

Surface critical field in superconductors with anisotropic pairing

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A microscopic derivation is given of the boundary conditions at a specular superconductor–vacuum (dielectric) boundary for the Ginzburg–Landau equations in superconductors with anisotropic pairing. Calculations were performed for a hexagonal crystal. The form of the boundary conditions in this case depends strongly on the orientation of the surface relative to the principal axes of the crystal lattice. The equations determining the dependence of the surface-superconductivity field for different types of order parameters are derived. The applicability of the results obtained to the identification of superconducting phases in $U\text{Pt}_3$ is discussed. © 1995 American Institute of Physics.

1. INTRODUCTION

The superconducting properties of compounds with heavy fermions, such as $U\text{Pt}_3$, CeCu_2Si_2 , UPe_{13} , and others, have been actively investigated experimentally and theoretically for the past ten years (see Refs. 1 and 2 and the literature cited therein). The data on the low-temperature behavior of the heat capacity, the thermal conductivity, the nuclear spin relaxation time, and so on show that in these materials nontrivial pairing of carriers occurs and the superconducting state has a more complicated structure than in the standard BCS theory.

Although the microscopic mechanisms responsible for the nontrivial pairing are still imperfectly understood, the phenomenological approach based on symmetry considerations has been found to be very fruitful.³ The basic idea consists of the following: the superconducting phase transition is accompanied by breaking of the symmetry of the normal-metal phase, described by the group $G = G_0 \times U(1) \times R$, where G_0 is the point group of the crystal, $U(1)$ is the gauge group, and R is the time reversal operation (the spin-orbit interaction in the materials considered is strong). Nontrivial (anisotropic) pairing occurs in superconductors in which the symmetry of the order parameter $\hat{\Delta}(\mathbf{k})$ is lower than $G_0 \times R$. Near the critical temperature T_c , the order parameter transforms according to an irreducible representation (one-, two-, or three-dimensional) of the group G_0 ; this makes it possible to construct a Ginzburg–Landau expansion of the free energy in powers of the components of the order parameter.^{1–3}

Great interest has recently been shown in the compound $U\text{Pt}_3$, in which the superconducting transition ($T_c \sim 0.5$ K) has been found to split into two close transitions with $\Delta T_c \sim 0.05$ K.⁴ The measurements show that the H – T – P phase diagram contains at least three different superconducting phases.⁵ The theoretical explanations of this fact are based on the assumption that $U\text{Pt}_3$ (hexagonal crystal with $G_0 = D_{6h}$) possesses a multicomponent order parameter corresponding either to a two-dimensional representation of the group D_{6h} (Ref. 6) or a combination of two- and one-dimensional^{7,8} or two one-dimensional^{9,10} representations. We shall not discuss here the advantages and deficiencies

of these models; we merely point out that only additional, more refined experiments will probably help to assess the faithfulness of these models (one such experiment would be to measure in this compound the anisotropy of the surface superconductivity field H_{c3} for different geometries of the samples; the measurement of H_{c3} for whiskers is discussed in Ref. 11).

The observation of a nontrivial dependence of the slope of the line $H_{c3}(T)$ on the orientation of the flat surface of the superconductor relative to the crystallographic axes in the basal plane would be decisive proof of anisotropic pairing; such a proof would make possible substantial progress in identifying the superconducting phases (see Sec. 3 below). In this connection, we recall that the manifestation of the nontrivial character of pairing as anisotropy of the upper critical field H_{c2} ,¹ which cannot be described by an effective-mass tensor, does not occur in hexagonal superconductors,¹² and it is therefore useless for determining the type of symmetry of the order parameter.

From a theoretical standpoint, to calculate the surface superconductivity field it is necessary to know the boundary conditions on the order parameter in the Ginzburg–Landau region.¹³ These conditions in turn can be introduced phenomenologically on the basis of a symmetry approach as follows.^{1,2} The boundary lowers locally (on a scale $\sim \xi_0$) the symmetry of the system to some subgroup G' of the group G , and this results in the appearance of a distinguished direction \mathbf{n} —the normal to the surface. This effect can be described quantitatively by adding to the Ginzburg–Landau functional terms which are localized near the surface (delta functions) and are invariant under transformations from G' ; these terms are constructed from the components of the order parameter and the vector \mathbf{n} . In this approach the boundary conditions are obtained by the standard method: by varying the complete functional and equating to zero the sum of the surface contributions originating from both the standard and the additional terms (see Ref. 2 for a more detailed discussion).

In the present paper we propose a derivation based on the microscopic theory of the boundary conditions for the Ginzburg–Landau equations in superconductors with aniso-

tropic pairing (this can be regarded as a method for calculating the coefficients in the phenomenological surface invariants). In so doing, we proceed, following Ref. 14, from a simple model with specular reflection of electrons from the crystal–vacuum interface, neglecting the splitting of the phase transition. The surface superconductivity field (for UPT₃) is calculated using the boundary conditions obtained, and the possibility of using measurements of H_{c3} to determine the representation according to which the order parameter in such superconductors transforms is also discussed.

This paper is organized as follows. A microscopic derivation of the boundary conditions of an order parameter of arbitrary symmetry in the Ginzburg–Landau region is given in Sec. 2. In Sec. 3 these boundary conditions, which turn out to be strongly anisotropic, are used to calculate $H_{c3}(T)$ for different representations of the group D_{6h} . One-dimensional representations are considered in Sec. 3.1; in addition, for the representations $B_{1,2}$ both the boundary conditions and H_{c3} have an anisotropy of sixth order and for the representation A_2 the anisotropy is of twelfth order. Two-dimensional representations for which the boundary conditions and the slopes of the lines $H_{c3}(T)$ are isotropic are studied in Sec. 3.2.

2. MICROSCOPIC DERIVATION OF THE BOUNDARY CONDITIONS

The order parameter, which transforms according to the a representation of the group G_0 , has the following form in superconductors with anisotropic pairing:³

$$\hat{\Delta}(\mathbf{k}, \mathbf{r}) = \sum_j \eta_j(\mathbf{r}) \hat{\Delta}_j^{(a)}(\mathbf{k}), \quad (1)$$

where $\hat{\Delta}_j^{(a)}$ are the basis functions of the chosen representation, which consists of 2×2 matrices in the spin space (more accurately, because of the strong spin-orbit interaction, in the pseudospin space²). For singlet pairing

$$\Delta_{j,\alpha\beta}^{(a)}(\mathbf{k}) = (i\hat{\sigma}_2)_{\alpha\beta} \psi_j^{(a)}(\mathbf{k}),$$

and for triplet pairing

$$\Delta_{j,\alpha\beta}^{(a)}(\mathbf{k}) = (i\hat{\sigma}_\mu \hat{\sigma}_2)_{\alpha\beta} d_j^{(a),\mu}(\mathbf{k}).$$

