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ORIGINAL PAPER

Fluctuation of Specific Heat in Two-Band Superconductors

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Abstract Analytical calculations of fluctuation part of specific heat conducted using two-band Ginzburg–Landau equations. Results applied to MgB_2, comparison with available experimental data, and theoretical calculations are conducted and agreement achieved.

Keywords Two-band superconductivity · Fluctuations · Specific heat · Magnesium diboride

1 Introduction

The discovery of superconductivity in MgB_2 [1] has attached a lot of attention in the solid state community. The magnesium diboride MgB_2 [2] structure consists of an alternative stacking of the boron layer and magnesium layer. This material is metallic, and hence they are promising in considering the application in the various fields [3]. The experimental study indicates a phonon mediated mechanism of superconductivity in MgB_2, for example, see [4, 5]. The relatively high T_c has motivated many studies, as has the observation that the detailed superconducting properties of MgB_2 show significant deviation from those calculated using the standard isotropic single-band three-dimensional Bardeen–Cooper–Schrieffer model. Theoretical calculations show that the Fermi surface has several pieces and is very anisotropic [6]. The electron-phonon interaction varies strongly on the Fermi surface [7, 8]. Unusual superconductivity in this compound is related with two distinct energy gaps associated with different parts of the Fermi surface. The larger gap ($\Delta_\sigma = 7$ meV) originates from hole-like carriers residing on two cylindrical Fermi surface sheets, derived from σ bonding of the p_{xy} boron orbital (σ-band). The smaller gap ($\Delta_\pi = 2$ meV) originates from the two three-dimensional sheets of electrons and holes derived from π bonding of the p_z orbitals (π-band) [9–11]. The two-band characteristic of the superconducting state in MgB_2 is clearly evident in the recently performed tunnel measurements [12, 13], and specific heat measurement [14].

Generalization of Ginzburg–Landau (GL) theory for the case two-band superconductors was conducted in [15–20]. As shown in these works, presence of two-order parameters give nonlinear temperature dependence of physical quantities. The description of superconducting fluctuations is one of the major fields for the application of GL theory [21]. Since the standard single-band GL approach turns to be insufficient for MgB_2, a two-band GL is required in order to describe its fluctuation properties. In this paper, we obtain an analytical result for specific heat in two-band superconductors. Firstly, we show that in our case of two-band GL theory is equivalent to single-band theory with effective parameters. Finally, we compare the results of calculations obtained with the available experimental data and other theoretical calculations.

2 Basic Equations

In the presence of two-order parameters in isotropic s-wave superconductors, the Ginzburg–Landau functional free en-

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ergy can be written as [15–17, 19, 20]:

$$F[\Psi_1,\Psi_2] = \int d^3r\big(F_1 + F_{12} + F_2 + H^2/8\pi\big), \tag{1}$$

with

$$F_i = \frac{\hbar^2}{4m_i}\left|\left(\nabla - \frac{2\pi i A}{\Phi_0}\right)\Psi_i\right|^2 + \alpha_i(T)\Psi_i^2 + \frac{\beta_i}{2}\Psi_i^4, \tag{2}$$

$$F_{12} = \varepsilon\big(\Psi_1\Psi_2^* + c.c.\big) + \varepsilon_1\left(\left(\nabla + \frac{2\pi i A}{\Phi_0}\right)\Psi_1^* \times \left(\nabla - \frac{2\pi i A}{\Phi_0}\right)\Psi_2 + c.c.\right). \tag{3}$$

Here, m_i denotes the effective mass of the carriers belonging to band i $(i = 1; 2)$. F_i is the free energy of separate bands. The coefficient α is given as $\alpha_i = \gamma_i(T - T_{ci})$, which depends on temperature linearly, γ is the proportionality constant, while the coefficient β is independent of temperature. $\vec{H}$ is the external magnetic field and $\vec{H} = curl\vec{A}$. The quantities ε and ε_1 describe interband interaction of two-order parameters and their gradients, respectively. Intergradient interaction term is equal to zero in free energy presented in [20]. However, a similar term was introduced by other authors [15]. As shown in [16–19], presence of this term leads to measurable effects in the study of H_{c1},H_{c2} and other physical quantities.

