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Multiple gaps and superfluid density from interband pairing in a four-band model of the iron oxypnictides

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We study a four-band model for the iron oxypnictides, in which the superconducting properties are assumed to be determined by the interband coupling between holelike and electronlike Fermi sheets. We show that reasonable parameters can account for the angle-resolved photoemission spectra, showing multiple gaps in $Ba_{1-x}K_xFe_2As_2$, and for the temperature dependence of the superfluid density. At the same time, the zero-temperature value of the superfluid density shows a conventional scaling with the number of carriers.

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The discovery of superconductivity in the family of compounds characterized by Fe-As layers[1] is intriguing and challenging. At the moment they are the only materials with T_c larger than 40 K beside the cuprates. While some properties of these materials are reminiscent of the cuprates (superconductivity induced by doping a magnetic parent compound with layered basic structure), the differences are also remarkable.

Among the peculiarities of the iron oxypnictides not found in cuprates, we mention the magnetic nature of Fe and the multiband character of the band structure. The effect of correlations seems to be weaker than for the cuprates[2] even if, also in the latter case, the correlation strength may be smaller than usually believed.[3] At the same time, the calculated electron-phonon coupling cannot account for the high critical temperatures,[4] and some more exotic mechanism is expected to be realized.

The initial efforts in the field focused on $RO_{1-x}F_xFeAs$ and $RO_{1-\delta}FeAs$ (R being a rare-earth atom), in which electrons are doped in the parent ROFeAs. Later on one more direction opened thanks to the synthesis of $Ba_{1-x}K_xFe_2As_2$ and $Sr_{1-x}K_xFe_2As_2$, which are doped by holes. The great advantage of this class of materials is the availability of very large single crystals that allows for a much more complete and reliable experimental analysis.

Density-functional theory (DFT) calculations of the band structure of oxypnictides show that the Fermi surface (FS) is formed by disconnected holelike pockets centered around the Γ point and electronlike pockets centered around the M points of the folded Brillouin zone of the FeAs planes. All the pockets essentially arise from the five d orbitals of Fe with three pockets belonging to the holelike manifold and two forming the electronlike one.[5] Such a FS topology, along with the magnetic character of the parent compound, motivated one of the proposals that assigned to the interband coupling between the two manifold of FSs the role of driving force behind the superconducting (SC) phenomenon.[5,6] From a microscopic point of view, the origin of the interband pairing can be associated to spin fluctuations. Indeed, the magnetic ordering vector of the parent compounds roughly connects the two sets of hole and electron FSs, leading to an (approximate) nesting, eventually giving rise to an effective pairing interaction. On the other hand, attractive phonon-induced intraband pairing (or the pairing between FSs of the same nature) is likely to be relatively small.[4] In this perspective, different nesting properties between the various FS sheets can be expected to lead to different strengths of the pairing interaction in the various bands.

Recent angle-resolved photoemission (ARPES) results for undoped[7] and hole-doped $x=0.4$ $BaFe_2As_2$ (Ref. 8) clearly show that this can indeed be the case. From a broad perspective, ARPES confirms the prediction of DFT about the existence of distinct electronlike and holelike pockets. However, only two out of the three holelike pockets may be resolved around the Γ point, with considerable different areas, and a significant mass renormalization is found in all the bands with respect to DFT.[9] The SC gap opens on all the FS sheets at the same temperature, with a nodeless structure essentially compatible with simple s-wave symmetry. More remarkably, the gap at the smallest holelike FS and the one at the electronlike sheets are almost identical while the largest holelike FS has half of this gap. As we shall see below, this effect is highly nontrivial, and requires a proper analysis of the multiband model and the role of interband interactions. The experimental situation is less clear for the electron-doped materials. A nodeless SC gap at the Γ-FS has been reported for $NdFeAsO_{0.9}F_{0.1}$ (Ref. 10) but no information is available to our knowledge about the gap in the electronlike pocket(s).

