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Effect of equatorial line nodes on the upper critical field and London penetration depth

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The upper critical field H_{c2} and its anisotropy are calculated for order parameters with line nodes at the equators, $k_z = 0$, of the Fermi surface of uniaxial superconductors. It is shown that characteristic features found in Fe-based materials (a nearly linear $H_{c2}(T)$ in a broad T domain, a low and increasing on warming anisotropy $\gamma_H = H_{c2,ab}/H_{c2,c}$) can be caused by competing effects of the equatorial nodes and of the Fermi surface anisotropy. For certain material parameters, $\gamma_H(T) - 1$ may change sign upon warming, in agreement with the recorded behavior of FeTeS systems. It is also shown that the anisotropy of the penetration depth $\gamma_\lambda = \lambda_c/\lambda_{ab}$ decreases upon warming to reach γ_H at T_c, in agreement with data available. For some materials $\gamma_\lambda(T)$ may change upon warming, from $\gamma_\lambda > 1$ at low Ts to $\gamma_\lambda < 1$ at high Ts.

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Iron-based superconductors are layered compounds with nearly cylindrical Fermi surfaces, which at first sight should have lead to high anisotropies of the upper critical field and the London penetration depth. This, however, is not the case. Most of these compounds have relatively low values of $\gamma_H = H_{c2,ab}/H_{c2,c}$ that *increase on warming* [1] and in some materials even change from $\gamma_H < 1$ at low temperatures to $\gamma_H > 1$ at high Ts [2,3]. The anisotropy of the London penetration depth is also low but *decreases on warming* [4]. Originally, such behavior was attributed to multiband physics similar to that of MgB_2 [5]. However, in MgB_2, $\gamma_H(T)$ decreases on warming whereas $\gamma_\lambda(T)$ increases, just the opposite to Fe-based materials.

Recently, the increasing $\gamma_H(T)$ had been associated with the order parameter modulated along the c axis [6], even in a single-band scenario, so that multiband effects *per se* are not necessary to explain the observed behavior of $H_{c2}(T)$ and $\lambda(T)$. It is also known that some Fe-based materials have gap nodes and there are models suggesting equatorial, $k_z = 0$, line nodes [7]. Such a gap structure is seen in the angle-resolved photoemission spectroscopy (ARPES) data on $BaFe_2(As_{0.7}P_{0.3})_2$ [8,9] and was also explored for other unconventional superconductors, for example, Sr_2RuO_4, to understand anisotropic thermal conductivity [10,11].

Here we show that the competing effects of equatorial nodes and the Fermi surface anisotropy might be responsible for the observed behavior of H_{c2} in these materials. Moreover, equatorial line nodes cause the anisotropy of the London penetration depth γ_λ to *decrease on warming*, the feature seen in a number of materials for which data on λ anisotropy are available [4]. The interplay of the Fermi surface effects and those due to line nodes can result in the temperature-dependent sign of $\gamma_\lambda - 1$, the prediction to be verified. In particular, this interplay causes the in-plane superfluid density to change with temperature in a "d-wave-like" fashion (linear at low Ts), while being rather flat at low Ts for the c direction.

Studying the orbital $H_{c2}(T)$, we employ a version of Helfand-Werthamer (HW) theory [12] generalized for clean anisotropic superconductors [6]. It is based on Eilenberger quasiclassical formulation of the superconductivity [13] with a weak-coupling separable potential $V(\mathbf{k},\mathbf{k}') = V_0\Omega(\mathbf{k})\Omega(\mathbf{k}')$ and the order parameter in the form $\Delta = \Psi(\mathbf{r},T)\,\Omega(\mathbf{k})$, where $\mathbf{k}$ is the Fermi momentum [14]. $\Omega(\mathbf{k})$ determines the $\mathbf{k}$ dependence of Δ and is normalized so that the average over the Fermi surface $\langle\Omega^2\rangle = 1$. This popular approximation works well for one-band materials with anisotropic coupling and can be generalized to a multiband case [6].

