Quasiclassical Eilenberger approach to the vortex state in pnictide superconductors

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Abstract. Quasiclassical Eilenberger equations are solved for $s^\pm$-wave superconductors in the mixed state. This symmetry has been proposed for multiband superconductors as pnictides. This mechanism can be realized because of Umklapp scattering between the electron and the hole Fermi surface pockets resulting in opposite sign of pairing gap in these pockets. The applicability of the phenomenological Hao-Clem theory is investigated. Magnetic, temperature and impurity scattering rate dependencies of vortex core size are calculated. It is found that the accuracy of the effective London model gets better with the presence of the impurity scattering and even near the second critical field it is below 6%. The model with the parameters of intraband and interband impurity scattering, describing well superfluid density in $\text{BaFe}_2\text{As}_2$, is also considered.

The discoveries of the superconductivity in the layered $\text{FeP}$ [1] and $\text{FeAs}$ [2] systems have ignited tremendous research activities for understanding of the superconductivity in $\text{Fe}$ pnictides. The superconducting transition temperature $T_c$ of electron-doped $\text{LaFeAsO}_{1-x}\text{F}_x$ ("1111") reaches 43 K under pressure [3], and $\text{NdFeAsO}_{1-x}\text{F}_x$ and $\text{SmFeAsO}_{1-x}\text{F}_x$ show $T_c$ higher than 40 K at ambient pressure [4]. $\text{BaFe}_2\text{As}_2$ ("122") also shows superconductivity by hole doping with the highest $T_c$ of 38 K in $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$ [5] and by electron doping with the highest $T_c$ of 25 K in $\text{Ba}(\text{Fe},\text{Co})_2\text{As}_2$ [6]. Stoichiometric iron pnictides such as $\text{LiFeAs}$ or $\text{NaFeAs}$ ("111") are also interesting because they become superconducting without doping [7]. These $\text{Fe}$ pnictides commonly have the $\text{FeAs}$ layers, where the $\text{Fe}$ ions form a square lattice and each $\text{Fe}$ ion is tetrahedrally coordinated by four $\text{As}$ ions.

One key feature for understanding the origin of the high critical temperature and the pairing mechanism in superconductors is the symmetry of the order parameter. For iron pnictides, one of the attractive idea is that antiferromagnetic spin fluctuations mediate interband pairing. The sign of the Umklapp scattering between the electron and the hole Fermi surface, which is responsible for the superconducting pairing, is positive and the order parameter is fully gapped but changes sign between different Fermi sheets [8]. This situation is referred to as the extended $s^\pm$ symmetry. Using an $s^\pm$ model for the superconducting gap, a good explanation of experimental results on penetration depth in electron-doped and hole-doped $\text{BaFe}_2\text{As}_2$ pnictides has been obtained [9, 10]. In this model the Fermi surface is approximated by two cylindrical pockets centered at $\Gamma$ (hole) and M (electron) points of the Fermi surface, i.e. two dimensional limit of five-band model is proposed. Recently, strong evidence of the $s^\pm$ symmetry in iron pnictides has been found by scanning tunneling microscopic measurements [11]. In spite of...
success of $s^\pm$ model, there are some indications, e.g. weak sensitivity of $T_c$ to the impurity concentration [12], that a conventional $s$-wave state without sign reversal (so called $s_{++}$-wave state) is also possible candidate for iron pnictides. It has been proposed that the moderate electron-phonon interaction due to $Fe$-ion oscillation can induce the critical orbital fluctuation, without being prohibited by the Coulomb interaction. These fluctuations give rise to the strong pairing interactions for the $s_{++}$-wave superconductivity [13].

The aim of our paper is to apply quasiclassical Eilenberger approach to the vortex state of stoichiometric and nonstoichiometric iron pnictides considering $s^\pm$ and $s_{++}$ pairing symmetries as presumable states [9] and to calculate magnetic coherence length $\xi_b$ [14, 15]. As described in Ref. [16], $\xi_b$ is important for the description of the muon spin rotation ($\mu$SR) experiments and can be directly measured. On theoretical ground, the magnetic coherence length can be found from the fitting of the calculated magnetic field distribution $h_{EGL}(r)$ to the Eilenberger - Ginzburg-Landau field distribution $h_{EGL}(r)$ [14, 15]