The boundary conditions for the order parameter at the specular superconductor–vacuum (dielectric) boundary are determined from the solutions of Gor'kov's equations, which in the region of applicability of the Ginzburg–Landau theory reduce to a linear integral equation:^{2,14}

$$\begin{aligned} \Delta_{\alpha\beta}(\mathbf{k}, \mathbf{q}_1) = T \sum_{\omega} \int \frac{d^3 k_1}{(2\pi)^3} \frac{d^3 k_2}{(2\pi)^3} \frac{d^3 q_2}{(2\pi)^3} V_{\alpha\beta,\gamma\delta}(\mathbf{k}, \mathbf{k}_1) \\ \times G_{\omega,\gamma\lambda} \left(\mathbf{k}_1 + \frac{\mathbf{q}_1}{2}, \mathbf{k}_2 + \frac{\mathbf{q}_2}{2} \right) G_{-\omega,\delta\nu} \\ \times \left(-\mathbf{k}_1 + \frac{\mathbf{q}_1}{2}, -\mathbf{k}_2 + \frac{\mathbf{q}_2}{2} \right) \Delta_{\lambda\nu}(\mathbf{k}_2, \mathbf{q}_2), \end{aligned} \quad (2)$$

where $\omega = (2n+1)\pi T$.

Let the normal to the surface be directed along the x axis and let the components η_i of the order parameter depend only on x , i.e., $\mathbf{q}_{1,2} = (q_{1,2}, 0, 0)$. Writing the pairwise interaction potential in the form¹⁾

$$\hat{V}(\mathbf{k}, \mathbf{k}_1) = g^{(a)} \sum_j \hat{\Delta}_j^{(a)}(\mathbf{k}) \hat{\Delta}_j^{(a)+}(\mathbf{k}_1),$$

and switching to the Fourier representation with respect to $q_{1,2}$, we obtain the following equation for the order parameter:

$$\eta_j(x_1) = \int_0^\infty dx_2 S_{ij}(x_1, x_2) \eta_j(x_2). \quad (3)$$

In the case of singlet pairing the kernel has the form (in what follows we drop the index a designating the representation)

$$\begin{aligned} S_{ij}(x_1, x_2) = gT \sum_{\omega} \int \frac{d^2 p}{(2\pi)^2} \frac{dK_1}{2\pi} \frac{dK_2}{2\pi} \frac{dq_1}{2\pi} \frac{dq_2}{2\pi} \psi_i^*(\mathbf{k}_1) \psi_j \\ \times (\mathbf{k}_2) G_{\omega,\mathbf{p}} \left(K_1 + \frac{q_1}{2}, K_2 + \frac{q_2}{2} \right) G_{-\omega,-\mathbf{p}} \\ \times \left(-K_1 + \frac{q_1}{2}, -K_2 + \frac{q_2}{2} \right) \exp(iq_1 x_1 - iq_2 x_2). \end{aligned} \quad (4a)$$

In the case of triplet pairing

$$\begin{aligned} S_{ij}(x_1, x_2) = gT \sum_{\omega} \int \frac{d^2 p}{(2\pi)^2} \frac{dK_1}{2\pi} \frac{dK_2}{2\pi} \frac{dq_1}{2\pi} \frac{dq_2}{2\pi} d_i^{\nu*}(\mathbf{k}_1) d_j^{\nu} \\ \times (\mathbf{k}_2) G_{\omega,\mathbf{p}} \left(K_1 + \frac{q_1}{2}, K_2 + \frac{q_2}{2} \right) G_{-\omega,-\mathbf{p}} \\ \times \left(-K_1 + \frac{q_1}{2}, -K_2 + \frac{q_2}{2} \right) \exp(iq_1 x_1 - iq_2 x_2). \end{aligned} \quad (4b)$$

The basis functions ψ and \mathbf{d} in these expressions depend on the direction of the vector $\mathbf{k}_i = (K_i, \mathbf{p})$ and are assumed to be orthonormal:

$$\int_0^\pi \sin \theta d\theta \int_0^{2\pi} \frac{d\varphi}{4\pi} \psi^2(\mathbf{n}) = 1$$

for singlet pairing and

$$\int_0^\pi \sin \theta d\theta \int_0^{2\pi} \frac{d\varphi}{4\pi} \mathbf{d}^2(\mathbf{n}) = 1$$

for triplet pairing.

The Green's functions appearing in Eq. (4) are the Matsubara Green's functions for a normal metal with an isotropic excitation spectrum for a half-space with a specularly reflecting boundary. It has the following form in the coordinate representation:²⁾

$$G_{\omega,\mathbf{p}}(x_1, x_2) = \sum_q \frac{\Phi_q(x_1, x_2)}{i\omega - \varepsilon(q, \mathbf{p})},$$

where

$$\Phi_q = \begin{cases} \sin qx_1 \sin qx_2, & x_1 > 0, x_2 > 0, \\ 0, & \text{otherwise.} \end{cases}$$

In the momentum representation we have

$$G_{\omega, \mathbf{p}}(k_1, k_2) = \sum_q \frac{1}{i\omega - \varepsilon(q, \mathbf{p})} \times \left(\frac{1}{k_1 + q - i0} - \frac{1}{k_1 - q - i0} \right) \times \left(\frac{1}{k_2 + q + i0} - \frac{1}{k_2 - q + i0} \right).$$

Substituting the last expression into Eq. (4), performing successive integrations first over \mathbf{p} , K_1 , and K_2 (i.e., with respect to the moduli of the vectors \mathbf{k}_i) and then over $q_{1,2}$, and dropping the rapidly oscillating (on atomic scales) contributions, we obtain the following expression for the kernel S_{ij} :

$$S_{ij}(x_1, x_2) = \frac{\pi\rho T_c}{v_0} \sum_{\omega} \int_0^1 \frac{ds}{s} \int_0^{2\pi} \frac{d\varphi}{2\pi} \times \left[\exp\left(-\frac{2|\omega|}{v_0 s} |x_1 - x_2|\right) f_{ij}^{(-)}(s, \varphi) + \exp\left(-\frac{2|\omega|}{v_0 s} |x_1 + x_2|\right) f_{ij}^{(+)}(s, \varphi) \right], \quad (5)$$

where $\rho = g\nu_0$, $\nu_0 = m_*^2 v_0 / \pi_2$ is the density of states at the Fermi level, and v_0 is the Fermi velocity. The functions of directions $f_{ij}^{\pm}(s, \varphi)$, where $s = \cos \theta$, are determined as follows. For fixed angles $0 \leq \varphi < 2\pi$ and $0 \leq \theta < \pi/2$, we introduce two unit vectors:

$$\mathbf{n}_{\pm} = (\pm \cos \theta, \sin \theta \cos \varphi, \sin \theta \sin \varphi) = (\pm s, \sqrt{1-s^2} \cos \varphi, \sqrt{1-s^2} \sin \varphi), \quad (6)$$

which are related via reflection in the plane of the boundary. Then

$$f_{ij}^{(+)} = \frac{1}{2}(\psi_i^*(\mathbf{n}_+) \psi_j(\mathbf{n}_-) + \psi_i^*(\mathbf{n}_-) \psi_j(\mathbf{n}_+)), \quad (7a)$$

$$f_{ij}^{(-)} = \frac{1}{2}(\psi_i^*(\mathbf{n}_+) \psi_j(\mathbf{n}_+) + \psi_i^*(\mathbf{n}_-) \psi_j(\mathbf{n}_-))$$

for singlet pairing and

$$f_{ij}^{(+)} = \frac{1}{2}[d_i^{\mu*}(\mathbf{n}_+) d_j^{\mu}(\mathbf{n}_-) + d_i^{\mu*}(\mathbf{n}_-) d_j^{\mu}(\mathbf{n}_+)], \quad (7b)$$

$$f_{ij}^{(-)} = \frac{1}{2}[d_i^{\mu*}(\mathbf{n}_+) d_j^{\mu}(\mathbf{n}_+) + d_i^{\mu*}(\mathbf{n}_-) d_j^{\mu}(\mathbf{n}_-)]$$

for triplet pairing.

We have shown that the form of the kernel S_{ij} is determined by the transformation properties of the basis functions of the representation in the case of reflection in the boundary plane.

We shall now find, using Eqs. (3), (5), and (7a,b), the boundary conditions for the components η_i of the order parameter for $x=0$. The case of a diagonal kernel is important for the applications discussed below. Specifically, let $S_{ij}=0$ for $i \neq j$ and $S_{ij}=S_i$ for $i=j$. We introduce the notation

$$F^{(\pm)}(s) = \int_0^{2\pi} \frac{d\varphi}{2\pi} f^{(\pm)}(s, \varphi).$$

Then

$$S_i(x_1, x_2) = \frac{\pi\rho T_c}{v_0} \sum_{\omega} \int_0^1 \frac{ds}{s} \left[\exp\left(-\frac{2|\omega|}{v_0 s} |x_1 - x_2|\right) \times F_i^{(-)}(s) + \exp\left(-\frac{2|\omega|}{v_0 s} |x_1 + x_2|\right) F_i^{(+)}(s) \right]. \quad (8)$$

For an infinite uniform superconductor, the kernel of the linear integral equation for the order parameter has the form

$$S_i^{(0)}(x_1, x_2) = \frac{\pi\rho T_c}{v_0} \sum_{\omega} \int_0^1 \frac{ds}{s} \times \exp\left(-\frac{2|\omega|}{v_0 s} |x_1 - x_2|\right) F_i^{(-)}(s).$$

We note the following important property of the volume kernel:

$$\int_{-\infty}^{+\infty} dx_1 S_i^{(0)}(x_1, x_2) = 1, \quad (9)$$

which is simply the definition of the critical temperature T_c :

$$\pi\rho T_c \sum_{\omega} \frac{1}{|\omega|} = 1,$$

where the summation extends up to some maximum frequency (ω_D in the BSC theory).

To obtain the boundary conditions for the Ginzburg-Landau equation, we must find the asymptotic solution (for $x \gg \xi_0 = v_0 / 2\pi T_c$) of the following integral equation¹³:

$$\eta_i(x_1) = \int_0^{\infty} dx_2 S_i(x_1, x_2) \eta_i(x_2) \quad (10)$$

(no summation over i). By direct substitution, using Eq. (9), we can verify that the linear function

$$\eta_i(x) = \eta_{i,0}(1 + x/b_i)$$

with real b_i (the physical meaning of the fact that b_i are real is that no current flows through the boundary) is the desired asymptotic solution. The effective boundary condition then has the following form:

$$\left. \frac{\partial \eta_i}{\partial x} \right|_{x=0} = \frac{1}{b_i} \eta_i \Big|_{x=0}. \quad (11)$$

The expression for b_i has the form

TABLE I.

A_{1g}	$a(n_x^2 + n_y^2) + bn_z^2$	A_{1u}	$a(\hat{x}n_x + \hat{y}n_y) + b\hat{z}n_z$
A_{2g}	$(n_x^3 - 3n_xn_y^2)(n_y^3 - 3n_yn_x^2)$	A_{2u}	$\hat{z}n_z(n_x^3 - 3n_xn_y^2)(n_y^3 - 3n_yn_x^2)$
B_{1g}	$n_z(n_x^3 - 3n_xn_y^2)$	B_{1u}	$\hat{z}(n_x^3 - 3n_xn_y^2)$
B_{2g}	$n_z(n_y^3 - 3n_yn_x^2)$	B_{2u}	$\hat{z}(n_y^3 - 3n_yn_x^2)$
E_{1g}	n_zn_x, n_zn_y	E_{1u}	$\hat{z}n_x, \hat{z}n_y$
E_{2g}	$2n_xn_y, n_x^2 - n_y^2$	E_{2u}	$\hat{x}n_y + \hat{y}n_x, \hat{x}n_x - \hat{y}n_y$

Note. $n_x = \cos \theta \sin \varphi$, $n_z = \sin \sigma \cos \varphi$; \hat{x}, \hat{y} , and \hat{z} are unit basis vectors in spin space.

$$\begin{aligned}
 \frac{b_i}{\xi_0} &= \frac{1}{7\zeta(3)} \frac{1}{\int_0^1 ds s^2 F^{(-)}(s)} \\
 &\times \left[\frac{\pi^4}{24} \int_0^1 ds s^3 (F^{(-)}(s) + F^{(+)}(s)) \right. \\
 &\left. + \frac{(7\zeta(3) \int_0^1 ds s^2 (F^{(-)}(s) + F^{(+)}(s)))^2}{2\pi^2 \int_0^1 ds s (F^{(-)}(s) - F^{(+)}(s))} \right]. \quad (12)
 \end{aligned}$$

A variational calculation of b_i is performed in the Appendix.

