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Enhancement of the London penetration depth in pnictides at the onset of SDW order under superconducting dome

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Recent measurements of the doping dependence of the London penetration depth λ(x) at low T in clean samples of isovalent BaFe2(As1−xP2)x near optimal doping x ≈ 0.3 [11–14] revealed a peak in λ(x) near optimal doping. The observation of the peak at T ≪ Tc, points to the existence of the quantum critical point (QCP) beneath the superconducting dome. We associate such a QCP with the onset of a spin-density-wave order and show that the renormalization of λ(x) by critical magnetic fluctuations, gives rise to the observed feature. We argue that the case of pnictides is conceptually different from a one-component Galilean invariant Fermi liquid, for which correlation effects do not cause the renormalization of the London penetration depth at T = 0.

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Introduction.— Properties of iron–based superconductors (FeSCs) have been at the forefront of research activities in correlated electron community over the last few years [1–4]. These materials have multiple Fermi pockets with electron-like and hole-like dispersion of carriers. It is well established that superconductivity in FeSCs emerges in close proximity to a spin-density-wave (SDW) order, and superconducting (SC) critical temperature Tc has dome-shaped dependence on doping, with Tc maximum near the onset of SDW order [5–8].

Several groups [9] put forward the scenario that superconductivity in FeSCs has s± symmetry and emerges because SDW fluctuations increase inter-pocket interaction, which is attractive for s± gap symmetry, to a level when it overcomes intra-pocket repulsion. Likewise, SC fluctuations tend to increase the tendency towards SDW.

Once the system develops long-range order, the situation changes because SDW and SC orders compete, and the order which sets first tends to block the development of the other. According to theory, such competition may give rise to a homogeneous coexistence of SDW and SC orders in some range of dopings [12–14]. A homogeneous coexistence of SDW and SC orders has been detected in 122 materials – electron-doped Ba(Fe1−xCo2)xAs2 [7, 8, 15–20] and hole-doped Ba1−xKxFe2As2 [21–23]. On the other hand, for EuFe2−xCo2xAs2 Mössbauer spectroscopy measurements [24] were interpreted in favor of phase separation, when SC has a filamentary character and is concentrated in non-magnetic regions. In the third class of 122 materials – an isovalent BaFe2(As1−xP2)x2, the coexistence between SDW and SC order has not been yet probed experimentally, but the odds are that the two orders do coexist because the phase diagram of BaFe2(As1−xP2)x2 is quite similar to that for Ba(Fe1−xCo2)x2As2 [25].

The coexistence implies that the SDW transition line extends into superconducting phase. If this line reaches T = 0, the system develops a magnetic quantum-critical point (QCP) beneath the superconducting dome [11], see Fig. 1. A magnetic QCP without superconductivity has been analyzed in great detail [27, 28], and it is known that quantum fluctuations near this point give rise to

\[ \lambda \approx \lambda_T \approx \lambda_{SDW} \approx \lambda_{SC} \approx \lambda_{QCP} \]

FIG. 1: [Color online] Lower panel: a theoretical phase diagram of 122-type iron-based superconductors in temperature vs doping plane. Critical temperatures TN and TC indicate transitions into pure SDW and SC phases respectively. A QCP lies beneath of the SC dome and separates pure SC and coexistence SC+SDW phases. Re-entrant behavior of TN under the SC dome has been detected in Co-doped 122 materials [10] but well may be non-universal [11–14]. Upper panel: the theoretical behavior of the penetration depth \( \lambda \) at \( T = 0 \). In the mean-field approximation (dashed line), \( \lambda \) diverges at the edges of the superconducting dome, flat inside pure SC phase and increases monotonically as system moves towards the pure SDW phase. Beyond mean-field, magnetic fluctuations give rise to a peak in \( \lambda \) at the onset of the SDW order (solid line). The peak in \( \lambda \) has been observed in Ref. [26].
non-Fermi liquid (NFL) behavior and to singularities in various electronic characteristics. An SDW instability inside the $d$-wave SC state has been analyzed in [29] and was shown to give rise to NFL behavior of nodal fermions.

