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Surface critical magnetic field $H_{c3}(T)$ of a bulk superconductor MgB_2 using two-band Ginzburg–Landau theory

I N ASKERZADE[1,2]
[1]Institute of Physics, Azerbaijan National Academy of Sciences, H. Cavid 33, Baku, 370143 Azerbaijan
[2]Department of Physics, Faculty of Sciences, Ankara University, 06100 Tandoğan, Ankara, Turkey
Email: iaskerzade@yahoo.com; solstphs@physics.ab.az

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Abstract. Two-band Ginzburg–Landau (TB G–L) equations for a bulk MgB_2 were solved analytically to determine the temperature dependence of surface critical magnetic field $H_{c3}(T)$. It is shown that $H_{c3}(T)$ has the same temperature dependence with $H_{c2}(T)$, similar to the case of a single-band superconductor, $H_{c3}(T) = 1.66\ H_{c2}(T)$. We use an elimination procedure for the decoupling of G–L equations of two-band superconductivity, which eases the calculations. It is expected that the temperature dependence for $H_{c3}(T)$ gives positive curvature near T_c.

Keywords. Magnesium diboride; two-band superconductivity; Ginzburg–Landau theory; surface superconductivity.

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1. Introduction

MgB_2, a recently discovered [1] superconductor not only holds highest critical temperature among the binary metallic superconductors but also has many unusual superconducting properties (for a comprehensive review, see [2]). The material shows a pronounced isotope effect [3]. Measurements of the nuclear spin-lattice relaxation rate [4] indicate that MgB_2 is a BCS type phonon mediated superconductor. Calculations of the band structure and the phonon spectrum predict a double energy gap [5,6], the larger gap attributed to two-dimensional p_{x-y} orbitals and the smaller gap attributed to three-dimensional p_z bonding and anti-bonding orbitals. Two-band characteristic of the superconducting state in MgB_2 is clearly evident in the recently performed tunnel measurements [7,8] and specific heat measurement [9].

Magnetic phase diagram for MgB_2 has also been of interest to researchers [10,11]. In contrast to conventional superconductors, the upper critical field for MgB_2 has a positive curvature near T_c. Similar behaviour was also observed for non-magnetic borocarbides

[12]. To understand the nature of the unusual behaviour at a microscopic level, a two-band Eliashberg model of superconductivity in MgB_2 was first proposed by Shulga *et al* [13]. The calculations of the specific heat using the first principles of Eliashberg theory were also given by Golubov *et al* [14]. The two-band Ginzburg–Landau model for MgB_2 was successfully applied to fit the experimental results of the temperature dependence of upper $H_{c2}(T)$ [15], lower $H_{c1}(T)$ [16], thermodynamic $H_{cm}(T)$ [17] magnetic fields and of London penetration depth $\lambda(T)$ [18].

In addition, the nature of the surface states of MgB_2 and their effect on superconductivity has attracted recent interest [19–21]. The existence of surface states for MgB_2 as well as surface superconductivity were predicted in [20,21]. It is well-known that in semi-finite single-band superconductors, surface critical field $H_{c3}(T)$ is larger than the bulk critical field $H_{c2}(T)$. Both $H_{c2}(T)$ and $H_{c3}(T)$ decrease with temperature with the same temperature dependence. In this paper, we present calculations for the surface magnetic field $H_{c3}(T)$ using two-band G–L theory for MgB_2.

2. Theory

Two-band G–L free energy functional with coupled order parameters in linear approximation on Ψ_1^2 and Ψ_2^2 can be written similarly as in [15–18]

$$F_{SC}[\Psi_1,\Psi_2] = \int \mathrm{d}^3 r \begin{pmatrix} \frac{\hbar^2}{2m_1^*}\left|\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_1\right|^2 + \alpha_1(T)\Psi_1^2 \\ +\frac{\hbar^2}{2m_2^*}\left|\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_2\right|^2 + \alpha_2(T)\Psi_2^2 + \varepsilon(\Psi_1^*\Psi_2 + \mathrm{c.c.}) \\ +\varepsilon_1\left\{\left(\nabla + \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_1^*\left(\nabla - \frac{2\pi i\vec{A}}{\Phi_0}\right)\Psi_2 + \mathrm{c.c.}\right\} \end{pmatrix}, \quad (1)$$

where m_i^* are the effective masses of electron pairs for the band i $(i = 1,2)$. F_i is the free energy of each band and F_{12} is the coupling energy term between the bands. α is given by $\alpha_i = \gamma_i(T - T_{ci})$, while the coefficient β_i is independent of temperature, γ_i being the proportionality constant. The quantities ε and ε_1 describe the coupling of two-order parameters and their gradients, respectively.