We call attention to two important properties of b_i . For $F^{(-)} = F^{(+)}$ [this occurs when the i th basis function remains unchanged under the reflection $x \rightarrow -x$, i.e., $\psi_i(\mathbf{n}_-) = \psi_i(\mathbf{n}_+)$ or $\mathbf{d}_i(\mathbf{n}_-) = \mathbf{d}_i(\mathbf{n}_+)$], we find that $b_i = \infty$, i.e., $\partial \eta_i / \partial x|_{x=0} = 0$. This important result is not an artifact of the variational (approximate) calculation, but rather it is exact. Indeed, in this case, extending the definition of the order parameter into the “unphysical” region $x < 0$ via $\eta_i(-x) = \eta_i(x)$, we find that the kernel (8) assumes the form of the uniform volume kernel $S^{(0)}$, and the equation (10) in the half-space becomes an equation in all space:

$$\eta_i(x_1) = \int_{-\infty}^{+\infty} dx_2 S_i^{(0)}(x_1 - x_2) \eta_i(x_2),$$

which determines the superconducting transition temperature for an infinite uniform crystal. The even solution of this equation is, by virtue of Eq. (9), simply a constant. Therefore, the boundary condition has the form

$$\frac{\partial \eta_i}{\partial x} \Big|_{x=0} = 0. \quad (13)$$

In the other limiting case, when the i th basis function changes sign upon reflection, we have $F^{(+)} = -F^{(-)}$, and we obtain $b_i = 0$ from Eq. (12). We shall show that this property

is also exact. The order parameter can now be continued into the region $x < 0$, but it is now odd: $\eta_i(-x) = -\eta_i(x)$. Then, Eq. (10) with the kernel (8) once again transforms into a volume equation, whose odd solution is a linear function of x . This gives the following boundary condition:

$$\eta_i|_{x=0} = 0. \quad (14)$$

It should be noted that the conditions (13) and (14) were obtained in Ref. 2 by the method of quasiclassical trajectories, and they are also essentially identical to the boundary conditions found in Ref. 14 for the components of the order parameter in the A phase of superfluid ^3He .

In the general case, if the basis functions do not have a definite parity under reflection in the boundary plane, the integral equation (3) does not reduce to a simple form and, correspondingly, the boundary conditions are different from (13) or (14). In this situation the general formula (12) should be used.

3. CALCULATION OF THE SURFACE-SUPERCONDUCTIVITY FIELD

We now consider the problem of surface superconductivity for nontrivial types of Cooper pairing. We confine our attention to the case of a hexagonal superconductor (UPt₃), i.e., $G_0 = D_{6h}$. The point group D_{6h} has twelve irreducible representations: eight one-dimensional (A_1, A_2, B_1, B_2) and four two-dimensional (E_1, E_2) of different parity.¹⁵ The basis functions of these representations are presented in Table I.³

3.1. One-dimensional representations

We consider first the order parameters corresponding to the one-dimensional representations [see Eq. (1)]. The

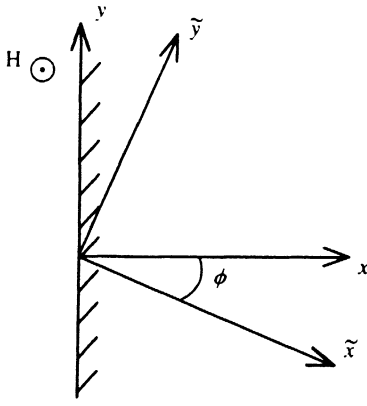


FIG. 1. Relationship between the flat surface of the sample and the principal axes ($\tilde{x}, \tilde{y}, \tilde{z}$) of the crystal lattice.

Ginzburg–Landau functional in an external magnetic field \mathbf{H} has the same form for all one-component order parameters $\eta(\mathbf{r})$:

$$F = a\tau|\eta|^2 + \frac{1}{2}\beta|\eta|^4 + K_1|D_k\eta|^2 + K_4|D_z\eta|^2 + \frac{1}{8\pi}\mathbf{B}^2 - \frac{1}{4\pi}(\mathbf{H}\mathbf{B}), \quad (15)$$

where

$$\tau = \frac{T - T_c}{T_c},$$

$$D_k = -i\nabla_k - \frac{2\pi}{\Phi_0}A_k, \quad k = x, y,$$

$$D_z = -i\nabla_z - \frac{2\pi}{\Phi_0}A_z, \quad \Phi_0 = \frac{hc}{2e},$$

$$\mathbf{B} = \text{curl } \mathbf{A}$$

(the z axis is directed along the six-fold axis). The critical temperature T_c and the coefficients α , β , and $K_{1,4}$ depend on the representation chosen.

The field $H_{c3}(T)$ is defined to be the field in which near the surface the normal state is absolutely unstable. Accordingly, we must solve the linearized Ginzburg–Landau equations in a half-space which follow from Eq. (15). Let the field \mathbf{H} be directed along the six-fold axis and let the normal to the boundary (which is assumed to be flat) lie in the basal plane and make an angle ϕ with the principal axes of the hexagonal lattice (see Fig. 1). Choosing the gauge

$$\mathbf{A} = (0, Hx, 0)$$

and substituting the order parameter in the form

$$\eta(\mathbf{r}) = f(x)\exp(ihx_0y),$$

where $h = 2\pi H/\Phi_0$, we obtain the following Ginzburg–Landau equation:

$$-K_1 \frac{d^2 f}{dx^2} + K_1 h^2 (x - x_0)^2 f + a\tau f = 0,$$

whose solution which decreases as $x \rightarrow +\infty$ has the form

$$f(x) = C \exp\left(-\frac{h}{2}(x - x_0)^2\right) H_\nu(\sqrt{h}(x - x_0)), \quad (16)$$

where $H_\nu(x)$ are Hermite functions^{3,16} with the index

$$\nu = -\frac{1}{2}(1 - \lambda), \quad \lambda = -\frac{a\tau}{K_1 h} = -\frac{a\Phi_0}{2\pi K_1} \frac{\tau}{H}. \quad (17)$$

The boundary condition for the order parameter at $x = 0$ has the form

$$\left. \frac{df}{dx} \right|_{x=0} = \frac{1}{b} f \Big|_{x=0},$$

where the parameter b is given by (12) and, in contrast to the ordinary isotropic superconductivity, can be strongly dependent on the angle ϕ in the case of anisotropic pairing. We find these dependences below. First, however, we make several general remarks.

Substituting the solution of the equations into the boundary condition, we obtain an equation for the parameter $\lambda = \lambda(r, h)$ (for convenience we set $r = \sqrt{hx_0}$):

$$2\nu \frac{H_{\nu-1}(-r)}{H_\nu(-r)} = -\left(r - \frac{1}{\sqrt{hb}}\right). \quad (18)$$

The derivation employs the property of the Hermite functions

$$H'_\nu(x) = 2\nu H_{\nu-1}(x).$$

The surface-superconductivity field is obtained from the solution of Eq. (18) by minimizing λ with respect to r , after which $\tau(h)$ is calculated from Eq. (17). For arbitrary values of b , the transcendental equation (18) cannot be solved analytically, but the problem can be simplified in two limiting cases.