The observation of coexistence brings about the new issue of whether there are electronic singularities at a magnetic QCP which develops in the presence of an $s^+$ SC order. Of particular interest are the singularities in quantities such as the penetration depth $\lambda(x)$, which measures electronic response averaged over the whole FS. Early experiments [30] on Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ found no special features in $\lambda(x)$ at the onset of SDW order, but recent measurements in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ (Ref. 26) found a peak in $\lambda(x)$ at the smallest $T < T_c$ at around optimal doping (see inset of Fig. 1). The authors of Ref. [26] speculated that the peak likely indicates that there is a QCP beneath a SC dome and argued that the peak in $\lambda(x)$ is a generic feature of 122 Fe-pnictides, but it is more difficult to detect it in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ because of greater degree of electronic disorder caused by Co doping. Another potential reason why the peak has been observed only in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ is that this material possess gap nodes [31] what generally leads to stronger effects due to quantum fluctuations.

In this communication, we analyze the behavior of $\lambda(x)$ under the assumption that the QCP is associated with the development of SDW order beneath a superconducting dome. A preemptive nematic order may also play a role [32], but we will not dwell into this.

London penetration depth near QCP. – In general, the peak in $\lambda(x)$ at a SDW QCP can emerge by three reasons: (i) a non-monotonic behavior of $\lambda$ near a QCP already within the mean-field theory (like the peak in the specific heat jump at $T_c$ at the onset of coexistence with SDW [33]); (ii) critical fluctuations at the onset of SDW, not specific to the form of the gap; (iii) critical fluctuations specific to the presence of the gap nodes. Besides, $\lambda$ can either diverge at a QCP, or get enhanced but stay finite. It was found recently [34] that, at the mean field level, the variation of $\lambda$ is smooth and cannot explain sharp feature observed in Ref. [26]. Here we investigate the effects of critical magnetic fluctuations. We find that fluctuations associated with SDW QCP beneath a SC dome give rise to the enhancement of the effective mass $m^*$. The mass does not diverge because SC order cuts infrared singularities, but nevertheless $m^*/m$ at the QCP is noticeably enhanced. We argue that the enhancement of $m^*$ gives rise to a sharp peak in $\lambda(x)$ at the onset of coexistence with SDW. We also find that the presence of the nodes in the gap is not sufficient to transform a peak into a divergence because the dominant contribution to $m^*$ comes from the region away from the nodes.

London penetration depth in a type-II superconductor with cubic symmetry is expressed via zero-momentum component of the electromagnetic response tensor $Q_{ij}(k) = (\delta_{ij} - k_i k_j / k^2) Q(k)$, which relates vector potential $A$ and the current density $j$: $j_i(k) = -Q_{ij}(k) A_j(k)$. The temperature and doping dependent penetration depth is given by $\lambda^{-2}(T, x) = (4\pi/e) Q(T, x)$, where $e$ is the velocity of light. The kernel $Q(T, x)$ is related to current-current correlation function in the limit of zero frequency and vanishing momentum and is expressed via the superfluid density $n_s(T, x)$ as $Q = e^2 n_s / mc$, where $m$ and $e$ are the mass and the charge of an electron. Then $\lambda^2 = mc^2 / (4\pi e^2 n_s)$. In Galilean invariant, one-component fermionic system superfluid density at $T = 0$ is equal to the total density of fermions $n(x)$. In this situation $\lambda(T = 0, x)$ does not depend on Fermi liquid corrections and remains the same as in a Fermi gas [35, 36]. Diagrammatically, superfluid density is given by the sum of two bubble diagrams made out of normal and anomalous Green’s function, and the independence of $n_s(T = 0, x)$ on the electron-electron interaction is the result of the cancelation between self-energy and vertex corrections to these diagrams. At $T > 0$ the $T$-dependent part of $n_s$ does depend on Fermi liquid parameters [36].

