Upper critical field in dirty two-band superconductors: Breakdown of the anisotropic Ginzburg-Landau theory

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We investigate the upper critical field in a dirty two-band superconductor within quasiclassical Usadel equations. The regime of very high anisotropy in the quasi-2D band, relevant for MgB_2, is considered. We show that strong disparities in pairing interactions and diffusion constant anisotropies for two bands influence the in-plane H_{c2} in a different way at high and low temperatures. This causes temperature-dependent H_{c2} anisotropy, in accordance with recent experimental data in MgB_2. The three-dimensional band most strongly influences the in-plane H_{c2} near T_c, in the Ginzburg-Landau (GL) region. However, due to a very large difference between the *c*-axis coherence lengths in the two bands, the GL theory is applicable only in an extremely narrow temperature range near T_c. The angular dependence of H_{c2} deviates from a simple effective-mass law even near T_c.

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I. INTRODUCTION

There is strong evidence of the multigap nature of superconducting state in the recently discovered[1] compound MgB_2. The concept of multiband superconductivity was introduced in Refs. 2,3 for the case of large disparity of the electron-phonon interaction for the different Fermi-surface sheets. Based on this concept, a general theory of the upper critical field in a clean two-band superconductor with overlapping *s* and *d* bands was developed (see Ref. 4, and references therein). For MgB_2, first-principles calculations of the electronic structure and the electron-phonon interaction[5–10] have revealed two distinct groups of bands, namely, strongly superconducting quasi-two-dimensional σ bands and weakly superconducting three-dimensional π bands. Quantitative predictions for various thermodynamic and transport properties of MgB_2 were made in the framework of the two-band model.[11–14]

A large number of experimental data, in particular tunneling,[15,16] point contact measurements,[17–19] and heat capacity measurements,[20] directly support the concept of a double gap MgB_2. Intraband impurity scattering in both bands may vary in large limits, while interband scattering is always weak due to the disparity of σ- and π-band wave functions.[14] This explains the extremely weak suppression of T_c by impurities and the weak correlation between T_c and the resistivity. Therefore, a unique feature of the MgB_2 is that the two-gap nature of superconductivity persists even in the dirty limit for the intraband scattering rates.

Superconductivity in the two bands is characterized by different energy and length scales which show up in several properties of a superconductor. Particularly interesting are the properties of the mixed state. The *c*-axis Abrikosov vortex structure in MgB_2 was studied by STM in Ref. 21, which probes mainly the weakly superconducting π band. A large vortex core size compared to estimates based on H_{c2} and the rapid suppression of the apparent tunneling gap by small magnetic fields has been reported. These observations can be naturally explained within the two-band model.[22,23]

One of the most spectacular consequences of the two-band superconductivity is the unusual behavior of anisotropy factors for different physical parameters.[24] It was demonstrated that in clean MgB_2 samples the anisotropy of the London penetration depth[25,26] γ_λ has to be very different from the anisotropy of the upper critical field[27,28] γ_{c2}. Both anisotropy factors should strongly depend on temperature and have opposite temperature dependencies: γ_λ is expected to increase and γ_{c2} is expected to decrease with temperature. Strong temperature dependence of γ_{c2} has been reliably confirmed by experiment.[29–34] Typically, γ_{c2} drops from 5–6 at low temperatures down to ~ 2 near T_c.

In this paper we consider in detail the behavior of the upper critical field for different field orientations for the case of a dirty two-band superconductor with weak interband scattering. The model is based on the multiband generalization of the quasiclassical Usadel equations.[35] The same model has been used recently to describe vortex core structure in MgB_2.[22] The general equations for determination of the upper critical field within this model have been derived in a recent paper.[36] However, calculations in this paper have been done only for the case of small band anisotropies. In this paper we address the case of very high anisotropy in the quasi-2D band, more suitable for MgB_2.

We demonstrate that the strong temperature dependence of the H_{c2}-anisotropy exists also in the dirty case and therefore represents a general property of a two-band superconductor. The main reason for this dependence is the strong reduction of the in-plane upper critical field by the weak π band in the very narrow temperature region near T_c. This also leads to the significant upward curvature of the temperature dependence of the in-plane upper critical field near T_c. This behavior illustrates the breakdown of the anisotropic

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Ginzburg-Landau (GL) theory for the description of this superconductor. We demonstrate that, due to the large difference between microscopic coherence lengths in the c direction for the two bands, the anisotropic GL theory is applicable only within the extremely narrow temperature range near T_c.

We analyze the angular dependence of the upper critical field and show that it strongly deviates from the standard "effective-mass" dependence predicted by the anisotropic GL theory. Contrary to naive expectations, these deviations are strongest for temperatures quite close to T_c (at $T \sim 0.9T_c$) and only vanish for temperatures extremely close to T_c [for $(T_c-T)/T_c \lesssim 1\%$]. The angular dependence of the upper critical field has been studied in Ref. 41 for a clean two-band superconductor. It was shown that for the case of two weakly deformed spherical Fermi surfaces with opposite anisotropies the angular dependence also strongly deviates from the "effective-mass" law.

The paper is organized as follows. In Sec. II we present Usadel equations for a two-band superconductor and introduce parameters relevant for MgB_2. In Sec. III we derive an equation for the upper critical field in the c direction and obtain the exact asymptotics at small and high temperatures. In Sec. IV we consider the in-plane upper critical field. We derive general equations for determination of this field and study the solutions of these equations in different regimes. We demonstrate that the GL result for the in-plane H_{c2} is valid only within a very narrow range of temperatures. We also numerically calculate in-plane H_{c2} and the anisotropy parameter γ_{c2} in the whole temperature range. In Sec. V we study the angular dependence of the upper critical field and analyze quantitatively the deviations from the effective-mass law.

II. THE MODEL: USADEL EQUATIONS FOR A TWO-BAND SUPERCONDUCTOR

We consider a two-band superconductor with weak interband impurity scattering and rather strong intraband scattering rates exceeding the corresponding energy gaps (dirty limit). In this case the quasiclassical Usadel equations[35] are applicable within each band. The mixed state in this case is described by the system of coupled Usadel equations[22,35]

$$\omega F_\alpha - \sum_j \frac{\mathcal{D}_{\alpha,j}}{2}\left[G_\alpha\left(\nabla_j - \frac{2\pi i}{\Phi_0}A_j\right)^2 F_\alpha - F_\alpha \nabla_j^2 G_\alpha\right] = \Delta_\alpha G_\alpha, \tag{1a}$$

$$\Delta_\alpha = 2\pi T \sum_{\beta,n} \Lambda_{\alpha\beta} F_\beta, \tag{1b}$$

where $\alpha = 1,2$ is the band index, $j = x,y,z$ is the coordinate index, $\hat{\Lambda}$ is the matrix of effective coupling constants, defined as $\Lambda_{\alpha,\beta} = \lambda_{\alpha,\beta} - \mu^*_{\alpha,\beta}$ where $\lambda_{\alpha,\beta}$ are the electron-phonon coupling constants and $\mu^*_{\alpha,\beta}$ are the renormalized Coulomb pseudopotentials, $\mathcal{D}_{\alpha,j}$ are diffusion constants, which determine the coherence lengths $\xi_{\alpha,j} = \sqrt{\mathcal{D}_{\alpha,j}/2\pi T_c}$, G_α, F_α, and Δ_α are normal and anomalous Green's functions and the pair potential, respectively, and $\omega = 2\pi T(s+1/2)$ are Matsubara frequencies. Bearing in mind the application to MgB_2, in our notation, index 1 corresponds to σ bands and index 2 to π bands. All bands are isotropic in the xy plane, $\mathcal{D}_{\alpha x} = \mathcal{D}_{\alpha y}$ and anisotropic in the xz plane with the anisotropy ratios $\gamma_\alpha = \sqrt{\mathcal{D}_{\alpha x}/\mathcal{D}_{\alpha z}}$. The multigap Usadel equations for general case, taking into account also interband scattering, have been recently derived in Ref. 36.