In the limit $b \rightarrow \infty$ [in the theory of ordinary superconductivity a boundary condition of this type is used to study the superconductor–vacuum (dielectric) boundary], we obtain an equation for $\lambda(r)$ that does not depend explicitly on h . Solving the equation numerically gives $\lambda_{\min} = 0.59$ and $r = 0.77$, i.e., from Eq. (17)

$$H_{c3}^{(0)}(T) = 1.69 H_{c2}(T) = 1.69 \frac{a\Phi_0}{2\pi K_1} (-\tau)$$

see Ref. 17.

For $b = 0$ we have $f(0) = 0$. Therefore, $\nu = 0$ ($r = \infty$), i.e., in this case the surface-superconductivity field is identical to the volume critical field H_{c2} .

For arbitrary $0 < b < \infty$, we expect that a superconducting state will arise near the surface in a field between $H_{c2}(T)$ and $H_{c3}^{(0)}(T)$; in addition, the surface-superconductivity field is no longer a linear function of the temperature because the right-hand side of Eq. (18), and therefore also λ , depend explicitly on h . It is easy to determine the asymptotic behavior of H_{c3} for weak and strong fields. As $h \rightarrow 0$, the second term on the right-hand side of Eq. (18) dominates, and we return effectively to the situation $b = 0$, i.e., in weak fields $H_{c3} = H_{c2}$. In strong fields, the first term remains on the right-hand side of Eq. (18) and the picture is similar to the

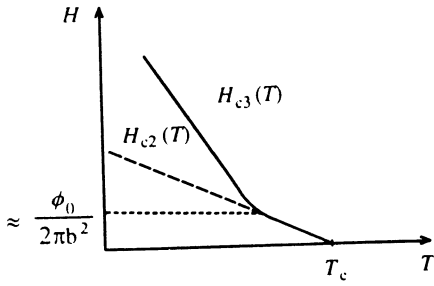


FIG. 2. Critical field of surface superconductivity as a function of temperature for boundary conditions of the general form $df(0)/dx=(1/b)f(0)$.

case $b \rightarrow \infty$, i.e., here the H_{c3} line is parallel here to the $H_{c3}^{(0)}$ line. A transition from one asymptotic behavior to another occurs in fields $h \propto b^{-2}$ (the section with negative curvature). The qualitative dependence of the surface-superconductivity field is displayed in Fig. 2 (see also Ref. 18). It should be kept in mind, however, that the theory presented here is valid only in the Ginzburg–Landau region, i.e., in sufficiently weak fields, and for this reason a dependence similar to that shown in Fig. 2 can be observed only for $b \gg \xi_0$.

Using Eq. (12), we shall now find the angular dependences of the parameter b for different one-dimensional representations.

A_{1g} . For the unit representation A_{1g} we can set, without loss of generality, $a = b = 1$ (see Table I), i.e., the basis function $\psi = 0$, and from Eq. (12) we obtain $b = \infty$. Therefore, the boundary condition for the Ginzburg–Landau equations is identical to Eq. (13); this leads to the ordinary isotropic surface superconductivity.

A_{1u} . In this case we obtain (setting, once again, $a = b = 1$)

$$f^{(+)}(s) = F^{(+)}(s) = 1 - 2s^2, \quad f^{(-)}(s) = F^{(-)}(s) = 1$$

and

$$b = 0.42 \xi_0.$$

Since the parameter b is of the order of ξ_0 , i.e., it is much less than the correlation length in the Ginzburg–Landau region, we can set $b = 0$ and therefore $H_{c3}(T) = H_{c2}(T)$.

A_{2g} . The basis function in the principal axes has the form (c is a normalization factor; see Table I):

$$\tilde{\psi}(\mathbf{n}) = c(n_x^3 - 3n_x n_y^2)(n_y^3 - 3n_y n_x^2).$$

To calculate the functions $f^{(\pm)}$ from (7) appearing in the kernel (5), the basis function must be rewritten in the coordinates (x, y, z) associated with the surface (Fig. 1). It is convenient to switch to the complex coordinates $\xi_{\pm} = n_x \pm i n_y$. Then

$$\tilde{\psi} = \frac{1}{4} i c (\tilde{\xi}_+^3 + \tilde{\xi}_-^3)(\tilde{\xi}_+^3 - \tilde{\xi}_-^3).$$

Since the complex coordinates ξ_{\pm} transform as follows accompanying a transformation from $(\tilde{x}, \tilde{y}, \tilde{z})$ to (x, y, z)

$$\tilde{\xi}_{\pm} = \exp(\mp i \phi) \xi_{\pm},$$

we have

$$\begin{aligned} \psi(\mathbf{n}_+) &= \frac{ic}{4} (\tilde{\xi}_+^6 - \tilde{\xi}_-^6) = \frac{ic}{4} (\cos 6\phi (\xi_+^6 - \xi_-^6) \\ &\quad - i \sin 6\phi (\xi_+^6 + \xi_-^6)). \end{aligned}$$

In the case of a reflection in the plane of the boundary $\xi_+ \leftrightarrow -\xi_-$, and therefore

$$\psi(\mathbf{n}_-) = \frac{ic}{4} (-\cos 6\phi (\xi_+^6 - \xi_-^6) - i \sin 6\phi (\xi_+^6 + \xi_-^6)).$$

Substituting the expressions found above into Eq. (7a), we obtain

$$f^{(\pm)} = \frac{c^2}{16} (\mp \cos^2 6\phi |\xi_+^6 - \xi_-^6|^2 + \sin^2 6\phi |\xi_+^6 + \xi_-^6|^2).$$

The algorithm for subsequent operations is obvious: the expressions for n_x and n_y must be substituted into the last formula, the integration over ϕ must be performed, the normalization factors must be taken into account, and the expressions obtained for $F^{(\pm)}(s)$ (in this case polynomials of degree 12 in s) must be substituted into Eq. (12). Carrying out these rather lengthy calculations, we obtain the final result presented in Table II.

We can see that the boundary condition on the order parameter is strongly anisotropic. Therefore, the field H_{c3} will also have an anisotropy of order 12, specifically, we have $b = 0$ for $\phi = 0, 2\pi/12, \dots$, i.e., H_{c3} takes on its minimum value, equal to H_{c2} . For $\phi = 2\pi/24, 2\pi/8, \dots$ we have $b = \infty$, and H_{c3} takes on its maximum value, equal to $H_{c3}^{(0)}$. For intermediate angles a nonlinear temperature dependence $H_{c3}(T)$ should be observed (see Fig. 2).

The remaining one-dimensional representations can be studied similarly. The corresponding values of $b(\phi)/\xi_0$ are summarized in Table II. We emphasize that although the expressions obtained are approximate (they are of an interpolatory character), they reflect correctly the important features of the functions $b(\phi)$. The final result is that for the order parameter transforming according to A_2 , the field H_{c3} has an anisotropy of order 12, and in the case of B_1 and B_2 the anisotropy is of order 6.