Somehow related to the issue of the multiband structure is the behavior of the superfluid density ρ_s both at zero and finite temperatures. The $T=0$ BCS value of ρ_s is indeed related to the filling and effective masses of the various bands while its temperature dependence probes via quasiparticle excitations the presence of distinct SC gaps. The aim of this paper is to study a simple model that can capture the main effects of the multiple-gap opening in $BaFe_2As_2$ superconductors. We will show that a reasonable description of ARPES results and superfluid density can be achieved within a four-band model with realistic parameters, and that a doping-dependent renormalization of the band structure should be envisaged. Finally, we show that the calculated $T=0$ BCS value of the superfluid density is in reasonable agreement with the experiments,[11–15] in striking contrast to cuprates where the anomalous scaling of ρ_s with doping can

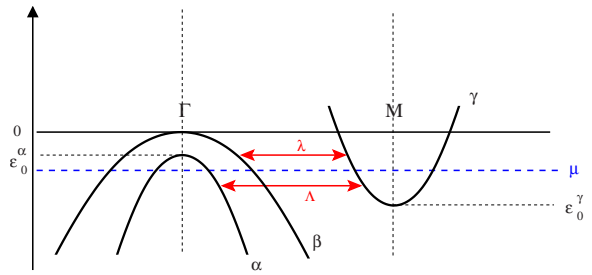

FIG. 1. (Color online) Schematic of the multiband model used in this work. The two hole bands α and β are centered around the Γ point while the electron γ bands are centered around the M point.

only be accounted for by including correlation effects.[16,17]

We consider a four-band model with parabolic dispersion, $\epsilon_i(\mathbf{k})=\epsilon_0^i \pm t_i(\mathbf{k}-\mathbf{k}_i)^2$, with the plus (minus) sign for the electron (hole) bands and t_i hopping parameter (we will use, unless explicitly stated, units $\hbar=a=1$, with a being the lattice spacing). For the two hole bands around the Γ point, labeled as α and β (according to the notation of Ref. 8), $\mathbf{k}_i=0$, while for the two electron bands γ around the M points $\mathbf{k}_i=(\pi,\pi)$. As we mentioned above, the third hole pocket predicted by DFT is not seen around the Γ point, possibly because this pocket is highly degenerate with the α one. Moreover, the two hole pockets are slightly split in the undoped system.[7] Thus, we choose the reference energy such that $\epsilon_0^\beta=0$ while ϵ_0^α and ϵ_0^γ are in general different from zero (see Fig. 1). For simplicity, we assume that the two electron bands are equal and isotropic around the M points even though both DFT and experiments show that they are slightly elongated along the k_x and k_y directions. Within a BCS-like approach, the pairing Hamiltonian can be written as

$$H=\sum_{i,\mathbf{k}\sigma}\epsilon_i(\mathbf{k})c^+_{i,\mathbf{k}\sigma}c_{i,\mathbf{k}\sigma}+\sum_{\substack{i\neq j\\ \mathbf{k},\mathbf{k}'}}V_{i,j}c^+_{i,\mathbf{k}\uparrow}c^+_{i,-\mathbf{k}\downarrow}c_{j,-\mathbf{k}'\downarrow}c_{j,\mathbf{k}'\uparrow}, \quad (1)$$

where $c^+_{i,\mathbf{k}}$ creates an electron in the ith band ($i=\alpha,\beta,\gamma$), and as we discussed above, we neglect intraband pairing. Moreover, the similar size of the FS for the α and γ bands suggests that the largest pairing acts between these two FS sheets, which are strongly nested, while the β and γ bands are less coupled. These conditions are implemented in Eq. (1) by taking $V_{\alpha\beta}=0$, $V_{\beta\gamma}=\lambda$, and $V_{\alpha\gamma}=\Lambda>\lambda$. As it has been noticed in Refs. 5 and 6, for interband mechanisms, it is not necessary that the interaction is attractive, as it happens for intraband mechanisms. However, if $\Lambda,\lambda>0$ one sees that the order parameters must have different signs on different kinds of FS sheets, i.e., sign $\Delta_{\alpha,\beta}=-$sign Δ_γ. The resulting set of self-consistent equations for the absolute values of the gaps is a straightforward extension of the usual BCS equations:

