is smaller, and the pairing gap has nodes on the electron FS. This is consistent with what is currently known about \( \text{FeP} \) 1111 material \( \text{LaOFeP} \) which does not display a SDW order and has a small \( T_c \sim 5K \).

This may explain diverse reports of the measured temperature dependence of the penetration length \( \Delta(T) \). The exponential \( T \) dependence of \( \Delta(T) \) in \( \text{SmFeAsO}\)\(^{15}\) is consistent with the nodeless \( \text{A}_{1g} \) gap; linear in \( T \) behavior in \( \text{LaOFeP}\)\(^{16}\) is consistent with line nodes. Measured \( \Delta(T) \) in \( K \) or \( Co \)-doped \( \text{BaFe}_2\text{As}_2 \) and in \( F \)-doped \( \text{La} (\text{Nd}) \text{FeAsO}\)\(^{17}\) scales roughly as \( T^2 \). The latter behavior is difficult to obtain from the momentum-dependence of the \( s^\pm \) gap alone, and likely originated from the effect of impurities: either inter-pocket impurity scattering \( \Gamma_\tau \) in an \( s^\pm \) superconductor without nodes\(^1\) or intra-pocket scattering \( \Gamma_\delta \) for an \( s^\pm \) SC with nodes.\(^2\)

**Comparison with other theories.** Our results are consistent with the numerical RG studies by Wang et al.\(^2\) who found an extended \( s^\pm \) wave state, but with a substantial modulation of the gap along the two electron FS. These authors found that the modulation increases with doping, what is in line with the idea that the up-turn renormalization of \( u_3 \), driven by a tendency towards a SDW order, decreases with doping. Our results and the reasoning are also consistent with RPA-based studies of the 5-orbital Hubbard model by Grasier et al.\(^3\) They considered the case of near-equal intra-orbital and inter-orbital Hubbard interactions, which in our notations corresponds to \( u_3 \approx u_4 \). They found that the gaps along electron FS have nodes and \( \Delta \propto (1 + r \cos 2\varphi) \) with \( r \approx 2.3 - 2.5 \). We also found the gap with nodes at \( u_3 = u_4 \), and our results are \( r = 2 \) at \( \delta = 0^\circ \), and \( r = 2.3 \) at \( \delta = 0.27 \). We recall that a small value of \( \delta \) is expected for small sizes of the pockets because \( \delta \propto E_F/W \). We re-iterate that the gap with no nodes appears only when \( u_3 \) flows to a higher value than \( u_4 \) under the parquet RG, due to non-ladder renormalizations originating from the mixing with the SDW channel. Such renormalizations are not included into the RPA formalism.

**Summary.** We showed here that the gap structure in iron-pnictides is sensitive to the interplay between intra-pocket repulsion and the pair hopping at energies \( O(E_F) \). If the pair hopping is larger, the system develops a gap without nodes but with different signs of the gap on electron and hole FSs. If the intra-pocket repulsion is larger, the pairing is still possible, but is now governed by the momentum-dependent part of the pair-hopping. Such pairing yields an extended \( s^\pm \) wave gap with nodes on the electronic FS, which allows the system to avoid a strong intra-pocket repulsion. We argue that the extended \( s^\pm \) wave channel always wins over a \( d^- \) wave channel and that the gap with nodes is more likely for the systems with less developed tendency towards a SDW order. This nodal state is, however, affected by intra-pocket impurity scattering.

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**Note added.** A day before this paper was submitted to arXiv, T. Maier et al posted arXiv 0903.5216 with their analysis of the gap anisotropy, based on numerical analysis of a 5 band model. They named the momentum dependence of the interaction and the need to overcome a repulsion within hole and electron pockets as the reasons for the gap anisotropy and the nodes. These are the same reasons that we found in our analytical study.

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