$$h_{EGL}(r) = \frac{\phi_0}{S} \sum_G \frac{F(G)e^{iGr}}{1 + \lambda_s^2G^2},$$

where $F(G) = uK_1(u)$, $K_1(u)$ is the modified Bessel function, $u = \xi_bG$, $G$ is a reciprocal lattice vector and $S$ is the area of the vortex lattice unit cell. It is important to note that $\xi_b$ in Eq. (1) is obtained from solving the Eilenberger equations and doesn’t coincide with the variational parameter $\xi_v$ (analytical Ginzburg-Landau (AGL) model), ”improved” analytical GL solution [17] or numerical GL solution [18]. We will call the obtained field distribution as an Eilenberger - Ginzburg-Landau field distribution $h_{EGL}(r)$. Using the GL type of the field distribution does not mean direct connection to the GL theory and it is taken as a reasonable starting point of the investigation similar to the empirical approach to the problem [16, 19]. In Eq. (1) $\lambda(T)$ is calculated in Ref. [9]

$$\frac{\lambda_L^2}{\lambda_s^2(T)} = 2\pi T \sum_{\omega_n > 0} \frac{\Delta_n^2}{\eta_n(\Delta_n^2 + \omega_n^2)^{3/2}}, \quad \eta_n = 1 + 2\pi \frac{\Gamma_0 + \Gamma_\pi}{\sqrt{\Delta_n^2 + \omega_n^2}}.$$  

where $\lambda_L$ is the London penetration depth at $T = 0$ K in the absence of the impurities. Here, $\Delta_n = \Delta(T) - 4\pi\Gamma_\pi\Delta_n/\sqrt{\Delta_n^2 + \omega_n^2}$ for the $s^\pm$ pairing and $\Delta_n = \Delta(T)$ for the $s_{++}$ pairing symmetry. The order parameter $\Delta(T)$ is determined by the selfconsistent equation

$$\Delta(T) = 2\pi T \sum_{0 < \omega_n < \omega_c} \frac{V^{SC}\Delta_n}{\sqrt{\Delta_n^2 + \omega_n^2}}.$$  

With the Riccati transformation of the Eilenberger equations quasiclassical Green functions $f$ and $g$ can be parameterized via functions $a$ and $b$ [20]

$$\tilde{f} = \frac{2a}{1 + ab}, \quad f = \frac{2b}{1 + ab}, \quad g = \frac{1 - ab}{1 + ab},$$

satisfying the nonlinear Riccati equations. In Born approximation for impurity scattering we have

$$u \cdot \nabla a = -a[2(\omega_n + G) + iu \cdot A] + (\Delta + F) - a^2(\Delta^* + F^*),$$

$$u \cdot \nabla b = b[2(\omega_n + G) + iu \cdot A] - (\Delta^* + F^*) + b^2(\Delta + F),$$

$$u \cdot \nabla \tilde{f} = \frac{2a}{1 + ab}[2(\omega_n + G) + iu \cdot A] - \frac{a}{1 + ab}(\Delta + F) + a^2(\Delta^* + F^*),$$

$$u \cdot \nabla \tilde{g} = \frac{2b}{1 + ab}[2(\omega_n + G) + iu \cdot A] - \frac{b}{1 + ab}(\Delta + F) - b^2(\Delta^* + F^*),$$

$$u \cdot \nabla F = \frac{1}{1 + ab}(\Delta + F - a^2(\Delta^* + F^*) - b^2(\Delta^* + F^*)),$$

$$u \cdot \nabla G = \frac{1}{1 + ab}(\alpha + \beta(\omega_n - a\Delta^* - b\Delta^*) + iu \cdot A - \Gamma_\pi G - \Gamma_0 G - \Gamma_\pi \alpha_{out}).$$
where $\omega_n = \pi T(2n + 1)$, $G = 2\pi \langle g \rangle (\Gamma_0 + \Gamma_\pi) \equiv 2\pi \langle g \rangle \Gamma^s$, $F = 2\pi \langle f \rangle (\Gamma_0 - \Gamma_\pi)$ for $s^\pm$ pairing symmetry and $F = 2\pi \langle f \rangle \Gamma^s$ for the $s_{++}$ pairing symmetry. Here, $\Gamma_0 = \pi n_i N_F |u_0|^2$ and $\Gamma_\pi = \pi n_i N_F |u_\pi|^2$ are the intra- and interband impurity scattering rates, respectively ($u_{0,\pi}$ are impurity scattering amplitudes with correspondingly small, or close to $\pi = (\pi, \pi)$, momentum transfer) and $\mathbf{u}$ is a unit vector of the Fermi velocity. The FLL create the anisotropy of the electron spectrum. Therefore the impurity renormalization correction in Eq. (5) and (6), averaged over Fermi surface, can be reduced to averages over the polar angle $\theta$, i.e. $\langle \ldots \rangle = (1/2\pi) \int \ldots d\theta$. To take into account the influence of screening the vector potential $\mathbf{A}(\mathbf{r})$ in Eqs. (5) and (6) is obtained from the equation $\nabla \times \nabla \times \mathbf{A}_E = \frac{4}{c^2} \mathbf{J}$, where the supercurrent $\mathbf{J}(\mathbf{r})$ is given in terms of $g(\omega_n, \theta, \mathbf{r})$

