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Superfluid density and penetration depth in the iron pnictides

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We consider the superfluid density $\rho_s(T)$ in a two-band superconductor with sign-changing extended s-wave symmetry (s^+) in the presence of nonmagnetic impurities and apply the results to Fe-pnictides. We show that the behavior of the superfluid density is essentially the same as in an ordinary s-wave superconductor with magnetic impurities. We show that, for moderate to strong interband impurity scattering, $\rho_s(T)$ behaves as a power law T^n with $n \approx 1.6 \div 2$ over a wide range of T. We argue that the power-law behavior is consistent with recent experiments on the penetration depth $\lambda(T)$ in doped $BaFe_2As_2$ but disagrees quantitatively with the data on LaFePO.

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I. INTRODUCTION

Recent discovery of iron-based pnictide superconductors instigated massive theoretical and experimental research efforts aimed at unveiling fundamental properties of these materials. Both oxygen containing '1111's materials (La, Nd, Pr, Sm)FeAsO, and oxygen-free '122's $(Ca,Ba,Sr)Fe_2As_2$ have high potential for the applications and may create a breakthrough in the field of superconductivity (SC).[1]

One of the central and still unsettled issues is the symmetry of the SC gap. An ordinary s-wave superconductivity due to phonons has been deemed unlikely because of too small electron-phonon coupling,[2] suggesting that the SC pairing is of electronic origin. Electronic structure of pnictides shows pairs of small hole and electron pockets centered at (0,0) and (π,π), respectively, in the *folded* Brillouin zone.[2–4] Most of parent compounds display an SDW order with momentum at, or near (π,π), and an early scenario was the pairing mediated by antiferromagnetic spin fluctuations.[5] For pnictide geometry, this mechanism yields an extended s-wave gap which changes sign between hole and electron pockets but remains approximately uniform along either of them (an s^+ gap). The s^+ gap symmetry has been found in weak coupling studies of two-band[6] and five-band[7] "g-ology" models of interacting low-energy fermions. Some other studies, however, found a gap with extended s-wave symmetry in the *unfolded* Brillouin zone.[8] Such gap has no nodes on the hole Fermi surface (FS) but has four nodes on the electron FS, such as a d-wave gap in the cuprates. The uncertainty arises from the fact that in pnictides there is a competition between the interpocket interaction with large momentum transfer and intrapocket repulsion. When interpocket interaction is stronger, the system likely develops a sign-changing s-wave gap without nodes; when intrapocket repulsion is stronger, the system develops an extended s-wave gap with nodes to minimize the effect of intrapocket repulsion.[9]

From experimental perspective, the situation is also unclear. Andreev spectroscopy[10] and angle resolved photoemission spectroscopy (ARPES) measurements[11] are consistent with the gap without nodes. NMR and Knight shift measurements[12] were originally interpreted as evidence of a gap with nodes, but it turns out that the data can be fitted equally well by a dirty s^+ superconductor.[6,13] The situation is further complicated by the fact that the two hole FSs are of different sizes and have different gaps.[14]

To truly distinguish between an s^+ gap and a gap with the nodes one should go to very low temperatures. Recently, two groups reported measurements of the penetration depth $\lambda(T)$ down to 10^{-2} T_c. The data seem to point to different directions. Ames group reported the data on Co- and K-doped $BaFe_2As_2$ (Ref. 15) and demonstrated that down to the lowest T and for all dopings the T dependence of $\lambda(T) = \lambda(0) + \Delta\lambda(T)$ can be fitted by $\Delta\lambda(T) \propto T^2$. In $SmFeAsO_{1-x}F_x$ (Ref. 16) and PrFeAsO (Ref. 17) penetration depth seems to have an exponential temperature dependence at low T, consistent with the gap without nodes. At the same time, in another 1111 material, LaFePO, the Bristol group has found $\Delta\lambda \propto T^{1.2}$ down to the lowest temperatures.[18] FS in this material has been reconstructed from magneto-oscillation measurements[19] and consists of weakly corrugated small-size cylinders making it unlikely that either hole or electron FSs extend to the points where s^+ order parameter changes sign.

