Electronic specific heat of two-band layered superconductors: Analysis within the generalized two-band α model

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The generalized two-band α model of superconductivity is consistently developed by taking into account the interband electron-phonon interaction. The model is applied to calculate the electronic contribution to the specific heat, superconducting gaps, and electron-phonon coupling constants of the multiband layered superconductors MgB_2 and $Ba(Fe_{0.925}Co_{0.075})_2As_2$. For both compounds, the energy gaps and electron-phonon coupling constants are determined, and the temperature behavior of the specific heat is obtained that describes the experimental data well. It is shown that the well-known two-band α model that assumes independent bands is formally valid only in the case of relatively strong interband scattering in the band with a smaller gap.

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I. INTRODUCTION

Interest to theoretical investigation of electronic specific heat of two-band superconductors has reemerged (see review[1] and references therein) after the discovery of layered superconductors—magnesium diboride and iron-pnictides/chalcogenides. In this new class of superconductors, as distinct from classical two-band superconductors (like Nb, V, and others), the two-band character of superconductivity reveals itself in an anomalous temperature behavior of the specific heat, $C_s(T)$.[2,3] The main peculiarities appear in the $C_s(T)$ dependences at relatively low temperatures, $T^* \ll T_c$, in the form of characteristic features whose origin can naturally be considered as caused by bumps in $C_s(T)$ coming from the band with a smaller superconducting (SC) gap $\Delta_{\min}$ (in the case of independent bands, these jumps would be real specific heat jumps at corresponding critical temperatures $T^* \sim T_{c\,\min}^{(0)} = \Delta_{\min}(0)/1.764$).

During the last 10 years, a large amount of theoretical papers has been published on the properties of layered superconductors. We briefly review some of them that are directly related to the present work. They include first-principles calculations of electron-phonon interaction (EPI) in single crystalline MgB_2,[4–6] fundamental investigations of the thermodynamics of two-band superconductors (Refs. 7 and 8 and detailed literature review therein), a paper,[9] where the role of various defects in MgB_2 is analyzed, and a more recent work.[10] In Refs. 7–9, calculations have been made both within the Eliashberg theory with the first-principles EPI and based on the model Bardeen–Cooper–Schrieffer (BCS) interaction. Here, detailed numerical studies of general properties (including specific heat) of two-gap superconductors were performed. However, the methods used could hardly be applied to theoretical analysis of real (polycrystalline and/or containing impurities/defects) and even of single crystalline samples. Comparison of EPI parameters obtained in first-principles calculations by various authors[4–6] shows that the absolute accuracy of the determination of EPI constants is less than 0.1. For interband constants that are of the order of Coulomb pseudopotential,[4–6] this uncertainty is definitely too large and does not allow correct calculation of the temperature variation of the smaller gap $\Delta_{\min}(T)$ and specific heat $C_s(T)$ at temperatures above T^* since these two quantities are strongly sensitive to the value of interband interaction (see for example Ref. 7). The problem becomes especially serious while calculating the Leggett modes $\Omega_L(T)$.[11] For example, on the basis of first-principles calculations of EPI, it has been concluded in Ref. 12 that the Leggett plasmons cannot propagate in MgB_2—in clear contradiction with experimental data.[13] An attempt[14] to calculate the specific heat of MgB_2 in the frame of classical two-band BCS theory can hardly be considered as successful.

In order to calculate the $C_s(T)$ dependences of real two-band superconductors, a calculation technique is frequently employed that is known as two-band α model ($2B\alpha$ model).[2] In some cases, the model allows one to relatively simply and determine rather well, basing on the specific heat $C_s(T)$ curve, the low temperature values of SC energy gaps. It is based on a straightforward application of the single-band α model[15] to each band and, thus, does not take into account the main feature of the two-band superconducting system—the interband interaction. This model takes into account empirical parameters $\alpha_{1,2} = \Delta_{1,2}(0)/T_c^{\exp}$, and the same dependence of reduced SC energy gaps $\delta_{1,2}(t) = \Delta_{1,2}(T/T_c)/\Delta_{1,2}(0)$ on the reduced temperatures $t = T/T_c^{\exp}$ is taken that is given by a standard BCS function $\delta_0(t)$.[15] In reality, this way of analysis is absolutely unacceptable, at least for the smaller gap $\delta_{\min}(t)$, that is strongly depending on the interband interaction and whose anomalous temperature variation determines specific behavior of $C_s(T)$ of two-band superconductors.

For a more correct calculation within the $2B\alpha$-like formalism of $\delta_{1,2}(t)$, one should use the BCS-like two-band equations that take into account some empirical parameters $\alpha_{1,2}$ in combination with self-consistency conditions on $\alpha_{1,2}$ that

follow from general properties of two-band BCS equations. We have successfully used this kind of generalization of the $2B\alpha$ model earlier to analyze the tunnel experimental data of $Mg_{1-x}Al_xB_2$ (Ref. 16) and the optical experiments on $Ba(Fe_{0.9}Co_{0.1})_2As_2$.[17] In this communication, we describe calculations of specific heat of a two-band superconductor by applying the BCS-like equations under a more general (compared to Refs. 16 and 17) assumption about weak coupling in one of the bands—an assumption that is valid for practically all layered Fe-based superconductors and for MgB_2. We first present a brief review of the main properties of two-band BCS equations (second section). Main attention is paid to an analytical exploration of reduced SC energy gaps and to the dependence on the interband interactions of the important parameters of empirical models α_J ($J = 1, 2$)—the ratios of the superconducting gaps to the critical temperature; simple analytical expressions for such dependences are derived that actually represent the self-consistence conditions for $\alpha_{1,2}$. Using these conditions, in the third section, we obtain the BCS-like equations with parameters $\alpha_{1,2}$ for the case of weak coupling in one of the bands. Finally, we apply the developed formalism to analyze experimental dependences $C_s(T)$ of $Mg^{11}B_2$ (Ref. 2) and $Ba(Fe_{0.95}Co_{0.075})_2As_2$ (Ref. 3) and to determine SC energy gaps and EPI constants of these compounds.