Corresponding system equations of two-band GL theory givens as for $A = (0, Hx, 0)$

$$-\frac{\hbar^2}{4m_1}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_2 + \beta_1\Psi_1^3 = 0, \tag{4}$$

$$-\frac{\hbar^2}{4m_2}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_1 + \beta_2\Psi_2^3 = 0, \tag{5}$$

where $l_s^{-2} = \frac{2eH}{\hbar c}$. Linearization of system equations leads to

$$-\frac{\hbar^2}{4m_1}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_1 + \alpha_1(T)\Psi_1 + \varepsilon\Psi_2 + \varepsilon_1\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_2 = 0, \tag{6}$$

$$-\frac{\hbar^2}{4m_2}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_2 + \alpha_2(T)\Psi_2 + \varepsilon\Psi_1 + \varepsilon_1\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi_1 = 0. \tag{7}$$

In the absence of any external magnetic field, i.e., $H = 0$, near T_c it is true the relation $\Psi_1(x) = C\Psi_2(x)$ [16, 17], which followed from (6) (7)

$$C = -\frac{\varepsilon}{\alpha_1(T)} = -\frac{\alpha_2(T)}{\varepsilon}. \tag{8}$$

Consequently, the critical temperature T_c of two-band superconductors is determined by the expression:

$$(T_c - T_{c1})(T_c - T_{c2}) = \frac{\varepsilon^2}{\gamma_1\gamma_2}. \tag{9}$$

Using (9), we can conclude that T_c is greater than T_{c1} and T_{c2} independently of the sign of interband interaction parameter ε. As followed from (8), in vicinity T_c, two-band G-L equations are equivalent to single-band G-L theory equation

$$-\frac{\hbar^2}{4m^*}\left(\frac{d^2}{dx^2} - \frac{x^2}{l_s^4}\right)\Psi + \alpha^*(T)\Psi + \beta^*\Psi^3 = 0, \tag{10}$$

with effective parameters:

$$m^* = \frac{m_1}{1 - \frac{4m_1\varepsilon_1}{C\hbar^2}}, \quad \alpha^*(T) = \alpha_1(T) + \frac{\varepsilon}{C}, \quad \beta^* = \beta_1. \tag{11}$$

We carried out calculations similar to a single-band case [22] with effective parameters (11). As a measure of the importance of fluctuations, we will evaluate the fluctuation contribution to the heat capacity ΔC and compare it to discontinuity occurring in GL theory near a critical temperature $C = \frac{\gamma^2}{\beta}V$, i.e., we introduce a normalized specific heat jump near critical temperature $\frac{\Delta C}{C}$. In the last expression, γ is the coefficient of proportionality in relation $\alpha_i = \gamma_i(T - T_{ci})$. We firstly calculate the fluctuation part of the free energy functional ΔF and then specific heat jump, which is given by the expression $\Delta C = -T\frac{\partial^2\Delta F}{\partial T^2}$.

$$\Delta F = -kT\sum_k \ln\left\{2\pi\int_0^\infty d|\psi_k| \times \exp\left(-\frac{V}{kT}\sum_k\left(\frac{\hbar^2k^2}{4m} + \alpha + 3\beta|\psi_e|^2\right)|\psi_k|^2\right)\right\} = -kT\sum_k \ln\left[\frac{16\pi kTm}{V\hbar^2}\frac{1}{k^2 + \xi^{-2}(T)}\right]. \tag{12}$$

Introducing cut-of parameter in momentum space (ultraviolet divergence) and ignoring all temperature dependencies except that arising from $\xi(T)$, for the normalized fluctuations of specific heat in a single-band superconductor, we have

$$\left(\frac{\Delta C}{C}\right)_{\mathrm{SB}} \succ m_1^{3/2}T_{c1}\frac{1}{\alpha_1^{1/2}(T)}. \tag{13}$$

Using parameters (11), for corresponding effective single-band GL theory, leads to similar expression for the two-band superconductors

$$\left(\frac{\Delta C}{C}\right)_{\mathrm{TB}} \succ m_1^{*3/2} T_{\mathrm{c}} \left(\frac{\alpha_2(T)}{\alpha_1(T)\alpha_2(T)-\varepsilon^2}\right)^{1/2}. \tag{14}$$

Using results (13) and (14), we receive a final expression for the normalized fluctuation part of two-band superconductors:

$$\frac{(\frac{\Delta C}{C})_{\mathrm{TB}}}{(\frac{\Delta C}{C})_{\mathrm{SB}}} = \frac{T_{\mathrm{c}}}{T_{\mathrm{c}1}} \frac{1}{(1+\frac{4m_1\varepsilon\varepsilon_1}{\hbar^2\alpha_2(T)})^{3/2}} \times \left(1+\frac{\varepsilon^2}{\alpha_1(T)\alpha_1(T)-\varepsilon^2}\right)^{1/2}. \tag{15}$$