The penetration depth in the clean limit was considered in Ref. 20 for an s^+ gap and in Ref. 21 for several other gap symmetries. For a gap without nodes, $\Delta\lambda(T)$ is obviously exponential at low T; for a gap with nodes it is linear in T. In this paper we discuss to what extent the existing data for $\lambda(T)$ can be described by a dirty SC with an s^+ gap symmetry and nonmagnetic impurities. We argue that the T^2 behavior observed by Ames group in 122 materials can be fitted over a wide temperature range for various dopings, and in this respect the results for the penetration depth are not in conflict with ARPES and other measurements which show SC gap without nodes. The existence of the two different gaps on the two hole FS makes the agreement between experiments even better. On the other hand, the linear in T behavior observed in LaFePO is not reproduced, and it is more likely that the gap in this material has nodes, as suggested in Ref. 8.

For a conventional s-wave SC the effect of nonmagnetic impurities on the temperature dependence of $\lambda(T)$ is small and mostly irrelevant for all T. For s^+ superconductors, the situation is qualitatively different because interband impurity scattering Γ_π mixes hole and electron states with opposite values of the order parameter $\pm\Delta$ and in this respect should be pairbreaking and act in the same way as a magnetic impurity in a conventional s-wave superconductor. Consequently, scattering by nonmagnetic impurities in s^+ SC affects T_c, the density of states, *and* the temperature dependence of the penetration depth. Over some range of Γ_π/Δ, the behavior at the lowest T is still exponential; however, when Γ_π/Δ becomes larger than a critical value, superconductivity becomes gapless, and the exponential behavior disappears.

II. METHOD

The London penetration depth $\lambda(T)$ scales as $1/\sqrt{\rho_s(T)}$, where $\rho_s(T)$ is the superfluid density. The latter is, up to a factor, the zero frequency value of the current-current correlation function and can be written in the form,[22]

$$\frac{\rho_s(T)}{\rho_{s0}} = \pi T \sum_m \frac{\tilde{\Delta}_m^2}{(\tilde{\Delta}_m^2 + \tilde{\omega}_m^2)^{3/2}}, \tag{1}$$

where ρ_{s0} is the superfluid density at $T=0$ in the absence of impurities. The integrand in Eq. (1) is defined in terms of impurity-renormalized Matsubara energy, $\tilde{\omega}_m$, and the superconducting vertex $\tilde{\Delta}_m$. In an s^+ superconductor the order parameters on the hole (c) and electron (f) FS pockets are related, $\tilde{\Delta}_m^c = -\tilde{\Delta}_m^f = \tilde{\Delta}_m$ and in Born approximation,

$$i\tilde{\omega}_m = i\omega_m - \Gamma_{\mathbf{0}} g^c(\tilde{\omega}_m, \tilde{\Delta}_m) - \Gamma_\pi g^f(\tilde{\omega}_m, \tilde{\Delta}_m), \tag{2a}$$

$$\tilde{\Delta}_m = \Delta + \Gamma_{\mathbf{0}} f^c(\tilde{\omega}_m, \tilde{\Delta}_m) + \Gamma_\pi f^f(\tilde{\omega}_m, \tilde{\Delta}_m), \tag{2b}$$

where $\omega_m = \pi T(2m+1)$, $\Gamma_{\mathbf{0}} = \pi n_i N_F |u_0|^2$, and $\Gamma_\pi = \pi n_i N_F |u_\pi|^2$ are the intra- and interband impurity scattering rates, respectively ($u_{0,\pi}$ are impurity scattering amplitudes with correspondingly small, or close to $\pi = (\pi, \pi)$, momentum transfer), Δ is the SC order parameter, and functions $g^{c,f}$ and $f^{c,f}$ are ξ-integrated normal and anomalous Green's functions for holes and electrons,

$$g^c = g^f = \frac{-i\tilde{\omega}_m}{\sqrt{\tilde{\omega}_m^2 + \tilde{\Delta}_m^2}}, \quad f^c = -f^f = \frac{\tilde{\Delta}_m}{\sqrt{\tilde{\omega}_m^2 + \tilde{\Delta}_m^2}}. \tag{3}$$

