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Anisotropic criteria for the type of superconductivity

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The classical criterion for classification of superconductors as type-I or type-II based on the isotropic Ginzburg-Landau theory is generalized to arbitrary temperatures for materials with anisotropic Fermi surfaces and order parameters. We argue that the relevant quantity for this classification is the ratio of the upper and thermodynamic critical fields, H_{c2}/H_c , rather than the traditional ratio of the penetration depth and the coherence length, λ/ξ . Even in the isotropic case, H_{c2}/H_c coincides with $\sqrt{2}\lambda/\xi$ only at the critical temperature T_c and they differ as T decreases, the long known fact. Anisotropies of Fermi surfaces and order parameters may amplify this difference and render false the criterion based on the value of $\kappa = \lambda/\xi$.

I. INTRODUCTION

The classification of superconductors as type-I and type-II introduced within the Ginzburg-Landau (GL) theory near T_c is based on the value of the GL parameter $\kappa = \lambda/\xi$ (λ is the weak field penetration depth and ξ is the coherence length).^{1,2} An isotropic bulk material is of the type-II if $\kappa > 1/\sqrt{2}$; in fields $H > H_{c1} \approx (\phi_0/4\pi\lambda^2)(\ln \kappa + 0.5)$ vortices are nucleated.³ The lower critical field H_{c1} is related to the line energy ε_l of a single vortex which is found by solving the GL equations for the order parameter and supercurrents: $H_{c1} = \phi_0\varepsilon_l/8\pi$. The mixed phase with vortices exists in fields up to $H_{c2} = \phi_0/2\pi\xi^2$ such that $H_{c1} < H_c < H_{c2}$, where the thermodynamic critical field is related to the condensation energy density $F = H_c^2/8\pi$. In the GL domain $H_c = \phi_0/2\sqrt{2}\pi\xi\lambda$. If $\kappa < 1/\sqrt{2}$, the bulk material is in the Meissner state in fields $H < H_c$ and is classified as type-I.

The question of this classification for low temperatures in isotropic materials was addressed by Eilenberger who evaluated the upper critical field H_{c2} along with H_c to show that $\kappa_1 = H_{c2}(T)/\sqrt{2}H_c(T)$ increases on cooling to $T = 0$ by about 30%.⁴ Hence, taking κ as governing material behavior in magnetic field, one concludes that if $\kappa > 1/\sqrt{2}$ at T_c , it certainly exceeds this value at all temperatures and, therefore, the GL classification should hold at any T . It is worth noting that this classification holds for Fermi spheres and constant order parameters (s-wave).

When anisotropic materials came forth, it was realized that a mere fact of anisotropy may cause λ/ξ to change with the field orientation. It became clear that in principle an anisotropic material can be type-I for one field orientation and type-II for another.⁵ This prediction had been confirmed in experiments with intercalated crystals of C_xK .^{6,7} Later, similar ideas were explored in Ref. 8

The situation is even more complicated with multi-band materials and with other than s-wave order parameters for which the temperature and angular behavior of H_{c2} (along with ξ) differs from that of λ , while both these quantities depend on the Fermi surface and on the order parameter anisotropy.

The general formalism for calculating H_{c2} and λ in

the clean case has recently been developed for arbitrary Fermi surfaces and order parameters.⁹⁻¹¹ We argue that minute details of the Fermi surfaces are usually of little effect on H_{c2} and λ because the equations governing these quantities contain only integrals over the whole Fermi surfaces. Therefore, one can consider the simplest Fermi shapes of spheroids (for tetragonal materials) for which the Fermi surface averaging is a well defined procedure. Hence, $\kappa(T)$ is now accessible for various anisotropies of Fermi surfaces and order parameters.

However, for anisotropic materials at arbitrary temperatures, the GL criterion based on the value of $\kappa = \lambda/\xi$ is questionable because the GL theory *per se* only works near T_c . We use in this text a different approach based on the fact that in type-II superconductors the two characteristic fields, H_{c1} at which vortices nucleate in the bulk material, and H_{c2} , the maximum field at which the mixed state exists, satisfy $H_{c1} < H_c < H_{c2}$. Either part of this inequality, $H_{c1} < H_c$ or $H_c < H_{c2}$ (or for this matter $H_{c1} < H_{c2}$), can be used to classify the material behavior as that of type-II. However, to have $H_{c1}(T)$ one should evaluate the vortex line energy within the microscopic theory, a difficult problem if at all doable. On the other hand, both $H_{c2}(T)$ and $H_c(T)$ can be evaluated for anisotropic Fermi surfaces and order parameters at any temperature. It is the criterion $H_c(T) < H_{c2}(T)$ that we study in this work.

Below we calculate the condensation energy for anisotropic situation at arbitrary temperatures. Then we review methods for evaluation of H_{c2} and λ and present numerical results to show that the criterion based on the ratio H_{c2}/H_c differs substantially from that employing λ/ξ .

II. CONDENSATION ENERGY

Perhaps, the simplest formally for our purpose is the approach based on the Eilenberger quasiclassical formalism that holds for a general anisotropic Fermi surface and for any gap symmetry.¹² The theory deals with two functions, f and g , which are integrated over the energy Gor'kov Green's functions. For a uniform state of clean

superconductors of interest here f, g satisfy:

$$\Delta g - \hbar\omega f = 0, \quad g^2 + f^2 = 1. \quad (1)$$

Here, $\hbar\omega = \pi T(2n+1)$ with an integer n . We employ the approximation of a separable coupling responsible for superconductivity: $V(\mathbf{k}, \mathbf{k}') = V_0 \Omega(\mathbf{k}) \Omega(\mathbf{k}')$, \mathbf{k} is the Fermi momentum.¹³ In this approximation the order parameter $\Delta(T, \mathbf{k}) = \Psi(T) \Omega(\mathbf{k})$. $\Omega(\mathbf{k})$ determines the \mathbf{k} dependence of Δ and is normalized so that the average over the Fermi surface $\langle \Omega^2 \rangle = 1$. Equations (1) give:

$$f = \Delta/\beta, \quad g = \omega/\beta, \quad \beta^2 = \Delta^2 + \omega^2. \quad (2)$$

The order parameter should satisfy the self-consistency equation of the theory, see, e.g., Ref. 9:

$$\frac{\Psi}{2\pi T} \ln \frac{T_c}{T} = \sum_{\omega>0} \left(\frac{\Psi}{\hbar\omega} - \langle \Omega f \rangle \right), \quad (3)$$

where $\langle \dots \rangle$ stands for averaging over the Fermi surface.