The self-consistency equation can be rewritten in the form

$$W_1\Delta_1 - W_{12}\Delta_2 = 2\pi T \sum_{\omega>0}\left(F_1 - \frac{\Delta_1}{\omega}\right) + \Delta_1 \ln\frac{T_c}{T}, \tag{2a}$$

$$-W_{21}\Delta_1 + W_2\Delta_2 = 2\pi T \sum_{\omega>0}\left(F_2 - \frac{\Delta_2}{\omega}\right) + \Delta_2 \ln\frac{T_c}{T}, \tag{2b}$$

with the following matrix $W_{\alpha\beta}$

$$W_1 = \frac{-A + \sqrt{A^2 + \Lambda_{12}\Lambda_{21}}}{\mathrm{Det}}, \quad W_2 = \frac{A + \sqrt{A^2 + \Lambda_{12}\Lambda_{21}}}{\mathrm{Det}},$$

$$W_{12} = \Lambda_{12}/\mathrm{Det}, \quad W_{21} = \Lambda_{21}/\mathrm{Det}, \tag{3}$$

$$A = (\Lambda_{11} - \Lambda_{22})/2, \quad \mathrm{Det} = \Lambda_{11}\Lambda_{22} - \Lambda_{12}\Lambda_{21},$$

$$W_1 W_2 = W_{12} W_{21}.$$

The electron-phonon interaction in MgB_2 was calculated from first principles in a number of papers.[7,11,12] Here we use the effective coupling constants $\Lambda_{\alpha,\beta}$ from Ref. 12: $\Lambda_{11} \approx 0.81$, $\Lambda_{22} \approx 0.278$, $\Lambda_{12} \approx 0.115$, $\Lambda_{21} \approx 0.091$, from which we obtain the values of $W_{\alpha\beta}$ used in numerical calculations

$$W_1 \approx 0.088, \quad W_2 \approx 2.56, \quad W_{12} \approx 0.535, \quad W_{21} \approx 0.424. \tag{4}$$

The relative role of the weak band is characterized by the ratio $S_{12} \equiv W_1/W_2$,[37] which in the case of MgB_2 is rather small, $S_{12} \approx 0.034$. This ratio will be used below as a small parameter in our model to derive various approximations for the upper critical field. Another important small parameter is the ratio of diffusion coefficients in the σ band $\mathcal{D}_{1z}/\mathcal{D}_{1x}$. We will show in this paper that these two parameters S_{12} and $\mathcal{D}_{1z}/\mathcal{D}_{1x}$ influence H_{c2} differently for parallel field at high and low temperatures thus causing the temperature dependence of the anisotropy. In the following we consider separately the cases when the field is parallel and perpendicular to the ab plane.

III. FIELD IN THE c-DIRECTION

Let us first study the case when the magnetic field is oriented along the c axis. The upper critical field is determined by the linearized Usadel equation

$$\omega F_\alpha + \frac{\mathcal{D}_{\alpha x}}{2}\left[-\nabla_x^2 F_\alpha + \left(\frac{2\pi H x}{\Phi_0}\right)^2 F_\alpha\right] = \Delta_\alpha \tag{5}$$

and self-consistency Eq. (2). Solving these equations, we arrive at the equation for $H_{c2}^\perp$ [symbol $\perp$ denotes the field direction perpendicular to the (ab)-plane]

$$\ln\frac{1}{t}-g\left(\frac{H_{c2}^{\perp}}{tH_1}\right)=-\frac{W_1\left[\ln\frac{1}{t}-g\left(\frac{H_{c2}^{\perp}}{tH_2}\right)\right]}{W_2-\left[\ln\frac{1}{t}-g\left(\frac{H_{c2}^{\perp}}{tH_2}\right)\right]}, \tag{6}$$

where $t=T/T_c$, $H_\alpha\equiv 2T_c\Phi_0/\mathcal{D}_{\alpha x}$, $g(x)=\psi(1/2+x)-\psi(1/2)$, and $\psi(x)$ is a digamma function. We also obtain a relation between Δ_{01} and Δ_{02} near $H_{c2}^{\perp}$

$$\Delta_{02}=\frac{W_{21}\Delta_{01}}{W_2-\ln\frac{1}{t}+g\left(\frac{H_{c2}^{\perp}}{tH_2}\right)}. \tag{7}$$

In the absence of coupling to the weak π band ($W_1=0$) or in the case of identical diffusion constants ($\mathcal{D}_{1x}=\mathcal{D}_{2x}$) the upper critical field H_{c2}^s is given by the standard Maki–de Gennes equation[39,40]

$$\ln(1/t)=g[H_{c2}^s/(tH_1)]. \tag{8}$$

The well-known asymptotic solutions of this equation at low and high temperatures are, respectively,

$$\frac{H_{c2}^s(t)}{H_1}=\begin{cases} e^{-\gamma_E}/4\approx 0.140, & t\ll 1,\\ 2(1-t)/\pi^2\approx 0.203(1-t), & 1-t\ll 1,\end{cases} \tag{9}$$

where $\gamma_E\approx 0.577$ is Euler constant. In the temperature range near T_c one can obtain from Eq. (6) the following simple expression for $H_{c2}^{\perp}$ for arbitrary ratio $S_{12}\equiv W_1/W_2$:

$$\frac{H_{c2}^{\perp}}{H_1}=\frac{2(1+S_{12})(1-t)}{\pi^2(1+S_{12}\mathcal{D}_{2x}/\mathcal{D}_{1x})}. \tag{10}$$

At small temperatures, $T\ll T_c$, Eq. (6) also has an exact solution (see also Ref. 36)

$$H_{c2}(0)=H_{c2}^s(0)\exp\left(-\frac{W_1+W_2-\ln(r_x)}{2}+\sqrt{\frac{(W_1+W_2-\ln(r_x))^2}{4}+W_1\ln(r_x)}\right) \tag{11}$$

with $r_x\equiv\mathcal{D}_{1x}/\mathcal{D}_{2x}$. For MgB_2 the parameter W_1 is small and typically the inequality $W_1\ln(r_x)\ll[W_2-\ln(r_x)]^2/4$ is valid. In this case we can expand Eq. (11) with respect to W_1 and obtain a much simpler result

$$H_{c2}(0)\approx H_{c2}^s(0)\left(1+\frac{W_1\ln(\mathcal{D}_{1x}/\mathcal{D}_{2x})}{W_2-\ln(\mathcal{D}_{1x}/\mathcal{D}_{2x})}\right). \tag{12}$$

The π band strongly influences the upper critical field only if it is very dirty, $\mathcal{D}_{2x}\ll\mathcal{D}_{1x}\exp(-W_2)$. In this limit we obtain[38]

$$H_{c2}(0)\approx H_{c2}^{(2)}(0)\exp(-W_2)$$

with $H_{c2}^{(2)}(0)\equiv[\exp(-\gamma_E)/4]H_2$.

For the case $W_1\ll W_2$ realized in MgB_2, the upper critical field is typically determined by the strong band (except for the limit of very small diffusivity $\mathcal{D}_{2x}$ in the second band). A small correction due to the weak band can be found from Eq. (6) using an expansion with respect to the small parameter $S_{12}\equiv W_1/W_2$. In particular, we found very simple expressions for the slope of H_{c2} at T_c and $H_{c2}(0)$:

$$\frac{dH_{c2}}{dT}\approx\frac{dH_{c2}^s}{dT}\left(1+S_{12}\frac{\mathcal{D}_{1x}-\mathcal{D}_{2x}}{D_{1x}}\right), \tag{13a}$$

$$H_{c2}(0)\approx H_{c2}^s(0)\left(1+S_{12}\ln\frac{\mathcal{D}_{1x}}{\mathcal{D}_{2x}}\right). \tag{13b}$$

The signs of the above corrections to the universal curve following from Eq. (8) are positive if $D_{2x}<D_{1x}$ and negative for $D_{2x}>D_{1x}$.