We find, however, that in iron–pnictides the situation is different because these systems have multiple Fermi pockets, and $s^+$ pairing originates from inter-pocket interaction. The interplay between self-energy and vertex corrections then depends on the orientation of Fermi velocities and the values of superconducting order parameters at different FSs. We find that self-energy and vertex corrections generally do not cancel, and the penetration depth is roughly proportional to $m^*/m$.

We followed earlier works [9] and assumed that the most relevant interaction in Fe-pnictides is between hole and electron pockets, separated by $Q = (\pi, \pi)$ in the folded Brillouin zone, and that the gap has $s^+$ symmetry and changes sign between electron and hole pockets. We calculated the leading interaction correction to $\lambda(x)$ in the one-loop approximation. This perturbative analysis is justified because renormalized $\lambda(x)$ does not diverge even at an SDW QCP. There are 16 diagrams with one-loop corrections to current-current correlator, half of them are self-energy and half are vertex corrections. We evaluated the diagrams and found that self-energy and vertex corrections are of the same order, and both decrease the superfluid density and increase the penetration depth [37]. To be brief, below we analyze how $\lambda(x)$ is affected by inserting fermionic self-energy into current correlation function. A straightforward calculation yields, at one-loop order

$$\lambda^2(T = 0, x) = \lambda^2_{BCS}(1 + \beta(x)), \quad (1)$$

where

$$\beta = \left< \sum_j (1 - Z_j(k_F)) \right> \equiv \left< \lim_{\omega \to 0} \partial_{\omega m} \Sigma_j(k_F, e^{i \omega m}) \right> \phi. \quad (2)$$

Here $j$ labels Fermi pockets, $\Sigma$ is a diagonal (normal) self-energy, which generally depends on the location of
Instead of \( \mathbf{k}_F \) on the corresponding Fermi surface, and \( \langle \ldots \rangle_m = \int_0^{2\pi} d\phi/2\pi \). In a situation when the dependence of \( \Sigma_j(\mathbf{k},\omega_m) \) on \( \mathbf{k} - \mathbf{k}_F \) can be neglected, the quasiparticle residue is related to mass renormalization as \( Z_j(\mathbf{k}_F) = m/m_j(\mathbf{k}_F) \).

A similar expression for \( \lambda \) has been earlier obtained for heavy-fermion superconductor UBe\(_{13} \) [38], which is a two-component system of conduction \( d^- \) electrons and localized \( f^- \)electrons, of which only the first carry the current. It is tempting to extend the one-loop result (1) to \( \lambda^{-2} \propto \sum_j m/m_j\), but we caution that non-cancellation of one-loop self-energy and vertex corrections to the current correlator does not necessarily imply that vertex corrections can be simply neglected. An example of more complex behavior beyond one-loop order has been recently considered in [39].

**Evaluation of the fermionic self-energy.** We consider the minimal three-band model of two elliptical electron Fermi surfaces and one circular hole Fermi surface. The basic Hamiltonian includes the free fermion part \( H_0 \) and pair fermion interactions in superconducting \( H_\Delta \) and magnetic \( H_\sigma \) channels [37]. These interaction are described by the local coupling constants \( g_{ec} \) and \( g_{sw} \) respectively. The phase diagram of the model has been obtained before [14]. We focus on the region where at \( T = 0 \) the system has a long-range SC order and is about to develop an SDW order. Renormalization of mass on all Fermi surfaces is of the same order, and for brevity we show the calculations of \( m^*/m \) for just one pocket.

Potentially singular self-energy comes from the exchange of near-critical SDW fluctuations. In the normal state, these fluctuations are overdamped and are slow compared to electrons. In a SC state, the dynamical exponent changes from \( z = 2 \) to \( z = 1 \) because fermions which contribute to bosonic dynamics become massive particle-like excitations. Such systems have been earlier discussed in the context of cuprates [27] and we follow the same approach in deriving the expressions for the self-energy and spin polarization operator in the SC state in our case.

