Small-q Phonon Mediated Unconventional Superconductivity in the Iron Pnictides

A. Aperis,1,2 P. Kotetes,1,2 G. Varelogiannis,1 and P. M. Oppeneer3

1Department of Physics, National Technical University of Athens, GR-15780 Athens, Greece
2Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany
3Department of Physics and Materials Science, Uppsala University, Box 530, S-751 21 Uppsala, Sweden

We report self-consistent calculations of the gap symmetry for the iron-based high-temperature superconductors using realistic small-q phonon mediated pairing potentials and four-band energy dispersions. When both electron and hole Fermi surface pockets are present, we obtain the nodeless $s_\pm$ state that was first encountered in a spin-fluctuations mechanism picture. Nodal $s_\pm$ as well as other gap structures such as $d_{x^2-y^2}$, $s_\pm + d_{x^2-y^2}$ and even a $p$-wave triplet state, are accessible upon doping within our phononic mechanism. Our results resolve the conflict between phase sensitive experiments reporting a gap changing sign attributed previously only to a non-phononic mechanism and isotope effect measurements proving the involvement of phonons in the pairing.

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One of the foremost issues in contemporary condensed-matter superconductivity is the nature of the medium-high-temperature superconductors. When both electron and hole Fermi surface pockets are present, we obtain the nodeless $s_\pm$ state that was first encountered in a spin-fluctuations mechanism picture. Nodal $s_\pm$ as well as other gap structures such as $d_{x^2-y^2}$, $s_\pm + d_{x^2-y^2}$ and even a $p$-wave triplet state, are accessible upon doping within our phononic mechanism. Our results resolve the conflict between phase sensitive experiments reporting a gap changing sign attributed previously only to a non-phononic mechanism and isotope effect measurements proving the involvement of phonons in the pairing.

In this Letter we propose a new picture for superconductivity in the iron pnictides on the basis of self-consistent calculations of the gap symmetry. We argue, first, that small-q electron-phonon scattering dominates the pairing. Second, we show that this solely phononic mechanism in the presence of strong Coulombic interactions can naturally produce the unconventional gap symmetries proposed for the pnictides. When both electron and hole FS pockets are present, the nodeless $s_\pm$ gap is obtained self-consistently, because of the intricate four band pnictide FS combined with strong interband scattering. Third, nodal gap structures may also develop when going from underdoped to overdoped regimes upon doping. These include $s_\pm$, $d_{x^2-y^2}$-wave, $s_\pm + d_{x^2-y^2}$ and even $p$-wave triplet SC.

The effective electron-phonon interaction may be dominated by the forward processes only when the Coulomb interaction is short range or Hubbard-like [21, 22], which is a requirement for antiferromagnetism as well. Therefore, the proximity of the AFM and small-q phonon mediated SC phases is natural, and this is indeed the case in the pnictides. Unconventional SC due to small-q phonon pairing has already been considered for high-$T_c$ cuprates [21, 23], heavy fermion [24], organic [25] and cobaltite [26] systems.

Our aim is to describe the electronic structure of the iron pnictides around the Fermi energy as realistic as possible. To this end we construct a four band tight-binding (TB) model which captures the essential physics of the
V-mediated interaction takes the form [23]:

\[ \epsilon_{1,2}^h = -t_{1}^{h_{1,2}} (\cos k_x + \cos k_y) - t_{2}^{h} \cos k_x \cos k_y - \epsilon_{F}^{h_{1,2}}, \]
\[ \epsilon_{1,2}^{e} = -t_{1}^{e_{1,2}} (\cos k_x + \cos k_y) - t_{2}^{e} \cos k_x \cos k_y - \epsilon_{F}^{e}, \]
\[ \pm t_{3}^{e} \sin k_x \sin k_y, \]

(1)

with \( t_{1}^{e} = -1.14, t_{2}^{e} = -0.2, t_{3}^{e} = 0.2, \epsilon_{F}^{e} = -1.5, \]
\( t_{1}^{h_{1}} = -0.3, t_{2}^{h_{2}} = -0.2, t_{2}^{h_{1}} = -0.24, \epsilon_{F}^{h_{1}} = 0.6 \) and
\( \epsilon_{F}^{h_{2}} = 0.4. \) We have verified that these TB dispersions are in good agreement with band structure calculations; not only the FS topology and the susceptibility are reproduced (see Fig.1 but also the angularly resolved density of states (arDOS) at any Fermi momentum \( k_F \) is properly given (arDOS \( \sim |\nabla \epsilon_{1,2}^{h}(K_F)|^{-1} \)). To probe the doping dependence of the gap symmetry in our self-consistent calculations, we have introduced a chemical potential \( \mu \) varying in the interval \(-0.6 \leq \mu \leq 1.4. \) When \( \mu > 0 \) (\( \mu < 0 \)), the system is electron (hole) doped. The Fermi surfaces at various chemical potentials as well as the corresponding arDOS are depicted in Fig. 2.