IV. FIELD IN THE *a* DIRECTION

A. General relations

The upper critical field in the a direction ($\equiv y$ direction) is determined by the linear equations for the Green's functions F_α in two bands

$$\omega F_\alpha-\frac{\mathcal{D}_{\alpha x}}{2}\nabla_x^2F_\alpha+\frac{\mathcal{D}_{\alpha z}}{2}\left(\frac{2\pi Hx}{\Phi_0}\right)^2F_\alpha=\Delta_\alpha \tag{14}$$

with $\omega=2\pi T(s+1/2)$ and the self-consistency conditions (2). A technical difficulty of this problem is that, due to the difference in the anisotropy factors for the two bands γ_α, the harmonic oscillator operators in Eq. (14) have unmatching sets of eigenstates. We will use an expansion with respect to the eigenfunctions (Landau levels) of the strong (first) band $\Psi_n(x)$, which are defined as solutions of the oscillator equation

$$\frac{\mathcal{D}_{1z}}{2}\left(\frac{2\pi H}{\Phi_0}\right)^2x^2\Psi_n-\frac{\mathcal{D}_{1x}}{2}\nabla_x^2\Psi_n=\varepsilon_n\Psi_n. \tag{15}$$

In particular, the eigenvalues ε_n and ground state eigenfunction are given by

$$\varepsilon_n=\sqrt{\mathcal{D}_{1z}\mathcal{D}_{1x}}\,\frac{2\pi H}{\Phi_0}(n+1/2), \tag{16}$$

$$\Psi_0(x)=\left(\frac{2H}{\gamma_1\Phi_0}\right)^{1/4}\exp\left(-\frac{\pi Hx^2}{\gamma_1\Phi_0}\right), \tag{17}$$

where $\gamma_\alpha=\sqrt{\mathcal{D}_{\alpha x}/\mathcal{D}_{\alpha z}}$ are the band anisotropies. In the case of MgB_2 the first band is quasi-two-dimensional, i.e., $\gamma_1\gg 1,\gamma_2$. Substituting expansions

$$\Delta_\alpha(x)=\sum_n\Delta_{\alpha,n}\Psi_n(x);\ F_\alpha=\sum_n F_{\alpha,n}\Psi_n(x)$$

into Eq. (14), we obtain

$$F_{1,n}=\frac{\Delta_{1,n}}{\omega+\varepsilon_n}, \tag{18a}$$

$$\omega F_{2,n}+\sum_{m=0}^{\infty}\epsilon_{nm}F_{2,m}=\Delta_{2,n} \tag{18b}$$

with $\epsilon_{nm}=\langle(\mathcal{D}_{2z}/2)(2\pi H/\Phi_0)^2x^2-(\mathcal{D}_{2x}/2)\nabla_x^2\rangle_{nm}$. The only nonzero matrix elements ϵ_{nm} are at $m=n$ and $m=n\pm 2$:

$$\epsilon_{nn}=\frac{\pi H}{\Phi_0}\sqrt{\mathcal{D}_{2x}\mathcal{D}_{2z}}\left(n+\frac{1}{2}\right)\left(\frac{\gamma_2}{\gamma_1}+\frac{\gamma_1}{\gamma_2}\right), \tag{19a}$$

$$\epsilon_{n-2,n}=\epsilon_{n,n-2}=\frac{\pi H\sqrt{\mathcal{D}_{2x}\mathcal{D}_{2z}}}{\Phi_0}\frac{\sqrt{n(n-1)}}{2}\left(\frac{\gamma_2}{\gamma_1}-\frac{\gamma_1}{\gamma_2}\right). \tag{19b}$$

Neglecting the small ratio γ_1/γ_2 in comparison with γ_2/γ_1 we obtain

$$\epsilon_{nn}\approx\left(n+\frac{1}{2}\right)w_2, \tag{20a}$$

$$\epsilon_{n-2,n}=\epsilon_{n,n-2}\approx-\frac{\sqrt{n(n-1)}}{2}w_2 \tag{20b}$$

with $w_2\equiv(\pi H/\Phi_0)\mathcal{D}_{2z}\gamma_1$. This approximation for the matrix elements is equivalent to the local approximation for the F function in the π band described in the Appendix. Therefore, we can rewrite the equation for F_{2n} as

$$\omega F_{2n}+\epsilon_{n,n-2}F_{2,n-2}+\epsilon_{n,n}F_{2,n}+\epsilon_{n,n+2}F_{2,n}=\Delta_{2,n}. \tag{21}$$

At $n=0$ the term $\epsilon_{n,n-2}F_{2,n-2}$ has to be skipped. This means that even Landau levels $n=2i$ do not mix with the odd Landau level $n=2i+1$. For the calculation of the upper critical field it is sufficient to consider only even Landau levels. The self-consistency equations in terms of the expansion coefficients are given by

$$W_1\Delta_{1,n}-W_{12}\Delta_{2,n}=2\pi T\sum_{\omega>0}\left(\frac{1}{\omega+\varepsilon_n}-\frac{1}{\omega}\right)\Delta_{1,n}+\Delta_{1,n}\ln\frac{1}{t}, \tag{22a}$$

$$-W_{21}\Delta_{1,n}+W_2\Delta_{2,n}=2\pi T\sum_{\omega>0}\left(F_{2,n}-\frac{\Delta_{2,n}}{\omega}\right)+\Delta_{2,n}\ln\frac{1}{t}. \tag{22b}$$

To simplify the analysis further we introduce the reduced variables

$$z=\omega/w_2=t_2(s+1/2),\quad \tilde{F}_{2,i}=w_2F_{2,2i}$$

with $t_2\equiv 2\pi T/w_2\equiv 2\Phi_0T/(H\mathcal{D}_{2z}\gamma_1)$ and s is the Matsubara index. Then equations for $\tilde{F}_{2,i}(z)$ are given by

$$\left(z+\frac{1}{2}\right)\tilde{F}_{2,0}-(1/\sqrt{2})\tilde{F}_{2,1}=\Delta_{2,0}, \tag{23a}$$

$$-\sqrt{i(i-1/2)}\tilde{F}_{2,i-1}+(z+2i+1/2)\tilde{F}_{2,i}-\sqrt{(i+1)(i+1/2)}\tilde{F}_{2,i+1}=\Delta_{2,2i}. \tag{23b}$$

The formal solution of Eq. (23) is given by

$$\tilde{F}_{2,i}(z)=\sum_{j=0}^{\infty}A_{i,j}(z)\Delta_{2,2j},$$

where the matrix $A_{i,j}(z)$ is defined as solution of equations

$$\left(z+\frac{1}{2}\right)A_{0,j}-\sqrt{1/2}A_{1,j}=\delta_{0,j}, \tag{24a}$$

$$-\sqrt{i(i-1/2)}A_{i-1,j}+(z+2i+1/2)A_{i,j}-\sqrt{(i+1)(i+1/2)}A_{i+1,j}=\delta_{i,j}. \tag{24b}$$

