

Superfluid density and penetration depth in Fe-pnictides

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We consider the superfluid density $\rho_s(T)$ in a two-band superconductor with extended s -wave symmetry (s^+) in the presence of non-magnetic 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 inter-band 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 BaFe_2As_2 , but disagree quantitatively with the data on LaFePO .

Introduction. Recent discovery of iron-based pnictide superconductors instigated massive theoretical and experimental research effort aimed at unveiling fundamental properties of these materials. Both oxygen containing ‘1111’s materials $(\text{La}, \text{Nd}, \text{Sm})\text{FeAsO}$, and oxygen free ‘122’s $(\text{Ba}, \text{Sr}, \text{Ca})\text{Fe}_2\text{As}_2$ have high potential for the applications and may create a breakthrough in the field of superconductivity.¹

One of the central and still unsettled issues is symmetry of the superconducting (SC) gap. An ordinary s -wave superconductivity due to phonons has been ruled out because of too small electron-phonon coupling,² suggesting that the SC pairing is possibly 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.^{2,3,4} Most of parent compounds display an SDW order with momentum at, or near (π, π) , and one of early suggestions was the pairing mediated by antiferromagnetic spin fluctuations.⁵ For pnictide geometry, this mechanism yields an extended s -wave gap symmetry (s^+), with $\Delta \propto \cos k_x + \cos k_y$. This gap changes sign between hole and electron pockets but remains approximately uniform along either of them. The same gap symmetry has been found in weak coupling studies of two-band⁶ and five-band⁷ “ g -ology” models of interacting low-energy fermions. Some other studies, on the contrary, found a gap with extended s -wave symmetry in the *unfolded* Brillouin zone.⁸ In the folded zone, such gap behaves as $\Delta \sim \cos \frac{k_x}{2} \cos \frac{k_y}{2}$ and has four nodes at the electron Fermi surface, like a d -wave gap in the cuprates.

Weak coupling studies found that the gap with the nodes at the Fermi surface has a higher energy than an s^+ -wave gap.⁷ The situation may change at stronger coupling, but only if superconductivity and antiferromagnetism are not correlated, otherwise (π, π) magnetic fluctuations favor s^+ gap. Below we assume that the SC gap has s^+ symmetry.

From experimental perspective, situation is far from clear. Andreev spectroscopy⁹ and ARPES measurements¹⁰ are consistent with the gap without nodes. NMR and Knight shift measurements¹¹ were originally interpreted as evidence of a gap with nodes, however they were done at relatively high temperatures, $T > 0.2 T_c$, and can

be fitted equally well by a dirty s^+ superconductor.^{6,12} To truly distinguish between s^+ gap and a gap with the nodes one should go to much lower temperatures. Recently, two groups reported measurements of the penetration depth $\lambda(T)$ down to $10^{-2} T_c$. The data seem to point into different directions. Ames group reported the data on Co-doped BaFe_2As_2 (Ref. 13) 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 $\Delta\lambda(T) \propto T^2$. They argued that this dependence is consistent with a 3D gap with point nodes and conjectured that hole and electron Fermi surfaces (FS) strongly evolve along z direction and at some particular z may include the points where the s^+ gap changes sign. Bristol group found¹⁴ that in $\text{SmFeAsO}_{1-x}\text{F}_x$, penetration depth has an exponential temperature dependence at low T , consistent with the gap without nodes. At the same time, in another 1111 material, LaFePO , the same group has found the behavior which can be reasonably well fitted by a power law $\Delta\lambda \propto T^{1.2}$ down to the lowest temperatures (Ref. 15). FS in this material have been reconstructed from magneto-oscillation measurements¹⁶ and consist 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.

In this paper we discuss to what extent the existing data can be described by a dirty SC with an s^+ gap symmetry, small hole and electron FS, and non-magnetic impurities. The input parameters for our fits are the ratio Γ_π/T_{c0} (Γ_π is the inter-band scattering rate and T_{c0} is the critical temperature of a clean sample), and the value of the penetration depth at $T = 0$, $\lambda(0)$. We argue that the T^2 behavior observed by Ames group can be fitted over a wide temperature range for various dopings using realistic $\lambda(0) \sim 400 - 700 \text{ nm}$. The smaller value of power in T^n , observed in LaFePO , is harder to reproduce and the low- T fit requires a rather large $\lambda(0) \sim 1000 \text{ nm}$.

