

Specific heat jump of two-band superconductor KFe₂As₂ using Ginzburg-Landau theory

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In this study specific heat jump using two-gap Ginzburg-Landau (GL) theory has been calculated. In contrast to the previous approaches, we have taken into account intergradient order parameters interaction in the GL free energy functional. The thermodynamic magnetic field revealed nonlinear temperature dependence due to interband interaction between order parameters and their gradients. The calculations showed that the specific heat jump in two-order parameter superconductors was smaller than that of single-order parameter superconductors. It has been shown that such a model is in good agreement with experimental data for KFe_2As_2 superconductors.

Keywords: Fe based superconductors; Ginzburg-Landau theory; specific heat jump; two-band superconductivity

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1. Introduction

The discovery of new Fe-based superconductors triggered intense studies in this field. Superconductivity in the LaOFeP compound was observed by Kamihara et al. [1] at $T_c = 4$ K. Up to now, a few types of these materials have been synthesized and investigated [2-8]. The highest superconducting transition temperature of the materials of the so-called 1111 class (ReFeAsO, Re = Sm, La, Dy, Eu, Th, Gd, etc.) is about $T_c = 50$ K. The 122 (Ba(K)Fe₂As₂) compound is transformed to the superconducting state at $T_c = 40$ K, while the transition temperature of the 111 superconductors (LiFeAs, NaFeAs) is 18 K. The 11 compound (FeS) with the lowest transition temperature $T_c = 8$ K is another representative of Fe-based superconductors. Like in cuprate superconductors, the Fe-based compounds are layered. In the spatially separated Fe layers electrons condense into Cooper pairs and the oxygen layers supply charge carriers in the case of deviation from stoichiometric composition. Detailed reviews

of the state of the art investigations of these materials are given in [9-13]. Comparison of the properties of cuprate superconductors and Fe-based superconductors reveals that there are certain elements of similarities as well as many differences. It is well known that the symmetry of the order parameters of cuprate superconductors is of *d*-wave nature, while the s±type symmetry is proposed for new compounds [12].

In contrast to cuprate superconductors the main peculiarity of Fe-based compounds is related to the multiband character of superconducting state [13– 15]. It is useful to note that the multiband Bardeen-Cooper-Schrieffer (BCS) theory for Fe-based compounds was suggested in studies [16, 17]. The multiband Eliashberg theory with antiferromagnetic spin fluctuations was considered in [18]. The four-band Eliashberg model was applied for the study of thermodynamic properties of optimally doped $Ba_{1-x}K_xFe_2As_2$ [19]. The two-band GL theory in application to recently discovered superconductors was developed in [20-24]. The obtained equations were applied to study different physical properties of MgB₂, nonmagnetic borocarbides, and good agreement with experimental data was

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achieved. In a recent study [25] analytical calculations of anisotropy parameters of upper and lower critical fields were conducted using two-band GL equations for layered systems, and the results applied to Fe based superconductor LiFeAs gave a good agreement.

Among various Fe-based superconductors KFe₂As₂, which critical temperature is about 3.5 K, stands out as a unique material [26]. The highest temperature of doped $Ba_{1-x}K_x$ Fe₂As₂ systems is 38 K for x = 0.4 [27, 28]. The Fermi surface of KFe₂As₂ is dominated by three concentric hole cylinders at the Γ point of Brillouin zone and a small hole cylinder near the zone boundary [29, 30]. It is generally accepted that the Fe-based superconductors are described by many band models. Multi-band character of superconducting state in KFe₂As₂ was confirmed by ARPES [30] and de Haas-van Alphen experiments [31]. The specific heat of KFe_2As_2 was measured using a relaxation technique [32]. The authors found that the electronic specific heat cannot be described by the standard BCS theory with a single isotropic energy band. Fitting the specific heat data with the two-band α -model indicates that the two superconducting energy gaps appear at about 0.54 meV and 0.16 meV, respectively [32]. As shown in [14], despite the five-band character of $Ba_{1-x}K_xFe_2As_2$ superconductors the tunnel microscopy measurements reveal two energy gaps. In the present work the specific heat jump in KFe₂As₂ was calculated using the two-gap GL theory. Fitting parameters for the calculation were taken from experimental data and from microscopic calculations for KFe₂As₂. Finally, the results of the calculations were compared with the available experimental data.