Using this solution we represent the self-consistency conditions for even Landau levels in the form

$$W_1\Delta_{1,2i}-W_{12}\Delta_{2,2i}=\Delta_{1,2i}\left[\ln\frac{1}{t}-g\left(\frac{H(4i+1)}{tH_1^{\parallel}}\right)\right], \tag{25a}$$

$$-W_{21}\Delta_{1,2i}+W_2\Delta_{2,2i}=\sum_{j=0}^{\infty}U_{i,j}(t_2)\Delta_{2,2j}+\Delta_{2,2i}\ln\frac{1}{t} \tag{25b}$$

with

$$H_1^{\parallel}\equiv\frac{2T_c\Phi_0}{\sqrt{\mathcal{D}_{1z}\mathcal{D}_{1x}}}, \tag{26}$$

where $\parallel$ denotes the field direction parallel to the (ab) plane and

$$U_{i,j}(t_2)=t_2\sum_{s=0}^{\infty}\left(A_{i,j}[t_2(s+1/2)]-\frac{\delta_{i,j}}{t_2(s+1/2)}\right). \tag{27}$$

We again used notations $t=T/T_c$ and $g(x)\equiv\psi(1/2+x)-\psi(1/2)$. We show in the Appendix that $U_{i,j}(t_2)$ can also be related with the oscillator matrix element of the function $g[x^2/t_2]$

$$U_{i,j}(t_2)=\int_{-\infty}^{\infty}dx\,\psi_{2i}(x)\psi_{2j}(x)g[x^2/t_2],$$

$$\psi_n(x)=\frac{\exp(-x^2/2)H_n(x)}{\pi^{1/4}\sqrt{2^n n!}},$$

where $H_n(x)$ are Hermite polynomials.

B. Temperatures not close to T_c: High-field approximation in the π band

The overall behavior is determined by the value of dimensionless parameter t_2, which depends on field and temperature. To evaluate this parameter we represent it in the form

$$t_2=\frac{\mathcal{D}_{1z}}{\mathcal{D}_{2z}}\frac{tH_1^{\parallel}}{H}. \tag{28}$$

Because $\mathcal{D}_{1z}\ll\mathcal{D}_{2z}$ and at low temperatures $H\lesssim H_1^{\parallel}$, the parameter t_2 is much smaller than unity almost in the whole temperature range except a very narrow region near T_c. The

parameter t_2 becomes of the order of one only at $(T_c - T)/T_c \sim \mathcal{D}_{1z}/\mathcal{D}_{2z} \ll 1$. Outside this region one can replace summation with respect to the Matsubara index s in Eq. (27) by integration, which allows us to reduce it to the following form:

$$U_{i,j}(t_2) \approx f_{i,j} + (\ln t_2 - \gamma_E - 2\ln 2)\,\delta_{i,j},$$

where

$$f_{i,j} = \int_0^\infty dz \left(A_{i,j}(z) - \frac{\delta_{i,j}}{z+1} \right) \tag{29}$$

$$= -4 \int_0^\infty dx\, \psi_{2i}(x)\, \psi_{2j}(x) \ln(x) \tag{30}$$

is the universal matrix of constants (in particular, $f_{0,0} = \gamma_E + 2\ln 2 \approx 1.96$). Using this representation, we transform Eq. (25b) to the form

$$-W_{21}\Delta_{1,2i} + W_2 \Delta_{2,2i} = \sum_{j=0}^{\infty} f_{i,j} \Delta_{2,2j} - \left[\ln\left(\frac{H}{H_1^\parallel} \frac{\mathcal{D}_{2z}}{\mathcal{D}_{1z}} \right) + \gamma_E + 2\ln 2 \right] \Delta_{2,2i}. \tag{31}$$

We refer to this approximation as the high-field regime in the π band. The last equation in combination with Eq. (25a) determines the upper critical field along the a direction within the "high-field in the π-band" regime, at $(T_c - T)/T_c \gg \mathcal{D}_{1z}/\mathcal{D}_{2z}$. Note that in this approximation the temperature dependence exists only in Eq. (25a). Therefore, once computed, matrix $f_{i,j}$ allows us to calculate the temperature dependence of $H_{c2}^\parallel$ in a wide temperature range.

Excluding $\Delta_{1,2i}$

$$\Delta_{1,2i} = \frac{W_{12}}{W_1 - \left[\ln\frac{1}{t} - g\left(\frac{H(4i+1)}{tH_1^\parallel} \right) \right]} \Delta_{2,2i}, \tag{32}$$

we also derive equations containing only $\Delta_{2,2i}$:

$$\left[\ln\left(\frac{H}{H_1^\parallel} \frac{\mathcal{D}_{2z}}{\mathcal{D}_{1z}} \right) + \gamma_E + 2\ln 2 + \frac{-W_2 \left[\ln\frac{1}{t} - g\left(\frac{H(4i+1)}{tH_1^\parallel} \right) \right]}{W_1 - \left[\ln\frac{1}{t} - g\left(\frac{H(4i+1)}{tH_1^\parallel} \right) \right]} \Delta_{2,2i} - \sum_{j=0}^{\infty} f_{i,j} \Delta_{2,2j} \right. = 0. \tag{33}$$

The upper critical field $H = H_{c2}^\parallel$ is given by the maximum root of the determinant of this linear system. An approximate solution can be obtained neglecting coupling to the higher Landau levels in the self-consistency equations leading to the following equation for $H_{c2}^\parallel$:

$$\ln\frac{1}{t} - g\left(\frac{H_{c2}^\parallel}{tH_1^\parallel} \right) = \frac{W_1 \ln\left(\frac{H_{c2}^\parallel}{H_1^\parallel} \frac{\mathcal{D}_{2z}}{\mathcal{D}_{1z}} \right)}{W_2 + \ln\left(\frac{H_{c2}^\parallel}{H_1^\parallel} \frac{\mathcal{D}_{2z}}{\mathcal{D}_{1z}} \right)}. \tag{34}$$

Since $W_1 \ll 1$, the right hand side of Eq. (34) is small. As a result, in the limit of small t_2 the parallel critical field is close to the solution of the Maki–de Gennes equation (8) with the effective parameter H_1 replaced by $H_1^\parallel$ from Eq. (26). A small correction from the weak band can be estimated at low temperatures

$$H_{c2}^\parallel(0) \approx H_{c2}^{s\parallel}(0) \left(1 - \frac{W_1(\ln(\mathcal{D}_{2z}/\mathcal{D}_{1z}) - 1.96)}{W_2 + \ln(\mathcal{D}_{2z}/\mathcal{D}_{1z}) - 1.96} \right) \tag{35}$$

with $H_{c2}^{s\parallel}(0) = [\exp(-\gamma_E)/4] H_1^\parallel$.

Combining Eqs. (12) and (35) we obtain an estimate for the anisotropy factor $\gamma_{c2}(T) = H_{c2}^\parallel(T)/H_{c2}^\perp(T)$ at low temperatures

$$\gamma_{c2}(0) \approx \gamma_1 \left(1 + \frac{W_1 \ln(\mathcal{D}_{2x}/\mathcal{D}_{1x})}{W_2 + \ln(\mathcal{D}_{2x}/\mathcal{D}_{1x})} - \frac{W_1(\ln(\mathcal{D}_{2z}/\mathcal{D}_{1z}) - 1.96)}{W_2 + \ln(\mathcal{D}_{2z}/\mathcal{D}_{1z}) - 1.96} \right). \tag{36}$$

As follows from this equation, the anisotropy of H_{c2} at $T = 0$ is very close to the anisotropy of the first band

$$\gamma_{c2}(0) \approx \gamma_1 \equiv \sqrt{\mathcal{D}_{1x}/\mathcal{D}_{1z}}. \tag{37}$$