Equations (1) and (3) can be obtained as minimum conditions for the energy functional:¹²

$$\frac{\mathcal{F}}{N(0)} = \Psi^2 \ln \frac{T_c}{T} + 2\pi T \sum_{\omega>0} \left[\frac{\Psi^2}{\hbar\omega} - 2 \langle \Delta f + \hbar\omega(g-1) \rangle \right] \quad (4)$$

where $g = \sqrt{1-f^2}$ and $N(0)$ is the density of states per spin on the Fermi level. Substituting here the solutions (2) and taking into account the self-consistency relation (3) one obtains the condensation energy density F :

$$\frac{F}{2\pi T N(0)} = \left\langle \sum_{\omega>0} \frac{(\beta - \hbar\omega)^2}{\beta} \right\rangle. \quad (5)$$

At $T = 0$ (replace $2\pi T \sum_{\omega} \rightarrow \int_0^\infty \hbar d\omega$),

$$F(0) = \frac{N(0)}{2} \langle \Delta^2(0) \rangle = \frac{N(0)}{2} \Psi^2(0) \quad (6)$$

(recall the isotropic result $F(0) = N(0)\Delta^2(0)/2$). To find the value of $\Psi(0)$ one considers the first sum in Eq. (3) as extended to $n_{\max} = \hbar\omega_D/2\pi T$, while the second is replaced with $\int_0^{\hbar\omega_D} d(\hbar\omega)/2\pi T$ (ω_D is the Debye frequency for the phonon mechanism or a proper cutoff for others):

$$\ln \frac{T_c}{T} = \ln \frac{2e^C \hbar\omega_D}{\pi T} - \left\langle \Omega^2 \ln \frac{2\hbar\omega_D}{\Psi|\Omega|} \right\rangle, \quad (7)$$

where $C \approx 0.577$ is the Euler constant. This gives:

$$\Psi(0) = \frac{\pi T_c}{e^C} e^{-\langle \Omega^2 \ln |\Omega| \rangle}. \quad (8)$$

Hence, we have $H_c(0) = 2\sqrt{\pi N(0)} \Psi(0)$.

Near T_c , Eq. (3) yields

$$\Psi^2 = \frac{8\pi^2 T_c^2 (1-t)}{7\zeta(3) \langle \Omega^4 \rangle}, \quad (9)$$

where $t = T/T_c$. The condensation energy is readily found:

$$F = \frac{7\zeta(3)N(0)\langle \Omega^4 \rangle \Psi^4}{16\pi^2 T_c^2} = \frac{4\pi^2 T_c^2 N(0)}{7\zeta(3) \langle \Omega^4 \rangle} (1-t)^2. \quad (10)$$

Given $F(T)$, it is straightforward to obtain the difference of specific heats $C_s - C_n$ at any T and in particular the specific heat jump at T_c .^{14,15}

$$\frac{\Delta C}{C_n} = \frac{12}{7\zeta(3) \langle \Omega^4 \rangle} = \frac{1.43}{\langle \Omega^4 \rangle}. \quad (11)$$

Near T_c , we have

$$H_c = 8\pi T_c \sqrt{\frac{\pi N(0)}{14\zeta(3) \langle \Omega^4 \rangle}} (1-t). \quad (12)$$

For the numerical work at arbitrary temperatures, we rewrite the energy as

$$F = 4\pi^2 T_c^2 N(0) t^2 S, \quad S = \sum_{n=0}^{\infty} \left\langle \frac{\left[\sqrt{(n+1/2)^2 + \psi^2 \Omega^2} - (n+1/2) \right]^2}{\sqrt{(n+1/2)^2 + \psi^2 \Omega^2}} \right\rangle \quad (13)$$

where $\psi = \Psi/2\pi T$. Thus, the general scheme of evaluation of the thermodynamic critical field consists of solving the self-consistency equation (3) for $\Psi(T)$ at each T and then evaluating F of Eq. (13) and $H_c = \sqrt{8\pi F}$.

As mentioned in Introduction, describing Fermi surface shapes within problems of H_c and H_{c2} , one can consider Fermi ellipsoids, for which the averaging is a well defined analytic procedure.^{11,16} Although straightforward, this procedure is quite involved, a brief description is given in Appendix A.

Hence we characterize Fermi surfaces for tetragonal materials by a single parameter ϵ , the squared ratio of the spheroid semi-axes. We consider only representative order parameters: s-wave ($\Omega = 1$), d-wave ($\Omega = \sqrt{2} \cos 2\varphi$ with φ being the azimuth of spherical coordinates with the polar axis along the c crystal direction, and order parameters of the form $\Omega = \Omega_0 \cos^n \theta$ with the polar angle θ . The latter were recently suggested as possibilities for at least some of the Fe-based materials;^{17,18} the ‘‘equatorial’’ node $n = 1$ has also been observed in the ARPES data on $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$.¹⁹

Numerical results for the thermodynamic critical field H_c in units of $2\pi T_c \sqrt{N(0)}$ are shown in Fig. 1. This normalization is chosen because for the s-wave order parameter on a sphere we have a close to 1 value of

$$h_{th}(0) = \frac{H_c(0)}{2\pi T_c \sqrt{N(0)}} = \frac{\sqrt{\pi}}{e^C} \approx 0.995 \quad (14)$$

(the notation h_{th} for the normalized H_c is to avoid confusion with the c direction). As is seen in Fig. 1, nodes suppress the condensation energy and H_c . Besides, we observe that while the shape of the Fermi surface does not affect H_c for s- and d-wave order parameters, the equatorial node clearly makes a difference.