2. Basic equations

We can write GL free energy functional for two order parameter superconductors as follows [20–25]

$$F_{SC} = \int d^3 r (F_1 + F_{12} + F_2 + H^2 / 8\pi) \quad (1)$$

where:

$$F_{i} = \frac{\hbar^{2}}{4m_{i}} \left| \left(\nabla - \frac{2\pi i \vec{A}}{\Phi_{0}} \right) \Psi_{i} \right|^{2} + \alpha_{i}(T) |\Psi_{i}|^{2} \quad (2)$$
$$+ \beta_{i} |\Psi_{i}|^{4} / 2$$

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

 m_i are the masses of electrons belonging to different bands (i = 1, 2); $\alpha_i = \gamma_i(T - T_{ci})$ are the quantities linearly dependent on the temperature; β_i and γ_i are constant coefficients; ε and ε_1 describe the interaction between the band order parameters and their gradients, respectively; H is the external magnetic field; and Φ_0 is the magnetic flux quantum. In equations 1 and 2 the order parameters $\Psi_{1,2}$ are assumed to be slowly varying in space. Minimization procedure of the free energy functional yields the system of GL equations. For an isotropic superconductor, in the case (without limiting the generality) of A = (0, Hx, 0), the time-independent GL equations take the following form:

$$-\frac{\hbar^{2}}{4m_{1}}\left(\frac{d^{2}}{dx^{2}}-\frac{x^{2}}{l_{s}^{2}}\right)\Psi_{1}+\alpha_{1}(T)\Psi_{1}+\varepsilon\Psi_{2}$$
$$+\varepsilon_{1}\left(\frac{d^{2}}{dx^{2}}-\frac{x^{2}}{l_{s}^{2}}\right)\Psi_{2}+\beta_{1}|\Psi_{1}|^{2}\Psi_{1}=0 \qquad (4)$$

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

where $l_s^{-2} = \frac{\hbar c}{2eH}$ is so-called magnetic length. In the general case, the signs of the parameters of interband interactions ε and ε_1 in equations 4 and 5 can be arbitrary. These signs are determined by the microscopic nature of the interaction of electrons belonging to different bands. If the inter-band interaction vanishes equations 4 and 5 convert into the usual GL equations with the critical temperatures T_{c1} and T_{c2} . In the general case (irrespective of the sign of ε), the superconducting transition takes place at a temperature T_c , which is higher than both T_{c1} and T_{c2} and is determined by the following equation **3.** [20–25]:

$$(T_c - T_{c1})(T_c - T_{c2}) = \frac{\varepsilon^2}{\gamma_1 \gamma_2}$$
 (6)

Using equations 4, 5 and 6 we can calculate the free-energy difference between a normal and superconducting state. Final result can be written as:

$$\Delta F = -\frac{\beta_1}{2} |\Psi_{1.0}|^4 - \frac{\beta_2}{2} |\Psi_{2.0}|^4 - 2\varepsilon |\Psi_{1.0}|^2 |\Psi_{2.0}|^2$$
(7)

where the equilibrium values of the order parameters are given by $|\Psi_{i,0}|^2$:

$$|\Psi_{1,0}|^{2} = -\frac{\alpha_{2}^{2}(T)(\alpha_{1}(T)\alpha_{2}(T) - \varepsilon^{2})}{\varepsilon^{2}\beta_{2}\alpha_{1}(T) + \beta_{1}\alpha_{2}^{3}(T)}$$
(8)

$$|\Psi_{2,0}|^{2} = -\frac{\alpha_{1}^{2}(T)(\alpha_{1}(T)\alpha_{2}(T) - \varepsilon^{2})}{\varepsilon^{2}\beta_{1}\alpha_{2}(T) + \beta_{2}\alpha_{1}^{3}(T)}$$
(9)

The last term in equation 7 is related to the interband interaction ε and causes an increase in free energy difference between the normal and superconducting state. For the calculation of specific heat jump we use the Ruthgers expression [33]:

$$\frac{\Delta C}{T_c} = \frac{1}{4\pi} \left(\frac{\partial H_c}{\partial T} \right)^2 \Big|_{T_c}$$
(10)

where thermodynamic magnetic field H_c is related to free energy differences as [33]:

$$\Delta F = -\frac{H_c^2}{8\pi} \tag{11}$$

Using equations 7, 8, 9 one can obtain the following expression for the thermodynamic magnetic field H_c :