To estimate the ratio $\mathcal{D}_{1x}/\mathcal{D}_{1z}$ we use the relation $\mathcal{D}_{1x,z} = v_{F1x,z}^2 \tau_{1x,z}$ between the diffusion coefficients $\mathcal{D}_{1x,z}$, Fermi velocities in the first band $v_{F1x,z}$ and scattering times $\tau_{1x,z}$ along x and z directions. If we assume the isotropic scattering, $\tau_{1x} \approx \tau_{1z}$, the value of $\gamma_{c2}(0)$ is determined by the anisotropy of Fermi velocities in the first band $\gamma_{c2}(0) \approx \sqrt{\mathcal{D}_{1x}/\mathcal{D}_{1z}} \approx v_{F1x}/v_{F1z}$, which for MgB_2 gives $\gamma_{c2}(0) \approx 6$ (see Ref. 13). The assumption of isotropic scattering can be violated if a sizable amount of p-wave scattering exists, i.e., γ_1 may depend on type of impurities. On the other hand, the isotropic-scattering value $\gamma_1 \approx 6$ is consistent with the experimental data on the H_{c2} anisotropy in MgB_2 single crystals.[29–33]

C. Ginzburg-Landau region

In the close vicinity of T_c (exact criterion will be established below) one can solve Eq. (14) using the gradient expansion

$$F_\alpha \approx \frac{\Delta_\alpha}{\omega} - \frac{1}{\omega^2} \left[-\frac{\mathcal{D}_{\alpha x}}{2} \nabla_x^2 \Delta_\alpha + \frac{\mathcal{D}_{\alpha z}}{2} \left(\frac{2\pi H x}{\Phi_0} \right)^2 \Delta_\alpha \right].$$

Substituting this expansion into the self-consistency conditions and using relation $2\pi T \Sigma_{\omega>0}(1/\omega^2) = \pi/4T$, we obtain

$$W_1\Delta_1 - W_{12}\Delta_2 = -\left(-\xi_{1x}^2\nabla_x^2\Delta_1 + \xi_{1z}^2\left(\frac{2\pi Hx}{\Phi_0}\right)^2\Delta_1\right) + \Delta_1\ln\frac{1}{t}, \tag{38a}$$

$$-W_{21}\Delta_1 + W_2\Delta_2 = -\left(-\xi_{2x}^2\nabla_x^2\Delta_2 + \xi_{2z}^2\left(\frac{2\pi Hx}{\Phi_0}\right)^2\Delta_2\right) + \Delta_2\ln\frac{1}{t} \tag{38b}$$

with $\xi_{\alpha i}^2 \equiv \pi\mathcal{D}_{\alpha i}/(8T)$. Near T_c we can look for solution for Δ_2 in the form

$$\Delta_2 \approx \frac{W_{21}}{W_2}\Delta_1 + \delta_2,$$

where δ_2 is a small correction, for which we obtain from Eq. (38b)

$$-W_{12}\delta_2 \approx -\left(-\xi_{1x}^2\nabla_x^2\Delta_1 + \xi_{1z}^2\left(\frac{2\pi Hx}{\Phi_0}\right)^2\Delta_1\right) + \Delta_1\ln\frac{1}{t}.$$

Substituting this result into Eq. (38a) we obtain the linear Ginzburg-Landau (GL) equation for Δ_1

$$-\xi_x^2\nabla_x^2\Delta_1 + \xi_z^2\left(\frac{2\pi Hx}{\Phi_0}\right)^2\Delta_1 - \Delta_1\ln\frac{1}{t} = 0, \tag{39}$$

in which the averaged coherence lengths ξ_i, with $i=x,z$, are defined as

$$\xi_i = \sqrt{\frac{\xi_{1i}^2 + S_{12}\xi_{2i}^2}{1+S_{12}}}. \tag{40}$$

From this equation we immediately obtain the usual GL result for the upper critical field at $T \to T_c$

$$H_{c2} = \frac{\Phi_0(1-t)}{2\pi\xi_x\xi_z}. \tag{41}$$

For comparison with numerical results at lower temperature we also provide $H_{c2}^{\parallel}$ in units of $H_1^{\parallel}$

$$\frac{H_{c2}^{\parallel}}{H_1^{\parallel}} = \frac{2\sqrt{\mathcal{D}_{1x}\mathcal{D}_{1z}}(1+S_{12})(1-t)}{\pi^2\sqrt{(\mathcal{D}_{1x}+S_{12}\mathcal{D}_{2x})(\mathcal{D}_{1z}+S_{12}\mathcal{D}_{2z})}} \approx \frac{2}{\pi^2\sqrt{1+S_{12}\mathcal{D}_{2z}/\mathcal{D}_{1z}}}(1-t) \tag{42}$$

for $W_1 \ll W_2$ and $\mathcal{D}_{1x} \sim \mathcal{D}_{2x}$. Due to the strong inequality $\mathcal{D}_{2z} \gg \mathcal{D}_{1z}$, in the vicinity of T_c the three-dimensional band strongly reduces the upper critical field. This reduction leads to a strong temperature dependence of the H_{c2} anisotropy γ_{c2}.

Let us compare anisotropy parameters at low T and near T_c. According to Eq. (37), the anisotropy of H_{c2} at low temperatures is close to the anisotropy of the σ band $\gamma_{c2}(0) \approx \sqrt{\mathcal{D}_{1x}/\mathcal{D}_{1z}}$, while the anisotropy ratio near T_c follows from Eqs. (10) and (42)

$$\gamma_{c2}(T_c) \equiv \gamma_{\rm GL} = \gamma_1\sqrt{\frac{1+S_{12}\mathcal{D}_{2x}/\mathcal{D}_{1x}}{1+S_{12}\mathcal{D}_{2z}/\mathcal{D}_{1z}}} \approx \frac{\gamma_1}{\sqrt{1+S_{12}\mathcal{D}_{2z}/\mathcal{D}_{1z}}}. \tag{43}$$

Thus the ratio $\gamma_{c2}(0)/\gamma_{c2}(T_c)$ is roughly given by

$$\frac{\gamma_{c2}(0)}{\gamma_{c2}(T_c)} \approx \sqrt{1+S_{12}\mathcal{D}_{2z}/\mathcal{D}_{1z}}. \tag{44}$$

The larger the ratio of transport constants $\mathcal{D}_{1z}/\mathcal{D}_{2z}$, the stronger the suppression of $\gamma_{c2}(T)$ with increasing temperature.

According to Eq. (44), strong temperature dependence of H_{c2} anisotropy appears as an interplay of two small parameters: pairing interaction ratio S_{12} and the ratio of diffusion constants $D_{1z}/D_{2z} \propto v_{1z}^2\tau_{1z}/(v_{2z}^2\tau_{2z})$. This important property was first pointed out in Refs. 27,28 within the clean limit. Therefore the above effect is quite general and does not depend on the details of the theoretical model. The main reason is the strong reduction of the in-plane upper critical field by the weak π band in the narrow temperature region near T_c.

We obtain now the applicability criterion for the GL expansion. Typical scales of the order parameter variation near T_c are given by the GL coherence lengths $\xi_i^{\rm GL}(T) = \xi_i/\sqrt{1-t}$, with $i=x,y$ and ξ_i given by Eq. (40). The GL expansion is valid until the GL coherence lengths are larger than the corresponding microscopic coherence lengths in both bands, $\xi_i^{\rm GL}(T) > \xi_{\alpha,i}$. Because of the strong inequality $\xi_{1,z} \ll \xi_{2,z}$, the most sensitive condition is

$$\xi_z^{\rm GL}(T) > \xi_{2,z} \tag{45}$$

leading to the following condition for the GL temperature range:

$$\frac{T_c - T}{T_c} < \max\left(\frac{\xi_{1z}^2}{\xi_{2z}^2}, S_{12}\right). \tag{46}$$

Because $\xi_{1z} \ll \xi_{2z}$ and $S_{12} \ll 1$, the applicability of the GL approach is limited to an extremely narrow temperature range near T_c, i.e., the situation is very different from the usual single-band superconductors. The comparison of the GL asymptotic with the exact solution is shown in Fig. 1, where the narrowness of the GL region is demonstrated in the inset.