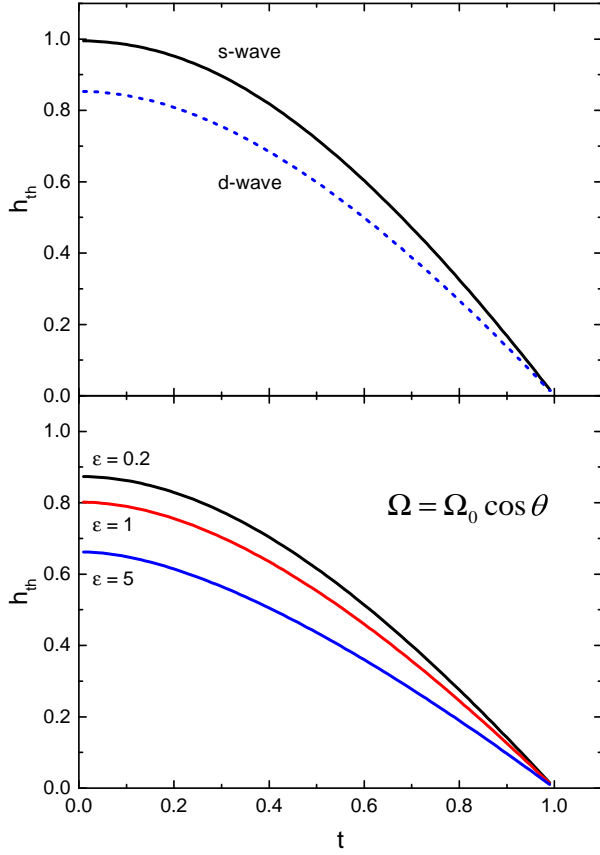


FIG. 1. (Color online) Dimensionless thermodynamic critical field $h_{th}(t) = H_c/2\pi T_c \sqrt{N(0)}$. Each curve on the upper panel in fact is three coinciding curves for Fermi sphere and prolate and oblate spheroids, $\epsilon = 1, 0.2$, and 5 . The lower panel is for the order parameter $\Omega \propto \cos \theta$ with the normalization Ω_0 evaluated separately for each Fermi shape, see Appendix A.

III. UPPER CRITICAL FIELD

The theory of the orbital H_{c2} of clean superconductors has recently been developed by the authors for arbitrary anisotropies of Fermi surfaces and order parameters.¹¹ Within this theory, $H_{c2}^{(c)}$ along the c axis of uniaxial crystals is found by solving an equation:

$$\ln t = 2h^{(c)} \int_0^\infty s \ln \tanh(st) \left\langle \Omega^2 \mu_c e^{-\mu_c h^{(c)} s^2} \right\rangle ds, \quad (15)$$

$$h^{(c)} = H_{c2}^{(c)} \frac{\hbar^2 v_0^2}{2\pi \phi_0 T_c^2}, \quad \mu_c = \frac{v_x^2 + v_y^2}{v_0^2}, \quad v_0^3 = \frac{2E_F^2}{\pi^2 \hbar^3 N(0)}. \quad (16)$$

Here, v_x, v_y are Fermi velocities in the a, b plane, E_F is the Fermi energy, the velocity $v_0 = v_F$ for the isotropic case. Hence, both μ_c depending on the Fermi surface and Ω describing the order parameter anisotropy, enter the equation for $h^{(c)}$ under the integral over the Fermi surface. This is the reason why the simple spheroid with the shape fixed by a single parameter, the ratio of semi-axes, suffices to describe major features of quantities of

interest here.

The theory of Ref. 11 allows one to evaluate also the anisotropy parameter $\gamma_H = H_{c2}^{(a)}/H_{c2}^{(c)}$. Given $h^{(c)}(t)$, one solves Eq. (15) in which μ_c is replaced with $\mu_a = (v_x^2 + \gamma_H^2 v_z^2)/v_0^2$.

In general, Eq. (15) can be solved numerically, but if $T = 0$ or $T \rightarrow T_c$, the solutions are exact:¹¹

$$h^{(c)}(0) = \exp(-C - \langle \Omega^2 \ln \mu_c \rangle),$$

$$h^{(c)}(t \rightarrow 1) = \frac{8(1-t)}{7\zeta(3) \langle \Omega^2 \mu_c \rangle}. \quad (17)$$

For the isotropic case, $\langle \mu_c \rangle = 2/3$, $\langle \ln \mu_c \rangle = 2 \ln(2/e)$, and one reproduces the Helfand-Werthamer clean limit results.²⁰

After simple algebra we obtain:

$$\frac{H_{c2}^{(c)}(0)}{H_c(0)} = \frac{\phi_0 T_c}{\hbar^2 v_0^2 \sqrt{\pi N(0)}} \exp \left\langle \Omega^2 \ln \frac{|\Omega|}{\mu_c} \right\rangle, \quad (18)$$

$$\frac{H_{c2}^{(c)}}{H_c} \Big|_{T_c} = \frac{2\sqrt{2}\phi_0 T_c}{\hbar^2 v_0^2 \sqrt{7\zeta(3)\pi N(0)}} \frac{\sqrt{\langle \Omega^4 \rangle}}{\langle \Omega^2 \mu_c \rangle}. \quad (19)$$

In the isotropic case near T_c , $H_{c2}/H_c = \sqrt{2} \kappa_{GL}$ with

$$\kappa_{GL} = \frac{3\phi_0 T_c}{\hbar^2 v_F^2 \sqrt{7\zeta(3)\pi N(0)}}, \quad (20)$$

see e.g. Ref. 21; this coincides with the isotropic limit of Eq. (19).

As mentioned above, if the ratio $R = H_{c2}/H_c > 1$, the material in question is of the type-II, if $R < 1$ it behaves as type-I. Using Eqs. (18) and (19) we compare these ratios at $T = 0$ and T_c for the c direction:

$$\frac{R^{(c)}(0)}{R^{(c)}(T_c)} = \sqrt{\frac{7\zeta(3)}{8}} \frac{\langle \Omega^2 \mu_c \rangle}{\sqrt{\langle \Omega^4 \rangle}} \exp \left\langle \Omega^2 \ln \frac{|\Omega|}{\mu_c} \right\rangle. \quad (21)$$

It is worth noting that this ratio depends on the Fermi surface shape and the order parameter symmetry, but not on other material characteristics.

As an example we take $\Omega = \sqrt{3} \cos \theta$ on a Fermi sphere to obtain $R^{(c)}(0)/R^{(c)}(T_c) \approx 1.365$. We note again that for the same order parameter anisotropy, say, for $\Omega = \Omega_0 \cos \theta$, the normalization $\langle \Omega^2 \rangle = 1$ imposes different Ω_0 for different Fermi surfaces, see Appendix A and Fig. 8. Hence, the criteria for type-I or -II behavior depend on the Fermi surface shape and the order parameter symmetry.