$$\Delta_\alpha=\Lambda\Delta_\gamma 2\Pi_\gamma, \quad (2)$$

$$\Delta_\beta=\lambda\Delta_\gamma 2\Pi_\gamma, \quad (3)$$

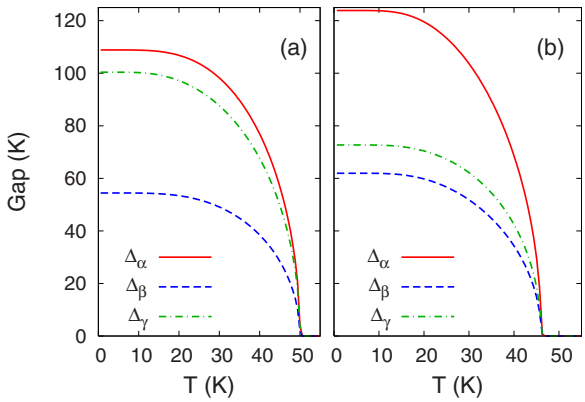

FIG. 2. (Color online) (a) Temperature dependence of the SC gaps in the hole and electron bands. The parameter values are optimized to obtain the same gap value in the α and γ bands (see the text). Moreover, we used $\lambda=\Lambda/2$ to have $\Delta_\beta=\Delta_\alpha/2$. (b) SC gaps for the hopping parameters estimated from ARPES measurements of Ref. 7 at half filling.

$$\Delta_\gamma=\Lambda\Delta_\alpha\Pi_\alpha+\lambda\Delta_\beta\Pi_\beta, \quad (4)$$

where Δ_i is the gap in the ith band, whose dispersion is now $E_{i,\mathbf{k}}=\sqrt{\xi_i^2(\mathbf{k})+\Delta_i^2}$, with $\xi_i\equiv\epsilon_i-\mu$. The Π_i are the particle-particle bubbles, given by $\Pi_i=N_i\int_0^{\omega_0}d\xi(1/E_i)\tanh(E_i/2T)$, where the pairing is only effective for states in a range of $|\xi|<\omega_0$ around the Fermi level and $N_i=1/4\pi t_i$ is the density of states (DOS) of each band. Here we use $\omega_0=20$ meV, i.e., of the order of the smallest Fermi energy in the different sheets. Along with Eqs. (2)–(4) we must solve self-consistently the equation for the particle number $n=n_\alpha+n_\beta+2n_\gamma$, where $n=4$ is the half filling. At the present stage the agreement between the experimental dispersion and the DFT band structure is hardly satisfactory;[9] therefore we extract the band parameters from the experimental data of Ref. 7 for undoped $BaFe_2As_2$. Here one has $t_\alpha=90$ meV, $t_\beta=39$ meV, and $t_\gamma=45$ meV with a band splitting $\epsilon_0^\alpha=-10$ meV and $\epsilon_0^\gamma=-45$ meV. However, in a rigid-band picture with these parameters at the doping $x=0.4$, the electron pockets would be empty. Moreover, as we shall see in Fig. 2(b), with these parameters the gap values in the α and γ bands would be quite different, in contrast to what is measured in Ref. 8. We thus proceed by assuming a band renormalization with respect to half filling to obtain $\Delta_\alpha\simeq\Delta_\gamma$ and $\Delta_\alpha=2\Delta_\beta$ from Eqs. (2)–(4), where the gap values depend only on the DOS and on the coupling. The latter condition is always realized for $\lambda=\Lambda/2$. The former condition instead can be obtained with slightly renormalized bands, i.e., we use $t_\alpha=65$ meV, $t_\beta=25$ meV, and $t_\gamma=60$ meV. Notice that if a third hole pocket of the same size as the α one is present, even if not explicitly observed by ARPES, this would just require one to slightly change the parameters to compensate for the substitution of $\Pi_\alpha\to 2\Pi_\alpha$ in Eq. (4).

Once the DOS are fixed by the gap values, we tune the band splitting according to the FS areas A_i measured in Ref. 8. In particular, it is observed that $A_\alpha/A_\beta=2/9$. Notice that if α and β bands were degenerate (or nearly degenerate) at the Γ point, this A_α/A_β ratio would require a very large aniso-