Within this theory, $H_{c2,c}$ along the c axis of uniaxial crystals is found by solving an equation [6]:

$$\ln t = 2h_c \int_0^\infty s\, \ln\tanh(st)\left\langle \Omega^2 \mu_c e^{-\mu_c h_c s^2}\right\rangle ds\,, \tag{1}$$

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

Here, $t = T/T_c$, v_x, v_y are Fermi velocities in the a,b plane, E_F is the Fermi energy, $N(0)$ is the total density of states at the Fermi level per spin, the velocity $v_0 = v_F$ for the isotropic case, and $\langle\ldots\rangle$ stands for the Fermi surface average.

In principle, Eq. (1) can be used to evaluate $h_c(t)$ for any order parameter anisotropy (any Ω) and any Fermi surface (any μ_c). Both Ω and μ_c enter Eq. (1) under the sign of the Fermi surface averaging and one does not expect fine details of the Fermi surface to strongly affect the $H_{c2,c}(T)$ shape. For this reason, describing Fermi surface shapes, we focus on the simplest version of Fermi spheroids, for which the averaging is a well-defined analytic procedure (see, e.g., [6,15]).

In general, Eq. (1) can be solved numerically, but if $T \to T_c$, the result is exact [6]:

$$h_c = \frac{8(1-t)}{7\zeta(3)\langle\Omega^2\mu_c\rangle}\,, \tag{3}$$

where $\zeta(3) \approx 1.202$. For the isotropic case $\Omega = 1$, $\langle\mu_c\rangle = 2/3$, and one reproduces the HW slope near T_c in the clean limit.

At $T = 0$, Eq. (1) was shown to yield [6]

$$h_c(0) = e^{-\boldsymbol{C}-\langle\Omega^2\ln\mu_c\rangle}\,, \tag{4}$$

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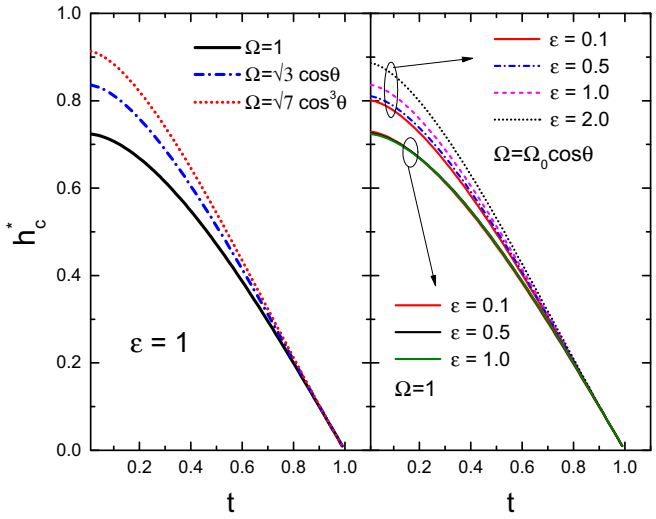

FIG. 1. (Color online) $h_c^*(t)$ for various Fermi surfaces and order parameters. (Left panel) Fermi sphere and $\Omega = \sqrt{2n+1}\cos^n\theta$ with $n = 0,1,3$. One sees that equatorial nodes cause a substantial increase of $h_c^*(0)$ and widen the domain of nearly linear behavior of $h_c^*(t)$. Note also a slight positive curvature at high Ts for $n = 1,3$. (Right panel) The lower group of three nearly coincident curves are for an s-wave order parameter on a Fermi sphere and two prolate spheroids. The upper group is for $\Omega \propto \cos\theta$, showing clearly that $h_c^*(0)$ increases with increasing ϵ, the ratio of effective masses m_c/m_{ab} (of a squared spheroid's semiaxes).