\[
\mathbf{J}(\mathbf{r}) = 2\pi T \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\theta}{2\pi} \mathbf{\hat{k}} g(\omega_n, \theta, \mathbf{r}).
\]

Here $\mathbf{A}$ and $\mathbf{J}$ are measured in units of $\phi_0/2\pi \xi_0$ and $2ev_FN_0T_c$, respectively. The self-consistent condition for the pairing potential $\Delta(\mathbf{r})$ is given by

\[
\Delta(\mathbf{r}) = V^{SC} 2\pi T \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\theta}{2\pi} f(\omega_n, \theta, \mathbf{r}),
\]

where $V^{SC}$ is the coupling constant and $\omega_c$ is the ultraviolet cutoff determining $T_{c0}$ [15].

All over this paper the energy, the temperature and the length are measured in units of $T_{c0}$ and the coherence length $\xi_0 = v_F/T_{c0}$, where $v_F$ is the Fermi velocity. The magnetic field $\mathbf{h}$ is given in units of $\phi_0/2\pi \xi_0$. The impurity scattering rates are in units of $2\pi T_{c0}$. In calculations the ratio $\kappa = \lambda_{T0}/\xi_0 = 10$ is used. It corresponds to $\kappa_{GL} = 43.3$ [20]. To obtain the quasiclassical Green function, the Riccati equations [Eq. (5, 6)] are solved by the Fast Fourier Transform (FFT) method for triangular FLL [15]. This method is reasonable for dense FLL discussed in this paper. In high field the pinning effects are weak and they are not considered in our paper. To study high field regime we should calculate upper critical field $B_{c2}(T)$. It can be found from the similarity of the considered model to the model of spin-flip superconductors [21].

Solid lines in Fig. 1 demonstrate magnetic field dependence $\xi_v(B)$ in reduced units for superconductors with impurity scattering at $T/T_{c0} = 0.5$ with $\Gamma_0 = \Gamma_\pi = 0; \Gamma_0 = 3, \Gamma_\pi = 0.03$ and $\Gamma_0 = 0.5, \Gamma_\pi = 0.01$. Dash line demonstrates the result of the AGL theory for $\xi_v[22]$

\[
\xi_v = \xi_{c2}(\sqrt{2} - 0.75) (1 + b^4)^{1/2}[1 - 2b(1-b)^2]^{1/2},
\]