tropy between the hole bands, $t_\beta = t_\alpha(2/9)$, which in turn would not allow the condition $\Delta_\alpha \simeq \Delta_\gamma$ to be fulfilled. Thus, to justify the ratios of the FS areas, we assume a splitting of the hole bands at the Γ point larger than what is measured at half filling.[7] This enhancement of the splitting can be associated with a different Hartree shift of the two bands, arising from a particle-hole decoupling of the interband interaction. Imposing the FS ratios suggested in Ref. 8, we determine $\epsilon_0^\alpha = -25$ meV and $\epsilon_0^\gamma = -71$ meV (so that $\mu \simeq -60$ meV). In Fig. 2(a) we show the results for the gaps using $\Lambda = 260$ meV, which at low T are in good agreement with the experimental results of Ref. 8, even though the ratios $2\Delta_\beta/T_c = 2$ and $2\Delta_\alpha/T_c = 4$ are smaller than what is found experimentally. Such a discrepancy can be ascribed to the role of fluctuations beyond BCS, which are expected to reduce T_c without affecting much the low-temperature gaps. Indeed, the (almost) two-dimensional (2D) structure of pnictides, and a relatively small value of the superfluid density (see below), naturally suggest an increased relevance of fluctuations on T_c. Both these issues are relevant also for the physics of high-temperature cuprate superconductors, and indeed they have been widely discussed in the literature in that context.[18] Finally, the idea that the enhanced $2\Delta/T_c$ ratios follow from the reduction in T_c is also experimentally supported by the sudden non-BCS-like drop of the gaps near T_c.[8]

When multiple gaps are present, one may expect a signature on the temperature behavior of the superfluid density ρ_s. For a generic lattice dispersion $\epsilon_{\mathbf{k}}$, the superfluid density at BCS level is given by

$$\rho_s = \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_\alpha^2} \left[1 - \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2T} \right) \right] + 2 \int \frac{d^2\mathbf{k}}{(2\pi)^2} \left(\frac{\partial \epsilon_{\mathbf{k}}}{\partial k_\alpha} \right)^2 \frac{\partial f(E_{\mathbf{k}})}{\partial E_{\mathbf{k}}}, \tag{5}$$

where $f(x) = [1 + \exp(x/T)]^{-1}$ is the Fermi function and $k_\alpha = k_{x,y}$. Let us first consider the electron bands γ: Since they are almost empty, we can approximate the full dispersion $\epsilon_{\mathbf{k}}$ with the parabolic band ϵ_γ introduced above so that the previous equation reduces to $\rho_s^\gamma = 2t_\gamma n_\gamma + 4t_\gamma N_\gamma \int d\epsilon \epsilon f'(E_\gamma)$. As $T \to 0$ the quasiparticle excitations vanish due to the derivative $f'(E_\gamma)$, and the usual result $\rho_s^\gamma = 2t_\gamma n_\gamma$ is recovered. For hole bands, a similar expression can be used after a particle-hole transformation, which insures that only the hole states at the top of the band contribute to the superfluid density, i.e., $\rho_s^\alpha = 2t_\alpha(2 - n_\alpha)$ at $T = 0$.

The results for the temperature dependence of the superfluid density for the same parameters of Fig. 2(a) are shown in Fig. 3, where we plot the total ρ_s together with the contributions from the single bands. In the β band, which has the smallest gap, the clear signature of the two different order parameters can be seen most clearly, while the two other bands have a more standard behavior. As we observed above, for the β band $2\Delta_\beta/T_c = 2$, i.e., it is smaller than the BCS value. This means that $\Delta(T)$ is finite and sizable in a regime of temperature where it would be zero if not coupled to another band. As a consequence, at low T, ρ_s^β decreases quite rapidly, as it would vanish at a temperature proportional to

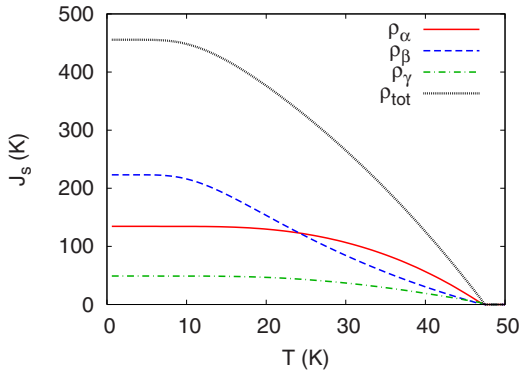

FIG. 3. (Color online) Temperature dependence of the superfluid density in units of Eq. (6) for the various bands.