For a conventional s -wave SC the effect of non-magnetic 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 inter-band 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 conven-

tional s -wave superconductor. Consequently, scattering by non-magnetic 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.

Conventional s -wave superconductors with magnetic impurities have been extensively studied in the past, although the T dependence of $\lambda(T)$ and superfluid density $\rho(T) \propto \lambda^{-2}(T)$ has not been investigated, to the best of our knowledge. We show that values of Γ_π similar to those used to fit Knight shift and NMR data^{6,12} in F-doped PrOFes give a reasonable fit of the penetration depth data for Ba(Fe_{1-x}Co_x)₂As₂, Ref. 13 (see Fig. 2a). On the other hand a fit to LaFePO data¹⁵ (Fig. 2b) is not good and requires very large $\lambda(T = 0)$. We further show that at low T the penetration depth demonstrates T^2 -behavior once superconductivity at $T = 0$ becomes gapless, and is non-analytic, $\propto T^{5/3}$, at the critical point where gapless superconductivity emerges at $T = 0$, strongly deviating from the exponential behavior in the clean limit.¹⁷

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 form¹⁸

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

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

$$\tilde{\omega}_m = \omega_m + \Gamma_0 g^c(\tilde{\omega}_m, \tilde{\Delta}_m) + \Gamma_\pi g^f(\tilde{\omega}_m, \tilde{\Delta}_m), \quad (2a)$$

$$\tilde{\Delta}_m = \Delta + \Gamma_0 f^c(\tilde{\omega}_m, \tilde{\Delta}_m) + \Gamma_\pi f^f(\tilde{\omega}_m, \tilde{\Delta}_m), \quad (2b)$$

where $\omega_m = \pi T(2m + 1)$, $\Gamma_0 = \pi n_i N_F |u_0|^2$ and $\Gamma_\pi = \pi n_i N_F |u_\pi|^2$ are the intra- and inter-band 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:

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

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 $\tilde{\Delta}_m = \tilde{\Delta}_m/\eta_m$ that satisfy

$$\eta_m = 1 + (\Gamma_0 + \Gamma_\pi) \frac{1}{\sqrt{\tilde{\Delta}_m^2 + \omega_m^2}}; \quad (4a)$$

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

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

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

where V^{sc} is the s^+ coupling constant and Λ is the ultraviolet cutoff. Notice that the last expression contains $\tilde{\Delta}_m$ and bare Matsubara frequencies ω_m .

Solutions of the system of Eqs. (4b) and (5) give the values of $\Delta(T)$ and $\tilde{\Delta}_m$. In particular, Eq. (4b) is an algebraic equation (valid at any T) which expresses $\tilde{\Delta}_m$ in terms of Δ . The latter itself depends on Γ_π , because the self-consistency equation (5) contains $\tilde{\Delta}_m$. Without inter-band scattering ($\Gamma_\pi = 0$) we have $\tilde{\Delta}_m = \Delta = \Delta_0 = 1.76 T_{c0}$, where T_{c0} and Δ_0 are the BCS transition temperature and the $T = 0$ gap in a clean superconductor. For $\Gamma_\pi \neq 0$, $\tilde{\Delta}_m$ differs from Δ , and Δ differs from Δ_0 . Converted to real frequencies, Eqs. (4b) and (5) yield a complex function $\tilde{\Delta}(\omega)$. For $2\Gamma_\pi \geq \Delta$, $\tilde{\Delta}(\omega = 0)$ vanishes, i.e., superconductivity becomes gapless.¹⁹ At the critical point $2\Gamma_\pi = \Delta$, $\tilde{\Delta}(\omega) \propto (-i\omega)^{2/3}$ at small ω , at larger Γ_π , $\tilde{\Delta}(\omega) = -i \text{const } \omega + O(\omega^2)$.

Results. We express the results using dimensionless parameter $\zeta = \Gamma_\pi/2\pi T_{c0}$. For $2\Gamma_\pi/\Delta < 1$, $y = \Delta/\Delta_0$ is the solution of $y = \exp[-\pi e^\gamma \zeta/y]$, where $\gamma \approx 0.577$ is the Euler constant.²⁰ 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^{19,20} $\ln(T_c/T_{c0}) = \Psi(1/2) - \Psi(1/2 + 2\zeta T_{c0}/T_c)$, where $\Psi(x)$ is a di-Gamma function. T_c decreases with ζ and vanishes at $\zeta_{cr} = e^{-\gamma}/8 \approx 0.07$ ($\Gamma_\pi/\Delta_0 = 1/4$). For $0.064 < \zeta < \zeta_{cr}$, $\tilde{\Delta}(T, \omega) \propto i\omega$ 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 $\Delta(0) = 0.46 \Delta_0$).