IV. PENETRATION DEPTH

The inverse tensor of squared penetration depth for the general anisotropic clean case is:^{9,10}

$$(\lambda^2)_{ik}^{-1} = \frac{16\pi^2 e^2 N(0) T}{c^2} \sum_{\omega > 0} \left\langle \frac{\Delta^2 v_i v_k}{\beta^3} \right\rangle. \quad (22)$$

Here $\Delta = \Psi\Omega$, $\beta = \sqrt{\Delta^2 + \hbar^2\omega^2}$, and $\Psi(T)$ satisfies the self-consistency equation:

$$-\ln t = \sum_{n=0}^{\infty} \left(\frac{1}{n+1/2} - \left\langle \frac{\Omega^2}{\sqrt{\psi^2\Omega^2 + (n+1/2)^2}} \right\rangle \right) \quad (23)$$

where $\psi = \Psi/2\pi T$.

The density of states $N(0)$, Fermi velocities \mathbf{v} , and the order parameter anisotropy Ω are the input parameters for evaluation of λ_{aa} and λ_{cc} . $N(0)$ is not needed if one is interested only in the anisotropy $\gamma_\lambda = \lambda_{cc}/\lambda_{aa}$:

$$\gamma_\lambda^2 = \frac{\lambda_{aa}^{-2}}{\lambda_{cc}^{-2}} = \frac{\sum_n \langle \Omega^2 v_a^2 / \eta^{3/2} \rangle}{\sum_n \langle \Omega^2 v_c^2 / \eta^{3/2} \rangle}, \quad \eta = \psi^2 \Omega^2 + (n+1/2)^2. \quad (24)$$

It is easy to show that this gives:^{9,22}

$$\gamma_\lambda^2(0) = \frac{\langle v_a^2 \rangle}{\langle v_c^2 \rangle}, \quad \gamma_\lambda^2(T_c) = \frac{\langle \Omega^2 v_a^2 \rangle}{\langle \Omega^2 v_c^2 \rangle}. \quad (25)$$

At first sight, γ_λ should approach T_c as a constant or at least as some power $(1-t)^p$ with $p > 1$. This would mean that $\gamma_\lambda \approx \text{const}$ in a practically finite GL domain. This, however, is not the case. To see this we evaluate γ_λ near T_c where

$$\eta^{3/2} = (n+1/2)^3 \left(1 + \frac{3\psi^2\Omega^2}{2(n+1/2)^2} \right) \quad (26)$$

since $\psi^2 \ll 1$. Expanding Eq. (24) for γ_λ in powers of ψ^2 we obtain the first correction:

$$\gamma_\lambda = \gamma_\lambda(T_c) - \frac{93\zeta(5)}{28\zeta(3)} \left(\frac{\langle \Omega^4 v_a^2 \rangle}{\langle \Omega^2 v_a^2 \rangle} - \frac{\langle \Omega^4 v_c^2 \rangle}{\langle \Omega^2 v_c^2 \rangle} \right) \psi^2. \quad (27)$$

Since $\psi^2 \propto (1-t)$, γ_λ approaches T_c with a non-zero slope for all order parameters except the s-wave with $\Omega = 1$.

We will see below that for general anisotropies the ratios H_{c2}/H_c and λ/ξ also attain their GL values only at T_c approaching them with finite slopes.²³

V. ISOTROPIC CASE

This well-studied case is worth recalling because already here one can see that the criterion based on the value of λ/ξ cannot be applied at arbitrary temperatures. We obtain using Eq. (21):

$$\frac{R(0)}{R(T_c)} = \sqrt{\frac{7\zeta(3)}{8}} e^{2-\ln 4} \approx 1.263, \quad (28)$$

the value originally obtained by Eilenberger.⁴ We thus see that if at T_c an isotropic material has $R(T_c) = \sqrt{2}\kappa_{GL} = 1$ at the boundary between type-I and type-II, it is of the type-II at $T = 0$. For the material to be of the type-I at all T 's, i.e., to have $R(t) < 1$ at all temperature, one needs $R(T_c) < 1/1.263 = 0.792$, or $\kappa_{GL} < 0.792/\sqrt{2} = 0.560$. Moreover, if $0.560 < \kappa_{GL} < 1/\sqrt{2} = 0.707$ at T_c ,

the material should undergo the transition from type-I to type-II at some temperature under T_c .

It is easy to see that at all temperatures $T \neq T_c$ the criterion based on the ratio H_{c2}/H_c differs from that based on $\kappa = \lambda/\xi$. To this end we take microscopically calculated values at $T = 0$:

$$\lambda^{-2}(0) = \frac{8\pi e^2 N(0) v_F^2}{3c^2}, \quad \xi^2(0) = \frac{\phi_0}{2\pi H_{c2}(0)} = \frac{\hbar^2 v_F^2}{\pi^2 T_c^2} e^{C-2}, \quad (29)$$

which give

$$\kappa^2(0) = \frac{3\pi c^2 T_c^2}{8e^2 N(0) \hbar^2 v_F^4} e^{2-C}. \quad (30)$$

Using the GL value for $\kappa(T_c)$ (20) we obtain:⁴

$$\frac{\kappa(0)}{\kappa(T_c)} = \sqrt{\frac{7\zeta(3)}{24}} e^{2-C} = 1.206, \quad (31)$$

This differs from $R(0)/R(T_c) = 1.263$ obtained above using the H_{c2}/H_c criterion. The difference is not large, still it shows that even in the isotropic case the value of $\kappa = \lambda/\xi$ is not a correct criterion for the type of superconductivity at any temperature except T_c . Basically, this is because $H_{c2}/H_c = \kappa\sqrt{2}$ only at T_c .

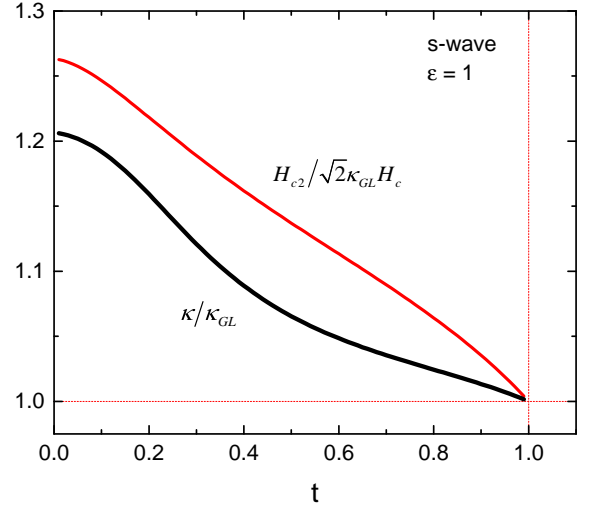


FIG. 2. (Color online) The upper curve is $H_{c2}(t)/\sqrt{2}\kappa_{GL}H_c(t)$ and the lower one is $\kappa(t)/\kappa_{GL}$ for the isotropic case. Note the different slopes of these quantities at T_c .

