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Cutoff parameter and vortex core size in d-wave superconductors

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Abstract. There is some evidence that the electron-phonon mechanism is not strong enough to produce observed high critical temperatures in unconventional superconductors; this is the case in both the cuprates and Fe-based superconductors. The d-wave pairing in strongly correlated systems is consistent with the observation of nodal quasiparticles in the heavily hole doped superconductor KFe_2As_2 with $T_c = 3$ K and high-T_c cuprates. In this work the Eilenberger equations are solved for anisotropic $d_{x^2-y^2}$-wave superconductors. The cutoff parameter ξ_h and vortex core size ξ_2 (the distance from the vortex center to the radius where the current density reaches its maximum value) in the mixed state are investigated numerically. The cutoff parameter determines the field distribution in the generalized London equation obtained as a projection of the quasiclassical theory. It can be used for the fitting of the μSR and small-angle neutron scattering (SANS) experimental data. Field and temperature dependences of ξ_h/ξ_{c2} in $d_{x^2-y^2}$-wave superconductors are similar to those in s-wave superconductors: $\xi_h/\xi_{c2}(B/B_{c2})$ dependence has minimum at high temperatures and shows monotonously increasing behavior at low temperatures. Here, ξ_{c2} is determined by the relation $B_{c2} = \Phi_0/2\pi\xi_{c2}^2$. The $\xi_2/\xi_{c2}(B/B_{c2})$ dependence is monotonously decreasing function at intermediate and high temperatures.

1 Introduction

It has become commonplace when a new class of superconductors is discovered to discuss electronic pairing mechanisms as soon as there is some evidence that the electron-phonon mechanism is not strong enough to produce observed critical temperatures; this was the case in both the cuprates and Fe-based superconductors. Among many candidates for electronic pairing, Berk-Schrieffer [1] type spin fluctuation theories are popular because they are relatively simple to express and they give some qualitatively correct results in the well-known cases of ^{3}He and the cuprates. This type of description cannot be regarded as the complete answer even in superfluid ^{3}He, where the true pairing interaction contains a significant density fluctuation component, while in the cuprates it is controversial whether the full pairing interaction can be described by a simple boson exchange theory at all. Nevertheless, spin fluctuation theories can explain the symmetry of the order parameter in both systems quite well, in part because other interaction channels are projected out in the ground state. For example, in the cuprates, the d-wave nature of the pair wave function follows from the strongly peaked spin susceptibility at $(\pi;\pi)$, characteristic of repulsive local interactions between electrons hopping on a square lattice [2]. In the Fe-based superconductors, the early realization that the Fermi surface consisted of small, nearly nested electron and hole pockets led to the analogous anticipation of a strongly peaked susceptibility near Q = $(\pi; 0)$, and a corresponding pairing instability with sign change between electron and hole sheets [3]. In the case of the nesting absence d-wave symmetry can be realized also in iron-based superconductors such as $K_xFe_{2-y}Se_2$ [4], $Rb_{0.8}Fe_{1.6}Se_2$ [5] and KFe_2As_2 [6]. Likewise, d-wave pairing is observed in heavy fermion $CeCoIn_5$ [7].

A nontrivial orbital structure of the order parameter, in particular the presence of the gap nodes, leads to an effect in which the disorder is much richer in $d_{x^2-y^2}$-wave superconductors than in conventional materials. For instance, in contrast to the s-wave case, the Anderson theorem does not work, and nonmagnetic impurities exhibit a strong pair-breaking effect. In addition, a finite concentration of disorder produces a nonzero density of quasiparticle states at zero energy, which results in a considerable modification of the thermodynamic and transport properties at low temperatures. For a pure superconductor in a d-wave-like state at temperatures T well below the critical temperature T_c, the deviation $\Delta\lambda$ of the penetration depth from its zero-temperature value $\lambda(0)$ is proportional to T. When the concentration n_i of strongly scattering impurities is nonzero, $\Delta\lambda \propto T^n$, where $n = 2$ for $T < T^* \ll T_c$ and $n = 1$ for $T^* < T \ll T_c$, where T^* is a crossover temperature [8]. Unlike s-wave superconductor, impurity scattering suppresses both the transition temperature T_c and the upper critical field $H_{c2}(T)$ [9].