To avoid misunderstanding, it should be noted that by anisotropy of the surface superconductivity we mean here the anisotropy of the slope of the $H_{c3}(T)$ line for a fixed direction of the external field—along the z axis—and different directions of the normal to the surface in the basal plane.

Another consequence of the anisotropy of the boundary conditions, which is more suitable from the standpoint of performing an experiment, is the appearance of lines of zeros of the order parameter on the surface of cylindrical samples oriented along the hexagonal axis [the order parameter vanishes at locations where $b(\phi) = 0$]. It is qualitatively clear that this in turn results in a corresponding “real” anisotropy of the surface critical field in the basal plane.

3.2. Two-dimensional representations

For a two-component order parameter, the Ginzburg–Landau functional, up to quadratic terms, has the form

TABLE II.

A_{1g}	$b = \infty$	A_{1u}	$b = 0.42\xi_0$
A_{2g}	$\sin^2 6\phi(0.80 + 0.65 \operatorname{tg}^2 6\phi)$	A_{2u}	$\sin^2 6\phi(0.75 + 0.61 \operatorname{tg}^2 6\phi)$
B_{1g}	$\sin^2 3\phi(0.72 + 0.56 \operatorname{tg}^2 3\phi)$	B_{1u}	$\sin^2 3\phi(0.79 + 0.62 \operatorname{tg}^2 3\phi)$
B_{2g}	$\cos^2 3\phi(0.72 + 0.56 \operatorname{ctg}^2 3\phi)$	B_{2u}	$\cos^2 3\phi(0.79 + 0.62 \operatorname{ctg}^2 3\phi)$
E_{1g}	$b_1 = 0, b_2 = \infty$	E_{1u}	$b_1 = 0, b_2 = \infty$
E_{2g}	$b_1 = 0, b_2 = \infty$	E_{2u}	$b_1 = b_2 = 0.21\xi_0$

$$\begin{aligned}
 F = & a\tau(|\eta_1|^2 + |\eta_2|^2) + K_1(D_x \eta_j)^*(D_x \eta_j) \\
 & + K_2(D_x \eta_i)^*(D_x \eta_j) + K_3(D_x \eta_j)^*(D_x \eta_i) \\
 & + K_4(D_z \eta_i)^*(D_z \eta_i). \quad (19)
 \end{aligned}$$

We require that the coefficients of the gradient terms satisfy the following boundary conditions¹⁹:

$$K_1 > |K_3|, \quad K_{123} > |K_2|, \quad K_4 > 0, \quad (20)$$

where $K_{123} = K_1 + K_2 + K_3$. These conditions follow from the requirement that the gradient part of Eq. (19) be positive definite.

The corresponding linearized equations (the order parameter does not depend on z) have the form

$$\begin{cases}
 (K_{123} \hat{D}_x^2 + K_1 \hat{D}_y^2) \eta_1 + (K_2 \hat{D}_x \hat{D}_y + K_3 \hat{D}_y \hat{D}_x) \eta_2 + a\tau \eta_1 = 0, \\
 (K_{123} \hat{D}_y^2 + K_1 \hat{D}_x^2) \eta_2 + (K_3 \hat{D}_x \hat{D}_y + K_2 \hat{D}_y \hat{D}_x) \eta_1 + a\tau \eta_2 = 0.
 \end{cases}$$

We now introduce, following Zhitomirskii,¹⁹ the new functions $\eta_{\pm} = \eta_1 \pm i \eta_2$ and the operators $\hat{D}_{\pm} = \hat{D}_x \mp i \hat{D}_y$, and we also use the fact that

$$[\hat{D}_x, \hat{D}_y] = ih \quad (h = 2\pi H / \Phi_0).$$

Then, the equations assume the form

$$\begin{cases}
 (a\tau + K_0(\hat{D}_x^2 + \hat{D}_y^2) + K_- h) \eta_+ + K_+ \hat{D}_-^2 \eta_- = 0, \\
 K_+ \hat{D}_+^2 \eta_+ + (a\tau + K_0(\hat{D}_x^2 + \hat{D}_y^2) - K_- h) \eta_- = 0,
 \end{cases} \quad (21)$$

where

$$K_0 = (K_{123} + K_1)/2, \quad K_{\pm} = (K_2 \pm K_3)/2.$$

In Ref. 19 these equations were used to find the upper critical field H_{c2} in an infinite volume. In this case the solution must decay as $x \rightarrow -\infty$. The solution of Eq. (21) can then be expressed in terms of Hermite polynomials. In our case, however, we do not fix the behavior of the solution at $-\infty$ and, correspondingly, we do not require positive definiteness or that the indices of the Hermite polynomials be integers. The Hermite polynomials thus become Hermite functions H_{ν} .¹⁶

We now seek the order parameter in the form

$$\eta_{\pm} = \exp(ihx_0 y) f_{\pm}(x).$$

The particular solution of Eq. (21) has the form

$$\begin{pmatrix} f_+(x) \\ f_-(x) \end{pmatrix} = C \begin{pmatrix} F_{\nu}(x-x_0) \\ qF_{\nu+2}(x-x_0) \end{pmatrix}, \quad (22)$$

where

$$F_{\nu}(x) = \exp\left(-\frac{h}{2} x^2\right) H_{\nu}(\sqrt{hx}).$$

The fact that Eq. (21) is indeed satisfied can be verified by using the following identities (see Ref. 16):

$$\begin{aligned}
 \hat{D}_-^2 F_{\nu} &= -4\nu(\nu-1)hF_{\nu-2}, \\
 \hat{D}_+^2 F_{\nu} &= -hF_{\nu+2}, \\
 (\hat{D}_x^2 + \hat{D}_y^2) F_{\nu} &= (2\nu+1)hF_{\nu}.
 \end{aligned}$$

Substituting Eq. (22) into Eq. (21) gives the following relation between τ , h , and ν :

$$\begin{aligned}
 \tau = & -(2\nu+3)K_0 \\
 & + \sqrt{(2K_0 - K_-)^2 + 4(\nu+1)(\nu+2)K_+^2} \frac{h}{a}. \quad (23)
 \end{aligned}$$

Then the order parameter q is given by

$$\begin{aligned}
 q(\nu) &= \\
 &= \frac{-(2K_0 - K_-) + \sqrt{(2K_0 - K_-)^2 + 4(\nu+1)(\nu+2)K_+^2}}{4(\nu+1)(\nu+2)K_+}.
 \end{aligned}$$

In contrast to the one-component case [see Eq. (17)], the expression (23) does not permit finding ν as a unique function of τ and h . Since it is quadratic in ν , this equation can have two roots with a fixed dimensionless ratio $\lambda = -a\tau/K_1 h$:

$$\nu_{1,2} = -\frac{3}{2} + \frac{\lambda K_0 K_1 \pm \sqrt{D}}{2(K_0^2 - K_+^2)}, \quad (24)$$

where

$$D = 4K_0^4 + K_+^4 - 5K_0^2 K_+^2 - K_- (K_0^2 - K_+^2)(4K_0 - K_-) + \lambda^2 K_+^2 K_1^2.$$

The corresponding values of $q_{1,2}(\lambda)$ are

$$q_{1,2} = \frac{K_+ (K_0^2 - K_+^2)}{(2K_0 - K_-)(K_0^2 - K_+^2) + \lambda K_1 K_+^2 \pm \sqrt{D} K_0}. \quad (25)$$

We assume below that the discriminant is positive, and $\nu_{1,2}$ and $q_{1,2}$ are real. Ignoring this requirement, by the way, does not introduce any fundamental difficulties, since the Hermite functions can be analytically continued to complex values of the index.¹⁶ We note that if $K_2 = K_3$,⁴⁾ it can be shown, taking Eq. (20) into account, that $D > 0$.