Since the f function has opposite signs in two bands, Γ_π has the same effect on anomalous self-energy as the scattering on magnetic impurities in an ordinary s-wave superconductor. Following the customary path one may introduce $\eta_m = \tilde{\omega}_m/\omega_m$ and $\bar{\Delta}_m = \tilde{\Delta}_m/\eta_m$ that satisfy

$$\eta_m = 1 + (\Gamma_{\mathbf{0}} + \Gamma_\pi) \frac{1}{\sqrt{\bar{\Delta}_m^2 + \omega_m^2}}, \tag{4a}$$

$$\bar{\Delta}_m = \Delta(T) - 2\Gamma_\pi \frac{\bar{\Delta}_m}{\sqrt{\bar{\Delta}_m^2 + \omega_m^2}}. \tag{4b}$$

The order parameter $\Delta(T)$ is determined by the self-consistency equation,

$$\Delta(T) = V^{\text{sc}} \pi T \sum_{\omega_m}^{\Lambda} f^c(\tilde{\omega}_m, \tilde{\Delta}_m) = \pi T \sum_{\omega_m}^{\Lambda} \frac{V^{\text{sc}} \bar{\Delta}_m}{\sqrt{\bar{\Delta}_m^2 + \omega_m^2}}, \tag{5}$$

where V^{sc} is the s^+ coupling constant and Λ is the ultraviolet cutoff. Notice that the last expression contains $\bar{\Delta}_m$ and *bare* Matsubara frequencies ω_m. Equations (2)–(5) can be extended to the case when the gaps on hole and electron FS have different magnitudes.

Solutions of the system of Eqs. (4b) and (5) give the values of $\Delta(T)$ and $\bar{\Delta}_m$. In particular, Eq. (4b) is an algebraic equation (valid at any T) which expresses $\bar{\Delta}_m$ in terms of Δ. The latter itself depends on Γ_π because the self-consistency equation, Eq. (5), contains $\bar{\Delta}_m$. Without interband scattering ($\Gamma_\pi = 0$) we have $\bar{\Delta}_m = \Delta = \Delta_0 = 1.76\ T_{c0}$, where T_{c0} and Δ_0 are the BCS transition temperature and the $T=0$ gap in a clean superconductor. For $\Gamma_\pi \neq 0$, $\bar{\Delta}_m$ differs from Δ, and Δ differs from Δ_0. Converted to real frequencies, Eqs. (4b) and (5) yield a complex function $\bar{\Delta}(\omega)$. For $2\Gamma_\pi \geq \Delta$, $\bar{\Delta}(\omega=0)$ vanishes, i.e., superconductivity becomes gapless.[23] At the critical point $2\Gamma_\pi = \Delta$, $\bar{\Delta}(\omega) \propto (-i\omega)^{2/3}$ at small ω, at larger Γ_π, $\bar{\Delta}(\omega) = -i$ const $\omega + O(\omega^2)$.

III. RESULTS

We express the results using dimensionless parameter $\zeta = \Gamma_\pi / 2\pi T_{c0}$. For equal gap magnitudes and $2\Gamma_\pi/\Delta < 1$, $y = \Delta/\Delta_0$ is the solution of $y = \exp[-\pi e^\gamma \zeta / y]$, where $\gamma \approx 0.577$ is the Euler constant.[24] At a given T a gapless superconductivity emerges, when y becomes smaller than $4\zeta e^\gamma$, i.e., for $\zeta > (1/4)\exp[-(\gamma + \pi/4)] \approx 0.064$. The transition temperature obeys[23,24] $\ln(T_c/T_{c0}) = \Psi(1/2) - \Psi(1/2 + 2\zeta T_{c0}/T_c)$, where $\Psi(x)$ is the di-Gamma function [Fig. 1(a)]. T_c decreases with ζ and vanishes at $\zeta_{\text{cr}} = e^{-\gamma}/8 \approx 0.07(\Gamma_\pi/\Delta_0 = 1/4)$. For $0.064 < \zeta < \zeta_{\text{cr}}$, $\bar{\Delta}(T, \omega) \propto i\omega$ for small ω, including $T=0$, and thus even $T=0$ zero-energy density of states becomes finite. (At the onset, at $\zeta = 0.064$, $T_c \approx 0.22 T_{c0}$, and $\Delta(0) = 0.46\Delta_0$). The ratio $2\Delta(0)/T_c$ increases with ζ and reaches 7.2 at the onset of the gapless behavior and 8.88 at $\zeta = \zeta_{\text{cr}}$).[24] A large value of $2\Delta(0)/T_c$ is often attributed to strong coupling[25] but, as we see, can also be due to impurities.

