PHYSICAL REVIEW B **77**, 064519 (2008)

In-plane magnetic field phase diagram of superconducting Sr_2RuO_4

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(Received 3 December 2007; published 27 February 2008)

We develop the Ginzburg–Landau theory of the upper critical field in the basal plane of a tetragonal multiband metal in two-component superconducting state. It is shown that typical for the two-component superconducting state, the upper critical field basal plane anisotropy and the phase transition splitting still exist in a multiband case. However, the value of anisotropy can be effectively smaller than that in the single band case. The results are discussed in the application to the superconducting Sr_2RuO_4.

DOI: 10.1103/PhysRevB.77.064519 PACS number(s): 74.20.De, 74.20.Rp, 74.25.Dw, 74.70.Pq

I. INTRODUCTION

The tetragonal compound Sr_2RuO_4 is an unconventional superconductor (see review[1]). It reveals properties typical for non-*s*-wave Cooper pairing: the suppression of superconducting state by disorder,[2] the presence of zeros in the superconducting gap discovered by the magnetothermalconductivity measurements,[3,4] and the odd parity of the superconducting state in respect of reflections in the (a,c) plane established by the Josephson interferometry method.[5] All these properties are equally possible for single or multicomponent order parameter superconducting state.

Other important observations demonstrate the appearance of spontaneous magnetization or time-reversal symmetry breaking in the superconducting state of this material. These are (i) the increase of μSR zero-field relaxation rate,[6] (ii) the hysteresis observed in field sweeps of the critical Josephson current,[7] and (iii) the Kerr rotation of the polarization direction of reflected light from the surface of a superconductor[8] (for the theoretical treatment, see Refs. 9 and 10).

A superconducting state possessing spontaneous magnetization is described by the multicomponent order parameter.[11] In a tetragonal crystal, the superconducting states with two-component order parameters (η_x, η_y) corresponding to singlet or to triplet pairing are admissible.[11] In application to Sr_2RuO_4, the time-reversal symmetry breaking form of the order parameter $(\eta_x, \eta_y) \propto (1, i)$ has been proposed first in Ref. 12.

The specific properties for the superconducting state with two-component order parameter in a tetragonal crystal under magnetic field in basal plane are (i) the anisotropy of the upper critical field[13–15] and (ii) the splitting of the phase transition to superconducting state in two subsequent transitions.[11] Both of these properties should manifest themselves starting from the Ginzburg–Landau temperature region $T \approx T_c$ but until now there is no experimental evidence for that. The in-plane anisotropy of the upper critical field has been observed only at low temperatures,[16] where it is a quite well known phenomenon for any type of superconductivity originating from the Fermi surface anisotropy.

Theoretically in application to Sr_2RuO_4, these properties have been investigated by Agterberg and co-workers.[17,18] They have found that one particular choice of the basis functions of a two-dimensional irreducible representation for a tetragonal point group symmetry is appropriate for the elimination of the basal plane upper critical field anisotropy but at the same time the considerable phase transition splitting occurs. Vice versa, another particular choice of the basis functions almost eliminates the phase transition splitting for one particular field direction but keeps the basal plane upper critical field anisotropy. Thus, the basal plane upper critical field properties seem incompatible with the multicomponent order parameter structure dictated by the experimental observations manifesting the spontaneous time-reversal breaking.

All the mentioned theoretical treatments of H_{c2} problem have been undertaken for the two-component superconducting state in a single band superconductor. On the other hand, in Sr_2RuO_4, we deal with three bands of charge carriers.[1] Hence, the formation of multiband superconducting state is quite probable. A microscopic theory of such a state was proposed in Ref. 19.

Here, we apply the Ginzburg–Landau equations for the multiband and multicomponent superconducting states in a superconductor with tetragonal symmetry to the basal plane upper critical field calculation. The coefficients in the Ginzburg–Landau equations obtained in the frame of weak coupling BCS theory are given.