By the minimization of free energy of eq. (1)

$$\delta F/\delta\Psi_1^* = 0, \quad \delta F/\delta\Psi_2^* = 0, \quad (2)$$

we obtain the usual basic equation for the description of the two-band superconductivity. To proceed further, we choose one dimension for simplicity, we write a vector potential $\vec{A} = (0, Hx, 0)$ and with this, eq. (4) gives two sets of equations of the following form [15–18]:

$$-\frac{\hbar^2}{2m_1^*}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^2}\right)\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^2}\right)\Psi_2 = 0, \quad (3)$$

$$-\frac{\hbar^2}{2m_2^*}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^2}\right)\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{x^2}{l_s^2}\right)\Psi_1 = 0, \quad (4)$$

where $l_s^2 = (\hbar c/2eH)$ is the so-called magnetic length. Here we assume that the order parameter $|\Psi_i|^2$ has weak spatial dependence. The signs of the coefficients ε_1 and ε can be taken as arbitrary, which are related to electronic configuration of the superconductor. Note that we ignore the magnetic field dependence of these coefficients for simplicity. This approximation implicitly assumes isotropic s-wave superconductivity. One can get identical equations for $\Psi_1(x)$ and $\Psi_2(x)$ from eqs (3) and (4) by elimination. Therefore, we can assume that $\Psi_1(x) = C\Psi_2(x)$. The coefficient C is obtained by solving eqs (3) and (4).

In the case of single-band superconductivity, the surface critical field $H_{c3}(T)$ is determined from the G–L equation with vector potential $A = H(x - x_0)$ as in [22]. This procedure allows one to obtain an exact value of $H_{c3}(T)$, but requires some sophisticated numerical calculations. However, a simple variational analysis provides us with an almost exact solution [23]. The accuracy of simple variational procedure is about 2% and can be improved by choosing trial function [25]. As a result, the problem of solving G–L equation may be presented as a variational problem of finding the minimum of free energy functional for the single band [24,25].

3. Results and discussions

For trial solutions, we substitute trial functions of $\Psi_1(x) = \exp(-(\delta x^2/2))$ and $\Psi_1(x) = C\Psi_2(x)$ into eq. (3) with appropriate boundary conditions of $\Psi_1(\infty) = 0$, $(\mathrm{d}\Psi_1/\mathrm{d}x)(0) = 0$ [23], we then obtain an expression for the coefficient C as

$$C = -\frac{\varepsilon - \varepsilon_1\delta}{(\hbar^2/2m_1^*)\delta + \alpha_1}. \tag{5a}$$

From eq. (4) we obtain

$$C = -\frac{(\hbar^2/2m_2^*)\delta + \alpha_2}{\varepsilon - \varepsilon_1\delta}. \tag{5b}$$

The coefficient δ must be determined from the minimum condition for the free energy functional eq. (1). Taking into account the expression for the vector potential $A = H(x - x_0)$ and using the trial functions, we can rewrite expression (1) as

$$\Delta F = \int_0^\infty \mathrm{d}x \left\{ \begin{array}{l} \frac{\hbar^2}{2m_1^*}\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \left(\frac{2\pi H}{\Phi_0}\right)^2 (x - x_0)^2 + \alpha_1(T)\right] \\ + \frac{1}{C^2}\frac{\hbar^2}{2m_2^*}\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \left(\frac{2\pi H}{\Phi_0}\right)^2 (x - x_0)^2 + \alpha_2(T)\right] \\ + \frac{2\varepsilon}{C} + \frac{2\varepsilon_1}{C}\left(\frac{2\pi H}{\Phi_0}\right)^2 (x - x_0)^2 \end{array} \right\} \mathrm{e}^{-\delta x^2}. \tag{6}$$

First we will find the minimum of the free energy (6) with respect to x_0 after integration. Differentiation with respect to x_0 gives a value

$$x_0 = \frac{1}{(\pi\delta)^{1/2}}. \tag{7}$$

Next we will find the minimum of energy functional eq. (6) with respect to δ. This gives a relation between δ and C as

$$C^2\frac{\hbar^2}{2m_1^*}(\alpha_1(T)+\delta)+2C(\varepsilon-\varepsilon_1\delta)+\frac{\hbar^2}{2m_2^*}(\alpha_2(T)+\delta)=0, \tag{8}$$

which is equivalent to the following equation:

$$\left(\frac{\hbar^2}{2m_2^*}\delta+\alpha_2\right)\left(\frac{\hbar^2}{2m_1^*}\delta+\alpha_1\right)=(\varepsilon-\varepsilon_1\delta)^2. \tag{9}$$