In terms of auxiliary $\bar{\Delta}_m$ and η_m,

$$\frac{\rho_s(T)}{\rho_{s0}} = \pi T \sum_{\omega_m} \frac{\bar{\Delta}_m^2}{\eta_m (\bar{\Delta}_m^2 + \omega_m^2)^{3/2}}. \tag{6}$$

In general, the value of $\rho_s(T=0)$ and the functional form of $\rho_s(T)$ depend on both Γ_π and Γ_0 because Γ_0 is explicitly present in Eq. (6) via η_m given by Eq. (4a). Impurity scattering amplitude is a decreasing function of momentum transfer, and, in general, $\Gamma_0 \gg \Gamma_\pi$. Since we are interested in $\Gamma_\pi \sim \Delta$, we have $\Gamma_0 \gg \Delta$ and

$$\rho_s(T) \approx BT \sum_{\omega_m} \frac{\bar{\Delta}_m^2}{\bar{\Delta}_m^2 + \omega_m^2}, \tag{7}$$

where $B = \pi\rho_{s0}/(\Gamma_0 + \Gamma_\pi)$. We see that Γ_0 only affects the overall factor B, and all nontrivial T dependence comes from frequency and temperature dependence of $\bar{\Delta}_m$.

Several results for $\rho_s(T)$ given by Eq. (7) can be obtained analytically. First, near T_c, $\rho_s(T) \propto \Delta^2(T) \propto T_c - T$, i.e.,

$$\frac{\rho_s}{\rho_s(T=0)} = B(\zeta)\left(1 - \frac{T}{T_c}\right), \tag{8}$$

where $\rho_s(T=0)$ is the actual zero-temperature value of ρ_s. In a clean BCS superconductor $B=2$. In the present dirty case

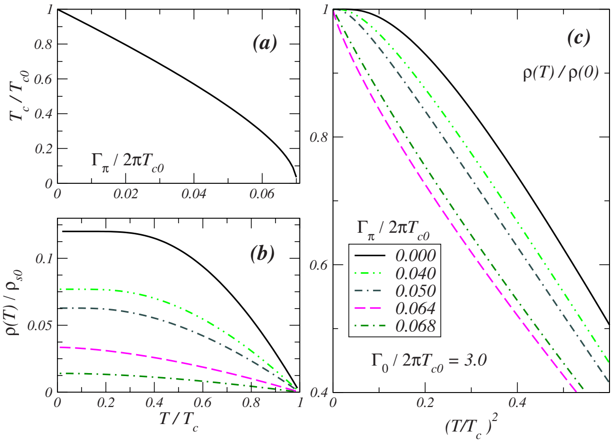

FIG. 1. (Color online) (a) Suppression of T_c by interband scattering in a two-band $(\Delta,-\Delta)$ model; (b) superfluid stiffness $\rho_s(T)$ in a dirty s^+ superconductor for fixed intraband impurity scattering $\Gamma_0/2\pi T_{c0}=3$ and various interband scatterings $\zeta=\Gamma_\pi/2\pi T_{c0}$; and (c) low-$T$ plot of ρ_s vs T^2 showing near $n=2$ power law around onset of gapless regime.