It will be shown that both properties, H_{c2} basal plane anisotropy and the phase transition splitting, still exist in a multiband case. However, quantitatively, the value of anisotropy can be smaller than that in the single band case.

II. UPPER CRITICAL FIELD

The order parameter in multiband tetragonal superconductor with singlet pairing is

$$\Delta(\mathbf{r},\hat{\mathbf{k}}) = \sum_{\lambda} \sum_{i} \eta_i^{\lambda}(\mathbf{r}) \psi_i^{\lambda}(\hat{\mathbf{k}}). \tag{1}$$

Here, $i=x,y$ numerates the components of the order parameter, λ is the band number, and $\psi_i^{\lambda}(\hat{\mathbf{k}})$ are the functions of the irreducible representation dimensionality 2 of the point symmetry group D_{4h} of the crystal in the normal state. Similar decomposition takes place for the vectorial order parameter function in triplet state,

$$\mathbf{d}(\mathbf{r},\hat{\mathbf{k}}) = \sum_{\lambda} \sum_{i} \eta_i^{\lambda}(\mathbf{r}) \boldsymbol{\psi}_i^{\lambda}(\hat{\mathbf{k}}). \tag{2}$$

Although our theory is applicable to the superconductor with arbitrary number of bands, we shall write all the concrete results for the two-band situation.

The system of the Ginzburg–Landau equations for the multiband multicomponent tetragonal crystal determined by the symmetry considerations has the form

$$g^{\lambda\mu}[K_1^\mu D_i^2\eta_j^\mu + K_2^\mu D_j D_i \eta_i^\mu + K_3^\mu D_i D_j \eta_i^\mu + K_4^\mu D_z^2 \eta_j^\mu + K_5^\mu(\delta_{xj}D_x^2\eta_x^\mu + \delta_{yj}D_y^2\eta_y^\mu) - \Lambda(T)\eta_j^\mu] + \eta_j^\lambda = 0. \quad (3)$$

Here,

$$D_i = -i\frac{\partial}{\partial r_i} + \frac{2e}{c}A_i(\mathbf{r})$$

is the operator of covariant differentiation; the Planck constant $\hbar$ is taken equal to unity throughout the paper.

The coefficients in these equations can be easily established in the frame of weak coupling BCS theory. Following the derivation given in Ref. 20, we find

$$\Lambda = \ln\frac{2\gamma\epsilon}{\pi T},$$

where $\ln\gamma=0,577,\ldots.$ is the Euler constant and ϵ is an energy cutoff for the pairing interaction. We assume here that it has the same value for the different bands. The matrix $g^{\lambda\mu}$ is

$$g^{\lambda\mu} = V^{\lambda\mu}\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle = V^{\lambda\mu}\langle|\boldsymbol{\psi}_y^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle. \quad (4)$$

Here, $V^{\lambda\mu}$ is the matrix of the constants of pairing interaction. The angular brackets mean the averaging over the Fermi surface and $N_0^\mu(\hat{\mathbf{k}})$ is the angular dependent density of electronic states at the Fermi surface of the band μ. The gradient term coefficients are

$$K_1^\mu = \frac{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})v_{Fy}^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}\frac{\pi T}{2}\sum_{n\geq 0}\frac{1}{|\omega_n|^3},$$

$$K_2^\mu = \frac{\langle\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})(\boldsymbol{\psi}_y^\mu(\hat{\mathbf{k}}))^* v_{Fx}^\mu(\hat{\mathbf{k}})v_{Fy}^\mu(\hat{\mathbf{k}})N_0^\mu(\hat{\mathbf{k}})\rangle}{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}\frac{\pi T}{2}\sum_{n\geq 0}\frac{1}{|\omega_n|^3},$$

$$K_3^\mu = K_2^\mu,$$

$$K_4^\mu = \frac{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})v_{Fz}^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}\frac{\pi T}{2}\sum_{n\geq 0}\frac{1}{|\omega_n|^3},$$