The eigenvalue is found to be doubly degenerate, and accordingly the general solution of Eq. (21) has the form

$$\begin{pmatrix} f_+(x) \\ f_-(x) \end{pmatrix} \sim \begin{pmatrix} F_{\nu_1}(x-x_0) \\ q_1 F_{\nu_1+2}(x-x_0) \end{pmatrix} + p \begin{pmatrix} F_{\nu_2}(x-x_0) \\ q_2 F_{\nu_2+2}(x-x_0) \end{pmatrix}, \quad (26)$$

where p is a free parameter, which we choose, without loss of generality, to be real. Substituting Eq. (26) into the boundary conditions yields a system of two transcendental equations for $\lambda(h, x_0, p)$. Minimizing λ with respect to the parameters x_0 and p makes it possible, in principle, to find the temperature dependence of the surface-superconductivity field $H_{c3}(T)$.

What are the boundary conditions on the components of the order parameter? In the case of two-dimensional representations of the hexagonal group, the second-order terms in the Ginzburg-Landau functional—both the uniform and gradient terms—have the continuous symmetry $D_{\infty h}$ in the basal plane (if the magnetic field is oriented along the z -axis). This allows us to choose the basis functions in the most convenient manner—specifically, so that the kernel (5) is diagonal and independent of ϕ , and so that we have independent integral equations for each component η_i .

E_1 . The basal functions of the representation E_{1g} are such that under the substitution $n_x \rightarrow -n_x$, $\psi_1 \sim n_z n_x$ changes sign and $\psi_2 \sim n_z n_y$ does not. Therefore, $F_1^{(-)}(s) = -F_1^{(+)}(s)$ and $F_2^{(-)}(s) = F_2^{(+)}(s)$, i.e., the boundary conditions have the form

$$\eta_1|_{x=0} = 0, \quad \left. \frac{\partial \eta_2}{\partial x} \right|_{x=0} = 0. \quad (27)$$

We stress that these expressions are isotropic in the basal plane.

Similarly, it is easy to see that for the representations E_{1u} , the boundary conditions are identical to (27), because in this case too, one basis function changes sign on reflection in the boundary plane and the other does not (see Table I).

Substituting Eq. (26) into Eq. (27) gives equations for $\lambda(h, x_0, p)$ from which, using the property

$$H_{\nu+1}(x) = 2xH_{\nu}(x) - 2\nu H_{\nu-1}(x)$$

of the Hermite functions and eliminating p , we obtain an equation for $\lambda(h, r)$ (once again, we set $r = \sqrt{h}x_0$):

$$g_1(r, \lambda) + g_2(r, \lambda) \frac{H_{\nu_1-1}(-r)}{H_{\nu_1}(-r)} + g_3(r, \lambda) \frac{H_{\nu_2-1}(-r)}{H_{\nu_2}(-r)} + g_4(r, \lambda) \frac{H_{\nu_1-1}(-r)H_{\nu_2-1}(-r)}{H_{\nu_1}(-r)H_{\nu_2}(-r)} = 0, \quad (28)$$

where

$$\begin{aligned} g_1 &= 4r((q_1 - q_2)(2r^2 - 3) - 2(q_1\nu_1 - q_2\nu_2) - 2q_1q_2(\nu_1 - \nu_2)(1 + 2r^2)), \\ g_2 &= -2\nu_1(1 - 4(q_1 - q_2)r^2 + 2(q_1\nu_1 - q_2\nu_2) + 4q_1 - 2q_2 - 4q_1q_2(2 + \nu_1 + 2\nu_2 + \nu_1\nu_2 - 2(\nu_1 - \nu_2)r^2)), \\ g_3 &= 2\nu_2(1 + 4(q_1 - q_2)r^2 - 2(q_1\nu_1 - q_2\nu_2) - 2q_1 + 4q_2 - 4q_1q_2(2 + 2\nu_1 + \nu_2 + \nu_1\nu_2 + 2(\nu_1 - \nu_2)r^2)), \\ g_4 &= 8\nu_1\nu_2r((q_1 - q_2) - 2q_1q_2(\nu_1 - \nu_2)). \end{aligned}$$

In these expressions $q_{1,2}$ and $\nu_{1,2}$ are related to λ by Eqs. (24) and (25).

An important property of Eq. (28) is that this equation does not contain an explicit dependence on h , i.e., $\lambda = \lambda(r)$, and therefore the function $H_{c3}(T)$, corresponding to λ_{\min} —the minimum solution of Eq. (28) with respect to r —is linear, but the coefficient cannot be determined analytically.

A numerical calculation for $K_1 = K_2 = K_3$ yields $\lambda_{\min} = 0.89$ and $r = 0.55$, i.e., $H_{c3}/H_{c2} = 1.24$.

E_2 . The situation in this case is different for the representations E_{2g} and E_{2u} .

The basis functions of E_{2g} (see Table I) behave oppositely under the reflection $n_x \rightarrow -n_x$, and therefore the boundary conditions have the form (27), and the equation for $H_{c3}(T)$ is identical to Eq. (28). For $K_2 = K_3 = 0$ (see footnote 4) the equations for η_1 and η_2 decouple, and therefore the components of the order parameter can be studied independently and similarly to the one-dimensional case (see Sec. 3.1). For η_1 we have $H_{c3}(T) = H_{c2}(T)$, and for η_2 we have $H_{c3}(T) = 1.69H_{c2}(T)$, i.e., for $H_{c2} < H < H_{c3}$ a phase of the type (0,1) appears.

We now substitute the basis functions of the representation of E_{2u} from Table I into Eq. (7b). These functions obviously do not have definite parity under reflection, and we obtain

$$F_{1,2}^{(-)}(s) = \frac{3}{4}(1 + s^2),$$

$$F_{1,2}^{(+)}(s) = \frac{3}{4}(1 - 3s^2).$$

The boundary conditions are identical for the two components of the order parameter and have the form

$$\left. \frac{\partial \eta_{1,2}}{\partial x} \right|_{x=0} = \frac{1}{b} \eta_{1,2} \Big|_{x=0},$$

where the parameter b , which is independent of direction in the basal plane, is presented in Table II.