$(\Gamma_0 \gg T_c, \Gamma_\pi)$ $B(\zeta)$ is nonmonotonic in ζ and equals $B(\zeta \to 0) \approx 2.65$, $B(\zeta=0.064) \approx 1.67$, and $B(\zeta \approx \zeta_{\text{cr}})=2.03$. This implies that a linear extrapolation of ρ_s from $T \approx T_c$ to $T=0$ still yields a significantly larger value than the actual $\rho_s(0)$. Second, at $\zeta < 0.064$, the T dependence of $\rho_s(T)$ remains exponential at low T, $\rho_s(T) \propto e^{-\bar{\Delta}(\omega=0)/T}$ with $\bar{\Delta}(\omega=0) = \Delta_0[1-(\zeta/\zeta_{\text{cr}})^{2/3}]^{3/2}$, but at the onset of gapless superconductivity, when $\bar{\Delta}(\omega) \propto (-i\omega)^{2/3}$, we have $\rho_s(T) \propto T^{5/3}$. Finally, in the gapless regime $0.064 < \zeta < \zeta_{\text{cr}}$, we found $\rho_s(T) \propto T^2$ at low T.

To obtain $\rho_s(T)$ at arbitrary T, we numerically self-consistently solved the gap equation, Eq. (5), together with equations for the impurity self-energies, Eqs. (2), and the Green's functions, Eq. (3); found $\Delta(T)$ and $\tilde{\Delta}_m$, substituted them into Eq. (1), and obtained $\rho_s(T)$. We present the results in Fig. 1 for several values of ζ.

We see that, once the interband impurity scattering increases, the range of exponential behavior of $\rho_s(T)$ progressively shrinks to smaller T [Fig. 1(b)]. Outside this low T range, the temperature dependence of ρ_s strongly resembles T^2 behavior [see Fig. 1(c)]. The $T^{5/3}$ behavior at the onset of gapless superconductivity is hard to see numerically as this power is confined to very low T, while for slightly larger T the behavior is again close to T^2. Overall, the behavior of the superfluid density in a relatively wide range of ζ is a power law T^n with n reasonably close to 2 down to quite low T. At the same time, we did not find conditions under which the superfluid density would be linear at low T.

IV. COMPARISON WITH EXPERIMENTS

Judging by the value of $2\Delta(0)/T_c$,[16] the material with the least amount of interband impurity scattering is $SmFeAsO_{1-x}F_x$, where $T_c \sim 55K$. In this compound it is difficult to expect a large ζ since the observed exponential BCS-type behavior of $\rho_s(T)$ at small T (Ref. 16) is consistent with extended s-wave gap and weak interband impurity scattering.[20]

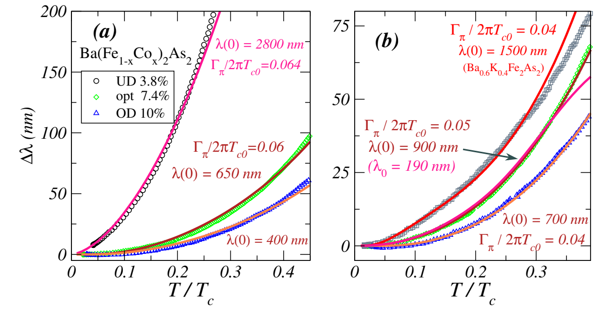

FIG. 2. (Color online) The fits to experimental data for $BaFe_2As_2$ (Ref. 15). We use only low-T data as at higher T the experimental $\lambda(T)$ may be influenced by sample geometry and fluctuations. (a) The data for electron-doped $BaFe_2As_2$ for optimally doped (x=7.4%) and overdoped (x=10%) samples can be fitted reasonably well using $(\Delta,-\Delta)$-model; (b) the fit of data for two Co-doped (x=7.3%, 10%) and one K-doped samples with a phenomenological extension of the presented two-band model to the case of four gaps. We set gaps to be $(\Delta,-\Delta;\Delta,-\Delta_h)$ with $\Delta_h=\Delta/3$, $\Delta/2$. In this case the pairbreaking parameter does not need to be large. The fitting values of $T=0$ penetration length are large, but for x=7.4% sample we show a fit with inclusion of Fermi-liquid effects that reduces this parameter to $\lambda_{\text{FL}}(0) \equiv \lambda_0 \sim 190$ nm in agreement with experimental values.

The data for electron- and hole-doped $BaFe_2As_2$ (Ref. 15) are fitted in Figs. 2(a) and 2(b). The measured $\rho_s(T)$ scales approximately as T^2, which is similar to behavior shown in Fig. 1(c). Left panel is the fit assuming that the gaps on two electron FSs and two hole FSs are Δ and $-\Delta$; right panel is a more realistic fit in which we assumed, guided by ARPES data,[14] that the gaps on the inner hole and the two electron FS are the same, but the gap on the outer hole FS is two to three times smaller.