The aim of our paper is to apply quasiclassical Eilenberger approach to the vortex state of d-wave supercon-

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ductors for the different level of impurity scattering rates Γ, to calculate the cutoff parameter ξ_h [10, 11] and vortex core size ξ_2 [12]. As described in Ref. [13], ξ_h is important for the description of the muon spin rotation (μSR) experiments and can be directly measured.

The London model used for the analysis of the experimental data does not account for the spatial dependence of the superconducting order parameter and it breaks down at distances of the order of coherence length from the vortex core centre − *i.e.* $B(r)$ logarithmically diverges as $r \to 0$. To correct this, the **G** sum in the expression for vortex lattice free energy can be truncated by multiplying each term by a cutoff function $F(G)$. Here, **G** is a reciprocal vortex lattice vector. In this method the sum is cut at high $G_{max} \approx 2\pi/\xi_h$, where ξ_h is the cutoff parameter. The characteristic length ξ_h accommodates a number of inherent uncertainties of the London approach, the question discussed originally by de Gennes' group [14] and in some detail in Ref. [15]. It is important to stress that the appropriate form of $F(G)$ depends on the precise spatial dependence of the order parameter in the the vortex core region, and this in general depends on temperature and magnetic field. Using a Lorentzian trial function for the order parameter of an isolated vortex, Clem found for stronger $\kappa_{GL} \gg 1$ that $F(G)$ is proportional to the modified Bessel function [16]. Hao *et al.* [17] extended the model [16] to larger magnetic fields up to B_{c2} through the linear superposition of the field profiles of individual vortices.

Strictly speaking, Ginzburg-Landau theory is valid only near T_c but it is often used in whole temperature range taking the cutoff parameter and penetration depth λ as fitting parameters. Recently an effective London model with the effective cutoff parameter $\xi_h(B)$ as a fitting parameter was obtained for clean [10] and dirty [11] superconductors, using self-consistent solution of quasiclassical nonlinear Eilenberger equations. In this approach λ is not a fitting parameter but is calculated from the microscopical theory of the Meissner state. In this case the effects of bound states in the vortex cores leading to Kramer-Pesch effect [18], their delocalization between the vortices [19] and non-local electrodynamic [20] are self-consistently included.

2 Model

Following the microscopical Eilenberger theory, the cutoff parameter, ξ_h, can be found from the fitting of the calculated magnetic field distribution $h_E(\mathbf{r})$ to the Eilenberger - Hao-Clem (EHC) field distribution $h_{EHC}(\mathbf{r})$ [10, 11]

$$h_{EHC}(\mathbf{r}) = \frac{\Phi_0}{S}\sum_{\mathbf{G}}\frac{F(\mathbf{G})e^{i\mathbf{G}\mathbf{r}}}{1+\lambda^2G^2}. \qquad (1)$$

Here, $F(\mathbf{G}) = uK_1(u)$, where $K_1(u)$ is modified Bessel function, $u = \xi_h G$, S is the area of the vortex lattice unit cell and $\lambda(T)$ is the penetration depth in the Meissner state. Because the magnetic field distribution is taken similar to the analytical solution of the Ginzburg-Landau model (AGL) [17], we will call this approach as Eilenberger-Hao-Clem (EHC) model and ξ_h as AGL cutoff parameter.

While the fitting analysis of the μSR data is performed entirely in time domain, one can reconstruct $B(r)$ by Eq. (1) using the physical parameters deduced from the fitting analysis. The vortex core size defined by $J(\xi_2) = J_{max}$ (where J_{max} denotes the maximum of $J(r)$) is considerably large than the magnetic cutoff parameter ξ_h. The result of a data analysis for various fields/temperatures indicates that ξ_2 is always proportional to ξ_h at low fields [21].