II. SOME GENERAL PROPERTIES OF TWO-BAND BCS SUPERCONDUCTORS

The two-band BCS equations that determine the temperature dependence of the SC gaps can be written as:[7]

$$\Delta_I(T) = \sum_{J=1,2} \lambda_{IJ}\Delta_J(T) \int_0^{\Omega_c} d\xi \tanh[E_J(\xi)/2T]/E_J(\xi), \tag{1}$$

$$E_J(\xi) = \sqrt{\xi^2 + \Delta_J^2(T)}. \tag{2}$$

Here Ω_c is the characteristic phonon frequency and $E_J(\xi)$ is the quasiparticles spectrum in the band J ($J = 1, 2$). The renormalized EPI coupling constants are expressed via BCS paring constants $\tilde{\lambda}^0_{IJ}$ as

$$\tilde{\lambda}^0_{IJ} = \lambda^0_{IJ} - \mu^*_{IJ}, \tag{3}$$

where λ^0_{IJ} ($I = 1, 2$ and $J = 1, 2$) is the EPI coupling constant and μ^*_{IJ} is the Coulomb pseudopotential

$$\lambda_{IJ} = \tilde{\lambda}^0_{IJ}/\left(1 + \lambda^0_{II} + \lambda^0_{I\neq J}\right). \tag{4}$$

It is convenient to rewrite Eq. (1) in the form[16]

$$\int_0^{\Omega_c} d\xi \tanh[E_1(\xi)/2T]/E_1(\xi) = \tilde{\lambda}_{22} - \tilde{\lambda}_{12}\theta(T), \tag{5}$$

$$\int_0^{\Omega_c} d\xi \tanh[E_2(\xi)/2T]/E_2(\xi) = (\tilde{\lambda}_{11} - \tilde{\lambda}_{21})/\theta(T), \tag{6}$$

$$\theta(T)\ln\theta(T) = -[\tilde{\lambda}_{11} - \tilde{\lambda}_{22} - \delta n_{12}(T)]\theta(T) - \tilde{\lambda}_{12}\theta^2(T) + \tilde{\lambda}_{21}, \tag{7}$$

where $\theta(T) = \Delta_2(T)/\Delta_1(T)$ is the gap ratio, $\delta n_{12}(T) = n_1(T) - n_2(T)$ and $n_J(T)$ is the normalized quasiparticles number for the band J:

$$n_J(T) = 2\int_0^{\infty} d\xi\, f[E_J(\xi)/T]/E_J(\xi) \tag{8}$$

with $f[E_J(\xi)/T]$ being the quasiparticles distribution function and $\tilde{\lambda}_{IJ}$ the effective coupling constant:

$$\tilde{\lambda}_{IJ} = \frac{\lambda_{IJ}}{\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}} = \frac{\lambda_{IJ}}{\lambda_{11}\lambda_{22}}\frac{1}{[1 - \lambda_{12}\lambda_{21}/(\lambda_{11}\lambda_{22})]}. \tag{9}$$

To obtain a self-consistent solution, any convenient pair of equations of Eqs. (5)–(7) can be taken. Obviously, the effective coupling constants $\tilde{\lambda}_{IJ}$ given in Eq. (9), and especially the interband ($I \neq J$) coupling constants, are strongly sensitive to the relative magnitude of the interband interaction. (Typical values of $\tilde{\lambda}_{IJ}$ are given in Table I.) The situation when the determinant of Eq. (1) vanishes, $\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} \to 0$, does not represent any special interest; in this case, the gap ratio does not depend on temperature, $\theta(T) = \lambda_{21}/\lambda_{11} = \lambda_{22}\lambda_{12} =$ const, as can easily be shown using Eq. (1).

Knowing the available data on the EPI in layered superconductors,[4–6] in the following, we consider only positive effective coupling constants $\tilde{\lambda}_{IJ}$, Eq. (9). Then for $T = 0$, the task is reduced to finding of a suitable $\theta(0)$ that provides the solution of Eq. (7)

$$\tilde{\lambda}_{11} - \tilde{\lambda}_{22} = -\ln\theta(0) - \tilde{\lambda}_{12}\theta(0) + \tilde{\lambda}_{21}/\theta(0) \tag{10}$$

with subsequent determination of the gaps $\Delta_{1,2}(0)$ according to the following expressions

$$\ln[2\Omega_c/\Delta_1(0)] = \tilde{\lambda}_{22} - \tilde{\lambda}_{12}\theta(0),$$
$$\ln[2\Omega_c/\Delta_2(0)] = \tilde{\lambda}_{11} - \tilde{\lambda}_{21}/\theta(0). \tag{11}$$

Below, we consider some general properties of the two-band superconductor that is described by Eqs. (5)–(7), at finite

TABLE I. Parameters of the superconducting state calculated for a superconductor in the weak coupling regime (1 and 2), a layered superconductor of the family $Mg_{1-x}Al_xB_2$ with $T_c = 32$ K (Ref. 16) (MgB_2), and an example that demonstrates the dependence of α_1 (and T_c) on interaction $\tilde{\lambda}_{12}$ (labeled "MgB_2").

Sample	λ^0_{11}	λ^0_{22}	λ^0_{12}	λ^0_{21}	μ^*	$\theta(0)$	$\tilde{\lambda}_{11}$	$\tilde{\lambda}_{22}$	$\tilde{\lambda}_{12}$	$\tilde{\lambda}_{21}$	α_1	$\alpha_1^{\rm exp}$
1	0.4	0.2	0.2	0.15	0.1	0.29	16.2	6.4	5.4	3.2	2.04	2.04
2	0.4	0.12	0.2	0.15	0.1	0.29	13.9	5.2	0.93	2.62	1.82	1.82
MgB_2	0.82	0.43	0.124	0.157	0.12	0.29	5.12	2.78	0.03	0.33	1.78	3.08
"MgB_2"						0.29			5.107	0.33	3.08	

temperatures and under the assumption $\Delta_1(0) > \Delta_2(0)$. It is easy to show that, in this case, due to different amounts of quasiparticles [Eq. (8)] in the bands, $n_1(t) < n_2(t)$, and during growth of the temperature, the gap ratio $\theta(T)$ will decrease down to its minimal value reached at T_c

$$\theta(T_c) = \frac{1}{2\tilde{\lambda}_{12}}[-\tilde{\lambda}_{11} + \tilde{\lambda}_{22} + \sqrt{(\tilde{\lambda}_{11} - \tilde{\lambda}_{22})^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}}] \tag{12}$$

with the critical temperature determined from

$$\ln\frac{2\gamma_E\Omega_c}{\pi T_c} = \frac{1}{2}[\tilde{\lambda}_{11} + \tilde{\lambda}_{22} - \sqrt{(\tilde{\lambda}_{11} - \tilde{\lambda}_{22})^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}}]. \tag{13}$$