where $C \approx 0.577$ is the Euler constant. Hence we obtain the HW ratio,

$$h_c^*(0) = \frac{H_{c2,c}(0)}{T_c H'_{c2,c}(T_c)} = \frac{h_c(0)}{h'_c(1)} = \frac{7\zeta(3)}{8e^C}\langle\Omega^2\mu_c\rangle e^{-\langle\Omega^2\ln\mu_c\rangle}, \tag{5}$$

where $H'_{c2,c}(T_c) \equiv dH_{c2,c}/dT$ at T_c and $h'_c(1) = (dh_c/dt)_{t=1}$. For the isotropic case this gives the clean limit HW value $h_c^*(0) = 7\zeta(3)/48e^{C-2} = 0.727$.

Thus both the order parameter symmetry and the Fermi surface affect $h_c^*(0)$. However, as shown at the right panel of Fig. 1, for s-wave order parameters on Fermi spheroids, $h_c^*(0)$ remains close to 0.7 for all ratios of the spheroid semiaxes [6]. We also note that $h_c^*(0)$ is nearly insensitive to the nonmagnetic transport scattering, but it decreases fast in the presence of pair breaking to reach 0.5 for the strong T_c suppression [16].

To study how the order parameter anisotropy affects $H_{c2,c}(T)$ and $h_c^*(0)$, we first consider the case of the Fermi sphere. We are interested in k_z-dependent order parameters, which on the Fermi sphere implies that Ω depends on the polar angle θ. We model equatorial nodes by setting $\Omega = \Omega_0\cos^n\theta$. Near the "equator" at $\theta = \pi/2$, $|\Delta|$ behaves as $|\theta - \pi/2|^n$. Clearly, the bigger the power n, the wider is the equatorial belt where the order parameter is close to zero (we call the power n the "node order"). It is readily shown that

$$\Omega_0 = \sqrt{2n+1}\,, \quad \langle\Omega^2\mu_c\rangle = \frac{2(2n+1)}{4n^2+8n+3}\,, \tag{6}$$
$$\langle\Omega^2\ln\mu_c\rangle = -\mathbf{C} - \psi(n+3/2)\,,$$

where ψ is the digamma function. Thus we have

$$h_c^*(0) = \frac{7\zeta(3)}{4}\frac{2n+1}{4n^2+8n+3}\,e^{\psi(n+3/2)}, \tag{7}$$

i.e., $h_c^*(0)$ increases with increasing n. On the other hand, a larger $h_c^*(0)$ translates to a broader temperature range where $h(t)$ is close to being linear. We then expect the curve $H_{c2,c}(T)$ to have an extended linear domain for increasing n. To check this we turn to the full temperature dependence $h_c(t)$ by solving Eq. (1) numerically. The results are shown in the left panel of Fig. 1. We estimate that $h_c^*(t)$ deviates from the straight line $h_c^{*\prime}(1)(t-1)$ by less than 1% in the domain $t > 0.6$ for $n = 0$ (the s wave), $t > 0.4$ for $n = 1$, and $t > 0.2$ for $n = 3$. Therefore increasing the node order causes "straightening" of $H_{c2,c}(T)$, observed in pnictides [17] and some other materials [18].

Performing calculations for Fermi spheroids, one should evaluate properly Fermi surface averages. Details of this procedure were worked out in [6,15]. Examples of $h_c^*(t)$ so obtained for a few values ϵ, the squared ratio of the semiaxes, are given in the right panel of Fig. 1.

Similar to Eq. (1) for $H_{c2,c}(T)$, one can obtain an equation for $H_{c2,ab}(T)$, or directly for the anisotropy parameter $\gamma_H = H_{c2,ab}/H_{c2,c}$ [6]. In fact, $\gamma_H(t)$ satisfies Eq. (1), in which, however, $h_c(t)$ is now known and μ_c is replaced with

$$\mu_b = \frac{v_x^2 + \gamma_H^2 v_z^2}{v_0^2}\,. \tag{8}$$

The left panel of Fig. 2 shows $\gamma_H(t)$ for equatorial line nodes with $n = 1,2,3$. One sees that for this type of node on a sphere (i) $\gamma_H < 1$, i.e., $H_{c2,c} > H_{c2,ab}$, and (ii) γ_H *increases on warming*, the feature ubiquitous for the Fe-based materials.