To consider the mixed state of a *d*-wave superconductor we take the center of the vortex as the origin and assume that the Fermi surface is isotropic and cylindrical. With the Riccati transformation of the Eilenberger equations quasiclassical Green functions f and g can be parameterized via functions a and b [22]

$$\bar{f} = \frac{2a}{1+ab},\ \ f^{\dagger} = \frac{2b}{1+ab},\ \ g = \frac{1-ab}{1+ab}, \qquad (2)$$

satisfying the nonlinear Riccati equations. The Riccati equations for $d_{x^2-y^2}$-wave superconductivity in Born impurity scattering are [23]

$$\mathbf{u}\cdot\nabla a = -a\left[2(\omega_n+G)+i\mathbf{u}\cdot\mathbf{A}_E\right]+\Delta-a^2\Delta^*, \quad (3)$$

$$\mathbf{u}\cdot\nabla b = b\left[2(\omega_n+G)+i\mathbf{u}\cdot\mathbf{A}_E\right]-\Delta^*+b^2\Delta, \quad (4)$$

where $G = 2\pi\langle g\rangle\Gamma$ and **u** is a unit vector of the Fermi velocity. In the new gauge vector-potential $\mathbf{A}_E = \mathbf{A} - \nabla\Phi$ is proportional to the superfluid velocity. It diverges as $1/r$ in the vortex center. The FLL creates the anisotropy of the electron spectrum. Therefore, the impurity renormalization correction in Eq. (3) and (4), averaged over the Fermi surface, can be reduced to averages over the polar angle θ, i.e. $\langle\ldots\rangle = (1/2\pi)\int\ldots d\theta$.

To take into account the influence of screening, the vector potential $\mathbf{A_E}(\mathbf{r})$ in Eqs. (3) and (4) is obtained from the equation

$$\nabla\times\nabla\times\mathbf{A_E} = \frac{4}{\kappa^2}\mathbf{J}, \qquad (5)$$

where the supercurrent $\mathbf{J}(\mathbf{r})$ is given in terms of Green function $g(\omega_n,\theta,\mathbf{r})$ by

$$\mathbf{J}(\mathbf{r}) = 2\pi T\sum_{\omega_n>0}\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\hat{\mathbf{k}}}{i}g(\omega_n,\theta,\mathbf{r}). \qquad (6)$$

Here $\mathbf{A_E}$ and $\mathbf{J}$ are measured in units of $\Phi_0/2\pi\xi_0$ and $2ev_FN_0T_c$, respectively. The spatial variation of the internal field $\mathbf{h_E}(\mathbf{r})$ is determined through

$$\nabla\times\mathbf{A_E} = \mathbf{h_E}(\mathbf{r}). \qquad (7)$$

The self-consistent condition for the pairing potential $\Delta(r)$ for *d*-wave pairing is

$$\Delta(\theta,\mathbf{r}) = V^{SC}_{d_{x^2-y^2}}2\pi T\cos(2\theta)\times$$

$$\times\sum_{\omega_n>0}^{\omega_c}\int_0^{2\pi}\frac{d\bar{\theta}}{2\pi}f(\omega_n,\bar{\theta},\mathbf{r})cos(2\bar{\theta}), \qquad (8)$$

where $V^{SC}_{d_{x^2-y^2}}$ is a coupling constant in the $d_{x^2-y^2}$ pairing channel and ω_c is the ultraviolet cutoff determining T_{c0}.

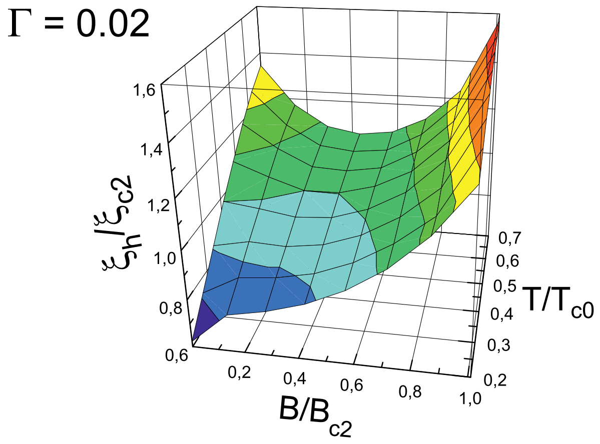

Figure 1. The three dimensional magnetic field dependence of the cutoff parameter ξ_h/ξ_{c2} with different temperatures for $d_{x^2-y^2}$ pairing symmetry with $\Gamma = 0.02$.