Near $\zeta = \zeta_{cr}$ both T_c and $\Delta(0)$ decrease as $T_c \approx 2.6 T_{c0} \sqrt{\zeta_{cr} - \zeta}$, $\Delta(0) = 6.54 \Delta_0 \sqrt{\zeta_{cr} - \zeta}$. The ratio $2\Delta(0)/T_c \approx 8.88$,²⁰ which is 2.5 times larger than the BCS value. A large value of $2\Delta(0)/T_c$ is often attributed to strong coupling,²¹ but, as we see, can also be due to impurities.

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

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

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

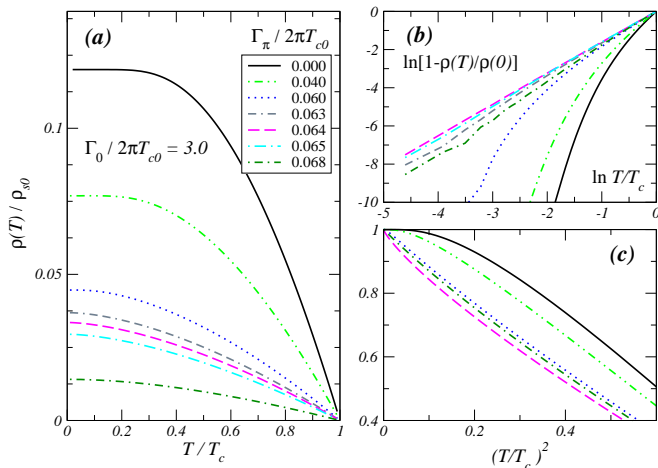


FIG. 1: (color online) (a) Superfluid stiffness $\rho_s(T)$ in a dirty s^+ superconductor with intra-band impurity scattering Γ_0 and inter-band scattering Γ_π , for fixed $\Gamma_0/2\pi T_{c0} = 3$ and various $\zeta = \Gamma_\pi/2\pi T_{c0}$. (b) Log-Log plot showing power-law behavior for $\zeta \gtrsim 0.06$; and (c) low- T plot of ρ_s vs. T^2 showing near $n = 2$ power-law around onset of gapless regime.

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

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

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

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

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

where $\rho_s(T=0)$ is the actual zero-temperature value of ρ_s . In a clean BCS superconductor $B = 2$. In the present case $B(\zeta)$ is non-monotonic in ζ and equals $B(\zeta \ll 1) \approx 2.65$, $B(\zeta = 0.064) \approx 1.67$, $B(\zeta \approx \zeta_{cr}) = 2.03$. 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 $\bar{\Delta}(\omega=0) = \Delta_0[1 - (\zeta/\zeta_{cr})^{2/3}]^{3/2}$, 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 $0.064 < \zeta < \zeta_{cr}$, we found $\rho_s(T) \propto T^2$ at low T .

To obtain $\rho_s(T)$ at arbitrary T , we solved the gap equation numerically, found $\Delta(T)$ and $\bar{\Delta}_m$, substituted them into Eq. (6) and obtained $\rho_s(T)$. We present the results in Fig. 1 for several values of ζ .