The values ζ=0.04–0.06 used in these fits correspond to $T_c/T_{c0} \sim 0.6-0.3$ which is consistent with the values of $T_c \sim 10-30K$ in this material if we assume that T_{c0} in the clean case is roughly the same as in SmFeAsO. The curves shown in Figs. 2(a) and 2(b) represent the best fits, but we emphasize that we do not need to adjust ζ to get a T^2 behavior—it persists over a range of ζ [see Fig. 1(c)]. However we note that $\lambda(0)$ used in the fits is rather large compared with the experimentally obtained values $\sim$200–300 nm.[15] We suggest that this discrepancy may be due to the omission of Fermi-liquid effects. The qualitative argument, supported by numerical estimates, is as follows. Assume, by analogy with the cuprates, that fermion-fermion interactions renormalize $\omega \to \omega Z_\omega$, where Z_ω is a decaying function of frequency, and further assume that $Z_\omega \approx 1$ at energies comparable to Δ so that it does not affect the relation between $\Delta(0)$ and T_c. Then we find that the low-temperature dependence $f(T/T_c)$ of the penetration length is rescaled $\Delta\lambda/\lambda_0 \sim f(Z_0 T/T_c)$ and the value of the fitting parameter $\lambda_0 \equiv \lambda_{\text{FL}}(0)$ decreases compared to what is obtained without Fermi-liquid effects. This Z factor is particularly relevant to heavily underdoped regime where it increases because of spin-density wave (SDW) fluctuations. We believe this is the reason why we have to use very large $\lambda(0)=2800$ nm to fit the data. At larger dopings, Z is smaller, but according to ARPES,[11] $Z\sim 2$ in optimally doped $Ba_{1-x}K_xFe_2As_2$. For $f\sim T^2$, from the analytic reasoning we get the effective λ_0 four times smaller than $\lambda(0)$, reducing it to $\lambda_0 \sim 150-400$ nm, in the range of what is experimentally extracted. The numerical analysis confirms this, and for $Z=2$ we show a fit for one of the electron-doped samples, which gives a reasonable value for the zero-temperature penetration length. We therefore conclude that the penetration depth data for 122 material can be fitted by a model of a dirty s^+ superconductor. Note in this regard that the data[26] show that T_c is almost insensitive to the value of residual resistivity. This was interpreted as the argument for a conventional s-wave gap. We note that this is also the case for extended s-wave gap as the dominant impurity scattering is intraband scattering, controlled by Γ_0, which affects residual resistivity but does not affect T_c.

We attempted to fit the data for LaFePO using this approach but the fit fails for all ζ and one has to assume unrealistically large $\lambda(0)$ to get even mediocre agreement with the data. From this perspective, it is likely that the linear in T behavior of $\lambda(T)$ in LaFePO is not related to impurities but rather is the consequence of the fact that the gap in this material has nodes.

V. CONCLUSIONS

In this paper we considered superfluid density $\rho_s(T)$ in a multiband superconductor with sign-changing s^+-symmetry in the presence of nonmagnetic impurities and applied the results to Fe-pnictides. We showed that the behavior of the superfluid density is essentially the same as in an ordinary s-wave superconductor with magnetic impurities. For a moderate *interband* impurity scattering, $\rho_s(T)$ over a wide range of T behaves roughly as T^2 and crosses over to exponential behavior only at very low T. When superconductivity becomes gapless at $T=0$, the T^2 behavior extends to the lowest T. We argue that this power-law behavior is consistent with recent experiments on penetration depth $\lambda(T)$ in hole and electron-doped $BaFe_2As_2$, but we find that the present model does not explain the data for LaFePO.

Several modifications of the model may improve the comparison with the experimental data. First, an extension beyond Born approximation may further flatten the T dependence of $\lambda(T)$, although recent study for a different model[27] did not find much changes beyond Born approximation. Second, we assumed that the surface of a superconductor sample is homogeneous. Defects on the surface may also modify the temperature dependence of the penetration depth.

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