We note that, in the above two expressions, the signs of the square roots correspond to the case $\tilde{\lambda}_{IJ} > 0$; otherwise, these signs should be inverted. Equations (10)–(13) allow one to determine the important parameters of the theory—the ratios of the superconducting gaps to the critical temperature $\alpha_J = \Delta_J(0)/T_c$:

$$\alpha_1 = \alpha_0 e^{\Lambda_1}, \quad \alpha_2 = \alpha_0 e^{\Lambda_2} \equiv \alpha_1\theta(0), \tag{14}$$

$$\Lambda_1 = \tilde{\lambda}_{12}\theta(0) - \frac{1}{2}[\sqrt{(\tilde{\Lambda}_{12})^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}} - \tilde{\Lambda}_{12}], \tag{15}$$

where $\alpha_0 = \pi/\gamma_E \approx 1.764$, and $\tilde{\Lambda}_{12}$ is the right part of Eq. (10). The so-determined parameters $\Lambda_{1,2}$ (and α_J) depend only on the values of $\theta(0)$ and of effective interband constant $\tilde{\lambda}_{IJ}$. In order to evaluate α_1, Eq. (14) has to be rewritten in a more visual form

$$\Lambda_1 = \tilde{\lambda}_{12}\{\theta(0) - \theta(T_c)\} > 0. \tag{16}$$

It is easily seen that, even in conditions of a relatively weak interband interaction when the parameter $\theta(0)$ depends mainly on intraband coupling constants and $\theta(T_c) \sim \lambda_{21}$, for $\lambda_{12} > \lambda_{21}$ the ratio α_1 of $\Delta_1(0)$ to the critical temperature can be rather large—even for weak coupling superconductors (see Table I). This means that, opposite to conventional regular superconductors, in the two-band superconductors, the large values of α_1, $\alpha_1 > 1.764$, are not unambiguously indicative of strong EPI.

The three parameters $\theta(0)$, $\tilde{\lambda}_{12}$, and $\tilde{\lambda}_{21}$ represent a complete set of the two-band BCS equations for the reduced gaps $\delta_J(t) = \Delta_J(t)/\Delta_J(0)$ at finite temperatures:

$$\ln\delta_1(t) = -n_1(t) - \tilde{\lambda}_{12}\theta(0)[1 - \delta_2(t)/\delta_1(t)], \tag{17}$$

$$\ln\delta_2(t) = -n_2(t) - \tilde{\lambda}_{21}/\theta(0)[1 - \delta_1(t)/\delta_2(t)], \tag{18}$$

$$n_J(t) = 2\int_0^\infty d\omega f[\alpha_J\varepsilon_J(\omega)/t]/\varepsilon_J(\omega), \tag{19}$$

$$\varepsilon_J(\omega) = \sqrt{\omega^2 + \delta_J^2(t)}. \tag{20}$$

In Eqs. (19) and (20), $\varepsilon_J(\omega)$ is the reduced spectrum of a superconductor and $t = T/T_c$ is the reduced temperature. It is seen that Eqs. (17) and (18) are much simpler than initial Eq. (1), and this allows one to easily determine the dependences of reduced gaps on the interband interaction.

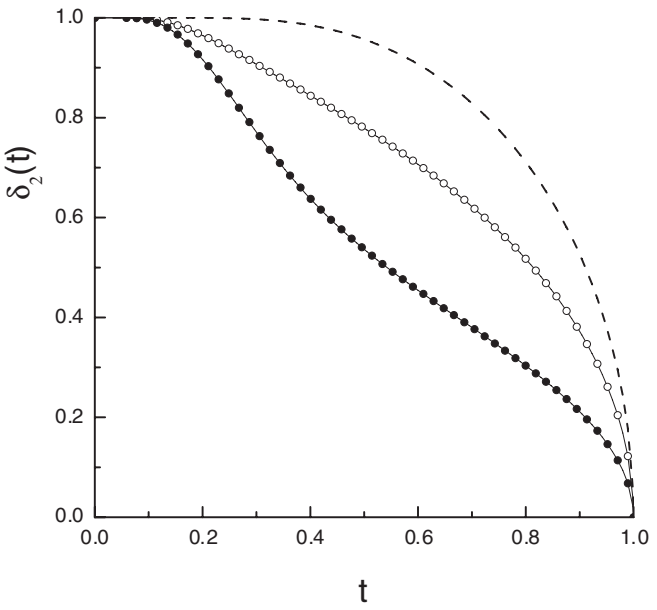

FIG. 1. Dependence of reduced gaps $\delta_2(t) = \Delta_2(t)/\Delta_2(0)$ on the reduced temperature $t = T/T_c$ calculated with $\theta(0) = 0.275$, $\alpha_1 = 1.78$ for two superconductors with different interband couplings, (a) $\tilde{\lambda}_{12} = 0.05$ and $\tilde{\lambda}_{21} = 0.1$ (filled symbols) and (b) $\tilde{\lambda}_{12} = 0.22$ and $\tilde{\lambda}_{21} = 0.8$ (open symbols). Dashed line shows the $\delta_0(t)$ dependence calculated according to the two-band α model that does not consider the interband interaction. [In the two cases, the reduced gaps $\delta_1(t)$ practically coincide with $\delta_0(t)$ and are not shown.]