D. Numerical solution in the whole temperature range

In the whole temperature range, for an arbitrary value of the parameter t_2, the problem can be solved numerically. The solution consists of three steps: (i) the matrix $A_{i,j}(z)$ has to be found from Eqs. (24) for the series of reduced Matsubara frequencies $z = t_2(s+1/2)$, (ii) the matrix $U_{i,j}$ has to be computed by summation over Matsubara indices s (27), and (iii) the upper critical field has to be found as the maximum root

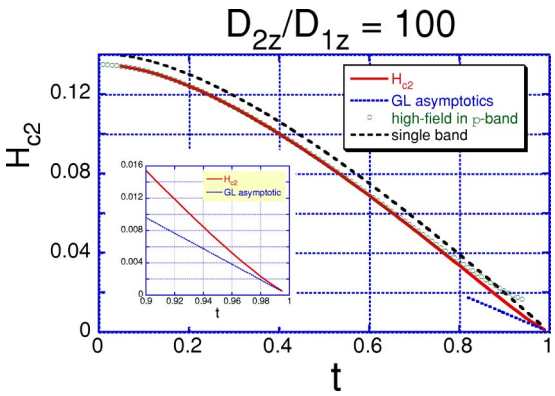

FIG. 1. Temperature dependence of the upper critical field in the a direction normalized to $H_1^{\parallel}$ defined in Eq. (26). Single-band curve is normalized to the corresponding scale H_1. Solid circles show the dependence obtained within the "high-field in the π-band" approximation [Eqs. (29) and (31)]. Inset: comparison between the exact solution and the GL asymptotics Eq. (42).

of the determinant of the linear system represented by Eqs. (25a) and (25b). Due to the fast decrease of the nondiagonal matrix elements $U_{i,j}$ for $|i-j|\gg 1$, sufficient accuracy is achieved for dimensions of a matrix of less than 30. The result of calculation of the parallel upper critical field is shown in Fig. 1 where the ratio $\mathcal{D}_{2z}/\mathcal{D}_{1z}=100$ relevant to MgB_2 was used. Note that when plotted in reduced units, the deviations of both ratios $H_{c2}^{\parallel}/H_1^{\parallel}$ and $H_{c2}^{\perp}/H_1^{\perp}$ from the universal single band curve are small (except from the region near T_c, in the GL region), in accordance with the above discussion. However, one should keep in mind the large difference in magnitudes of the characteristic scales $H_1^{\parallel}$ and $H_1^{\perp}$.

Numerically calculated temperature dependence of the anisotropy factor for several ratios $\mathcal{D}_{2z}/\mathcal{D}_{1z}$ is shown in Fig. 2. The anisotropy ratio drops with the increase of temperature, in accordance with the estimate (44). This result agrees qualitatively with the calculations within the clean limit model in Refs. 27,28 and with recent measurements of temperature-dependent anisotropy in MgB_2.[29–33] In experiment the change in anisotropy typically is distributed over wider temperature range than it is suggested by the theory.

V. TILTED FIELDS

The upper critical field for magnetic field tilted at angle θ with respect to the z axis in the (zy) plane is determined by

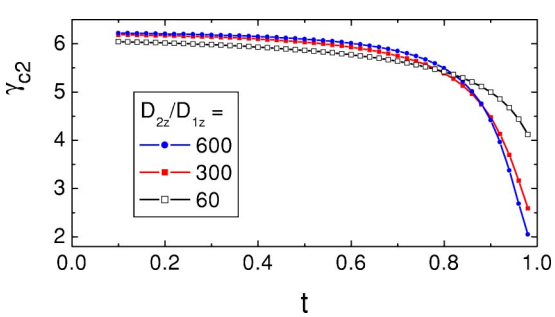

FIG. 2. Temperature dependence of the anisotropy of the upper critical field for several ratios $\mathcal{D}_{2z}/\mathcal{D}_{1z}$.

the coupled linear equations for the Green's functions F_α in two bands

$$\omega F_\alpha - \frac{\mathcal{D}_{\alpha x}}{2}\nabla_x^2 F_\alpha + \frac{\mathcal{D}_\alpha(\theta)}{2}\left(\frac{2\pi H x}{\Phi_0}\right)^2 F_\alpha = \Delta_\alpha \tag{47}$$

with

$$\mathcal{D}_\alpha(\theta) = \mathcal{D}_{\alpha x}\cos^2\theta + \mathcal{D}_{\alpha z}\sin^2\theta \tag{48}$$

and the self-consistency conditions (2).

Therefore the H_{c2} problem of the upper critical field in tilted field reduces to the in-plane H_{c2} problem by substitution $\mathcal{D}_{\alpha z}\to\mathcal{D}_\alpha(\theta)$. It is convenient to introduce the angular-dependent anisotropy parameters

$$\gamma_\alpha(\theta) \equiv \sqrt{\frac{\mathcal{D}_{\alpha x}}{\mathcal{D}_\alpha(\theta)}} = \frac{\gamma_\alpha}{\sqrt{\gamma_\alpha^2\cos^2\theta + \sin^2\theta}}. \tag{49}$$

Such defined anisotropy parameters vary from 1 to γ_α when angle varies from 0 to $\pi/2$.

Following the route of the previous section, we again use expansion with respect to the Landau levels of the strong band, defined by Eq. (17) with $\mathcal{D}_{1z}\to\mathcal{D}_1(\theta)$. The F function of the strong band is given by

$$F_{1,n} = \frac{\Delta_{1,n}}{\omega + \varepsilon_n(\theta)}$$

with the eigenvalue

$$\varepsilon_n(\theta) = 2\pi T\frac{H}{tH_1(\theta)}(2n+1),$$

$$H_1(\theta) = \frac{2T_c\Phi_0}{\sqrt{\mathcal{D}_1(\theta)\mathcal{D}_{1x}}}.$$

The matrix elements for the harmonic oscillator operator of the weak band are given by

$$\epsilon_{nn} = \frac{\pi H}{\Phi_0}\mathcal{D}_2(\theta)\gamma_1(\theta)\left(n+\frac{1}{2}\right)\left[1+\left(\frac{\gamma_2(\theta)}{\gamma_1(\theta)}\right)^2\right]$$
$$= \frac{2\pi T}{t_2(\theta)}[1+\alpha_\gamma(\theta)]\left(n+\frac{1}{2}\right)$$

$$\epsilon_{n,n-2} = -\frac{\pi H}{\Phi_0}\frac{\sqrt{n(n-1)}}{2}\mathcal{D}_2(\theta)\gamma_1(\theta)\left[1-\left(\frac{\gamma_2(\theta)}{\gamma_1(\theta)}\right)^2\right]$$
$$= -\frac{2\pi T}{t_2(\theta)}[1-\alpha_\gamma(\theta)]\frac{\sqrt{n(n-1)}}{2}$$

with

$$t_2(\theta) = \frac{2T\Phi_0}{H\mathcal{D}_2(\theta)\gamma_1(\theta)} = \frac{2T\Phi_0\sqrt{\cos^2\theta+\gamma_1^{-2}\sin^2\theta}}{H\mathcal{D}_{2x}(\cos^2\theta+\gamma_2^{-2}\sin^2\theta)},$$

$$\alpha_\gamma(\theta) = \left(\frac{\gamma_2(\theta)}{\gamma_1(\theta)}\right)^2 = \frac{1+\gamma_1^{-2}\tan^2\theta}{1+\gamma_2^{-2}\tan^2\theta}.$$

Note that at arbitrary angle we cannot use inequality $\gamma_2(\theta)/\gamma_1(\theta)\ll 1$ any more. The system of equations for the reduced F function at even Landau levels $\tilde{F}_{2,n}=[2\pi T/t_2(\theta)]F_{2,2i}$ at arbitrary tilt angle is given by

$$-(1-\alpha_\gamma)\sqrt{i(i-1/2)}\tilde{F}_{2,i-1}+\left[z+(1+\alpha_\gamma)\left(2i+\frac{1}{2}\right)\right]\tilde{F}_{2,i}$$
$$-(1-\alpha_\gamma)\sqrt{(i+1/2)(i+1)}\tilde{F}_{2,i+1}=\Delta_{2,2i} \tag{50}$$

with $z=t_2(\theta)(s+1/2)$.

