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 ($s^\pm$) 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 $n = 1.6 \pm 0.2$ 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$_2$As$_2$ 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$_2$As$_2$ have high potential for the applications and may create a breakthrough in the field of superconductivity (SC).

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, suggesting that the SC pairing is of electronic origin. Electronic structure of pnictides shows pairs of small hole and electron pockets centered at $(\pi, \pi)$, respectively, in the folded Brillouin zone. Most of parent compounds display an SDW order with momentum at $(\pi, \pi)$, and an early scenario was the pairing mediated by antiferromagnetic spin fluctuations. 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 $s^\pm$ gap). The $s^\pm$ gap symmetry has been found in weak coupling studies of two-band and five-band $\pi$-olgy models of interacting low-energy fermions. Some other studies, however, found a gap with extended $s$-wave symmetry in the unfolded Brillouin zone. 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.

From experimental perspective, the situation is also unclear. Andreev spectroscopy and angle resolved photoemission spectroscopy (ARPES) measurements are consistent with the gap without nodes. NMR and Knight shift measurements 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 $s^\pm$ superconductor. The situation is further complicated by the fact that the two hole FSs are of different sizes and have different gaps.
ever, when $\Gamma_\pi/\Delta$ 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,

$$\rho_s(T) = \frac{\alpha T}{\sum_m \Delta_m^2 + \omega_m^2}$$

(1)

where $\rho_s$ 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, $\omega_m$, and the superconducting vertex $\Delta_m$. In an $s^+$ superconductor the order parameters on the hole ($c$) and electron ($f$) FS pockets are related, $\Delta_m = -\Delta^f_m = \Delta_m$ and in Born approximation,

$$i\tilde{\omega}_m = i\omega_m - \Gamma_0 g^f(\tilde{\omega}_m, \Delta_m) - \Gamma_0 s^f(\tilde{\omega}_m, \Delta_m) \approx \Delta_m$$

(2a)

$$\Delta_m = \Delta + \Gamma_0 g^f(\tilde{\omega}_m, \Delta_m) + \Gamma_0 s^f(\tilde{\omega}_m, \Delta_m)$$

(2b)

where $\omega_m = \pi T (2m + 1)$, $\Gamma_0 = m N_F |\epsilon_0|^2$, and $\Gamma_\pi = m N_F |\epsilon_\pi|^2$ are the intra- and interband impurity scattering rates, respectively ($\epsilon_0, \pi$ are impurity scattering amplitudes, correspondingly small, or close to zero, $\epsilon_\pi - \pi$, momentum transfer). $\Delta$ is the SC order parameter, and functions $g^f$ and $s^f$ are $\xi$-integrated normal and anomalous Green’s functions for holes and electrons,

$$g^f = g^f = \frac{-i\tilde{\omega}_m}{\sqrt{\omega_m^2 + \Delta_m^2}} \quad f^f = -f^s = \frac{-\Delta_m}{\sqrt{\omega_m^2 + \Delta_m^2}}$$

(3)

Since the $f$ function has opposite signs in two bands, $\Gamma_\pi$ 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 $\tilde{\Delta}_m = \Delta_m/\eta_m$ that satisfy

$$\eta_m = 1 + (\Gamma_0 + \Gamma_\pi) \frac{1}{\sqrt{\omega_m^2 + \Delta_m^2}}$$

(4a)

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

(4b)

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

$$\Delta(T) = V^S \pi T \sum_m \Delta_m^2 \frac{\Delta_m}{\sqrt{\omega_m^2 + \Delta_m^2}}$$

(5)

where $V^S$ is the $s^+$ coupling constant and $\Delta$ is the ultraviolet cutoff. Notice that the last expression contains $\tilde{\Delta}_m$ and bare Matsubara frequencies $\omega_m$. Equations (2)–(5) can be extended to the case when 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 $\tilde{\Delta}_m$. In particular, Eq. (4b) is an algebraic equation (valid at any $T$) which expresses $\tilde{\Delta}_m$ in terms of $\Delta$. The latter itself depends on $\Gamma_\pi$ because the self-consistency equation, Eq. (5), contains $\tilde{\Delta}_m$. Without interband scattering ($\Gamma_\pi = 0$) we have $\tilde{\Delta}_m = \Delta = 1.76 T_c$, where $T_c$ and $\Delta$ are the BCS transition temperature and the $T=0$ gap in a clean superconductor. For $\Gamma_\pi \neq 0$, $\tilde{\Delta}_m$ differs from $\Delta$, and $\Delta$ differs from $\Delta_0$. Converted to real frequencies, Eqs. (4b) and (5) yield a complex function $\tilde{\Delta}(\omega)$. For $2\Gamma_\pi = \Delta$, $\tilde{\Delta}(\omega = 0)$ vanishes, i.e., superconductivity becomes gapless. At the critical point $2\Gamma_\pi = \Delta$, $\tilde{\Delta}(\omega = 0) = \tilde{\Delta}(\omega) = (-\omega)^{2/3}$ at small $\omega$, at larger $\Gamma_\pi$.