The quantities $\alpha_{1,2}$, $\tilde{\lambda}_{12}$, and $\tilde{\lambda}_{21}$ that enter Eqs. (17) and (18) characterize the intraband and the interband fluctuations, respectively. Let us consider the contribution of interband fluctuations. The ratio $\delta_2(t)/\delta_1(t) = \theta(t)/\theta(0) < 1$ and decreases with increasing temperature. For that reason, the contribution of interband fluctuations leads to the decrease of the gap $\delta_1(t)$ and to an increase of $\delta_2(t)$; this contribution, however, will never overcome the intraband one. This implies that, for large interband constants, $\lambda_{21} > \lambda_{22}$, the gaps values become equal: $\delta_2(t) \to \delta_1(t)$ and $\alpha_1 \to \alpha_0$ [see Eq. (16)], and the values of both reduced gaps approach $\delta_0(t)$—the solution of a standard BCS equation. Note that the amplitudes of reduced gaps, $\delta_{1,2}(t)$, at any temperature do not exceed the value $\delta_0(t)$, and their temperature dependences at $t \to 1$ are weaker compared with the dependence $\delta_0(t)$.

Figure 1 shows the dependence of the reduced gap $\delta_2(t)$ on interband constants values $\tilde{\lambda}_{IJ}$; the data in this figure are calculated for two kinds of superconductors, (a) and (b), that have the same ratios of the gaps $\theta(0)$ and the same ratios $\alpha_{1,2}$ of the gaps to the critical temperature, but different interband interactions: (a) $\tilde{\lambda}_{12} = 0.05, \tilde{\lambda}_{21} = 0.1$; (b) $\tilde{\lambda}_{12} = 0.22, \tilde{\lambda}_{21} = 0.8$. For comparison, also the reduced gap is plotted calculated according to the well-known two-band α model that assumes $\delta_{1,2}(t)$ equal to $\delta_0(t)$. The crucial role played by interband interaction is clearly seen.

The temperature dependence of the specific heat C_s of a superconductor is usually characterized by the ratio $C_s(T)/\gamma_n T_c$. For a two-band superconductor, the specific heat can be calculated in a usual manner.[1,15] Writing down the

expression for the entropy $S_J(T)$ [or normalized entropy $s_J(t) \equiv S_J(t)/\gamma_J T_c$] of a free Fermi gas with the spectrum given by Eqs. (2) and (20)

$$S_J(T) = 2N_J(0)\int_{-\infty}^{\infty} d\xi([E_J(\xi)/T]f[E_J(\xi)] - \ln\{f[-E_J(\xi)]\}), \quad (21)$$

$$s_J(t) = 3\alpha_J/\pi^2 \int_{-\infty}^{\infty} d\omega([\alpha_J\varepsilon_J(\omega)/t]f[\alpha_J\varepsilon_J(\omega)/t] - \ln\{f[-\alpha_J\varepsilon_J(\omega)/t]\}), \quad (22)$$

where $\gamma_J = 2\pi^2 N(0)/3$ is the coefficient of normal electronic specific heat of the band J ($\gamma_n = \gamma_1 + \gamma_2$), we get

$$[c_s(t)/\gamma_n T_c]/t = \frac{d}{dt}\left[\frac{\gamma_1}{\gamma_n}s_1(t) + \frac{\gamma_2}{\gamma_n}s_2(t)\right]. \quad (23)$$

The dependences of the electronic specific heat on interband interaction, again for the two kinds of superconductors, (a) and (b), are shown in Figs. 2 and 3. For comparison, these figures contain also the correspondent curves calculated within the standard (no interband interaction considered) two-band α model[2] with the same values of $\alpha_{1,2}$ as in (a) and (b). Figure 2 clearly demonstrates all peculiarities of the temperature behavior of the specific heat of a two-band superconductor. There is a feature around $T^*(\alpha_2)$—a smeared (by the interaction $\tilde{\lambda}_{21}$) kink in the specific heat of the band with a smaller gap. In the limit $\tilde{\lambda}_{21} \gg 1$ [corresponding to $\delta_2(t) \to \delta_0(t)$, as we have seen, i.e. to the standard two-band α model] the kink becomes much smoother. In the same manner, the interaction $\tilde{\lambda}_{12}$ smoothes the kink around T_c that is connected to the first band. From Eq. (23), it is seen that the feature

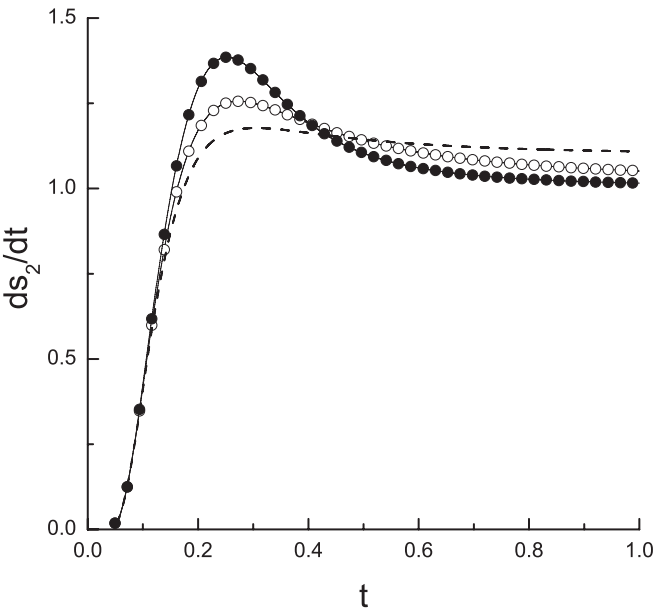

FIG. 2. Temperature dependence of normalized electronic specific heat of the band with smaller gap calculated with $\theta(0) = 0.275$, $\alpha_1 = 1.78$ for two superconductors with different interband coupling, (a) $\tilde{\lambda}_{12} = 0.05$ and $\tilde{\lambda}_{21} = 0.1$ (filled symbols) and (b) $\tilde{\lambda}_{12} = 0.22$ and $\tilde{\lambda}_{21} = 0.8$ (open symbols). Dashed line shows calculation according to the two-band α model that does not consider the interband interaction.