These arguments are supported by the numerical calculation at arbitrary temperatures shown in Fig. 2, where the upper curve is the ratio $R(t) = H_{c2}(t)/H_c(t)$ for $\kappa_{GL} = 1/\sqrt{2}$; the lower curve is $\kappa(t)/\kappa_{GL}$. A feature worth noting in this figure is that the two curves have *finite* and *different* slopes at T_c . In other words, in fact there is no however small temperature interval in the

immediate vicinity of T_c in which the GL “ κ -criterion” works, except T_c itself.

This feature is related to the mentioned above accuracy of GL theory: the energy expansion within GL is accurate up to terms of the order τ^2 with $\tau = 1 - t$, the order parameter $\Psi^2 \sim \tau$ along with λ^{-2} , H_{c2} , and H_c , all $\sim \tau$. Their ratios - within the GL theory - should be considered as constant. To get next corrections to these constants one has to overstep the accuracy of the GL theory, i.e., to go to the microscopic theory which shows that these ratios approach T_c with finite slopes.

VI. NUMERICAL RESULTS

The situation for anisotropic materials is, of course, more involved. To begin, we recall the standard notation. Introducing the geometric average $\lambda = (\lambda_a^2 \lambda_c)^{1/3}$ and $\gamma_\lambda = \lambda_c / \lambda_a$ one obtains $\lambda_a = \lambda \gamma_\lambda^{-1/3}$ and $\lambda_c = \lambda \gamma_\lambda^{2/3}$ (for brevity we use the notation λ_a instead of λ_{aa} for the square root of one of diagonal elements of the tensor $(\lambda^2)_{ik}$). For the coherence lengths we have $\xi_a = \xi \gamma_H^{1/3}$ and $\xi_c = \xi \gamma_H^{-2/3}$, where $\gamma_H = H_{c2}^{(a)} / H_{c2}^{(c)} = \xi_a / \xi_c$ and $\xi^3 = \xi_a^2 \xi_c$. In general, $\gamma_H(T) \neq \gamma_\lambda(T)$, but at T_c the anisotropies of both λ and H_{c2} are determined by the same “mass tensor” so that $\gamma_H(T_c) = \gamma_\lambda(T_c)$.^{16,22–24} Different $\gamma_H(T)$ and $\gamma_\lambda(T)$ demonstrate particularly well the common but misleading association of superconducting anisotropies with the effective mass tensor of the band theory.

Direct calculations of the thermodynamic critical field $H_c(T_c)$, either using the microscopic theory or the anisotropic GL equations, yield

$$H_c(T_c) = \frac{\phi_0}{2\sqrt{2}\pi\lambda_a\xi_a} = \frac{\phi_0}{2\sqrt{2}\pi\lambda_c\xi_c} = \frac{\phi_0}{2\sqrt{2}\pi\lambda\xi}. \quad (32)$$

Hence, we have:

$$\left. \frac{H_{c2}^{(c)}}{H_c} \right|_{T_c} = \sqrt{2} \frac{\lambda\xi}{\xi_a^2} = \sqrt{2} \frac{\lambda_a}{\xi_a} = \sqrt{2} \kappa_a. \quad (33)$$

because $\gamma_\lambda / \gamma_H = 1$ at T_c . Using known λ_a and ξ_a we obtain skipping the algebra:

$$\kappa_a = \frac{\phi_0 T_c}{\hbar^2 v_0} \sqrt{\frac{2\langle\Omega^4\rangle}{7\zeta(3)\pi N(0)\langle\Omega^2 v_a^2\rangle\langle\Omega^2 \mu_c\rangle}}. \quad (34)$$

In the isotropic case κ_a reduces κ_{GL} of Eq. (20) i.

For the in-plane field we have:

$$\left. \frac{H_{c2}^{(a)}}{H_c} \right|_{T_c} = \sqrt{2} \frac{\lambda\xi}{\xi_a\xi_c} = \sqrt{2} \frac{\lambda_c}{\xi_a} = \sqrt{2} \kappa_\parallel. \quad (35)$$

Hence, for this field orientation, one should operate with parameter $\kappa_\parallel = \lambda_c / \xi_a$. This choice is also dictated by the surface energy of the S-N boundary, say, in (c, b) plane in field along b ; the screening currents flow along c whereas

the order parameter is changing along a . Thus the relevant lengths in this case are λ_c and ξ_a . We obtain:

$$\begin{aligned} \kappa_\parallel &= \frac{\lambda_c}{\lambda_a} = \gamma_\lambda \kappa_a = \sqrt{\frac{\langle\Omega^2 v_a^2\rangle}{\langle\Omega^2 v_c^2\rangle}} \kappa_a \\ &= \frac{\phi_0 T_c}{\hbar^2 v_0} \sqrt{\frac{2\langle\Omega^4\rangle}{7\zeta(3)\pi N(0)\langle\Omega^2 v_c^2\rangle\langle\Omega^2 \mu_c\rangle}}. \end{aligned} \quad (36)$$

For an arbitrary T , we have:

$$\frac{H_{c2}^{(c)}}{H_c} = \frac{h^{(c)}(t)}{h_{th}} \frac{\phi_0 T_c}{\hbar^2 v_0^2 \sqrt{N(0)}}, \quad (37)$$

$$\frac{H_{c2}^{(a)}}{H_c} = \frac{h^{(a)}(t)}{h_{th}} \frac{\phi_0 T_c}{\hbar^2 v_0^2 \sqrt{N(0)}}. \quad (38)$$

Presenting the numerical results we normalize the ratio $R^{(c)} = H_{c2}^{(c)} / H_c$ to its value at T_c , i.e., to $\sqrt{2} \kappa_a$ whereas for the in-plane direction $R^{(a)} = H_{c2}^{(a)} / H_c$ is normalized to $\sqrt{2} \kappa_\parallel$. Figure 3 shows $R^{(c)} = H_{c2}^{(c)} / H_c$ for s- and d-wave order parameters for three Fermi surfaces: prolate spheroid $\epsilon = 0.2$, sphere, and oblate spheroid $\epsilon = 5$.