Δ_β, while at higher temperature the depletion softens in a tail which closes at the higher T_c determined by the interband coupling. The possibility to observe a clear change of curvature in the total superfluid response ρ_s^{tot} depends on the relative filling of the band with the smaller gap. In Fig. 3 we show that the presence of the multiple gaps leads to deviations of $\rho_s^{\mathrm{tot}}(T)$ with respect to the single-band case but with no upward curvature as in $\rho_s^\beta(T)$. We notice that ρ_s^{tot} strongly resembles the one reported recently in Ref. 11 in a $Ba_{0.55}K_{0.45}Fe_2As_2$ compound with similar doping of the one studied by ARPES in Ref. 8.

More intriguing is the temperature dependence observed in electron-doped $LaO_{1-x}F_xFeAs$ (Refs. 12 and 13) and $NdO_{1-x}F_xFeAs$ (Ref. 14) compounds, where the measured ρ_s resembles the one we find for the β band. This effect is particularly pronounced in $LaO_{1-x}F_xFeAs$ for $x > 0.1$, and suggests that the smaller gap is formed on the electron part of the FS, which is expected to give the larger contribution to the superfluid response in electron-doped compounds. Even though some indications of multiple gaps in $LaO_{1-x}F_xFeAs$ (Ref. 19) already exist, a clear experimental observation of the gap opening on the different FS sheets is still lacking.

We finally comment on the $T = 0$ value of the superfluid density, which is proportional to the Fermi energy within our BCS scheme, and it is therefore of the order of several hundreds of kelvin. This energy scale is comparable to the values currently available from penetration-depth measurements in both hole-doped[11,15] and electron-doped[12–14] oxypnictides. To make a direct comparison with the experiments, we recall that in two dimensions the quantity $J_s = \hbar^2 n_s^{2d}/m$ is an energy, where n_s^{2d} is a two-dimensional density of superfluid carriers. By considering each plane as the basic 2D unit, one can relate n_s^{2d} and J_s to the measured penetration depth λ as

$$J_s = \frac{\hbar^2 n_s^{2d}}{m} = \frac{\hbar^2 c^2}{4\pi e^2} \frac{d}{\lambda^2} = 2.48 \frac{d[\text{Å}]}{\lambda^2[(\mu\text{m})^2]} K, \tag{6}$$

where d is the interlayer spacing, which ranges between 6.6–8.7 Å in oxypnictides. The penetration depth of a $Ba_{0.6}K_{0.4}Fe_2As_2$ sample has been estimated in Ref. 15 from infrared measurements as $\lambda = 0.208$ μm. This gives according to Eq. (6) $J_s \simeq 380$ K, which is not much lower than the value we estimated above assuming the clean limit. More-

over, since the optical-conductivity measurements of Ref. 15 suggest that the sample is in the dirty limit, we would expect that only a fraction of the ρ_s estimated from the (renormalized) band structure will actually condense in the SC phase. We can then conclude that the measured superfluid-density values are quite consistent with BCS calculations. For this reason, the observed similarity of the relation of $1/\lambda^2$ vs T_c in oxypnictides and cuprates superconductors[12] should *not* be taken as a signature of similar unconventional behavior in the two classes of materials. Indeed, in cuprate superconductors the number of carriers is large because one is doping the system with respect to half filling, where the superfluid density is expected to attain its maximum value in a hypothetical uncorrelated system. In other words, one would expect $\rho_s \sim (1-x)t$ while one measures values of order $\rho_s \sim xt$, where x is the doping and t the typical hopping parameter. For this reason, correlation effects, as the proximity to a Mott insulator[16] or enhanced phase fluctuations,[17] have been invoked as a possible explanation of the low superfluid density in cuprates. Instead, in oxypnictides the system has a low superfluid density because an almost full hole band has a vanishing contribution to ρ_s, and one expects $\rho_s \sim xt$, which is indeed near to the experimental values.

In conclusion, we have presented calculations in a four-band model built on the basis of the experimental results on $BaFe_2As_2$, assuming that the pairing arises from the interaction between holelike and electronlike Fermi surfaces with different strengths due to different nesting properties of the various FS sheets. Within our multiband BCS approach we determine parameters that account for the multiple gaps recently observed by Ding *et al.*[8] Using the same parameters, we compute the superfluid density, which does not show striking signatures of the multiple gaps, in agreement with experiments. The same agreement holds for its zero-temperature value, which scales with the small density of carriers. This has to be contrasted to the case of cuprates, where the smallness of ρ_s is associated to correlation effects.

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