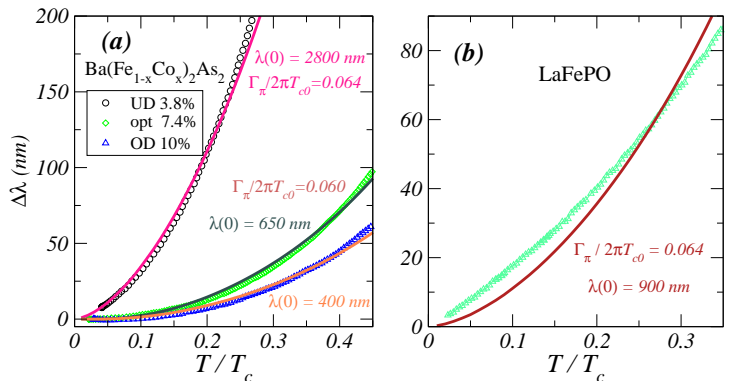


FIG. 2: (color online) The fits to experimental data for $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (Ref.13) and LaFePO (Ref.15). We use only low- T data as at higher T the experimental $\lambda(T)$ may be influenced by sample geometry and fluctuations. (a) The data for BaFe_2As_2 for optimally doped ($x = 7.4\%$) and overdoped ($x = 10\%$) samples can be fitted reasonably well using realistic $\lambda(0) \sim 400 - 700 \text{ nm}$ (in the underdoped material $\lambda(T)$ is likely influenced by SDW magnetism). (b) The power-law dependence of λ for LaFePO can not be reproduced well, and a rather large $\lambda(0)$ is required for the best quantitative fit.

We see that, once the inter-band impurity scattering increases, the range of exponential behavior of $\rho_s(T)$ progressively shrinks to smaller T (see the evolution of $\rho_s(T)$ between $\zeta = 0$ and $\zeta = 0.06$ in Fig. 1(a)). 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 the near-gapless and gapless regimes is a power-law T^n with n reasonably close to 2 down to the lowest T available with our numerical precision, see Fig. 1(b).

Comparison with the data. Judging by the value of $2\Delta(0)/T_c$, the material with the least amount of inter-band impurity scattering is $\text{SmFeAsO}_{1-x}\text{F}_x$, where $T_c \sim 55 \text{ K}$, and $2\Delta(0)/T_c$ is even smaller than the BCS value, possibly indicating multiple gaps in this material.¹⁴ In any way, it is difficult to expect a large ζ . The observed exponential BCS-like behavior of $\rho_s(T)$ at small T (Ref. 14) is consistent with extended s -wave gap and weak inter-band impurity scattering.¹⁷ In LaFePO , measured by the same group,¹⁵ $T_c \sim 6 \text{ K}$ is much lower, the jump of the specific heat $\Delta C/C(T_c)$ is around 0.5 of the BCS result.^{15,22} The ratio $2\Delta(0)/T_c$ has not been reported, but $\Delta C/C(T_c)$ decreases with increasing ζ , and the reduction by a factor 2 corresponds to $\zeta = 0.05$ (using results from Ref. 20). The low- T behavior of $\rho_s(T)$ in this material has been fitted by a power-law T^n with $n = 1.2$, down to very low T .¹⁵ Such behavior is *quantitatively* inconsistent with our theory – we couldn't find any regime where the power is smaller than 1.6. The closest fit we could achieve is for onset of gapless regime $\zeta = 0.064$ and quite large $\lambda(0) \sim 1000 \text{ nm}$. The situation

may change beyond Born approximation, but we do not focus on this at present.

The data on $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (Ref. 13) can be fitted by a more realistic $\lambda(0) \sim 400 - 700 \text{ nm}$ and a smaller value of Γ_π , see Fig.2(a). T_c in this material is rather small: it varies between 10 and 20K, depending on doping x . This could imply that intra-band impurity scattering is strong, although this can also be attributed to strong-coupling effect due to electron-boson interaction.²³ The measured $\rho_s(T)$ scales approximately as T^2 , which is similar to behavior shown in Fig. 1(c). Apart from the underdoped regime, where SDW magnetism interferes, the prefactor for the T^2 term only weakly depends on doping, which also agrees with the scenario based on inter-band impurity scattering. We therefore conclude that the penetration depth data for 122 material can be fitted by a model of a dirty s^+ superconductor.

A comment is in order here. The data²² 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 intra-band scattering, controlled by Γ_0 , which affects residual resistivity but does not affect T_c .

To conclude, in this paper we considered superfluid density $\rho_s(T)$ in a two-band superconductor with ex-

tended s -wave symmetry in the presence of non-magnetic 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. We showed that for a moderate *inter-band* 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 the power-law behavior is consistent with recent experiments on penetration depth $\lambda(T)$ in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ and in general LaFePO, but for the case LaFePO the theoretical fit requires large $\lambda(T = 0)$ and lower power than what is obtained in this model. An extension on the model beyond Born approximation may improve the comparison with the data for LaFePO. Also note that we assumed that the surface of a superconductor is homogeneous. Defects on the surface may modify the temperature dependence of the penetration depth.

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