By substituting eqs (7) and (8) into (6) with $\Delta F=0$, we obtain a formula for the critical field

$$\left(\frac{2\pi H}{\Phi_0}\right)^2\left(1-\frac{2}{\pi}\right)=\delta^2, \tag{10}$$

where δ is determined from eq. (9), which is consistent with the result found in [15]. Finally, the surface critical field can be given as

$$H_{c3}(T)=\left(\frac{\pi}{\pi-2}\right)^{1/2}\frac{\Phi_0\delta}{2\pi}=1.66H_{c2}(T), \tag{11}$$

where $H_{c2}(T)$ is the upper critical field of two-band superconductivity [15], which was given as

$$H_{c2}(T)=h_{c2}\frac{cT_c(\gamma_1m_1^*+\gamma_2m_2^*)}{\hbar e}, \tag{12}$$

$$h_{c2}=a_0^{-1}(-\theta-c_0+(A\theta^2+B\theta+c_0)^{1/2}), \tag{13}$$

$$A=\frac{(x-1)^2}{(x+1)^2}+A_1\eta^2;\quad A_1=64a_1a_2\frac{x^2}{(x+1)^2},\quad \theta=\frac{T}{T_c}-1,\quad x=\frac{\gamma_1m_1^*}{\gamma_2m_2^*}, \tag{13a}$$

$$B=\frac{2(x-1)(a_1x-a_2)}{(x+1)^2}+(a_1+a_2)A_1\eta^2+2B_1\eta,\quad B_1=8a_1a_2\frac{x}{x+1}, \tag{13b}$$

$$c_0=\frac{(a_1x+a_2)}{(x+1)}+B_1\eta;\quad a_0=1-16x\eta^2(\varepsilon/T_c)^2/\gamma_1\gamma_2,\quad a_i=1-\frac{T_{ci}}{T_c}. \tag{13c}$$

Note that the temperature dependence of $H_{c3}(T)$ in two-band G–L theory is dominantly determined by the interaction parameters ε_1 and ε. We have used the same parameters presented in [15–18]. Here, mass ratio parameter x is equal to 3, obtained from band structure calculations of MgB_2 [13]. When the carriers have different effective masses $(m_1^*\gg m_2^*)$ in different bands, the surface magnetic field $H_{c3}(T)$, as well as $H_{c2}(T)$ can effectively be determined by the larger mass m_1^*, in contrast to $H_{c1}(T)$ [16]. The contribution to $H_{c3}(T)$

from the smaller mass is insignificant in this case, while the kinetic properties are determined by the smaller mass m_2^*.

From the equations one can see that the surface critical field $H_{c3}(T)$ has the same temperature dependence with $H_{c2}(T)$ for both single-band and two-band G–L calculations. The calculations favour the existence of the surface critical field. The first angle-resolved photoemission spectroscopy measurements on a MgB_2 single crystal were reported in [26]. They observed several surface states. The effect of surface states for the superconductivity has been discussed in Servedio *et al* [27]. They claimed that the surface critical magnetic field would not exist. The surface electronic states can be responsible for the non-existence of the surface critical field [27]. However, Welp *et al* [28] presented data of $H_{c3}(T)$ for a single crystal of MgB_2 very recently. In their *c*-axis measurements, the surface critical field has a linear dependence, while it has a positive curvature for *ab*-plane measurements. Note that there exists anisotropy for the measurements. However, the calculations presented here assume isotropic superconductivity for two-band G–L theory. Although influence of surface state on superconductivity is still controversial, it has been suggested that superconductivity at *ab*-surfaces is suppressed, while superconductivity along *c*-axis is unaffected.

According to [15], in the framework of isotropic TB G–L theory the upper critical field $H_{c2}(T)$ reveal positive curvature at temperatures close to T_c. With the parameters of TB G–L theory presented in [15–18], one can observe a surface critical field H_{c3} in experiments with positive curvature similar to H_{c2} for a bulk MgB_2 superconductor. In our opinion preparation of bulk samples with smooth and clean surfaces would be enough for the measurements of $H_{c3}(T)$ in MgB_2. Paramagnetic Meissner effect, associated with the existence of the surface critical field was observed for the first time in finite-sized MgB_2 pellets and superconducting cores of the iron-sheathed MgB_2 wires in ref. [29]. The paramagnetic Meissner effect can be obtained in the framework of self-consistent solution of single-band G–L equations for a cylinder of finite size [30].

4. Conclusions

In summary, surface critical magnetic field of two-band superconductors is studied using the two-band G–L equations. It is shown that, relation between upper critical field and surface critical field is the same as in single-band G–L theory. Temperature dependence of surface critical field of two-band superconductors reveal positive curvature near T_c.