At small tilt angles, $\theta\ll 1$, one can solve Eq. (50) using perturbation theory with respect to θ^2. The quadratic angular correction can be obtained neglecting coupling to the higher Landau level. This leads to equation similar to Eq. (6) with replacements

$$H_1\to H_1(\theta)=\frac{2T_c\Phi_0}{\sqrt{\mathcal{D}_{1x}\mathcal{D}_1(\theta)}},$$

$$H_2\to H_2(\theta)=\frac{4T_c\Phi_0}{\mathcal{D}_2(\theta)\gamma_1(\theta)(1+\alpha_\gamma)}.$$

At small angles we obtain quadratic in θ corrections to typical fields

$$H_1(\theta)\approx H_1\left(1+(1-\gamma_1^{-2})\frac{\theta^2}{2}\right),$$

$$H_2(\theta)\approx H_2\left(1+(1-\gamma_2^{-2})\frac{\theta^2}{2}\right).$$

At low temperature one can derive an exact formula for small-angle correction

$$\frac{H_{c2}(\theta)-H_{c2}(0)}{H_{c2}(0)}\approx\frac{\theta^2}{2}\left[1-\frac{1}{2}\left(\gamma_1^{-2}+\gamma_2^{-2}-\frac{(\gamma_2^{-2}-\gamma_1^{-2})(W_2-W_1-\ln r_x)}{\sqrt{(W_2+W_1-\ln r_x)^2+4W_1\ln r_x}}\right)\right] \tag{51}$$

with $r_x\equiv\mathcal{D}_{1x}/\mathcal{D}_{2x}$. In the case of small correction from the weak band $4W_1\ln r_x\ll(W_2-\ln r_x)^2$, we obtain a simpler formula for $\theta\ll 1$

$$\frac{H_{c2}(\theta)-H_{c2}(0)}{H_{c2}(0)}\approx\frac{\theta^2}{2}\left(1-\gamma_1^{-2}+\frac{W_2W_1(\gamma_1^{-2}-\gamma_2^{-2})}{(W_2-\ln r_x)^2}\right). \tag{52}$$

For parameters of MgB_2 this formula gives an estimate almost identical to the exact result.

At large tilt angles, $\cos\theta\ll 1$, inequality $\gamma_2(\theta)\ll\gamma_1(\theta)$ is restored and we can utilize the approximations used for the case of in-plane field. In particular, at low temperatures the approximate angular dependence is given by a formula similar to Eq. (35):

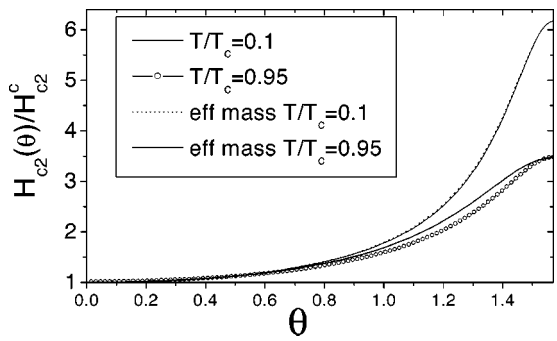

FIG. 3. Examples of angular dependence of the upper critical field at low and high temperatures. Fits to the effective-mass dependence are also shown.

$$H_{c2}(\theta)\approx\frac{H_{c2}^{(1)}(0)}{\sqrt{\cos^2\theta+\gamma_1^{-2}\sin^2\theta}}\times\left(1-\frac{W_1\left(\ln\frac{\mathcal{D}_{2z}}{\mathcal{D}_{1x}\cot^2\theta+\mathcal{D}_{1z}}-1.96\right)}{W_2+\ln\frac{\mathcal{D}_{2z}}{\mathcal{D}_{1x}\cot^2\theta+\mathcal{D}_{1z}}-1.96}\right). \tag{53}$$

In the whole angular range we calculated the upper critical field numerically following the procedure outlined in Sec. IV D. As input parameters we have used the values $\gamma_1=6.325$, $\gamma_1=0.816$ which follow from the electronic band-structure calculations in MgB_2. We have also used the relation $\mathcal{D}_{1x}=0.2\mathcal{D}_{2x}$—the reason for this choice was discussed in Ref. 22. The examples of the calculated angular dependence for $T/T_c=0.1$ and 0.95 are shown in Fig. 3. We also show fits to a simple effective-mass law, routinely used to describe angular dependence of H_{c2} in anisotropic superconductors $H_{c2}(\theta)=H_{c2,c}/\sqrt{\cos^2\theta+\gamma_{c2}^{-2}\sin^2\theta}$. Due to the contribution from the π band, one can see significant deviations from this law at high temperature. To enhance these deviations we plot in Fig. 4 the angular dependence of the combination $\mathcal{A}(\theta)=[H_{c2,z}(\theta)/H_{c2,c}]^2+[H_{c2,x}(\theta)/H_{c2,a}]^2$ for several temperatures [for the effective-mass law $\mathcal{A}(\theta)=1$ for all θ]. We find that $\mathcal{A}(\theta)<1$ always and the maximum de-

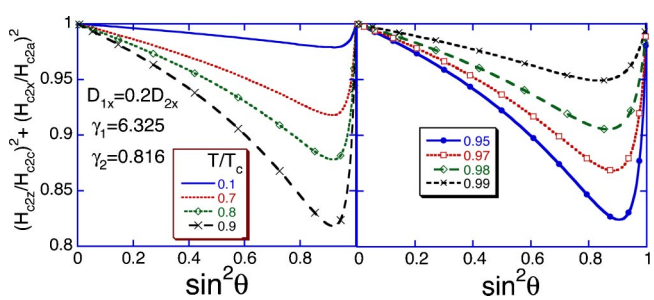

FIG. 4. Plots of the parameter $\mathcal{A}(\theta)=[H_{c2,z}(\theta)/H_{c2,c}]^2+[H_{c2,x}(\theta)/H_{c2,a}]^2$ vs $\sin^2\theta$ at different temperatures revealing deviations from the simple effective-mass law. Left panel: temperatures not very close to T_c. Right panel: temperature region near T_c.