Fig. 4 is for the order parameter with an equatorial node, $\Omega = \Omega_0 \cos \theta$. Note that $R^{(a)}(t)$ increases on cooling slower than $R^{(c)}(t)$ and can even go through a maximum as it is in the oblate case of $\epsilon = 5$. This behavior is related to the fact that $R^{(a)} = \gamma_H R^{(c)}$ and $\gamma_H(t)$ decreases on cooling for this order parameter, see Ref. 23 and references therein. One should bear in mind that for

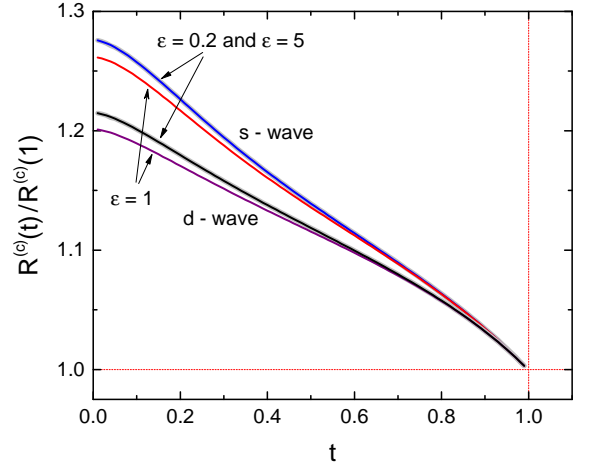


FIG. 3. (Color online) The ratio $R(t)/R(T_c)$ for s- and d-waves; $R(t) = H_{c2}(t)/H_c(t)$. Although the effect of the Fermi surface anisotropy is weak, in both cases it results in increasing ratio of H_{c2}/H_c at low- T 's

determining the material type at a particular temperature and for a given field orientation one should know not only the ratio $R(t)/R(1)$, but the value of $R = H_{c2}/H_c$ itself, i.e., $R(T_c)$ or the material parameters κ_a and κ_\parallel .

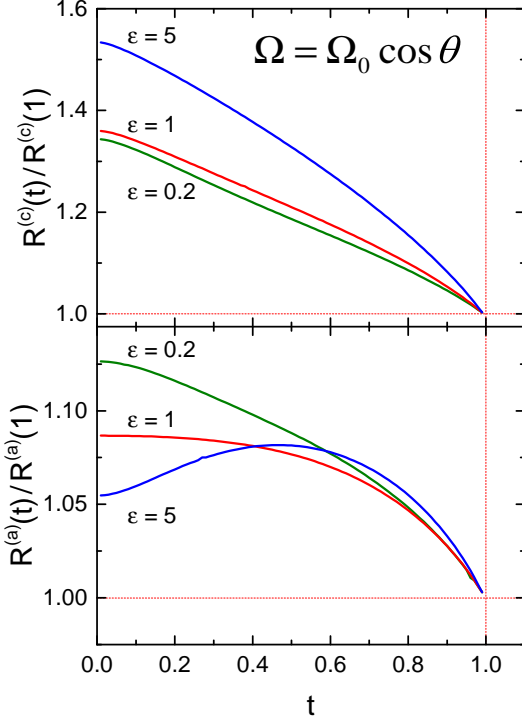


FIG. 4. (Color online) The ratio $R(t)/R(1)$ for two principal directions and three Fermi surface shapes: prolate spheroid $\epsilon = 0.2$, sphere, and oblate spheroid $\epsilon = 5$. The order parameter has an equatorial node, $\Omega = \Omega_0 \cos \theta$.

Other interesting possibilities are depicted in Fig. 5, which shows the ratios $h^{(c)}/h_{th}$ and $h^{(a)}/h_{th}$ for the s-wave order parameter, $\Omega = 1$, and the prolate (oblate) Fermi spheroid at the upper (lower) panel. According to Eq. (38) to get the ratio of actual $H_{c2}^{(c)}/H_c$ one has to multiply $h^{(c)}/h_{th}$ by a material specific dimensionless constant C which is roughly estimated as

$$C = \frac{\phi_0 T_c}{\hbar^2 v_F^2 \sqrt{N(0)}} \approx 0.1 T_c(K), \quad (39)$$

where we took $v_F \approx 10^8 \text{ cm/s}$ and $N(0) \approx 10^{33} \text{ 1/erg cm}^3$. For Fig. 5 this constant is chosen as $C = 1$ just for simplicity. Clearly, varying this constant one obtains different material behavior. For example, taking $C \approx 1.4$ we obtain type-I behavior for $H \parallel c$, but for in-plane fields we have type-I at high temperatures and type-II at low temperatures. For $C \approx 0.6$, the situation is different: type-II behavior for $H \parallel ab$ at all temperatures, but a change from type-I to type-II on cooling.

In Fig. 6 the ratios $h^{(c)}/h_{th}$ and $h^{(a)}/h_{th}$ for the order parameter $\Omega = \Omega_0 \cos \theta$ on a Fermi spheroid with $\epsilon = 5$ are plotted vs temperature. If, for example, $C \approx 0.2$, according to Fig. 6 the ratio $H_{c2}^{(c)}/H_c > 1$, while $H_{c2}^{(a)}/H_c < 1$ for all temperatures. In other words, in this hypothetical situation the material is of type-II in

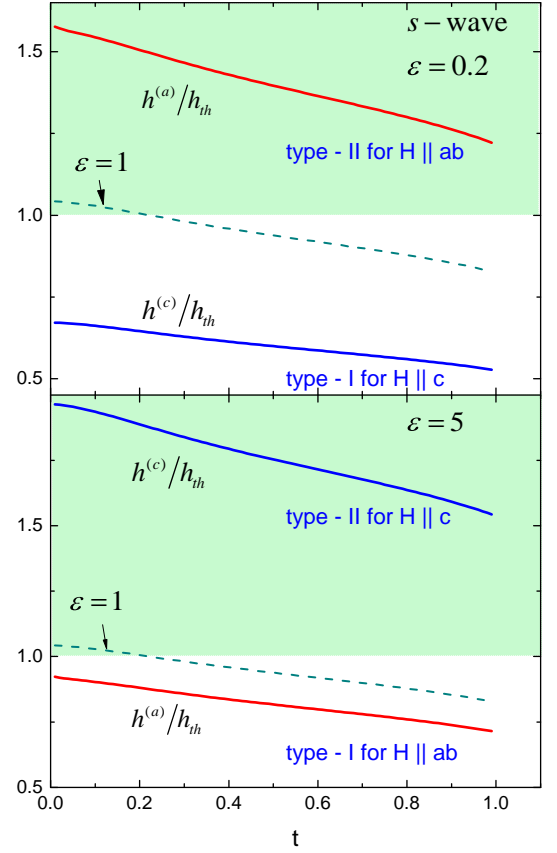


FIG. 5. (Color online) The ratios $h^{(c)}/h_{th}$ and $h^{(a)}/h_{th}$ for the s-wave order parameter $\Omega = 1$ on a Fermi spheroid with $\epsilon = 0.2$, the upper panel. For $C \approx 1$, Eq. (39). A hypothetical superconductor with such characteristics is of type-II in magnetic field along the ab plane and of type-I in fields along the c axis. The lower panel shows the situation for $\epsilon = 5$. For comparison we also show the ratio H_{c2}/H_c for the isotropic case.

fields along the c axis and of type-I in fields perpendicular to c .