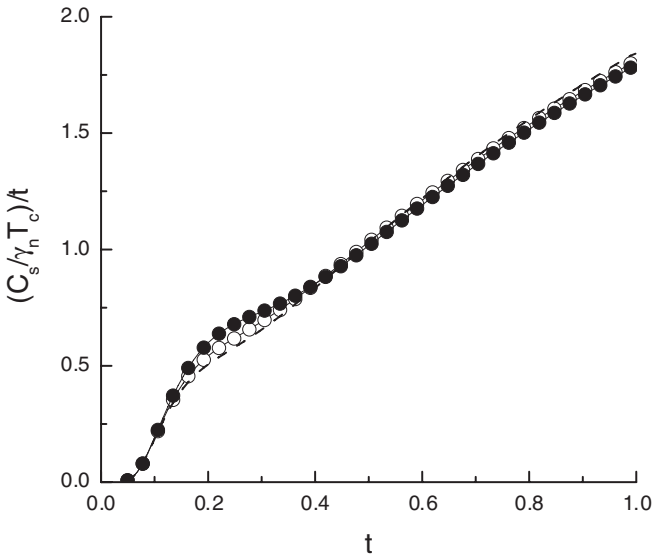

FIG. 3. Temperature dependence ($t = T/T_c$)of normalized electronic specific heat calculated with $\theta(0) = 0.275$, $\alpha_1 = 1.78$ for two superconductors with different interband couplings, (a) $\tilde{\lambda}_{12} = 0.05$ and $\tilde{\lambda}_{21} = 0.1$ (filled symbols) and (b) $\tilde{\lambda}_{12} = 0.22$ and $\tilde{\lambda}_{21} = 0.8$ (open symbols). Dashed line corresponds to calculations according to the two-band α model with $\gamma_1/\gamma_n = 0.55$ and $\gamma_2/\gamma_n = 0.45$.

originating from the band with a smaller gap is more developed when the weight γ_2/γ_n of this band is large enough and when $\theta(0) \ll 1$ (at $T^* \ll T_c$).

We conclude this section by briefly discussing how the two-band α approach can be used for determination of the gaps values from the temperature dependences of the specific heat. One of the merits of the two-band α model is the possibility to correctly determine the value of the smaller gap (α_2) by considering the experimental data at lower temperatures; after that, the larger gap (α_1) can also be found from the jump of the specific heat within the temperature interval closer to T_c. The amplitude of this jump is easily found within the two-band α model by direct calculations of the normalized specific heat, Eq. (22) $\tilde{C}_s$ at the transition point by using the known dependence from the BCS theory $\delta_0(t \to 1)$ (Ref. 18)

$$\tilde{C}_{sJ} = 1 + \frac{12}{7\zeta(3)}\left(\frac{\alpha_J}{\alpha_0}\right)^2, \quad (24)$$

$$\tilde{C}_s = 1 + 1.426\left(\frac{\alpha_1}{\alpha_0}\right)^2 \frac{\gamma_1 + \gamma_2\theta^2(0)}{\gamma_n}. \quad (25)$$

Here, ζ is the zeta-function. According to Eqs. (17) and (18), the two-band α approach is indeed theoretically correctly describing the temperature dependences of the gaps values (and of the specific heat) at temperatures $T \ll T^*$ (see also Figs. 2 and 3 where the symbols represent the accuracy that could be obtained in experiment). However, in order to approximate the experimental curve in a larger temperature interval up to $T \sim T^*$, one would have, generally speaking, to decrease the magnitude of the smaller gap (α_2) relative to its real value. Note, however, that even with this kind of fitting, the data can be realized only in the case of

relatively strong interband interaction (or in dirty enough superconductors). Due to a weaker temperature dependence of $\delta_{1,2}$ compared to $\delta_0(t)$, the specific heat jump in the two-band BCS superconductor appears to be smaller than the jump obtained within the two-band α model. This means that, in order to approximate the curve $C_s(t)$ with the two-band α model at temperatures around T_c, the larger gap has to be reduced relative to its real value. Formally, in the two-band α model, the gaps values can be determined more precisely only for interaction strengths $\lambda_{21} > \lambda_{22}$. This model, still, can describe the experimental data rather well (depending on experimental uncertainty) and provide reasonable estimates of $\alpha_{1,2}$ values also under more soft condition $\lambda_{21} \sim \lambda_{22}$. However, it is not able at all to deliver a correct temperature variation of energy gaps (Fig. 1) and more so the values of the EPI constants of the considered compounds.

III. ELECTRONIC SPECIFIC HEAT OF LAYERED TWO-BAND SUPERCONDUCTORS

The properties of conventional superconductors at low temperatures are well described within the BCS approach where the EPI coupling constants and the energy Ω_c are determined by the EPI spectral function $\alpha^2(\omega)F(\omega)$. (A detailed discussion is presented in Ref. 19.) However, at finite temperatures, the properties of real superconductors can be noticeably different from those predicted by the BCS theory, Eq. (1). In particular, application of the BCS formalism to the strong coupling superconductors overestimates the value of T_c (and correspondingly underestimates the value of α), see Table I. Nevertheless, while calculating the properties of conventional strong-coupling superconductors, the BCS theory can be successfully applied also for finite temperatures according to an empirical recipe given by the α model.[15] In particular, to calculate the electronic specific heat within the α model, one has to use the BCS expression Eq. (22) with the spectrum $\varepsilon(\omega) = \sqrt{\omega^2 + \delta_0^2(t = T/T_c^{\exp})}$ and to set $\alpha = \alpha^{\exp}$.

The success of the α model is based on the fact that its results can be obtained theoretically by formally introducing the kernel of the correction term $k_\alpha = T_c^{\exp}/T_c^0$ into the BCS equation

$$\ln[\Delta(T)/\Delta(0)] = -2\int_0^{\Omega_c} d\xi\, f\left\{\left(T_c^{\exp}/T_c^0\right)[E_J(\xi)/T]\right\}/E_J(\xi). \quad (26)$$

This guarantees that the correct value of $T_c = T_c^{\exp}$ is then obtained. Along with that, the BCS-like Eq. (26) looks exactly the same as the BCS equation for the reduced gap dependent on the reduced temperature, $\delta(t)$. To make a clear distinction to the empirical α model, this kind of theoretical approach should more appropriately be named as α approximation.