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References

[1] J Nagamatsu, N Nakagawa, T Muranaka,Y Zenitani and J Akimitsu, *Nature* **410**, 63 (2001)
[2] C Buzea and T Yamashita, *Supercond. Sci. Technol.* **14**, R115 (2001)
[3] S L Bud'ko, G Lapertot, C Petrovic, C E Cunningham, N Anderson and P C Canfield, *Phys. Rev. Lett.* **86**, 1788 (2001)

[4] H Kotegawa, K Ishida, Y Kitaoka, T Muranaka and J Akimitsu, *Phys. Rev. Lett.* **87**, 127001 (2001)
[5] J Kortus, I I Mazin, K D Belashchenko, V P Antropov and L L Boyer, *Phys. Rev. Lett.* **87**, 4656 (2001)
[6] A Liu, I I Mazin and J Kortus, *Phys. Rev. Lett.* **87**, 087005 (2001)
[7] X K Chen, M J Konstantinovich, J C Irwin, D D Lawrie and J P Frank, *Phys. Rev. Lett.* **87**, 157002 (2001)
[8] H Giublio, D Roditchev, W Sacks, R Lamy, D X Thanh, J Kleins, S Miraglia, D Fruchart, J Markus and P Monod, *Phys. Rev. Lett.* **87**, 177008 (2001)
[9] F Bouquet, R A Fisher, N E Phillips, D G Hinks and J D Jorgensen, *Phys. Rev. Lett.* **87**, 047001 (2001)
[10] S L Bud'ko, V G Kogan and P C Canfield, *Phys. Rev.* **B64**, 180506 (2001)
[11] M Angst, R Puzniak, A Wisniewski, J Jun, S M Kazakov, J Karpinski, J Roos and H Keller, condmat/0112166 (2001) (preprint)
[12] S V Shulga, S-L Drechsler, K-H Muller, G Fuchs, K Winzer, M Heinecke and K Krug, *Phys. Rev. Lett.* **80**, 1730 (1998)
[13] S V Shulga, S-L Drechsler, H Eschrig, H Rosner and W Pickett, condmat/0103154 (2001) (preprint)
[14] A A Golubov, J Kortus, O V Dolgov, O Jepsen, Y Kong, O K Andersen, R J Gibson, K Ahn and R K Kremer, *J. Phys. Condens. Matter* **14**, 1353 (2002)
[15] I N Askerzade, A Gencer and N Güçlü, *Supercond. Sci. Technol.* **15**, L13 (2002)
[16] I N Askerzade, A Gencer, N Güçlü and A Kılıc, *Supercond Sci. Technol.* **15**, L17 (2002)
[17] I N Askerzade and A Gencer, *J. Phys. Soc. Jpn.* **71(7)**, 1637 (2002)
[18] I N Askerzade and A Gencer, *Solid State Commun.* **123(1)**, 63 (2002)
[19] E Bascones and F Guinea, *Phys. Rev.* **B64**, 214508 (2001)
[20] V M Silkin, E V Chulkov and P M Echenique, *Phys. Rev.* **B64**, 172512 (2001)
[21] I N Gee Kim, J I Lee, B I Min and A J Freeman, *Phys. Rev.* **B64**, 020508 (2001)
[22] D Saint-James and P G De Gennes, *Phys. Rev. Lett.* **7**, 306 (1963)
[23] A A Abrikosov, *Fundamentals of the theory of metals* (Amsterdam, North-Holland, 1988)
[24] A A Abrikosov, *Zh. Eksp. Teor. Fiz.* **47**, 720 (1964)
[25] M Tinkham, *Introduction to superconductivity*, 2nd ed. (McGraw-Hill, New York, 1996)
[26] H Uchiyama, K M Shen, S Lee, A Damascelli, D H Lu, D L Feng, Z-X Shen and S Tajima, *Phys. Rev. Lett.* **88**, 175002 (2002)
[27] V D P Servedio, S-L Drechsler and T Mishonov *Int. J. Mod. Phys.* **B16**, 1613 (2002)
[28] U Welp, G Karapetrov, W K Kwok, G W Grabtee, Ch Marcenat, L Paulus, K H P Kim, C U Jung, H-S Lee, B Kang and S-I Lee, condmat/0203337 (2002) (preprint)
[29] J Horvat, X-L Wang, S Soltanian and S X Dou, *Appl. Phys. Lett.* **80**, 829 (2001)
[30] G F Zharkov, *Phys. Rev.* **B63**, 214502-1 (2001)