$$K_5^\mu = \frac{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2[(v_{Fx}^\mu(\hat{\mathbf{k}}))^2 - (v_{Fy}^\mu(\hat{\mathbf{k}}))^2]N_0^\mu(\hat{\mathbf{k}})\rangle}{\langle|\boldsymbol{\psi}_x^\mu(\hat{\mathbf{k}})|^2 N_0^\mu(\hat{\mathbf{k}})\rangle}\frac{\pi T}{2}\sum_{n\geq 0}\frac{1}{|\omega_n|^3},$$

where $\omega_n=\pi T(2n+1)$ is the Matsubara frequency and the components of the Fermi velocity of the band μ are given by $v_{Fx}^\mu(\hat{\mathbf{k}})$, $v_{Fy}^\mu(\hat{\mathbf{k}})$, and $v_{Fz}^\mu(\hat{\mathbf{k}})$. The definition of K^μ coefficients accepted here differs from the tradional one[17,20] by the terms in the denominators.

Neglecting the gradient terms and taking the determinant of the system [Eq. (3)] equal to zero, we obtain the critical temperature

$$T_c = \frac{2\gamma\epsilon}{\pi}\exp(-1/g), \quad (5)$$

where g is defined by

$$g = (g^{11}+g^{22})/2 + \sqrt{(g^{11}-g^{22})^2/4 + g^{12}g^{21}}. \quad (6)$$

The matrix $g^{\lambda\mu}$ in tetragonal crystal determined by Eq. (4) has the common value for x and y components of the order parameter. Hence, the phase transition to superconducting state occurs at the same critical temperature for all the components of the order parameter in all the bands.

In the case of a magnetic field in the basal plane,

$$\mathbf{H} = H(\cos\varphi, \sin\varphi, 0),$$

$$\mathbf{A} = Hz(\sin\varphi, -\cos\varphi, 0),$$

we obtain from Eq. (3),

$$g^{\lambda\mu}\left[-(K_4^\mu\partial_z + \Lambda)\delta_{ij} + h^2z^2\begin{pmatrix} K_1^\mu + K_{235}^\mu\sin^2\varphi & -K_{23}^\mu\sin 2\varphi \\ -K_{23}^\mu\sin 2\varphi & K_1^\mu + K_{235}^\mu\cos^2\varphi\end{pmatrix}_{ij}\right]\eta_j^\mu + \eta_j^\lambda = 0. \quad (7)$$

Here, we have introduced notations $h=2\pi H/\Phi_0$, $K_{23}^\mu=K_2^\mu+K_3^\mu$, and $K_{235}^\mu=K_2^\mu+K_3^\mu+K_5^\mu$.

Making use of the orthogonal transformation

$$\tilde{\eta}_p^\mu = \begin{pmatrix}\cos\beta^\mu & \sin\beta^\mu \\ -\sin\beta^\mu & \cos\beta^\mu\end{pmatrix}_{pl}\eta_l^\mu, \quad \tan 2\beta^\mu = \frac{K_{23}^\mu}{K_{235}^\mu}\tan 2\varphi, \quad (8)$$

we obtain

$$g^{\lambda\mu}\left[-(K_4^\mu\partial_z + \Lambda)\delta_{ij} + h^2z^2\begin{pmatrix} b_x^\mu & 0 \\ 0 & b_y^\mu\end{pmatrix}_{ij}\right]\tilde{\eta}_j^\mu + \tilde{\eta}_j^\lambda = 0. \quad (9)$$

Here,

$$b_{x,y}^\mu = K_1^\mu + \frac{K_{235}^\mu \pm \sqrt{(K_{235}^\mu\cos 2\varphi)^2 + (K_2^\mu\sin 2\varphi)^2}}{2}. \quad (10)$$