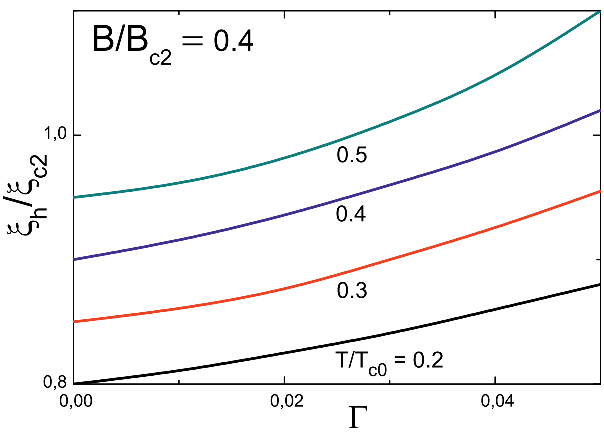

Figure 2. The impurity scattering rate dependence of the cutoff parameter ξ_h/ξ_{c2} with different temperatures at $B/B_{c2} = 0.4$ for $d_{x^2-y^2}$ pairing symmetry.

The obtained solution of $\mathbf{h_E}(\mathbf{r})$ is fitted to Eq. (1) giving the value of cutoff parameter ξ_h for $d_{x^2-y^2}$-wave pairing symmetry.

To study the obtained $\xi_h(B, T, \Gamma)$ dependences it is convenient to use normalization to the coherence length ξ_{c2}, determined from the upper critical field $B_{c2} = \Phi_0/2\pi\xi_{c2}^2$ (in our units $\xi_{c2} = 1/\sqrt{B_{c2}}$). In equations, Γ is impurity scattering rate. For $d_{x^2-y^2}$-wave, $B_{c2}(T)$ is given as in Ref. [9] and $\lambda(T)$ in Eq. (1) is given as [24]

$$\frac{\lambda_{L0}^2}{\lambda^2(T)} = 2\pi T \oint \frac{d\theta}{2\pi} \sum_{\omega_n>0} \frac{|\tilde{\Delta}(\theta)|^2}{(\tilde{\omega}_n^2 + |\tilde{\Delta}(\theta)|^2)^{3/2}}, \quad (9)$$

where

$$\tilde{\omega}_n = \omega_n + \Gamma \langle \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}(\vec{p}_f'; \omega_n)|^2}} \rangle_{\vec{p}_f'}, \quad (10)$$

$$\tilde{\Delta}(\vec{p}_f; \omega_n) = \Delta(\vec{p}_f) + \Gamma \langle \frac{\tilde{\Delta}(\vec{p}_f'; \omega_n)}{\sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}(\vec{p}_f'; \omega_n)|^2}} \rangle_{\vec{p}_f'}, \quad (11)$$

$$\Delta(\vec{p}_f) = \int d\vec{p}_f' V(\vec{p}_f, \vec{p}_f') \pi T \times \\ \times \sum_{\omega_n}^{|\omega_n|<\omega_c} \frac{\tilde{\Delta}(\vec{p}_f')}{\sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}(\vec{p}_f')|^2}}. \quad (12)$$

3 Results

Fig. 1 demonstrates magnetic field dependence of cut-off parameter ξ_h/ξ_{c2} at different temperatures ($T/T_{c0} = 0.2, 0.3, 0.4, 0.5, 0.7$) for $d_{x^2-y^2}$ pairing with $\Gamma = 0.02$. Kramer-Pesch effect obtained for single vortex [25] remains also for vortex lattice in $d_{x^2-y^2}$-wave superconductors. Field and temperature dependences of ξ_h/ξ_{c2} are similar to those in s-wave superconductors [26]: $\xi_h/\xi_{c2}(B/B_{c2})$ dependence has minimum at high temperatures and shows monotonously increasing behavior at low temperatures.

