

Generalized BCS Equations and the Iron-Pnictide Superconductors

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ABSTRACT

A detailed quantitative study of the pnictide composite superconductor (CS) $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ is presented in the framework of the recently derived set of generalized BCS equations. Invoking multiple Debye temperatures to take into account anisotropy of the CS, we address the current experimental data on its T_c and the (not so clear-cut) gap-values via different theoretical scenarios that attempt to identify the ion species responsible for pairing in it. This is done with the aid of the Bogoliubov's restriction on the BCS dimensionless electron-phonon coupling constant. Significantly, our study sheds light on the gaps which have recently been observed in different iron-pnictide CSs as nodes or line-nodes on the Fermi surface and have evinced considerable interest.

Keywords: Generalized BCS Equation; Iron-Pnictide Superconductors; Multiple Gaps

1. Introduction

Iron-pnictide superconductors (SCs) [1-4] constitute a promising new family because its members have rather high critical temperatures (T_c s); additionally, they readily allow a variety of chemical substitutions to be made. These attributes of the family suggest the possibility in the foreseeable future of fabricating SCs that might meet specific technological needs. It is therefore imperative to develop a theoretical understanding of these materials. To this end, we present in this paper the results of a detailed study, based on the new framework of the generalized BCS equations (GBCSEs) [5], concerned with a prominent member of the family, namely $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ (Ba-As henceforth). We believe that our findings will help in the current flurry in the field.

This paper is organized as follows. In §2 we summarize the main experimental features of Ba-As. §3 recalls the salient features of GBCSEs, which are then applied to this SC in §4 by taking into account different scenarios allowed by the current experimental situation. §5 sums up our findings.

2. Salient Experimental Features of Ba-As

The features of Ba-As that concern us here are its T_c and

the values of its multiple gaps. The experimental situation with regard to the first of these is easily summarized because the values quoted for it in the literature are more or less consistent: $T_c = 36.5$ K [3,6]; 38 K [4,6] and 37 K [7]. The situation with regard to the gap-values, however, is not so clear cut.

A broad statement about the $T = 0$ gap-values in question was made by [3] on the basis of angle-resolved photoemission spectroscopy (ARPES) measurements reported by [8]. The values so quoted are: 6 and 12 MeV. While reporting a gap at about 6 MeV and the absence of a gap at about 12 MeV, it was remarked in [6] that this discrepancy (the absence of the larger gap) may be induced by the difference in the methods adopted for determining the gap/s—a remark borne out by what follows. Gaps of single Ba-As crystals were determined both via scanning tunneling microscopy (STM) and spectroscopy in [7] and via penetration-depth measurements in [9]. While the latter of these approaches led to the values of 2.5 and 9.0 MeV, the values yielded by the former method are 3.3 and 7.6 MeV. The situation is further compounded because: 1) based on specific-heat data, three gap-values have been reported [10] at 3.6, 8.5 and 9.2 MeV, whereas 2) the recent ARPES experiment [11] has led to three gaps at 4, 7, and 12 MeV on hole-like

Fermi surfaces with an additional gap at 9.5 MeV on the electron-like Fermi surface.

For the application of GBCSEs to Ba-As, one requires, first of all, its Debye temperature. Then, in the two-gap scenario, given any two parameters from the set $S = \{\Delta_1(0), \Delta_2(0), T_c\}$, one is enabled to calculate the remaining parameter. In the scenario in which Ba-As is characterized by two gaps, guided by [7], we adopt for it the set $S = \{3.05 \text{ MeV}, 8.3 \text{ MeV}, T_c = 38 \text{ K}\}$ as our *starting point*. Also included in this study is an account of our findings in the scenario in which Ba-As may be characterized by three gaps different values for which have been quoted above.

In concluding this summary of the experimental features of Ba-As we note that its Debye temperature is an essential input in this study. This is a parameter rarely quoted for the class of SCs addressed here. The value 274 K adopted by us is the one quoted in [6]. This will be further discussed below.

3. Salient Features of GBCSEs

1) They are based on the premise that superconductivity arises from the formation of Cooper pairs (CPs). CPs in *composite superconductors* (CSs), however, are regarded as bound via not only one-phonon exchanges, but also via exchanges of two or more species of phonons: these lead to GBCSEs [5]. This implies that CPs in a binary SC, for example, may be bound via two kinds of “glues” or “springs”—leading to two binding energies for the CPs and hence to two gaps.

2) They bypass the issue of the underlying mechanism that brings about pairing. This is so because a two-gap SC requires the specification of two dimensionless interaction parameters λ_1^c and λ_2^c which occur in three GBCSEs: two for the gaps and one for the T_c . It is this feature of GBCSEs that enables one to calculate any one of the parameters of the set $S = \{\Delta_1(0), \Delta_2(0), T_c\}$, given the other two.