On the other hand, in materials such as pnictides, the Fermi surfaces are warped cylinders and $H_{c2,ab} > H_{c2,c}$; $\gamma_H(t) > 1$

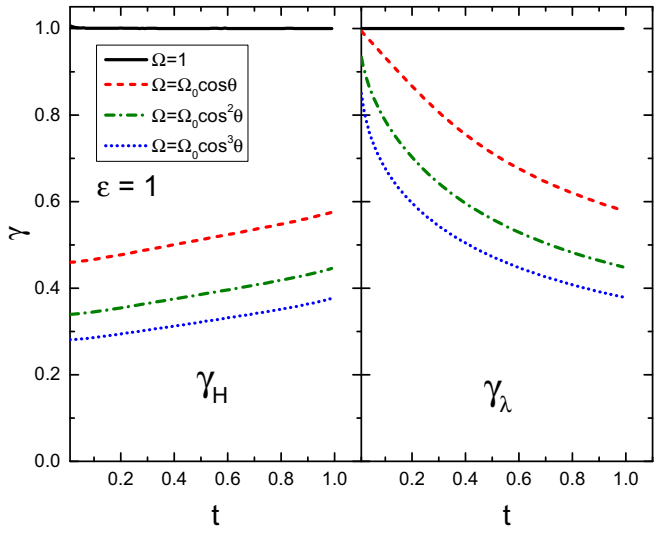

FIG. 2. (Color online) $\gamma_H = H_{c2,ab}/H_{c2,c}$ and $\gamma_\lambda = \lambda_c/\lambda_{ab}$ for the Fermi sphere and order parameters shown in the legend. Thus the values of both γ_H and γ_λ are suppressed by equatorial line nodes; the suppression is stronger for higher node orders. Besides, the nodes cause $\gamma_H(T)$ to increase upon warming, whereas γ_λ decreases with increasing T, the feature reported, e.g., for Nd-1111 [4].