$$H_{c}(T) = -\sqrt{4\pi} \frac{(\alpha_{1}(T)\alpha_{2}(T) - \varepsilon^{2})}{(\varepsilon^{2}\beta_{1}\alpha_{2}(T) + \beta_{2}\alpha_{1}^{3}(T))} \times \left\{\beta_{1}\varepsilon^{4} +\beta_{2}\alpha_{1}^{4}(T) - 2\varepsilon^{2}\alpha_{1}(T)\frac{\varepsilon^{2}\beta_{1}\alpha_{2}(T) + \beta_{2}\alpha_{1}^{3}(T)}{\alpha_{1}(T)\alpha_{2}(T) - \varepsilon^{2}}\right\}^{\frac{1}{2}}$$

$$(12)$$

As equation 12 suggests, thermodynamic magnetic field reveals nonlinear temperature dependence due to interband interaction between order parameters and their gradients.

8. Results and discussion

The expressions 10, 11 and 12 have been used for the calculation of specific heat jump at the critical temperature of the KFe₂As₂ superconductor. In these calculations the following values of parameters have been used: $T_c = 3.5$ K; $T_{c1} = 2.6$ K; $T_{c2} = 1.55$ K; $\frac{\varepsilon^2}{\gamma_1 \gamma_2 T_c^2} = 0.148$; $\frac{\gamma_1 m_1}{\gamma_2 m_2} = 0.3$. These parameters have been chosen using equation 5 for the critical temperature of two-gap superconductor KFe₂As₂. Critical temperatures of different bands T_{c1} and T_{c2} correspond to measurable pecularities of specific heat [32]. Accordingly to equation 5, at crtical temperature $T_c = 3.5$ K, the interband interaction parameter $\frac{\varepsilon^2}{\eta \gamma T_c^2}$ is calculated as 0.148. The ratio of effective masses in different bands in KFe₂As₂ compound is predicted by the ab-initio band structure calculations [29, 30]. This choice leads to specific heat jump at the critical temperature to the value 0.743, which is close to the value 0.76 obtained from the experimental study [32]. As it follows from the single-band GL theory, the normalized specific heat jump in this superconductors is equal to 1 [33]. This result shows that the specific heat jump in two-order parameter superconductors is smaller than that of single-order parameter superconductors.

Similar calculations for $Ba_{1-x}K_xFe_2As_2$ (x = 0.4) compound were conducted with the twogap GL theory using the parameters $T_c = 32.2$ K; $T_{c1} = 19.2$ K; $T_{c2} = 7.3$ K; $\frac{\varepsilon^2}{\eta \gamma_c T_c^2} = 0.327;$ $\frac{\gamma_1 m_1}{m_1} = 0.35$. The estimation using equations 10 – $\frac{\gamma_2 m_2}{\gamma_2 m_2}$ = 0.55. The estimation using equations 10 12 with these parameters gives the specific heat jump of 0.787, while the corresponding experimental data is around 0.81 [36]. Measurement of specific heat jump in another Fe-based $Ba(Fe_{1-x})$ $Co_x)_2As_2$ compound was carried out in [37]. Based on these results [36, 37] in the study [38] it was pointed out that specific heat jump at a critical temperature is consistent with the quantum critical nature of the normal state of Fe-based ²⁾ superconductors using BCS approach.

It is useful to note that the calculations of specific heat jump in two-order parameter superconductors in the framework of the BCS theory lead to [34]:

$$\frac{\Delta C}{C_N} = 1.43A(\chi), A(\chi) = \frac{8\chi^4 + 8\chi^2 + 2}{8\chi^4 + 24\chi^2 + 3} \quad (13)$$

where the parameter χ is the ratio of the order parameters at the critical temperature. Such a result also supports our remark on the smaller value of specific heat jump in two-band superconductors using GL theory in comparison with the single bands ones. The influence of the carrier density on the specific heat jump in two-band superconductors was analyzed in [35] using BCS theory. It is useful to note that the influence of multiband character and anisotropy order parameter of superconducting state on the specific heat jump reveals similar tendency [34]. In both cases specific heat jump at critical temperature is reduced.

4. Conclusions

In this study two-gap GL theory to calculate the specific heat jump at critical temperature for KFe₂As₂ superconductor has been used. The results show that specific heat jump is reduced in comparison with single-band superconductors. This reduction is determined by the parameters of the two-gap GL theory and is consistent with the available experimental data. In contrast to the previous approaches, intergradient order parameters interaction in the GL free energy functional has been taken into account here. In the author's opinion the presented theory can be used for the interpretation of specific heat jump measurements in many band superconductors via choosing corresponding parameters properly.

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