The one-loop self-energy due to spin-fluctuation exchange is a convolution of spin-fluctuation and fermionic propagators, both taken in the superconducting state:

\[
\Sigma_j(\mathbf{k},\omega_n) = 3T \sum_{\Omega_m} \int \frac{d\mathbf{q}}{4\pi^2} L(q,\Omega_m)G_j(\mathbf{k} - \mathbf{q},\omega_n - \Omega_m)
\]

(3)

where \( \Omega_m = 2\pi T(n + 1/2) \) and \( \Omega_m = 2\pi m T \) are fermionic and bosonic Matsubara frequencies respectively. The normal and anomalous components of the Green’s function in the SC are

\[
G_j(\mathbf{k},\omega_n) = \frac{-i\omega_n - \xi_j}{\xi_j^2 + \omega_n^2 + \Delta_j^2}, \quad F_j(\mathbf{k},\omega_n) = \frac{-\Delta_j}{\xi_j^2 + \omega_n^2 + \Delta_j^2}
\]

(4)

where \( \xi_j = \xi_j(\mathbf{k}) = v_{j,F}(k - k_F) \), and the energy gap \( \Delta_j \) is equal to \( \Delta_h \) on the hole Fermi surfaces and \( \Delta_e(\phi) = -\Delta_e(1 + \alpha \cos 2\phi) \) on the two electrons Fermi surfaces (we choose \( \Delta_h, \Delta_e > 0 \)). The gaps on electron pockets have nodes when \( \alpha > 1 \). We emphasize that the SC gap can be treated as doing-independent only in the paramagnetic state. Once SDW order sets in, the value of the gap changes [12–14].

The spin-fluctuation propagator is given by

\[
L(q,\Omega_m) = \frac{1}{g_{sw}^{-1} + \Pi(q,\Omega_m)}, \quad (5)
\]

where the polarization operator \( \Pi(q,\Omega_m) \) is (see [37] for details)

\[
\Pi = N_f \int \frac{d\xi}{\omega_n} \left[ \frac{[i\omega_+ - \xi_+][i\omega_- - \xi_-] + \Delta_h \Delta_e}{[\xi_+^2 + \omega_n^2 + \Delta_h^2][\xi_-^2 + \omega_n^2 + \Delta_e^2]} \right] \phi^\dagger \phi.
\]

(6)

Here \( \omega_\pm = \omega_n \pm \Omega_m/2, \xi_\pm = \xi \pm \delta/2 \), and we replaced the integration over momentum \( \mathbf{k} \) by \( \int d^2k/4\pi^2 = N_f \int d\xi d\phi/(2\pi) \), where \( N_f \) is the density of states. Parameter \( \delta = \delta_0 + \delta_a \) accounts for the doping-induced modification of the Fermi surfaces. The term \( \delta_0 = \delta_0 + \delta_2 \cos 2\phi \) describes changes in the Fermi surfaces radii and overall shape (ellipticity), while the term \( \delta_2 = v_F q \cos(\phi - \psi) \) describes the relative shift in the centers of Fermi surfaces, where \( \phi \) and \( \psi \) are the directions of \( \mathbf{k}_F \) and \( \mathbf{q} \). The magnetic SDW critical point is determined in terms of doping parameters \( \delta_0 \) and \( \delta_2 \) from the condition \( \Gamma = 0 \), where \( \Gamma = (g_{sw}^{-1} + \Pi(0,0))N_f^{-1} \).

We first consider the case of equal gaps on both Fermi surfaces (\( \alpha = 0 \), \( \Delta_h = \Delta_e = \Delta \)) and then discuss how the results are modified in the case when the gaps on electron pockets have nodes. Earlier calculations show [13] that there is a broad parameter range \( 0.8 \leq \delta_2/\delta_0 \leq 4.7 \) for which SDW order emerges gradually, and its appearance does not destroy SC order, i.e. SDW and SC orders coexist over some range of dopings. Since we are interested in \( T = 0 \) limit, it is sufficient to evaluate the propagator of magnetic fluctuations Eq. (5) only at small frequencies and momenta. A straightforward expansion leads to [37]