In the two-band case, the α approximation, Eq. (26), also provides a correct value of T_c keeping the form of Eqs. (17) and (18) unchanged. Such approach, however, is not universal because the strong coupling corrections are different for the two bands. This can be easily shown taking as an example the nearly independent ($\tilde{\lambda}_{12} \to 0$, $\tilde{\lambda}_{21} \to 0$) bands with strong and weak coupling $\Delta_1(0) > \Delta_2(0)$. In such case $\alpha_1 \to \alpha_0$ and $\alpha_2 \to \alpha_0(T_{c2}^0/T_{c1}^0)$, implying that for reduced temperatures $t \geqslant t^* = T_{c2}^0/T_{c1}^0 < 1$ the gap value $\delta_2(t) \to 0$. Thus, the critical temperatures T_{c1} and $T_{c2} \approx T^*$ in independent bands appear to be equal to $T_{c1} = T_c^{\exp}$ and $T_{c2} = T_{c2}^0(T_c^{\exp}/T_{c1}^0) \ll T_{c2}^0$, respectively. This example shows that in order to improve the α approximation-like Eqs. (17) and (18), the two correction coefficients of the type $k_{1,2} = \beta_{1,2}(\lambda_{IJ})k_\alpha$ have to be taken into account, providing on the one hand the correct values of $T_c = T_c^{\exp}$ and on the other hand the correct behavior of the weak-coupling band in the limit of independent bands. In Eqs. (17) and (18), this will lead to the formal redefinition of $\alpha_{1,2}$, i.e. of $\Delta_{1,2}(0)$ and $\theta(0)$, since T_c [Eq. (13)] depends only on the coupling constants and is not changed during such redefinition. In the general case, this kind of procedure is difficult to realize. At the same time, for the bands with strong and weak coupling in the limit $\tilde{\lambda}_{12} \ll 1$ the correction coefficients are easily found: $k_1 = k_\alpha$, $k_2 = 1$. Here, $\alpha_1 = \alpha_0$, $\alpha_2 = \alpha_2^{\exp}$, and assuming independent bands, the critical temperatures become $T_{c1} = T_c^{\exp}$ and $T_{c2} = T_{c2}^0$.

The above example can easily be generalized to the case of finite $\tilde{\lambda}_{12}$ by redefining the parameters in Eqs. (17) and (18): $\alpha_2 = \alpha_2^{\exp}$ and $\alpha_1 \to \alpha'$, where α' is determined by Eq. (14) and by a self-consistency condition $\alpha'_1\theta'(0) = \alpha_2^{\exp}$. This approximation can be named an α' approximation. Here, the parameter t keeps the meaning of a reduced temperature [$\delta_{1,2}(t = 1) = 0$, $t = T/T_c^{\exp}$] and the auxiliary parameters α' and $\theta'(0)$ are purely formal and carry no particular physical sense. (We note that the BCS-like equations within the α and α' approximations keep the same form of the BCS equations whose properties are described in detail in Sec. II). Now, the spectral functions $\varepsilon_J(\omega) = \sqrt{\omega^2 + \delta_J^2(t)}$, found with the help of two-band BCS-like equations, can be used for generalization of the standard two-band α model.

We have applied the so-generalized two-band α model in Ref. 16 to analyze the tunnel experiments on the two-gap superconductors $Mg_{1-x}Al_xB_2$. The EPI seed coupling constants have been unambiguously calculated for $\Omega_c = 67.76$ meV and for $\mu_{IJ}^* \approx 0.12$ based on the experimental values of $\Delta_{1,2}(0)$ and of Leggett mode energy $\Omega_L(0)$ (Ref. 11) with the values of $\theta(T \to T_c)$ considered; note that the Leggett mode energy is extremely sensitive to the interband as well as the intraband interactions. Calculations within the α' approximation give a very good agreement with experimental results presented in Ref. 13 and obtained not only for the temperature variation of both gaps $\Delta_{1,2}(T)$ but also for the Leggett mode energy $\Omega_L(T)$ (see Fig. 4). We have applied the same technique for calculations of the temperature variation of the superconducting condensate density and of the London penetration depth determined for $Ba(Fe_{0.9}Co_{0.1})_2As_2$ in Ref. 20. The results of our calculations according to the α and α' approximations are presented in Figs. 4 and 5, together with the results obtained according to the standard two-band α model. We see that the experimental data are well reproduced by calculations performed within the α' approximations. Unfortunately, there are no specific heat data for the samples measured in Refs. 13 and 20, and a comparison with our calculations is not possible.

Up to now, the properties of most layered superconductors are not studied in all details, and rather often, their char-

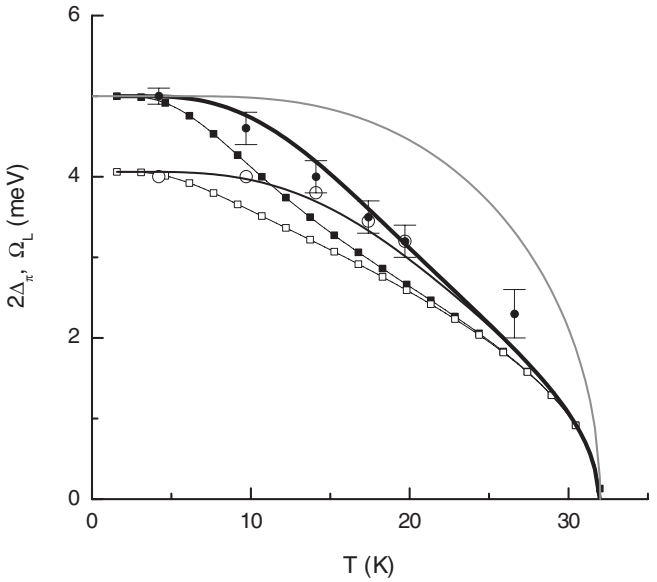

FIG. 4. Temperature dependence of the gap $2\Delta_\pi$ (filled symbols) and of the Leggett mode energy Ω_L (empty symbols) of $Mg_{1-x}Al_xB_2$ with $T_c = 32$ K (Ref. 13). Thick and thin solid lines are calculations within the α' approximation of the gap and Leggett mode energies, respectively. Lines with filled and empty square symbols are calculations according to the α approximation of the gap and Leggett mode energies, respectively. Grey line shows calculation according to α approximation.