where $\xi_{c2}$ is determined from the relation $B_{c2} = \Phi_0/2\pi \xi_{c2}^2$ (in our units $\xi_{c2} = 1/\sqrt{B_{c2}}$). This dependence with $\xi_{c2}$ as a fitting parameter is used often for the description of the $\mu$SR experimental results [16, 19]. As can be seen from Fig. 1 (a) the magnetic field dependence of $\xi_v/\xi_{c2}$ is nonuniversal because it depends not only from $B/B_{c2}$ (as in the AGL theory, dash line in Fig. 1 (a)), but also on interband and intraband impurity scattering parameters. In the case when, $\Gamma_0 = \Gamma_\pi = 0$, the results are the same for $s^\pm$ and $s_{++}$ pairing symmetries. We mark this curve as “clean” one. In this figure is considered the case $\Gamma_0 \gg \Gamma_\pi$ and the value of $\xi_v$ is reduced considerably in comparison with clean case. One can compare the observed behavior with that in $s_{++}$ pairing model. In $s_{++}$ pairing symmetry the intraband and interband scattering rates act in similar way and $\xi_v/\xi_{c2}$ decreases always with impurity scattering. In contrast, in $s^\pm$ model $\xi_v/\xi_{c2}(B/B_{c2})$ dependences show different behavior with $\Gamma_\pi$: $\xi_v/\xi_{c2}$ increases with $\Gamma_\pi$ at $B/B_{c2} < 0.8$ and decreases at higher fields, i.e. the curves are getting more flat. A crossing point appears in the dependences $\xi_v/\xi_{c2}(B/B_{c2})$ for $s^\pm$ and $s_{++}$ pairing. This can be explained by the fact that in superconductors without interband pair breaking the increasing in high field is
Figure 1. (a) The magnetic field dependence of $\xi_\mathrm{h}/\xi_{c2}$ for superconductors with impurity scattering. Dashed line demonstrates the result of the AGL theory for $\xi_c$ from Eq. 9. Solid lines represent our solution of Eilenberger equations at $T/T_0 = 0.5$ for the “clean” case ($\Gamma_0 = \Gamma_\pi = 0$) and $s^\pm$ model ($\Gamma_0 = 0.5$, $\Gamma_\pi = 0.04$ and $\Gamma_0 = 3$, $\Gamma_\pi = 0.03$). Dotted lines show result for $s_{++}$ model ($\Gamma^* = 0.5$ and $\Gamma^* = 3$). (b) Magnetic field dependence of mean square deviation of the $h_{\text{EGL}}$ distribution from the Eilenberger distribution normalized by the variance of the Eilenberger distribution, $\varepsilon$, for $T/T_0 = 0.5$ for the “clean” case, $\Gamma_0 = 3$, $\Gamma_\pi = 0.03$ and $\Gamma_0 = 0.5$, $\Gamma_\pi = 0.04$ for the $s^\pm$ model.

connected with field-dependent pair breaking under approaching to the upper critical field. We also calculate magnetic field dependence of mean square deviation of the $h_{\text{EGL}}$ distribution of the magnetic field from the Eilenberger distribution normalized by the variance of the Eilenberger distribution $\varepsilon = \sqrt{(h_E - h_{\text{EGL}})^2 / (h_E - B)^2}$, where average over unit vortex cell. Fig. 1 (b) demonstrates $\varepsilon(B)$ dependence for $T/T_0 = 0.5$ at $\Gamma_0 = 0$, $\Gamma_\pi = 0$; $\Gamma_0 = 3$, $\Gamma_\pi = 0.03$ and $\Gamma_0 = 0.5$, $\Gamma_\pi = 0.04$. It can be seen from this figure that accuracy of effective London model getting worse with increasing magnetic field, but in superconductors with impurity scattering the accuracy is below 6% even near the second critical field (Fig. 1 (b)).

The superfluidity density in pnictides shows often a power law dependence with exponent approximately equal to two at low temperatures [9, 10]. This law was explained by $s^\pm$ model with parameters $\Gamma_0 = 3$ and $\Gamma_\pi = 0.04 - 0.06$. Fig. 2 (a) shows $\xi_\mathrm{h}/\xi_{c2}(B/B_{c2})$ dependence with $\Gamma_0 = 3$ and $\Gamma_\pi = 0.06$ at different temperatures. All curves demonstrate growing behavior with values much less that one in whole field range, i.e. they are under the AGL curve of $\xi_c$. This shows strong effect of interband scattering. The inset to Fig. 2 (a) presents $\xi_\mathrm{h}/\xi_{c2}(B/B_{c2})$ results for $\Gamma_0 = 3$, $\Gamma_\pi = 0.06$ ($s^\pm$ pairing) and $\Gamma^* = 3$ ($s_{++}$ pairing) at $T/T_0 = 0.15$. This type of the behavior is cut off by the impurity pair breaking and introducing characteristic field $B^*$. The field dependence by the substitution $B/B_{c2} \rightarrow (B + B^*(\Gamma_\pi))/B_{c2}(\Gamma_\pi)$. There is additional low-field crossing point between $s^\pm$ and $s_{++}$ curves in this low-temperature case comparing with $T/T_0 = 0.5$ (Fig. 1 (a)). It can be explained by the restoration of the Usadel dirty limit behavior (where $\Gamma \gg 1$ and monotonously decreasing $\xi_\mathrm{h}(B)$ is expected [20, 23]) which is not realized for $s^\pm$ symmetry due to the pair breaking there. Opposite, slowly increasing $\xi_\mathrm{h}/\xi_{c2}(B/B_{c2})$ function is obtained for $s^\pm$ case in low-field range (Fig. 2 (a) main plot). It can be explained by the field-dependent splitting of the low-energy spectrum of bound state in the vortex core similar to the case of the surface bound states in $d$-wave superconductors [24]. The same effect is realized for extended state in high-field (for $B/B_{c2} > 0.5$ in Fig. 2 (a)).
Figure 2. (a) The magnetic field dependence of coherence length $\xi_h$ with different temperatures $T_c/T_{c0}$ for $\Gamma_0 = 3$, $\Gamma_\pi = 0.06$. The inset shows the magnetic field dependence of $\xi_h/\xi_{c2}$ for $s^\pm$ model ($\Gamma_0 = 3$, $\Gamma_\pi = 0.06$) and $s_{++}$ model ($\Gamma^* = 3$, dotted line) at $T_c/T_{c0} = 0.15$. (b) The interband scattering $\Gamma_\pi$ dependence of $\xi_h/\xi_{c2}$ at different temperatures $T_c/T_{c0}$ (intraband scattering $\Gamma_0 = 3$ and $B = 5$) for the $s^\pm$ pairing.