III. RESULTS

We express the results using dimensionless parameter $\xi = \Gamma_\pi/2\pi T_c$. For equal gap magnitudes and $2\Gamma_\pi/\Delta < 1$, $\gamma = \Delta/\Delta_0$ is the solution of $\gamma = \exp[-\pi y^2/(\gamma + y^2)]$, where $y = 0.577$ is the Euler constant. At a given $T$ a gapless superconductivity emerges, when $y$ becomes smaller than $4\xi e^2$, i.e., for $\gamma > (1/4) \exp[-(\gamma + y^2)/4] = 0.064$. The transition temperature obeys, $\Gamma_0 = \psi(1/2) - \psi(1/2 + 2\pi T_c/T_c)$, where $\psi(x)$ is the di-Gamma function [Fig. 1(a)]. $T_c$ decreases with $\xi$ and vanishes at $\xi = e^{-\gamma}/8 = 0.07(\Gamma_\pi/\Delta_0 = 1)/4$. For $0.064 < \xi < \xi_c$, $\tilde{\Delta}(\omega, T_c) \approx \omega$ for small $\omega$, including $T=0$, and thus even $T=0$ zero-energy density of states becomes finite. (At the onset, at $\xi = 0.064$, $T_c = 0.22 T_{c0}$, and $\Delta(0) = 0.46 \Delta_0$). The ratio $2\Delta(0)/T_c$ increases with $\xi$ and reaches 7.2 at the onset of the gapless behavior and 8.88 at $\xi = \xi_c$. A large value of $2\Delta(0)/T_c$ is often attributed to strong coupling but, as we see, can also be due to impurities.

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

$$\rho_s(T) = \frac{\alpha T}{\sum_m \omega_m \eta_m^{2} \frac{\Delta_m^2}{\sqrt{\omega_m^2 + \Delta_m^2}}}$$

(6)

In general, the value of $\rho_s(T=0)$ and the functional form of $\rho_s(T)$ depend on both $\Gamma_\pi$ and $\Gamma_0$, because $\Gamma_0$ is explicitly present in Eq. (6) via $\eta_m$ 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

$$\rho_s(T) \approx B T \sum_m \frac{\Delta_m^2}{\omega_m^2 \Delta_m^2 + \omega_m^2}$$

(7)

where $B = \pi \rho_s(0)/(\Gamma_0 + \Gamma_\pi)$. We see that $\Gamma_0$ only affects the overall factor $B$, and all nontrivial $T$ dependence comes from frequency and temperature dependence of $\Delta_m$.

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

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

(8)

where $\rho_s(T=0)$ is the actual zero-temperature value of $\rho_s$. In a clean BCS superconductor $B = 2$. In the present dirty case
This implies that a linear extrapolation of \( f \) is difficult to expect a large \( \Delta /H20849 \) to
\[ B(\xi) = B' \xi. \]
We see that, once the interband impurity scattering in-
\[ \Gamma/2\pi T0 = 3 \text{ and various interband scatters } \xi = \Gamma/2\pi T0, \text{ and} \]
\( \Gamma/2\pi Tc \approx \frac{2\pi Tc}{2\pi Tc} \approx 2.65, B(\xi=0.064) = 1.67, \text{ and } B(\xi = \xi_c) = 2.03. \]
This implies that a linear extrapolation of \( \rho_s \) from \( T = Tc \) to \( T = 0 \) still yields a significantly larger value than the actual \( \rho_s(0) \). Second, at \( \xi < 0.064 \), the \( T \) dependence of \( \rho_s(T) \) re-
\[ \Delta(\omega=0) \propto (-\omega)^{5/3}, \text{ we have } \rho_s(T) \propto T^{5/3}. \]
Finally, in the gapless regime \( 0.064 < \xi < \xi_c \), 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 
\[ \Gamma(0) = Tc, \text{ and } \Gamma(\xi) = \Gamma(0) = Tc, \]
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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 $\text{Ba}_2\text{K}_x\text{Fe}_2\text{As}_2$. For $f \sim T^2$, from the analytic reasoning we get the effective $\lambda_0$ 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 $\Gamma_0$, 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 $\xi$ 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$_2$As$_2$, 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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