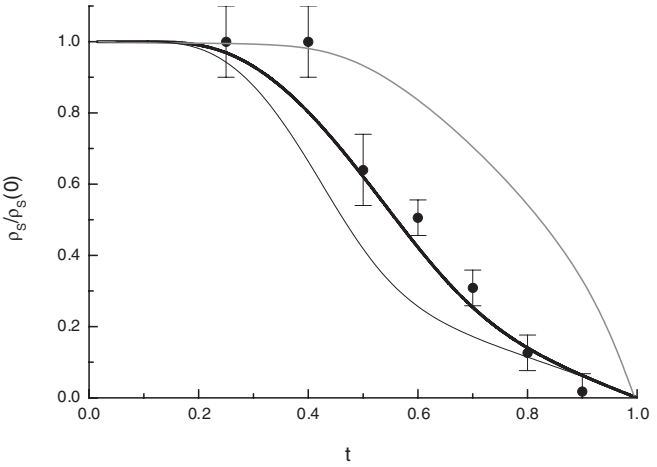

FIG. 5. Temperature dependence of normalized superconducting condensate density of $Ba(Fe_{0.9}Co_{0.1})_2As_2$ (Ref. 20) (symbols). Lines correspond to calculations according to the α' approximation with $\tilde{\lambda}_{12} \sim \tilde{\lambda}_{21} \sim 0.1$ (thick), α approximation (thin) and two-band α model (grey).

acteristics are determined by using indirect methods based on theoretical models. For example, in Refs. 2 and 3, the two-band α model was employed to determine the gaps values $\Delta_{1,2}(0)$ from the temperature variation of the specific heat $C_s(T)$. In these publications, surprisingly, a good agreement has been found in the whole temperature interval, between the two-band α calculations and experimental dependences $C_s(T)$ for $Mg^{11}B_2$ ($T_c = 38.7$ K) (Ref. 2) and $Ba(Fe_{0.95}Co_{0.075})_2As_2$ ($T_c = 21.4$ K).[3] As was discussed in Sec. II, such good agreement can be achieved in the two-band BCS-model (and in generalized two-band α model) under condition $\lambda_{21} \geqslant \lambda_{22}$, i.e. within the whole range of EPI constants. This assumes some uncertainty in the definition of EPI constants from experimental data in such cases. Calculation of electronic specific heat of such superconductors allows one to estimate potentialities of the generalized two-band α model when analyzing available experimental data of the specific heat $C_s(T)$.

We have used the α' approximation to calculate the specific heat of $Mg^{11}B_2$ and of $Ba(Fe_{0.95}Co_{0.075})_2As_2$ [referred to as Ba(FeCo)As in Table II]. The results are presented by Figs. 6 and 7 and in Tables II and III. It can be seen that within the experimental accuracy the specific heat data obtained in Refs. 2 and 3 are very well approximated by a set of curves with effective coupling constants $\tilde{\lambda}_{12} \leqslant \tilde{\lambda}_{12}^{\max}$, $\tilde{\lambda}_{21} \geqslant \tilde{\lambda}_{21}^{\min}$ and parameters $\alpha_{1,2}$ that are changing from the values indicated in Table II (fit max-min) to the values calculated within the two-band α model. These latter values are obtained for the interband interaction $\tilde{\lambda}_{12} \sim 0.1 \ll \tilde{\lambda}_{21} \sim 3.5$ (fit min-max). According to the formal approximation criteria, the parameters of the min-max fit are close to optimal. In Figs. 6 and 7, the fit min-max curves are shown with empty symbols. The fit min-max curves that are coinciding with those obtained within the two-band α model are not shown here.

A comparison of the gaps $\Delta_{1,2}(0)$ in $Mg^{11}B_2$ ($T_c = 38.7$ K) given in Table II with their values in MgB_2 ($T_c = 40.5$ K) $\Delta_1(0) \approx 10$ meV, $\Delta_2(0) \approx 2.6$ meV (Ref. 13) indicate different degrees of imperfection of the samples studied in Refs. 2 and 13. The difference, however, cannot be accounted for by elastic interband scattering on impurities that would lead to an increase of the smaller gap.[9] It looks more probable that the difference should be connected to the different electron-phonon scattering caused by defects in the crystal structure. The smaller gap in $Ba(Fe_{0.925}Co_{0.075})_2As_2$ ($T_c = 21.4$ K) agrees well with the values reliably determined from the optical experiments[20] $Ba(Fe_{0.9}Co_{0.1})_2As_2$ ($T_c \approx 20$ K): $\Delta_2(0) \approx 15$ cm^{-1} (1.85 meV) and $\Delta_1(0) \approx 30$ cm^{-1} (3.9 meV).

TABLE II. Gap values and coupling and other parameters characterizing superconducting $Mg^{11}B_2$ (Ref. 2) and $Ba(Fe,Co)_2As_2$ (Ref. 3).

Sample/reference	Fit	$\tilde{\lambda}_{12}^{\max}$	$\tilde{\lambda}_{21}^{\min}$	$\alpha_1(\tilde{\lambda}_{12}^{\max},\tilde{\lambda}_{21}^{\min})$	$\alpha_2(\tilde{\lambda}_{12}^{\max},\tilde{\lambda}_{21}^{\min})$	Δ_1 meV	Δ_2 meV
$Mg^{11}B_2$ (Ref. 2)	α'	1.9	2.75	2.3088	0.6	7.77	2.0
	Two-band α			2.2	0.6	7.337	2.0
$Ba(Fe,Co)_2As_2$ (Ref. 3)	α'	0.45	0.25	2.4875	0.9748	4.587	1.797
	Two-band α			2.2	0.95	4.057	1.752

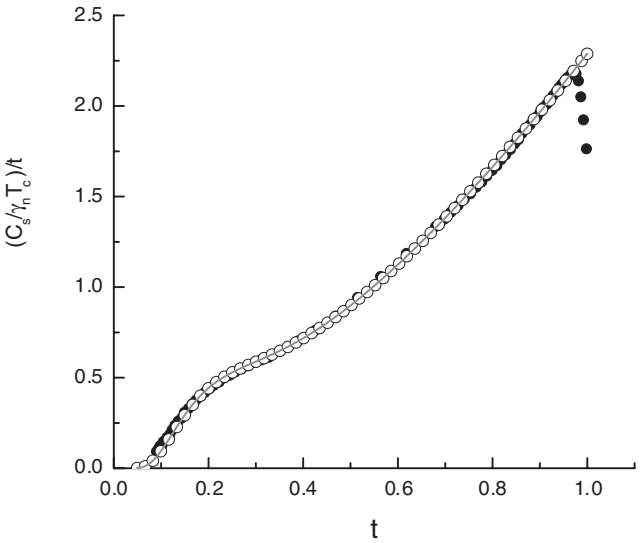

FIG. 6. Temperature dependence of electronic specific heat of $Mg^{11}B_2$ (Ref. 2) (filled symbols). Grey line shows calculations according to the two-band α model; open symbols represent calculation according to the α' approximation with parameters given in Table II.