It follows from Eq. (9) that in finite magnetic field, the phase transition to superconducting state splits on two subsequent phase transitions. Indeed, the system of equations for the x components of the order parameter from the different bands is proved to be independent of the corresponding system for the y omponents. Hence, they have independent and nonequal eigenvalues. The corresponding upper critical fields can be found only numerically. Here, we solve this problem following a variational approach, which is known to give a good accuracy in similar cases.[21] So, we look for a solution for the x component of the order parameter in the form

$$\tilde{\eta}_x^\mu = \begin{pmatrix} \tilde{\eta}_x^1 \\ \tilde{\eta}_x^2 \end{pmatrix} = \left(\frac{\lambda_x}{\pi}\right)^{1/4} \begin{pmatrix} C_x^1 \\ C_x^2 \end{pmatrix} e^{-\lambda_x z^2/2}. \tag{11}$$

The similar formula and the following calculations are valid for the y component of the order parameter.

After substitution of Eq. (11) into Eq. (9), multiplication of it by $\exp(-\lambda_x z^2/2)$, and spatial integration, we obtain

$$g^{\lambda\mu}(E_x^\mu - \Lambda)C_x^\mu + C_x^\mu = 0, \tag{12}$$

where

$$E_x^\mu = \frac{K_4^\mu \lambda_x^2 + h^2 b_x^\mu}{2\lambda_x}. \tag{13}$$

The transition field is determined by the condition of vanishing the determinant of the system [Eq. (12)]. Particularly, we are interested in upper critical field behavior near the critical temperature. Obviously, $E_x^\mu \propto h$; hence, it tends to zero at $T \to T_c$. So, in the vicinity of critical temperature, we receive after the simple calculations

$$\ln \frac{T_c}{T} = \frac{E_x^1(1+a) + E_x^2(1-a)}{2}, \tag{14}$$

where T_c is determined by Eq. (5) and

$$a = \frac{g^{11} - g^{22}}{\sqrt{(g^{11} - g^{22})^2 + 4g^{12}g^{21}}}. \tag{15}$$

The maximum of critical temperature at nonzero magnetic field is accomplished at following λ_x value:

$$\lambda_x|_{\max} = h\lambda_x^0, \quad \lambda_x^0 = \sqrt{\frac{\tilde{b}_x}{\tilde{K}_4}}, \tag{16}$$

where

$$\tilde{b}_x = b_x^1(1+a) + b_x^2(1-a), \tag{17}$$

$$\tilde{K}_4 = K_4^1(1+a) + K_4^2(1-a). \tag{18}$$

So, after the substitution of Eqs. (13) and (16)–(18) into Eq. (14), we obtain

$$h_{x,y} = \frac{2(1 - T/T_c)}{\sqrt{\tilde{K}_4 \tilde{b}_{x,y}}}. \tag{19}$$

In the case of single band superconductivity, our variational solution is exact and we obtain from Eq. (18) dropping out all the terms with index $\mu = 2$,

$$h_{x,y} = \frac{1 - T/T_c}{\sqrt{b_{x,y}^1 K_4^1}}. \tag{20}$$

So, the situation for the two-band and one-band superconducting states is characterized by the same properties: the basal plane anisotropy of the upper critical field corresponding to the largest of two eigenvalues (h_y) and two consecutive phase transitions to the superconducting state, first with y component and with x and y components of the order parameter.

It is worth noting that in the multiband case due to the compensation of the different band contributions,[17] the actual value of the anisotropy of H_{c2} can be smaller than that in the one-band situation. The phase transition splitting, however, still persists in the multiband case. The absence of experimental evidence of this phenomenon argues in support of one-component superconducting state in Sr_2RuO_4.

III. CONCLUSION

We have demonstrated that for a two-component superconducting state in a tetragonal crystal, the basal plane anisotropy of the upper critical field and the phase transition splitting are inherent properties both for the one-band and multiband superconductivity. Thus, the experimentally established[16] absence of these phenomena in Sr_2RuO_4 stays opposite to the possibility of existence of a two-component superconducting state in this material.

ACKNOWLEDGMENTS

I am indebted to M. Zhitomirsky, Y. Liu and D. Agterberg for the discussions of the problem of upper critical field in the multicomponent multiband superconducting state.

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