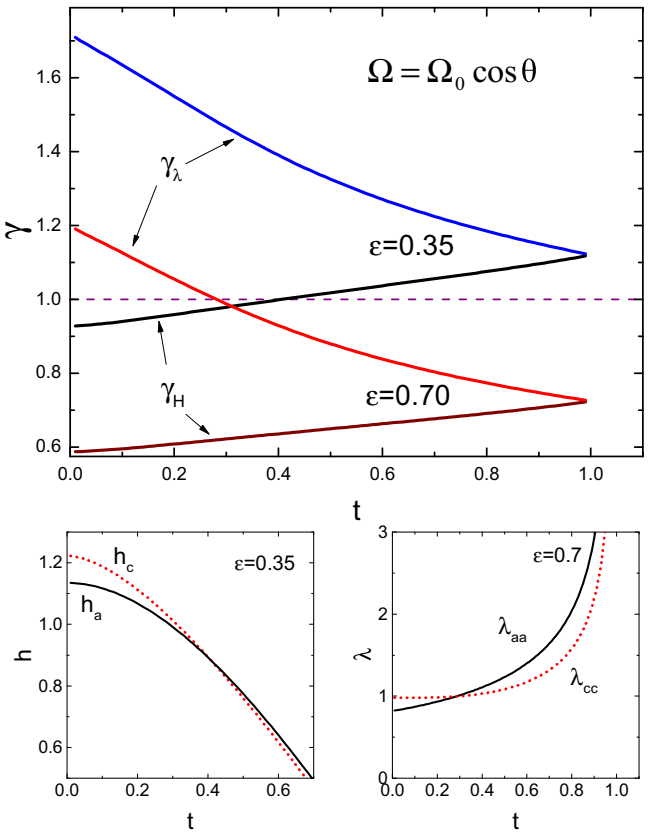

FIG. 3. (Color online) (Upper panel) Anisotropy parameters γ_λ and γ_H for the order parameter $\propto \cos\theta$ for two spheroidal Fermi surfaces, $\epsilon = 0.35$ and 0.70. (Lower left panel) The crossing of $h_c(t)$ and $h_a(t)$ near $t^* = 0.4$ for $\epsilon = 0.35$. (Lower right panel) The crossing of $\lambda_{aa}(t)$ and $\lambda_{cc}(t)$ near $t^* = 0.3$ for $\epsilon = 0.70$; both $\lambda_{aa}(t)$ and $\lambda_{cc}(t)$ are in units of $c/ev_0\sqrt{2\pi N(0)}$. Note the linear temperature dependence of λ_{aa} at low Ts and a flat "s-wave-like" behavior of λ_{cc}.

but it is not large. Qualitatively, one can model these Fermi surfaces as prolate spheroids, for which it was shown that $\gamma_H > 1$ for s-wave order parameters [6,15]. Thus the effect of equatorial nodes on γ_H is the opposite to that of prolate Fermi surfaces. It is of interest therefore to study order parameters $\propto \cos^n\theta$ on prolate spheroids. Figure 3 shows examples for spheroids with $\epsilon = 0.35$ and 0.70 and the order parameter $\propto \cos\theta$. Remarkably, for $\epsilon = 0.35$, $\gamma_H - 1$ changes sign near $t^* \approx 0.4$ so that $h_a < h_c$ for $t < 0.4$ and otherwise at higher temperatures.

We now turn to the London penetration depth. The inverse tensor of squared penetration depth for the general anisotropic clean case reads [19,20]

$$(\lambda^2)^{-1}_{ik} = \frac{16\pi^2 e^2 N(0) T}{c^2} \sum_{\omega>0} \left\langle \frac{\Delta^2 v_i v_k}{\beta^3} \right\rangle. \tag{9}$$

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

$$-\ln t = \sum_{n=0}^{\infty} \left(\frac{1}{n+1/2} - \left\langle \frac{\Omega^2}{\sqrt{\psi^2\Omega^2 + (n+1/2)^2}} \right\rangle \right), \tag{10}$$

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

Fermi velocities $\mathbf{v}$, $N(0)$, and $\Omega(\mathbf{k})$ are the input parameters for evaluation of λ_{aa} and λ_{cc}. $N(0)$ is not needed if one is interested only in the ratio $\gamma_\lambda = \lambda_{cc}/\lambda_{aa}$:

$$\gamma_\lambda^2 = \frac{\lambda_{aa}^{-2}}{\lambda_{cc}^{-2}} = \frac{\sum_n \langle \Omega^2 v_a^2/\eta^{3/2}\rangle}{\sum_n \langle \Omega^2 v_c^2/\eta^{3/2}\rangle}, \qquad \eta = \psi^2\Omega^2 + (n+1/2)^2. \tag{11}$$

In particular, this gives

$$\gamma_\lambda^2(0) = \frac{\langle v_a^2\rangle}{\langle v_c^2\rangle}, \quad \gamma_\lambda^2(T_c) = \frac{\langle \Omega^2 v_a^2\rangle}{\langle \Omega^2 v_c^2\rangle}, \tag{12}$$

showing that the order parameter anisotropy causes γ_λ to depend on T in a one-band situation [19,21], the property commonly associated with many bands.