\[
L(q,\Omega_m) = \frac{1}{N_f \eta v_F^2 q^2 + \chi\Omega_m^2 + \Gamma}, \quad (7)
\]

where

\[
\Gamma = \ln \left( \frac{T_{c,0}}{T_{N,0}} \right) - \left( \frac{\langle \delta_0 \rangle \text{arccosh} \sqrt{1 + \delta_0^2/\Delta^2}}{\sqrt{\delta_0^2 + \Delta^2}} \right) \phi, \quad (8a)
\]

\[
\chi(\Delta,\delta) = \frac{1}{8} \left[ \frac{\Delta^2}{\Delta^2 + \delta_0^2} + \left( \frac{\Delta^2 \text{arccosh} \left( 1 + \delta_0^2/\Delta^2 \right)}{\langle \delta_0 \rangle (\Delta^2 + \delta_0^2)^{3/2}} \right) \phi \right], \quad (8b)
\]
and
\[
\eta(\Delta, \delta, \psi) = \frac{1}{8} \left( \cos^2(\phi - \psi) \left[ \frac{2\Delta^2 - \delta_0^2}{(\Delta^2 + \delta_0^2)^{3/2}} \right] - 3\Delta^2|\delta_0| \arccosh\left( \frac{1 + \delta_0^2/\Delta^2}{(\Delta^2 + \delta_0^2)^{5/2}} \right) \right) \phi.
\]

In Eq. (8a) we absorbed coupling constants $g_{sdw}$ ($g_{sc}$) into the corresponding critical temperatures $T_{N,0}$ ($T_{c,0}$) for the transitions into a pure SDW (SC) state.

Without superconductivity, $\eta < 0$, and a magnetic transition at $T = 0$ is into an incommensurate phase [14, 32]. In the presence of SC order, the commensurate $(\pi, \pi)$ magnetic order is stabilized ($\eta > 0$), provided that relevant $\delta_0^2 \leq \Delta^2$, which we assume to hold. By order of magnitude, $\chi \sim \eta \sim 1/\Delta^2$.

Substituting Eqs. (4) and (7) into Eq. (2) and integrating explicitly over the momentum transfer $q$, we find the (non-singular) angular dependence and is normalized such that $\phi_k = 1$, where $\phi_k$ is the direction of a hot spot (a $k_F$ point for which $k_F + Q$ is also on another Fermi surface, see Fig. 2(a), and $F$ accounts for the dependence on the distance to hot spot, measured by $\Gamma$, and on the system parameters $\delta_0$ and $\delta_2$. In explicit form $F = (F(\kappa(\psi)), \gamma(\psi))\phi$, where $\kappa(\psi) = \chi/\eta(\psi)$, $\gamma = \Gamma/\eta(\psi)\Delta^2$, and

\[
F(\kappa, \gamma) = \frac{3}{8\pi^2\eta N_F u_F^2 \Delta} \int_{-\infty}^{+\infty} \frac{\kappa z^2 dz}{(1 - \kappa)z^2 + 1 - \gamma} \\
\times \left[ \frac{\kappa z^2 + \gamma}{\sqrt{\kappa z^2 + 1}} \right] \arccosh\left( \frac{\kappa z^2 + 1}{\sqrt{\kappa z^2 + 1}} \right) \phi.
\]

Using Eqs. (1) and (2) we find

\[
\beta = \lambda^2/\lambda_{BCS}^2 - 1 = F(I(\phi))
\]

Because angular integrals over $\phi$ in $I(\phi)$ and over $\psi$ in $F$ are non-singular, the dependence of $\beta$ on the distance to the critical point and on system parameters can be approximated by $\beta \sim F(\kappa, \gamma)$. It is apparent from the integral in (9) that $F(\kappa, \gamma)$ is finite even in the limit $\gamma \to 0$, which implies that the penetration depth remains finite at the SDW QCP. Still, $F(\kappa, \gamma)$ is peaked at the SDW QCP (when $\gamma = 0$), and decreases as $F(\kappa, \gamma) \propto \ln \gamma/\sqrt{\gamma}$ at $\gamma \gg 1$. We illustrate this behavior in Fig. 2. Because $\delta \lambda \sim F(\kappa, \gamma)$, the penetration depth is also peaked at the QCP. This behavior is in agreement with the data for isovalent $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ [26].