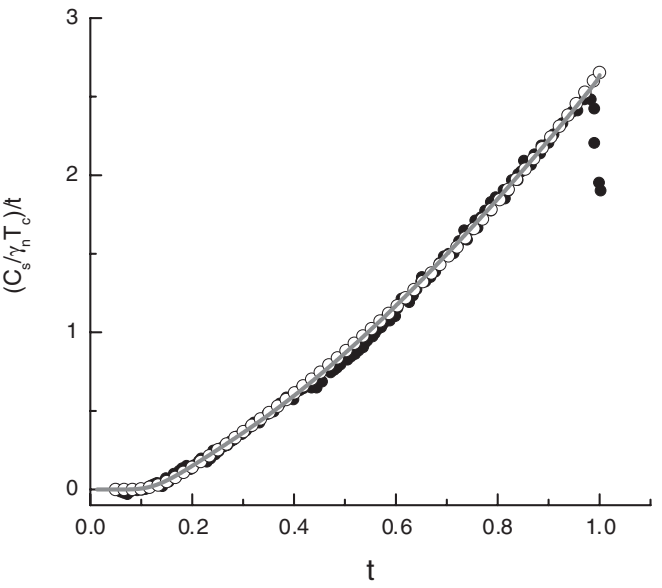

FIG. 7. Temperature dependence of electronic specific heat of $Ba(Fe_{0.925}Co_{0.075})_2As_2$ (Ref. 3) (filled symbols). Grey line shows calculations according to the two-band α model; open symbols represent calculations according to the α' approximation with parameters given in Table II.

The method we have used for our calculations allows one to determine not only the effective interband coupling constants, but also all EPI coupling constants of the samples. Assuming $\Omega_c = 67.76$ meV ($Mg^{11}B_2$), $\Omega_c \approx 30$ meV [Ba(FeCo)As],[21] $\mu^* = 0.12$ and using Eqs. (11), (9), and (4), we find the EPI seed constants λ^0_{IJ} that are given in Table III. It is seen from the table that the lowest accuracy of EPI constants determination that can be reached in the generalized two-band α model is not better than the best accuracy of the first-principles calculations,[4–6] and this fact in our opinion is quite a good result. In this table, we also present for comparison the data for MgB_2 ($T_c = 40.5$ K) determined in our early tunnel experiments.[16] Comparison of the EPI strengths in $Mg^{11}B_2$ (data from Ref. 2) and in MgB_2 (data from Ref. 16), really reveals significant differences. First, the interband EPI is much larger in $Mg^{11}B_2$ (Ref. 2) compared to MgB_2 (Ref. 16; see Table III). Second, an appreciable increase (actually an equalization) of interband and intraband scattering in the π band is observed in $Mg^{11}B_2$.[2] These kinds of effects can be caused by the defects in the magnesium plane.[9] In $Ba(Fe_{0.925}Co_{0.075})_2As_2$, the calculated value of the intraband constant $\lambda^0_{22} \leqslant 0.53$ is in good accordance with the value estimated from the optical experiments $\lambda^0_{22} \approx 0.45$.[17] We note that the optimal EPI constants (fit min-max) determined by us satisfy, as expected, the applicability criteria of the $2B\alpha$ model.

IV. CONCLUSIONS

The well known two-band α model considering independent bands is generalized by consistently taking into account the interband electron-phonon interaction. The validity of the obtained generalized BCS-like equations is verified by analyzing different experiments on different compounds—the data of the tunnel experiments on $Mg_{1-x}Al_xB_2$ and optical experiments on $[Ba(Fe_{0.9}\ Co_{0.1})_2As_2]$. It is demonstrated that the two-band α model that leaves out the interband interaction is formally valid only in the case of relatively strong interband scattering (when it is larger or of the order of intraband scattering) in the band with a smaller superconducting gap and that the values of the gaps determined within this model are understated. Within the developed formalism, the temperature dependences of the electronic specific heat of $Mg^{11}B_2$ and $Ba(Fe_{0.95}Co_{0.075})_2As_2$ are analyzed, and the values of energy gaps and coupling constants of the compounds are determined

TABLE III. Electron-phonon interaction constants of superconductors MgB_2 (Ref. 6), $Mg^{11}B_2$ (Ref. 2), and Ba(FeCo)As (Ref. 3). For comparison, the data obtained for MgB_2 ($T_c = 40.5$ K) determined from the tunnel experiments results (Ref. 16) is also presented.

Sample/reference	Fit	λ^0_{11}	λ^0_{22}	λ^0_{12}	λ^0_{21}	μ^*	Ω_c (meV)	$\theta(0)$	T_c (K)
MgB_2 (Ref. 16)		0.921	0.43	0.124	0.157	0.12	67.76	0.25	40.5
$Mg^{11}B_2$ (Ref. 2)	Max-min	0.78	0.228	0.205	0.209	0.12	67.76	0.26	38.7
	Min-max	0.767	0.204	0.124	0.22				
Ba(FeCo)As (Ref. 3)	Max-min	0.889	0.531	0.204	0.157	0.12	≈30.0	0.39	21.4
	Min-max	0.85	0.289	0.128	0.275				

basing on the known specific heat data. The values of obtained parameters are close to those of analogous compounds studied by us earlier, with the EPI constants in bands with smaller gaps fitting the criteria of applicability of the $2B\alpha$ model to the case of superconducting $Mg^{11}B_2$ and $Ba(Fe_{0.95}Co_{0.075})_2As_2$.

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