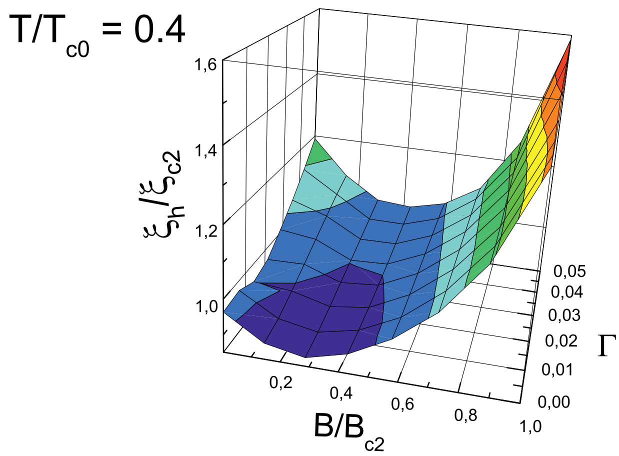

Figure 3. The three dimensional magnetic field dependence of the cutoff parameter ξ_h/ξ_{c2} with different impurity scattering rates Γ with $T/T_{c0} = 0.4$ for $d_{x^2-y^2}$ pairing symmetry.

Figs. 2 and 3 show the impurity scattering Γ dependences of ξ_h/ξ_{c2} for $d_{x^2-y^2}$ pairing at different temperatures and different fields, respectively. In contrast to s-wave superconductors [27, 28] the pair breaking effect in d-wave symmetry gives rise to growth of ξ_h/ξ_{c2}.

Fig. 4 presents the magnetic field dependence of ξ_2/ξ_{c2} with different impurity scattering rates Γ at $T/T_{c0} = 0.5$ (main panel) and $T/T_{c0} = 0.9$ (inset) for $d_{x^2-y^2}$ pairing symmetry. A similar increasing in field dependence of the vortex core size has been found in the framework of Bogoliubov - de Gennes equations for clean superconductors [29]. Our consideration includes effects of impurity. It shows that the core size increases with Γ similar to the cut-off parameter behavior (Fig. 3). Monotonously decreasing behavior of $\xi_2/\xi_{c2}(B/B_{c2})$ is often observed experimentally in different superconductor compounds [13, 30].

4 Conclusions

Eilenberger equations have been solved for superconductors with $d_{x^2-y^2}$ pairing symmetry in the mixed state.

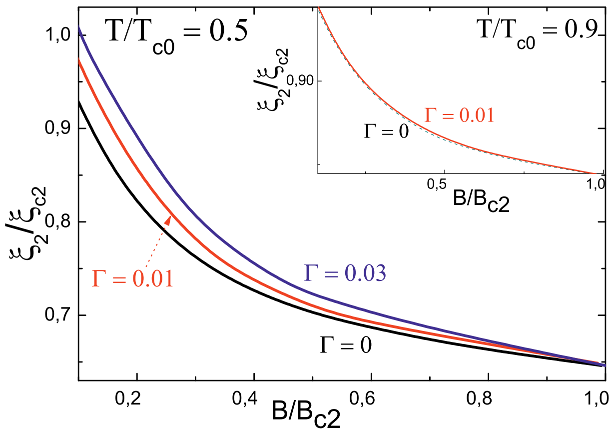

Figure 4. The magnetic field dependence of ξ_2/ξ_{c2} with different impurity scattering rates Γ at $T/T_{c0} = 0.5$ (main panel) and $T/T_{c0} = 0.9$ (inset) for $d_{x^2-y^2}$ pairing symmetry.

This symmetry can be realized in superconductors with spin-fluctuation mediation mechanism such as high-T_c cuprates, iron-based superconductors and heavy fermions. It is found that Eilenberger equations can be reduced to London model with only one parameter, $\xi_h(B)$. This length determines the form factor of FLL, which can be obtained in μSR and SANS experiments. It is found that normalized value of ξ_h/ξ_{c2} decreases with temperature due to Kramer-Pesch effect. In clean superconductors, the shape of $\xi_h/\xi_{c2}(B)$ for d-wave is similar to that in s-wave symmetry. In d-wave superconductors ξ_h/ξ_{c2} always increases with the scattering rate Γ. The vortex core size ξ_2, determined as a distance, where current has its maximum, is also calculated. In is found that ξ_2/ξ_{c2} increases with pair breaking impurity scattering.