The right panel of Fig. 2 shows γ_λ evaluated with the help of Eq. (11) for a Fermi sphere and $\Omega \propto \cos^n\theta$ with $n = 0,1,2,3$. Hence the equatorial line nodes cause $\gamma_\lambda(t)$ to *decrease on warming*, a behavior opposite to the increasing $\gamma_H(t)$ shown in the left panel. One also sees that the two anisotropy parameters meet at T_c, thus confirming consistency of the analytic and numerical procedures for evaluation of two physically different quantities: the high field $H_{c2}(T)$ at the second-order phase transition and the low-field penetration depth $\lambda(T)$.

The combined effect of the Fermi surface shape and of the order parameter $\Omega = \Omega_0\cos\theta$ on both γ_λ and γ_H is shown on the upper panel of Fig. 3. The Fermi surface parameters ϵ are chosen to demonstrate interesting situations: while $\gamma_\lambda > 1$ at all temperatures for $\epsilon = 0.35$, the anisotropy γ_H, being less than unity under $t^* \approx 0.4$, exceeds 1 above this temperature. Such a behavior has been recorded for FeTeS [2,3].

For $\epsilon = 0.7$ we have $\gamma_H < 1$ at all temperatures, whereas $\gamma_\lambda > 1$ at $t^* < 0.3$, but becomes less than unity above this temperature. The transverse magnetization of a material in the mixed state with such γ_λ placed in a field tilted relative to the principal crystal directions should change sign at t^* [22]. The same is true for the torque experienced by the crystal. In other words, the sign change of $\gamma_\lambda - 1$ can be detected by measuring the sign and angular dependence of the transverse magnetization or torque [23,24].

Figure 4 shows that temperatures t^*, at which $\gamma_H - 1$ and $\gamma_\lambda - 1$ change sign, vary as functions of the Fermi surface shape ϵ: with increasing ϵ these temperatures grow if one goes to a "less prolate" Fermi shape.

A popular quantity in analysis of penetration depth data is the superfluid density defined as λ^{-2} normalized on its value at $T = 0$. This quantity for two principal directions is plotted in Fig. 5 for an equatorial node, $\Omega = \Omega_0\cos\theta$, on a sphere and spheroid with $\epsilon = 0.5$. Interestingly, the node presence results in $\rho_{aa}(t)$ being qualitatively similar to the known d-wave linear low-temperature behavior, whereas a direct numerical check shows that $\rho_{cc} - 1 \propto t^3$. In fact, this behavior has been discussed considering properties of UBe_{13} [25].

Interestingly, the order parameter $\Omega = \Omega_0\cos\theta$ on prolate Fermi surfaces causes suppression of the specific heat jump at T_c, $\Delta C/C_n = 1.43/\langle\Omega^4\rangle$ [26,27]. For example, if $\epsilon = 0.1$, we estimate $\Delta C/C_n \approx 1.07$. Also, since for this type of order parameters $\langle\Omega\rangle = 0$, similar to the d wave, T_c should be suppressed in the same manner by magnetic and

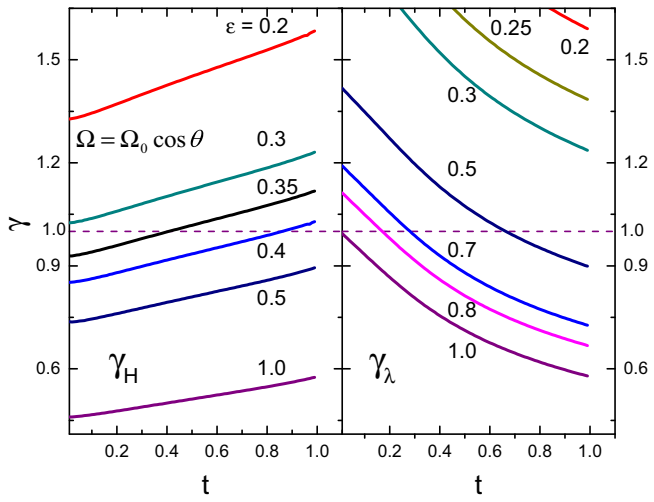

FIG. 4. (Color online) $\gamma_H(t)$ and $\gamma_\lambda(t)$ for the order parameter $\propto \cos\theta$ and the Fermi surface shapes ϵ indicated. One sees that $\gamma_H - 1$ changes sign in the domain $0.3 < \epsilon < 0.45$, whereas $\gamma_\lambda - 1$ in the region $0.45 < \epsilon < 1$.