Given these results, it is interesting to mention the data on superconductivity of potassium intercalated graphite, C_xK . As reported in Ref. 7, changing x between 8 and 14.7 does not affect T_c of this compound, but in fields along c the material is of type-I, whereas for $H \parallel ab$ the superconducting characteristics change from type-I to type-II. The Fermi surface of these compounds consists of nearly cylindrical piece attributed to graphite and a three-dimensional part presumably due to K. Our one band model is not directly applicable to this case, not to speak about unknown symmetry of the order parameter. Still, variety of possibilities demonstrated in Figs. 5 and 6 suggest that our theory (generalized for two bands and given needed input parameters) is potentially able to explain a quite complicated behavior of these and related compounds.

The lower panel of Fig. 4 shows that when the field is in

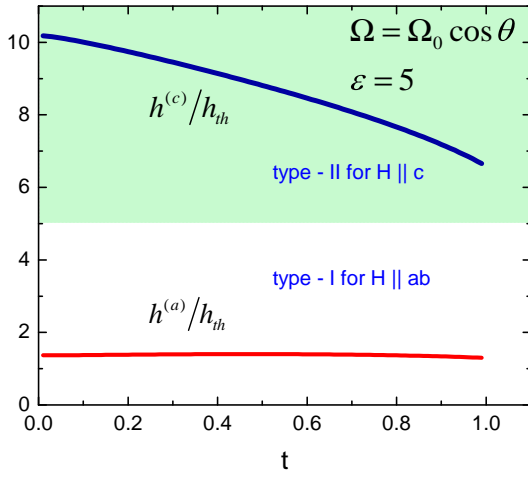


FIG. 6. (Color online) The ratios $h^{(c)}/h_{th}$ and $h^{(a)}/h_{th}$ for the order parameter $\Omega = \Omega_0 \cos \theta$ on a Fermi spheroid with $\epsilon = 5$ vs reduced temperature. For $C \approx 0.2$, Eq. (39), this corresponds to $H_{c2}^{(c)}/H_c|_{T_c} = \sqrt{2}\kappa_a(T_c) \approx 1.32$ and $H_{c2}^{(a)}/H_c|_{T_c} = \sqrt{2}\kappa_{||}(T_c) \approx 0.26$. A hypothetical superconductor with such characteristics is of type-II in magnetic field along the c axis and of type-I in fields along the ab plane.

the ab plane the ratio $R^{(a)} = H_{c2}^{(a)}/H_c$ is a non-monotonic function of t for an oblate Fermi spheroid. The source of this behavior is in the fact that $R^{(a)} = \gamma_H R^{(c)}$ and, as shown in Ref. 23, for the order parameter $\propto \cos \theta$, γ_H increases on warming. To verify that this behavior is not accidental we have calculated this ratio for $\epsilon \gg 1$ which corresponds to nearly one-dimensional situation, Fig. 7. This example shows that, in principle, situations are possible for which two transitions from type-I to type-II and back happen with changing temperature.

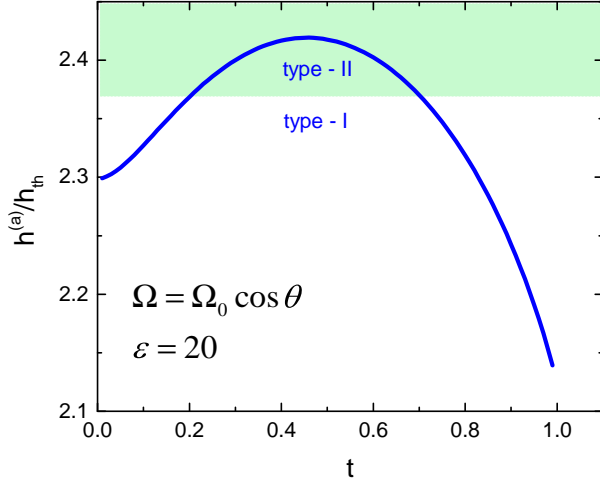


FIG. 7. (Color online) The ratio $h^{(a)}/h_{th} = (H_{c2}^{(a)}/H_c)/C$ vs t for $\epsilon = 20$, $\Omega = \Omega_0 \cos \theta$. The boundary between the type-II and type-I corresponds to the constant of Eq. (39) $C \approx 0.42$.

VII. DISCUSSION

We have shown that the criterion for the type of superconductivity based on the value of λ/ξ established for the GL domain near T_c cannot be used at arbitrary temperatures. The criterion based on the inequality $H_{c1} < H_c$ is not convenient since there is apparently no straightforward way to calculate the line energy of a single vortex at arbitrary T which is directly related to H_{c1} . On the other hand, both the upper critical field H_{c2} and the thermodynamic one, H_c , can be evaluated exactly at any T for any anisotropy. This qualifies the inequality $H_{c2}(T) > H_c(T)$ as an exact criterion for the type-II superconductivity.

While evaluating $R = H_{c2}/H_c$ within the microscopic theory, we do not observe any peculiarities near $R(T_c) = 1$ of the sort discussed in literature in the frame of extended GL equations for $\kappa_{GL} \approx 1/\sqrt{2}$, see Ref. 25 and references therein. Of course, if the curves of $H_{c2}(T)$ and $H_c(T)$ cross at some $T^* < T_c$, the material should undergo transition from type-I to type-II or otherwise so that in the vicinity of T^* one should take fluctuations into account (along with the sample shape and possibility of hysteresis), which are beyond the mean-field BCS theory. We, however, note that the argument for existence of a broad region of the HT phase diagram well under T_c with degenerate vortex configurations²⁶ in materials with $\kappa_{GL} \approx 1/\sqrt{2}$ is essentially mean-field as well.²⁵