Figure 3. The magnetic field dependence of coherence length at $T_c/T_{c0} = 0.5$ with the similar values of intraband $\Gamma_0$ and interband $\Gamma_\pi$ scattering $\Gamma$ ($\Gamma = 0$ for "clean" case and $\Gamma = 0.02, 0.03, 0.04$ for the $s^\pm$ pairing). Dotted line shows result for $s_{++}$ model ($\Gamma^* = 0.5$).

Study of the field dependence $\xi_h/\xi_{c2}(B/B_{c2})$ can clarify the both branches [25] of the energetic spectrum of the mixed state which can not be done in the phenomenological GL theory. Thus, the field-dependent suppression of $\xi_h/\xi_{c2}$ is expected in $s^\pm$ model in comparison to $s_{++}$ one in nonstoichiometric iron pnictides with high $\Gamma_\pi$ (like doped 122 compounds). Also nonmonotonous $\xi_h/\xi_{c2}(\Gamma_\pi)$ dependence is possible in general as is shown in Fig. 2 (b).

We also study the case of weak intraband scattering. This case can be realized in stoichiometric pnictides such as $LiFeAs$. Fig. 3 presents the $\xi_h/\xi_{c2}$ magnetic field dependence with scattering parameters $\Gamma_0 = \Gamma_\pi = \Gamma$ equal to 0, 0.02, 0.03 and 0.04. Dotted line shows the result for $s_{++}$ model ($\Gamma^* = 0.5$). The $\xi_h(B)$ dependence shifts upward from the "clean" curve and have higher values in $s^\pm$ model. In contrast, $\xi_h/\xi_{c2}$ curve shifts downward with impurity...
scattering in $s_{++}$ model. The high values of $\xi_h$ observed in $\mu$SR measurements in $LiFeAs$ [7] supports the $s^\pm$ pairing.

To conclude, Eilenberger equations have been solved in the mixed state for superconductors with $s^\pm$ pairing symmetry. This symmetry is proposed to realize in iron pnictide superconductors. Effects of interband ($\Gamma_0$) and intraband ($\Gamma_\pi$) impurity scattering on coherence length $\xi_h$ are investigated. It is found that $\xi_h/\xi_{c2}(B/B_{c2})$ dependence is nonuniversal and different from the GL theory prediction. In the case of intraband scattering $\xi_h/\xi_{c2}$ decreases with $\Gamma_0$. The effects of interband scattering on $\xi_h$ depends on $\Gamma_0$. The predictions for $\xi_h/\xi_{c2}(B/B_{c2})$ for doped 122 compounds (nonstoichiometric iron pnictides), where $\Gamma_0 \gg \Gamma_\pi$, are done. These dependencies demonstrate growing behavior defined by $\Gamma_0$ with values much less that one in whole field range, i.e. they are under the ”clean” ($\Gamma_0 = \Gamma_\pi = 0$) curve. In the case of weak impurity scattering, $\Gamma_0 = \Gamma_\pi \ll 1$, the $\xi_h/\xi_{c2}$ dependence shifts upward from the ”clean” curve. This case can be realized in stoichiometric 111 compounds. A comparison with $s_{++}$ pairing model is done. Opposite tendencies with interband scattering for $\xi_h/\xi_{c2}(B/B_{c2})$ dependences are found for $s^\pm$ and $s_{++}$ models for stoichiometric and nonstoichiometric iron pnictides. The predictions can be tested by $\mu$SR experiments.

This work was supported by the Finnish Cultural Foundation.

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