By order of magnitude $F(\kappa, 0) = O(1)$, hence $\beta = O(1)$. The enhancement of $\lambda^2 = \lambda_{BCS}^2(1 + \beta)$ at the SDW QCP is larger if magnetic order remains commensurate $(\pi, \pi)$ even in the absence of superconductivity. In this situation, $\delta_0$ and $\delta_2$ are not restricted to be smaller than $\Delta$, and, if they are larger, $\beta$ is enhanced by $(\delta/\Delta)^2$.

We caution, however, that once $\beta$ becomes large, the one-loop approximation is no longer applicable, and, in particular, vertex corrections has been analyzed in more detail [39].

We next computed $F(\kappa, \gamma)$ for the case when SC gap has nodes on electron pockets. We found that, roughly, the angular dependence of the gap renormalizes $\kappa$ downwards. This, however, does not change $\lambda$ qualitatively – at a magnetic QCP $F(\kappa, 0)$ increases when $\kappa$ decreases, but still remains finite. We illustrate this in Fig. 2(b). The reasoning is simple: the nodes of $s^\pm$ gap are located at accidental $k_F$ points which generally differ from hot spots. In the special case when the gap nodes coincide with hot spots, $Z$ at a hot spot diverges logarithmically at a SDW QCP, but momentum integral of $Z(\phi)$ is still finite, hence $\lambda$ remains finite even in this case.

Conclusions. In this paper we considered the behavior of the penetration depth $\lambda(x)$ in a clean Fe-based $s^\pm$ superconductor at the onset of a commensurate SDW order inside the SC phase at $T = 0$. We found that the penetration depth remains finite but has a peak at the onset of SDW order. The magnitude of the peak is larger when $s^\pm$ gap has accidental nodes, but still remains finite at the onset of SDW order. Our results agree with the measurements [26] of the penetration depth in the isovalent $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ inside the superconducting phase. Experiment [26] shows that that $\lambda$ has a peak at roughly the same doping where the Neel temperature $T_N$ intersects with $T_c$. Our results supports the scenario.

![FIG. 2: Color online] Scaling function $F(\kappa, \gamma)$ which accounts for the interaction correction to the London penetration depth $\lambda^2/\lambda_{BCS}^2 - 1 \propto F(\kappa, \gamma)$ is plotted versus $\gamma$ which measures the distance to the quantum critical point for three different combinations of the system parameters encoded by $\kappa = 0.1, 0.25, 0.5$. (see text). Inserts – (a) hole (circular) and electron (elliptical) Fermi surfaces, $\phi_k$ marks the location of a hot spot; (b) the dependence of $F(\kappa, 0)$, normalized to the pre-factor in Eq. 9, on $\kappa$. 

\[\text{FIG. 2: [Color online] Scaling function } F(\kappa, \gamma) \text{ which accounts for the interaction correction to the London penetration depth } \lambda^2/\lambda_{BCS}^2 - 1 \propto F(\kappa, \gamma) \text{ is plotted versus } \gamma \text{ which measures the distance to the quantum critical point for three different combinations of the system parameters encoded by } \kappa = 0.1, 0.25, 0.5. \text{ (see text). Inserts – (a) hole (circular) and electron (elliptical) Fermi surfaces, } \phi_k \text{ marks the location of a hot spot; (b) the dependence of } F(\kappa, 0), \text{ normalized to the pre-factor in Eq. 9, on } \kappa.\]
that SDW order in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ persists into SC phase, as it happens in other Fe-based superconductors, and that the peak in the penetration depth occurs at a magnetic quantum-critical point inside the SC dome. Whether SDW and SC orders co-exist microscopically or phase separate, remains to be seen.

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