Clearly, models based on extended GL functional are perfectly legitimate for systems described by this functional, provided this functional is considered as exact. However, for superconductors, the GL theory is an approximation which holds for $T \rightarrow T_c$ within certain accuracy. To study superconductors behavior in extended T domain, one should use, if possible, the microscopic theory instead of considering exact consequences of an approximate GL functional. As far as relative values of H_{c2} and H_c are concerned, this has been done for isotropic bulk materials by Eilenberger,⁴ who found that even if $H_{c2}(T_c) = H_c(T_c)$ or $\kappa_{GL} = 1/\sqrt{2}$, H_{c2} increases faster than H_c when T decreases, $dH_{c2}/dT|_{T_c} > dH_c/dT|_{T_c}$. Hence, there is no finite region of temperatures near T_c where $H_{c2}(T) = H_c(T)$. This in fact contradicts the claim of Ref. 25 that such a region does exist. For anisotropic one-band superconductors considered here, the microscopic approach also does not give an indication of peculiarities of the system properties for $R(T_c) = 1$ (such as degeneracy of different vortex configurations²⁶ in a broad region of the HT phase diagram).

VIII. ACKNOWLEDGEMENT

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Appendix A: Averaging over Fermi spheroids

Consider an uniaxial superconductor with the electronic spectrum

$$E(\mathbf{k}) = \hbar^2 \left(\frac{k_x^2 + k_y^2}{2m_{ab}} + \frac{k_z^2}{2m_c} \right), \quad (\text{A1})$$

so that the Fermi surface is a spheroid with z being the symmetry axis. In spherical coordinates (k, θ, ϕ) we have

$$E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_{ab}} \left(\sin^2 \theta + \frac{m_{ab}}{m_c} \cos^2 \theta \right) = \frac{\hbar^2 k^2}{2m_{ab}} \Gamma(\theta), \quad (\text{A2})$$

so that

$$k_F^2(\theta) = \frac{2m_{ab}E_F}{\hbar^2 \Gamma(\theta)}. \quad (\text{A3})$$

The Fermi velocity is $\mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}} E(\mathbf{k})$, with the derivatives taken at $\mathbf{k} = \mathbf{k}_F$:

$$\begin{aligned} v_x &= \frac{v_{ab} \sin \theta \cos \phi}{\sqrt{\Gamma(\theta)}}, \quad v_y = \frac{v_{ab} \sin \theta \sin \phi}{\sqrt{\Gamma(\theta)}}, \\ v_z &= \epsilon \frac{v_{ab} \cos \theta}{\sqrt{\Gamma(\theta)}}, \quad \epsilon = \frac{m_{ab}}{m_c}, \quad v_{ab} = \sqrt{\frac{2E_F}{m_{ab}}}. \end{aligned} \quad (\text{A4})$$

The value of the local Fermi velocity, $v = (v_x^2 + v_y^2 + v_z^2)^{1/2}$, is given by

$$v = v_{ab} \sqrt{\frac{\sin^2 \theta + \epsilon^2 \cos^2 \theta}{\sin^2 \theta + \epsilon \cos^2 \theta}} = v_{ab} \sqrt{\frac{\Gamma_1(\theta)}{\Gamma(\theta)}}. \quad (\text{A5})$$

The density of states is:

$$N(0) = \int \frac{\hbar^2 d^2 \mathbf{k}_F}{(2\pi\hbar)^3 v} = \frac{m_{ab}^2 v_{ab}}{2\pi^2 \hbar^3} \int \frac{d\Omega}{4\pi \sqrt{\Gamma(\theta) \Gamma_1(\theta)}}, \quad (\text{A6})$$

where the integration is over the solid angle $d\Omega = \sin \theta d\theta d\phi$.

The Fermi surface average of a function $A(\theta, \phi)$ is

$$\langle A(\theta, \phi) \rangle = \frac{1}{D} \int \frac{d\Omega A(\theta, \phi)}{4\pi \sqrt{\Gamma(\theta) \Gamma_1(\theta)}}, \quad (\text{A7})$$

$$D = \int \frac{d\Omega}{4\pi \sqrt{\Gamma(\theta, \epsilon) \Gamma_1(\theta, \epsilon)}} = \frac{F(\cos^{-1} \sqrt{\epsilon}, 1 + \epsilon)}{\sqrt{1 - \epsilon}} \quad (\text{A8})$$

where F is an Incomplete Elliptic Integral of the first kind. If A depends only on the polar angle θ , one can employ $u = \cos \theta$:

$$\langle A(\theta) \rangle = \frac{1}{D(\epsilon)} \int_0^1 \frac{du A(u)}{\sqrt{\Gamma(u, \epsilon) \Gamma_1(u, \epsilon)}}, \quad (\text{A9})$$

$\Gamma = 1 + (\epsilon - 1)u^2$, $\Gamma_1 = 1 + (\epsilon^2 - 1)u^2$. (A10)
It is useful to have a relation between $v_{ab} = \sqrt{2E_F/m_{ab}}$ and v_0 of Eq. (16) for a one-band situation:

$$v_{ab}^3 = D(\epsilon) v_0^3. \quad (\text{A11})$$

As an example we show in Fig. 8 how the averaging over Fermi spheroids affects the normalization constant Ω_0 for the order parameter of the form $\Omega = \Omega_0 \cos \theta$.

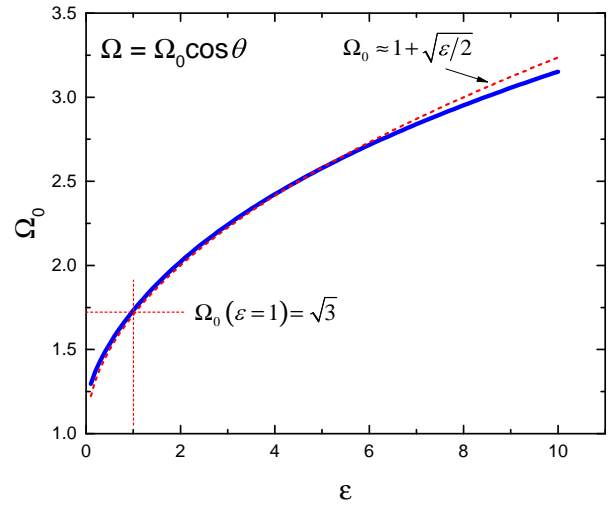


FIG. 8. (Color online) The normalization constant Ω_0 for the order parameter $\Omega = \Omega_0 \cos \theta$ as a function of the Fermi surface shape parameter ϵ . The dashed curve is a convenient approximation to $\Omega_0(\epsilon)$.

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