3 Results

As followed from (15), the main difference between single-band GL and a two-band GL results in the temperature dependence of the fluctuation heat capacity. Results of the calculation using expression (12) are shown in Fig. 1 (circles). Here, we use the following values for various parameters: $T_{\mathrm{c}} = 40$ K, $T_{\mathrm{c}1} = 20$ K, $T_{\mathrm{c}2} = 10K$, $\frac{\varepsilon^2}{\gamma_1\gamma_2 T_c^2} = \frac{3}{8}$, $\frac{m_1}{m_2} = 3$, $\eta = \frac{T_{\mathrm{c}} m_2 \varepsilon_1 \gamma_2}{\hbar^2 \varepsilon} = -0.16$. The same parameters were also used in [16–19] to determine the temperature dependence of superconducting state parameters. Experimental data for the fluctuations of specific heat in the two-band superconductor $\mathrm{MgB_2}$ taken from [23] (square symbols). Result of single-band GL calculations [22] in Fig. 1 presented by straight solid line $\frac{1}{(T_{\mathrm{c}}-T)^{1/2}}$. As it is clear from Fig. 1 that in the case of the two-band superconductors, the fluctuation part of specific heat grows. If take into account above presented values of fitting parameters, the ratio $T_{\mathrm{c}}/T_{\mathrm{c}1}$ became equal to 2, which lead to enhancement of fluctuations. It means that as result of interaction between order parameters (see (9)), the critical temperature of the two-band system increases, and as result, the fluctuations part of specific heat also increases. An additional source of enhancement of fluctuations in a two-band case related with sign of product $\varepsilon\varepsilon_1$. It is necessary to note that a normalized specific heat jump in two-band superconductors without fluctuations is smaller than in a single-band case [19, 24]. Taking into account this moment, we can make a conclusion that the increasing of critical temperature does not necessary lead to an increase in the fluctuation part of the jump. However, fluctuational parts of other physical quantities such as magnetization and diamagnetic susceptibility [25] in two-band superconductors does not need normalization and also grows. On the another hand, in Fig. 1, we present a nonnormalized fluctuational part of specific heat in two-band superconductors. As shown in [16–19], in the case of $\mathrm{MgB_2}$ for the fitting of experimental data, we use $\varepsilon\varepsilon_1 < 0$. As one can see from Fig. 1, two-band GL theory better describe experimental results. Presented calculations in the framework in two-band GL theory are in agreement with calculations in [26, 27]. In analogy with the results of this paper [26], specific heat in two-band superconductors depends on the temperature in complicated way, than in the case of single-band superconductors $\frac{1}{(T_{\mathrm{c}}-T)^{1/2}}$. Anisotropy parameters of fluctuation enhancement $\frac{\xi_{1z}}{\xi_z} \gg 1$ introduced in [26], is replaced by the factor $\frac{T_{\mathrm{c}}}{T_{\mathrm{c}1}} > 1$ in our approach. Enhancement of the fluctuations part of specific heat in two-band superconductors in comparison with single-band superconductors was also shown in [27]. Our study seems more in detail and in contrast to [26, 27], we use a free energy functional with an intergradient interaction parameter.

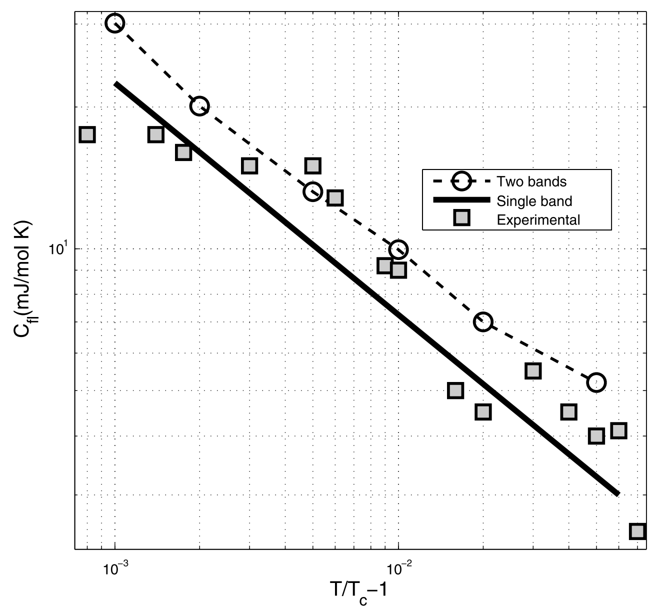

Fig. 1 The fluctuational specific heat versus reduced temperature on a log–log scale

Thus, in this study, we derive analytical expression for the fluctuation part of specific heat using a two-band GL theory. Using the value of fitting parameters for $\mathrm{MgB_2}$, we show nonlinear temperature dependence of specific heat near T_{c}. We also conclude that superconducting fluctuations grows in the case of two-band superconductors. Agreement with existing experimental data and other theoretical calculations is obtained.

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