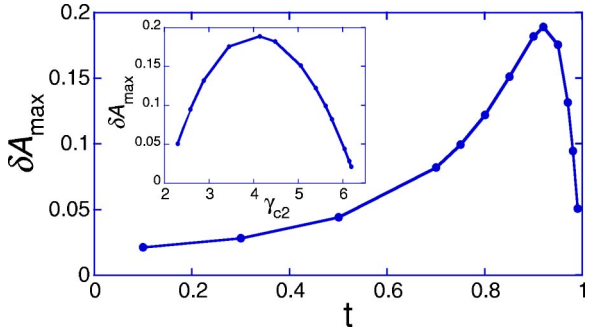

FIG. 5. Temperature dependence of the parameter $\delta\mathcal{A}_{\max} = \max_\theta |1-\mathcal{A}(\theta)|$ characterizing deviations from the effective-mass dependence of H_{c2}. Inset shows the dependence of this parameter on the H_{c2} anisotropy.

viation from unity is achieved around $\theta \sim 74°$. At high temperatures one can derive a very simple formula for $\mathcal{A}(\theta)$ at small angles $\theta \ll 1$, $\mathcal{A}(\theta) \approx 1-(1/\gamma_{\rm GL}^2 - 1/\gamma_{c2}^2)\theta^2$. Quantitatively, the deviations from the effective-mass law can be characterized by the parameter $\delta\mathcal{A}_{\max} = \max_\theta |1-\mathcal{A}(\theta)|$. Figure 5 shows the temperature dependence of this parameter. At low temperatures deviations from the effective-mass law are at the level of several percents. These deviations progressively grow with the temperature reaching $\sim 19\%$ at $T/T_c = 0.92$ and then rapidly decrease when the temperature approaches the narrow GL region near T_c. As the deviations from the effective-mass dependence have exactly the same origin as the temperature dependence of the anisotropy, it is interesting to correlate these deviations with the anisotropy change. The inset in the Fig. 5 shows plot of the parameter $\delta\mathcal{A}_{\max}$ vs the H_{c2} anisotropy. One can see that the distortion of the angular dependence is maximum when the anisotropy is approximately at the midpoint between the low-temperature and GL limits. Experimentally, it was found that the angular dependence of H_{c2} in MgB_2 indeed deviates from the effective mass law[44,45] and the shape of these deviations qualitatively agrees with our calculations.

VI. CONCLUSIONS

We have calculated the upper critical field in a dirty two-band superconductor within the quasiclassical Usadel equations, bearing in mind the regime of the very high anisotropy in the quasi-2D band relevant for MgB_2. Following Ref. 14, we have assumed that the interband scattering is negligible even in the dirty limit in both bands. Most of the MgB_2 samples are in the dirty limit, except for single crystals, where the dirty limit conditions are fulfilled in the π band but not fulfilled in the σ band.[42] Still, as argued in Ref. 22, our results should be qualitatively applicable to MgB_2 single crystals, if one considers the coherence length ξ_1 as a phenomenological parameter instead of expressing it via the diffusion constant $\mathcal{D}_1$.

We have considered the cases when the field is parallel and perpendicular to the basal plane separately. We have found that at low temperatures both critical fields are mainly determined by the strong band and only weakly deviate from the universal Maki–de Gennes result. The low-temperature anisotropy is mainly determined by the anisotropy of diffusion constants in a quasi-two-dimensional band. However, the anisotropy is suppressed at high temperatures. The reason is that there are two important parameters, anisotropy of pairing interaction and of diffusion constants, which enter the expression for the parallel H_{c2} in a different way at high and low temperatures. This property can be expressed as the anisotropy of coherence length ξ_{ab}/ξ_c which decreases with increasing temperature. The same effect was earlier pointed out in Refs. 27,28 within the clean limit and is in accordance with the experimental data in MgB_2. Note that the anisotropy of the penetration depth λ_c/λ_{ab} increases with increasing temperature,[25,26] which is another manifestation of the two-band model.

We have also studied quantitatively the dependence of H_{c2} on the angle θ between the c axis and the magnetic field direction. We have derived approximate expressions for H_{c2} for small and large tilt angles of magnetic field. In the whole angular range the dependence $H_{c2}(\theta)$ has been calculated numerically using parameters typical for MgB_2. This dependence deviates from the effective-mass dependence even in vicinity of transition temperature demonstrating the breakdown of anisotropic GL theory. Further, we have shown that the temperature range of applicability of the GL theory is extremely narrow in the considered two-band case.

An important issue is strong coupling corrections to H_{c2}. In this paper the weak coupling approach was used. On the other hand, it is known from work on isotropic superconductors[43] that strong coupling corrections renormalize the absolute value of H_{c2} by the factor $(1+\lambda)^\alpha$, where λ is the coupling constant and $\alpha \simeq 2$. Since electron-phonon coupling in MgB_2 is relatively strong (according to Ref. 12, $\lambda_{11} \simeq 1$), these corrections are important for calculation of absolute values of H_{c2}. However, we do not expect qualitative changes in the temperature and angle dependencies of the anisotropy ratio calculated in the present paper. Extension of our results to the strong coupling Eliashberg regime is an interesting subject for future work.

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APPENDIX: LOCAL APPROXIMATION FOR THE π BAND

Let us consider equation for the F function in the weak π band

$$\omega F_2 + \frac{\mathcal{D}_{2z}}{2}\left(\frac{2\pi H x}{\Phi_0}\right)^2 F_2 - \frac{\mathcal{D}_{2x}}{2}\nabla_x^2 F_2 = \Delta_2. \qquad \text{(A1)}$$

The typical scale of $\Delta_2(x)$ variation is imposed by the strong σ band. This scale is given by $x_1 = \sqrt{\gamma_1 \Phi_0/2\pi H}$ and, due to inequality $\gamma_1 \gg \gamma_2$, it is much larger than the length scale $x_2 = \sqrt{\gamma_2 \Phi_0/2\pi H}$ of the oscillator operator in the left side of

the Eq. (A1). For relevant ω's the typical length scale of F_2 variation is much larger than x_2. This allows us to neglect the gradient term in Eq. (A1). This approximation is equivalent to the approximation for the matrix elements used in Eqs. (20). Then the π-band F function is given by

$$F_2=\frac{\Delta_2}{\omega+\frac{\mathcal{D}_{2z}}{2}\left(\frac{2\pi Hx}{\Phi_0}\right)^2}. \tag{A2}$$

Substituting this expression into the second self consistency equation, we represent it in the form

$$-W_{21}\Delta_1+W_2\Delta_2=\left(\ln\frac{1}{t}-g\left[\frac{\mathcal{D}_{2z}}{4\pi T}\left(\frac{2\pi Hx}{\Phi_0}\right)^2\right]\right)\Delta_2. \tag{A3}$$

It has to be solved together with equations for F_1 and the first self-consistency equation. Using expansion with respect to eigenfunctions of the σ band $\Psi_n(x)$, this equation reduces to the form of linear equation (25b), in which the matrix $U_{i,j}$ is given by the matrix elements

$$U_{i,j}=-\int dx\Psi_{2i}(x)\Psi_{2j}(x)g\left[\frac{\mathcal{D}_{2z}}{4\pi T}\left(\frac{2\pi Hx}{\Phi_0}\right)^2\right].$$

Introducing the dimensionless oscillator wave functions $\psi_n(\tilde{x})$, $\Psi_n(x)=\psi_n(x/x_1)/\sqrt{x_1}$, we present these matrix elements in the dimensionless form

$$U_{i,j}(t_2)=\int_{-\infty}^{\infty}d\tilde{x}\psi_{2i}(\tilde{x})\psi_{2j}(\tilde{x})g[\tilde{x}^2/t_2],$$

where, again $1/t_2\equiv(\mathcal{D}_{2z}/\mathcal{D}_{1z})(H/tH_1)$. In particular, $\psi_0(\tilde{x})=\pi^{-1/4}\exp(-\tilde{x}^2/2)$. In the "high-field in π-band" regime, $t_2\ll 1$, one can use asymptotics $g[\tilde{x}^2/t_2]\approx 2\ln(\tilde{x})-\ln t_2+\gamma_E+2\ln 2$ and obtain

$$U_{i,j}(t_2)=f_{i,j}+(\ln t_2-\gamma_E-2\ln 2)\delta_{n,m}$$

$$f_{i,j}=-4\int_0^{\infty}d\tilde{x}\psi_{2i}(\tilde{x})\psi_{2j}(\tilde{x})\ln(\tilde{x}).$$

In particular,

$$f_{0,0}=-\frac{4}{\sqrt{\pi}}\int d\tilde{x}\exp(-\tilde{x}^2)\ln(\tilde{x})=\gamma_E+2\ln 2\approx 1.9635.$$

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