Since b is small ($b < \xi_0$), we can employ the following boundary conditions for the Ginzburg–Landau equations:

$$\eta_1|_{x=0} = \eta_2|_{x=0} = 0. \quad (29)$$

Substituting Eq. (26) into Eq. (29), we arrive at an equation similar to Eq. (28), where the functions $g_i(r, \lambda)$ assume the form

$$g_1 = (4r^2 - 2)(q_1 - q_2) - 2(q_1\nu_1 - q_2\nu_2),$$

$$g_2 = 4q_1\nu_1r,$$

$$g_3 = -4q_2\nu_2r,$$

$$g_4 = 0.$$

In the special case $K_2 = K_3 = 0$ (see footnote 4), the components of the order parameter become independent, and we verify that $H_{c3}(T) = H_{c2}(T)$ by substituting into the boundary conditions (29). In the general case, the slope of the H_{c3} line can be determined numerically.

4. CONCLUSIONS

In summary, measurements of the surface-superconductivity field $H_{c3}(T)$ make it possible in principle to identify the superconducting phases in UPT_3 . Even in the case of the simplest geometry investigated in the present paper, specifically, when the field is oriented parallel to a smooth superconductor–dielectric boundary passing through a six-fold axis, observation of the anisotropy of the slope of the $H_{c3}(T)$ line as a function of the angle between the normal to the surface and the principal axes of the crystal lattice would make it possible to narrow substantially the range of models which purport to explain the experimental phase diagram (see introduction).

The isotropic linear dependence $H_{c3}(T) = 1.69H_{c2}(T)$ means that we are dealing with the unit representation A_{1g} . The absence of surface superconductivity, i.e., the fact that the lines of H_{c3} and H_{c2} coincide, points toward the representation A_{2u} . Different values of the ratios of the slopes of the straight lines $H_{c3}(T)$ and $H_{c2}(T)$ may correspond to the two-dimensional representations E_1 or E_2 .

The anisotropy of the $H_{c3}(T)$ line indicates the existence of a one-component (nontrivial) order parameter, corresponding to B_1 or B_2 in the case of anisotropy of order six and A_2 in the case of anisotropy of order 12.

It is clear that the types of behavior of H_{c3} listed above also remain, at least qualitatively, in a different geometry of the problem, corresponding better to experiment, specifically, when the field rotates in the basal plane. In the present case, however, the anisotropy of H_{c3} can arise because of effects associated with the shape of the sample (existence of flat boundaries), as a result of the “beak-shape” dependence, known from the theory of ordinary superconductivity, of H_{c3} on the angle between the direction of the field and the plane of the boundary. It is periodic dependences of this type that were recently observed in whiskers.¹¹ Therefore, to eliminate

such effects as much as possible, H_{c3} should be measured on samples of different shape, specifically, cylindrical samples. The observation of surface superconductivity anisotropy in this case would be a strong argument for one or another one-dimensional representation.

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APPENDIX

We employ the variational method proposed in Ref. 20 to calculate the coefficient b_i in the linear asymptotic form of the order parameter.

We transform in Eq. (8) to the dimensionless variable $X = x/\xi_0$. Then

$$S_i(X_1, X_2) = \frac{1}{2} \rho \sum_n \int_0^1 \frac{ds}{s} \left(F_i^{(-)}(s) \times \exp\left(-\frac{|2n+1|}{s} \left| X_1 - X_2 \right| \right) + F_i^{(+)}(s) \exp\left(-\frac{|2n+1|}{s} \left| X_1 + X_2 \right| \right) \right).$$

Since $\eta(X)$ is asymptotically ($X \gg 1$) linear, we seek a solution in the form (dropping the subscript i)

$$\eta(X) = C(X + q(X)),$$

and

$$b/\xi_0 = \lim_{X \rightarrow \infty} q(X).$$

The equation for $q(X)$ has the form

$$q(X_1) = \frac{1}{2} E(X_1) + \int_0^\infty dX_2 S(X_1, X_2) q(X_2), \quad (A1)$$

$$E(X_1) = \rho \sum_n \frac{1}{(2n+1)^2} \int_0^1 ds s (F^{(-)}(s) + F^{(+)}(s)) \exp\left(-\frac{|2n+1|}{s} X_1\right).$$

To formulate the variational principle, we note that the integral equation (A1) is derived by varying the functional

$$\delta\Phi/\delta q(X_1) = 0,$$

where

$$\Phi[q] = \frac{\int_0^\infty dX q(X) (q(X) - \int_0^\infty dX' S(X, X') q(X'))}{[\int_0^\infty dX q(X) E(X)]^2}. \quad (A2)$$

Then, the extremum (minimum) of the functional is

$$\Phi_{\min} = \frac{1}{2 \int_0^\infty dX E(X) q(X)}.$$

We now show that the required limiting value, of the solution of Eq. (A1) as $X \rightarrow \infty$ can be expressed directly in terms of Φ_{\min} . Let

$$q(X) = b/\xi_0 + Q(X),$$

where $Q(X) \rightarrow 0$ as $X \rightarrow \infty$. Substituting into Eq. (A1), we obtain an equation for $Q(X)$. Next, multiplying both sides of this equation by X_1 and integrating over X_1 from 0 to ∞ , we obtain finally

$$\frac{b}{\xi_0} = \frac{1}{7\zeta(3)} \frac{1}{\int_0^1 ds s^2 F^{(-)}(s)} \left\{ \frac{\pi^4}{24} \int_0^1 ds s^3 (F^{(-)}(s) + F^{(+)}(s)) + \frac{1}{\rho \Phi_{\min}} \right\}.$$

The quantity Φ_{\min} can be calculated by the variational principle. Choosing a constant as the trial function and substituting it into Eq. (A2), we arrive at Eq. (12) (see Ref. 20 for a discussion of how to improve computational accuracy).

¹⁾As indicated in the Introduction, here we are considering the single (a)th representation with the maximum transition temperature, thereby neglecting effects associated with the possible coexistence of different symmetry in a system of two order parameters, which gives rise to splitting of the superconducting transition.

²⁾The Green's function is proportional to the unit matrix, in spite of the strong spin-orbit interaction.

³⁾The functions $f(x)$ can also be expressed directly in terms of Weber functions (parabolic cylinder functions).

⁴⁾In the weak-coupling theory, assuming exact electron-hole symmetry, we have $K_1 = K_2 = K_3$ for the representation E_1 and $K_2 = K_3 = 0$ for the representation E_2 .⁶

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