References

1. N. Berk, J. Schrieffer, Phys. Rev. Lett. **17**, 433 (1966)
2. C.C. Tsuei, J.R. Kirtley, Rev. Mod. Phys. **72**, 969 (2000)
3. P.J. Hirschfeld, M.M. Korshunov, I.I. Mazin, Rep. Prog. Phys. **74**, 124508 (2011)
4. T. Maier, S. Graser, P. Hirschfeld, D. Scalapino, Phys. Rev. B **83**, 100515 (R) (2011)
5. F. Kretzschmar, B. Muschler, T. Böhm, A. Baum, R. Hackl, H.H. Wen, V. Tsurkan, J. Deisenhofer, A. Loidl, Phys. Rev. Lett. **110**, 187002 (2013)
6. J.P. Reid, M.A. Tanatar, A. Juneau-Fecteau, R.T. Gordon, S.R. de Cotret, N. Doiron-Leyraud, T. Saito, H. Fukazawa, Y. Kohori, K. Kihou et al., Phys. Rev. Lett. **109**, 087001 (2012)
7. K. An, T. Sakakibara, R. Settai, Y. Onuki, M. Hiragi, M. Ichioka, K. Machida, Phys. Rev. Lett. **104**, 037002 (2010)
8. P.J. Hirschfeld, N. Goldenfeld, Phys. Rev. B **48**, 4219 (1993)
9. G. Yin, K. Maki, Physica B **194**, 2025 (1994)
10. R. Laiho, M. Safonchik, K.B. Traito, Phys. Rev. B **76**, 140501(R) (2007)
11. R. Laiho, M. Safonchik, K.B. Traito, Phys. Rev. B **78**, 064521 (2008)
12. J.E. Sonier, J. Phys.: Condens. Matter **16**, S4499 (2004)
13. J.E. Sonier, Rep. Prog. Phys. **70**, 1717 (2007)
14. P. de Gennes, Superconductivity of Metals and Alloys pp. Addison–Wesley, New York (1989)
15. V.G. Kogan, A. Gurevich, J.H. Cho, D.C. Johnston, M. Xu, J.R. Thompson, A. Martynovich, Phys. Rev. B **54**, 12386 (1996)
16. J.R. Clem, J. Low Temp. Phys **18**, 427 (1975)
17. Z. Hao, J.R. Clem, M.W. McElfresh, L. Civale, A.P. Malozemoff, F. Holtzberg, Phys. Rev. B **43**, 2844 (1991)
18. L. Kramer, W. Pesch, Z. Phys. **269**, 59 (1974)
19. M. Ichioka, A. Hasegawa, K. Machida, Phys. Rev. B **59**, 184 (1999)
20. V.G. Kogan, A. Gurevich, J.H. Cho, D.C. Johnston, M. Xu, J.R. Thompson, A. Martynovich, Phys. Rev. B **54**, 12386 (1996)
21. R. Kadono, W. Higemoto, A. Koda, M.I. Larkin, G.M. Luke, A.T. Savici, Y.J. Uemura, K.M. Kojima, T. Okamoto, T. Kakeshita et al., Phys. Rev. B **69**, 104523 (2004)
22. P. Miranović, M. Ichioka, K. Machida, Phys. Rev. B **70**, 104510 (2004)
23. A. Zare, A. Markowsky, T. Dahm, N. Schopohl, Phys. Rev. B **78**, 104524 (2008)
24. D. Xu, S.K. Yip, J.A. Sauls, Phys. Rev. B **51**, 16233 (1995)
25. M. Ichioka, N. Hayashi, N. Enomoto, K. Machida, Phys. Rev. B **53**, 15316 (1996)
26. R. Laiho, M. Safonchik, K.B. Traito, Phys. Rev. B **75**, 174524 (2007)
27. P. Belova, K.B. Traito, E. Lähderanta, J. Appl. Phys. **110**, 033911 (2011)
28. P. Belova, I. Zakharchuk, M. Safonchik, K.B. Traito, E. Lähderanta, Physica C **426**, 1 (2012)
29. W.A. Atkinson, J.E. Sonier, Phys. Rev. B **77**, 024514 (2008)
30. V.G. Kogan, R. Prozorov, S.L. Bud'ko, P.C. Canfield, J.R. Thompson, J. Karpinski, N.D. Zhigadlo, P. Miranović, Phys. Rev. B **74**, 184521 (2006)