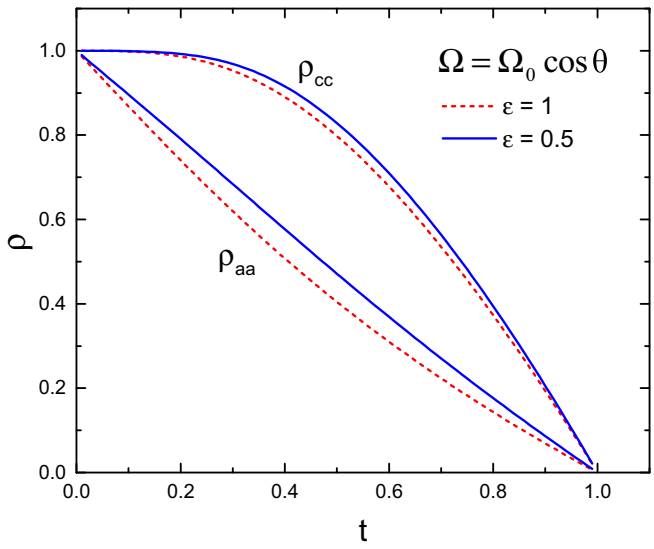

FIG. 5. (Color online) Superfluid densities $\rho_{aa} = \lambda_{aa}^2(0)/\lambda_{aa}^2(t)$ (the lower curves) and $\rho_{cc} = \lambda_{cc}^2(0)/\lambda_{cc}^2(t)$.

nonmagnetic impurities [28]. The data on electron-irradiated crystals of $Ba(Fe_{1-x}Ru_x)_2As_2$ ($x = 0.24$) qualitatively support this statement, although multiband Fermi surfaces complicate the picture [29].

Concluding, we reiterate that despite profound simplifications, such as a single-band ellipsoidal Fermi surface and the order parameter with equatorial nodes, our model reproduces qualitative features of anisotropic $H_{c2}(T)$ and $\lambda(T)$ often seen in real materials, notably, Fe-based superconductors. We do not claim that our model describes all properties of this diverse family of materials. We do, however, point to the potentially important role of competing equatorial nodes and Fermi surface anisotropy. Fine details of Fermi surfaces and order parameters enter the theory of $H_{c2}(T)$ and $\lambda(T)$ only as averages over the Fermi surface and thus do not justify the formal complications of taking them into account. Also, as far as $H_{c2}(T)$ and $\lambda(T)$ are concerned, the single- and multiband scenarios give similar results, as shown in our previous study [6]. Here we reproduced a number of features ubiquitous for Fe-based superconductors, the origin of which until now was not even questioned. In particular, we find that the equatorial line node causes an extended domain of nearly *linear* $H_{c2}(T)$, anisotropy of which *increases on warming*. By studying competing effects of equatorial nodes and of the Fermi surface anisotropy, we find that, nearly cylindrical Fermi shapes notwithstanding, materials with equatorial nodes can be only weakly anisotropic. For certain combinations of material parameters both $\gamma_H - 1$ and $\gamma_\lambda - 1$ may *change sign on warming* so that $H_{c2,ab} < H_{c2,c}$ at low Ts while $H_{c2,ab} > H_{c2,c}$ at high Ts. A similar situation may occur for the anisotropy of the London penetration depth, which can be probed by torque or transverse magnetization measurements in large fields. We also find that the nodes in question cause different T dependencies of different components of the superfluid density tensor. These predictions call for experimental verification.

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