We solve the most general multiband Bardeen-Cooper-Schrieffer (BCS) equation at zero temperature [28],

\[ \Delta_n(k) = -\sum_{n',k'} V_{nn'}(k,k') \frac{\Delta_{n'}(k')}{2E_{n'}(k')}, \]

(2)

where \( \Delta_n(k) \) is the momentum dependent superconducting gap and \( E_n(k) = \sqrt{\epsilon_n^2(k) + \Delta_n^2(k)} \) the quasiparticle excitation spectrum of the \( n \)th band. The pairing potentials \( V_{nn'}(k,k') \) can support intra \( (n=n') \) and interband \( (n \neq n') \) scattering. As a first approximation, we will take \( V_{nn'}(k,k') = V(k,k') \). This yields a ”global” SC gap symmetry valid over the entire B.Z., which is nevertheless driven by the characteristics of each separate band, such as the arDOS distribution.

The effective pairing potential of the small-q phonon-mediated interaction takes the form [23]:

\[ V(k,k') = V_c = \Delta_{\text{ph}} \frac{V_{\text{ph}}}{q_0^2 + |k-k'|^2} \]

properly continued periodically, where a repulsive Coulomb pseudopotential \( V_c \) is responsible for screening at short distances whereas the negative term is the attractive phonon part. The pairing kernel is characterized by a smooth momentum cutoff \( q_c \) which selects the small wave vectors in the attractive phonon part while at larger wave vectors the repulsive Coulomb pseudopotential may prevail. Decreasing the cutoff \( q_c \) leads to a situation that has been named momentum decoupling (MD) [21]. In the MD regime there is a tendency for superconductivity to decorrelate in the various FS regions; the gap function gradually loses its rigidity in momentum space. In regions of the FS with high arDOS we observe higher gap amplitudes, whereas in the low arDOS regions the gap is smaller. This arDOS driven anisotropy of the gap is the fingerprint of MD [21] and may be behind multiple gap signatures in the experiments.

To solve the BCS equation self-consistently with the momentum dependent pairing kernel, we perform the convolution integral in Eq. (2) by utilizing an FFT cyclic convolution technique. The k-summation was performed over a 512 x 512 grid in a thin shell around the FS, in order to get maximal resolution. In the results presented here, the Coulomb pseudopotential is fixed at \( V_{\text{ph}} = 0.09 V_{\text{ph}} \) and the pairing amplitude at \( V_{\text{ph}} = 2 \). Several values of the cutoff parameter \( q_c \) were considered varying from \( \pi \) to \( \pi/8 \) and various values of the chemical potential were explored.

When \( q_c \geq \pi/5 \), anisotropic s-wave, sign-preserving solutions are found at all dopings. Further reducing \( q_c \) yields interesting doping-induced transitions between different gap symmetries. When \( \pi/5 \geq q_c \geq \pi/8 \) we get remarkable self-consistent solutions of the gap, depending on the doping level, that include nodal \( d_{\pm x^2-y^2} \)-wave, \( s_{\pm} \), \( d_{\pm x^2-y^2} \)-wave and \( p \)-wave symmetries. Here we present calculations for \( q_c = \pi/6 \) as a representative example of our results. Fig. 2 depicts the evolution of the FS, colored by arDOS to as a function of doping. In the same plots, the lines where the respective self-consistently calculated SC gap vanishes are drawn.

Starting from the electron doped side, we find an anisotropic \( d_{\pm x^2-y^2} \)-wave gap in the regime \( 1.4 \geq \mu \geq 1.0 \) as shown in Fig. 4a. In this doping region, the high-DOS hole pockets lie away from the Fermi level, and only the electron pockets drive superconductivity. The SC gap contains nodes intersecting the FS in the lowest arDOS points (Fig. 2). The arDOS distribution at these dopings is highly anisotropic with the points where the gap nodes intersect the FS having considerably lowest DOS. Thus, gapping the rest of the FS while having nodes at the lowest DOS points is energetically favorable for SC.

Decreasing \( \mu \) shrinks the electron pockets and makes the SC more isotropically distributed. When \( 0.95 \geq \mu \geq 0.65 \), a structure of the \( p \)-wave (sin \( k_z \)) type develops with nodes at the locations where the electron pockets cross (Figs. 2 and 4b). Although these FS points have maximal arDOS this is only approximately two times larger than the minimum arDOS on the FS. The sys-

FIG. 1. (Color online) a) Fermi surface contour of the undoped pnictide compounds in our four-band model. b) Wavevector dependence of the static spin susceptibility along high symmetry lines. The peak indicates well nested electron-hole pockets at \( \mathbf{Q} = (\pi, \pi) \).
The superconductivity in our approach originates from particle-particle pairing in the same band, the symmetry of the gap function implies a spin-triplet order parameter. Such a state has already been proposed for the iron pnictides in a different context [29]. However, a spin-singlet $p$-wave order parameter is also possible if one considers interband pairing [30].

In the interval $0.6 \geq \mu \geq 0.25$ a nodeless $s_{\pm}$ gap is found, yet with the nodal lines close to the electron pockets (Fig. 2). The anisotropy of the $s_{\pm}$ gap is further reduced and any node on the FS is not the preferred configuration. This $s_{\pm}$ solution is mainly a superposition of $s_{\pm}$ solutions, this mechanism results in a sign alternating gap reported in several experiments [5–7].

Upon further doping the system with holes, $−0.35 \geq \mu \geq −0.55$, the nodes of the $s_{\pm}$ gap intersect the outer hole FS (Fig 2f). Finally, at $\mu = −0.6$ the FS and the arDOS distribution become as shown in Fig. 4. The gap amplitude varies over different regions through parameter $\mu$ 

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