3) They take into account the *anisotropy* of CSs by characterizing them via multiple Debye temperatures (MDTs). These were first introduced by Born and von Karman in connection with a refinement of the Debye theory of specific heat by observing that elastic waves in an anisotropic solid travel with different velocities in different directions. For a review of this and other similar work, we refer to the textbook [12]. In the context of superconductivity, MDTs were resurrected in [13], and subsequently applied [14,15] to a variety of CSs.

4. GBCSEs Applied to Ba-As

4.1. Two-Gap Scenario

The steps [14] to be followed are:

1) Identify the ion species responsible for pairing in

the CS. For Ba-As we assume that these are the Ba and the Fe or/and the Ba and As ions.

2) Fix the Debye temperatures of the ions identified in 1) via the following equations meant to take into account the anisotropy of the CS:

$$x\theta_2^c + (1-x)\theta_1^c = \theta(x) \quad (1)$$

$$\frac{\theta_1^c}{\theta_2^c} = \left[\frac{1 + \sqrt{m_2/(m_1 + m_2)}}{1 - \sqrt{m_2/(m_1 + m_2)}} \right]^{1/2} \quad (2)$$

These are to be applied to both the $\text{Ba}_{0.6}\text{K}_{0.4}$ and the Fe_2As_2 layers. In (1) $\theta(x)$ is Debye temperature of the CS; in (2) m_1, m_2 are the atomic masses of A, B if the layer is designated as A_xB_{x-1} . A derivation of (2) is given in [5] where it is assumed that the modes of vibration of the two ions in any layer of the SC are simulated by the modes of vibration of the two bobs of a double pendulum. Note that the ratio of the Debye temperatures in (2) depends on the relative positions of A and B in the double pendulum. In principle, therefore, each ion species may be characterized by *two* values of the Debye temperature. The values of θ_i^c ($i = \text{Ba, Fe, As}$) thus obtained appear in **Table 1**, where they are marked from (1) to (6).

3) To determine the values of λ_1^c and λ_2^c , employ the following GBCSEs [5] in which $W_1(0)$ and $W_2(0)$ are to be identified with $\Delta_1(0)$ and $\Delta_2(0)$ [14,15], respectively

$$1 = \lambda_1^c \ln \left[1 + \frac{2\hbar(\omega_D)_1^c}{|W_1(0)|} \right] \quad (3)$$

$$1 = \lambda_1^c \int_0^{\theta_1^c/2T_c} \frac{\tanh(x)}{x} dx + \lambda_2^c \int_0^{\theta_2^c/2T_c} \frac{\tanh(x)}{x} dx \quad (4)$$

$$1 = \lambda_1^c \ln \left[1 + \frac{2\hbar(\omega_D)_1^c}{|W_2(0)|} \right] + \lambda_2^c \ln \left[1 + \frac{2\hbar(\omega_D)_2^c}{|W_2(0)|} \right], (\hbar\omega_D = k_B\theta) \quad (5)$$

where k_B is the Boltzmann constant. The λ s can be determined with the input of: a) $\Delta_1(0)$ and $\Delta_2(0)$ into (3) and (5); b) $\Delta_1(0)$ and T_c into (3) and (4); c) T_c and $\Delta_2(0)$ into (4) and (5). One is then enabled to calculate T_c via (4), or $\Delta_2(0)$ via (5), or $\Delta_1(0)$ via (3).

4) Regardless of how $\lambda_{1,2}^c$ are determined, impose on them the Bogoliubov upper bound on λ [16] that each dimensionless coupling constant be positive definite and satisfy

$$\lambda_{1,2}^c < 0.5 \quad (6)$$

As will be seen, this criterion is an invaluable guide in this study.

5) If one follows either approach a) or b) of paragraph

Table 1. In the first three columns are given the Debye temperatures (θ) of Ba, Fe and As ions obtained via Equations (1) and (2) with $\theta(x) = 274$ K [6]. For each pair of Debye temperatures given in column (4), λ s given in column (6) are calculated with the initial input of $W_2 = 8.3$ MeV and $T_c = 38$ K. Since these λ -values (e.g., 28.61, -25.87 against the pair of Debye temperature (1, 3)) in each case violate the constraint given in Equation (6), we first vary $W_2(0)$ (retaining $T_c = 38$ K) till λ -values that satisfy constraint (6) are obtained. This procedure is repeated by varying T_c (retaining $W_2(0) = 8.3$ MeV). Each pair of such acceptable λ -values leads via Equation (3) to two possible values for the smaller gap, one of which ($\sim 10^{-2}$ MeV) seems to be a signature of the node or line-node reported in [17-19].

Debye Temperatures [K]			Ba + Fe scenario				Ba + As scenario			
θ_{Ba} [K]	θ_{Fe} [K]	θ_{As} [K]	Debye temps used	W_2, T_c [MeV, K]	$\lambda_{Ba}, \lambda_{Fe}$	$W_{1(Ba)}, W_{1(Fe)}$ [MeV]	Debye temps used	W_2, T_c [MeV, K]	$\lambda_{Ba}, \lambda_{As}$	$W_{1(Ba)}, W_{1(As)}$ [MeV]
				8.3, 38	28.61, -25.87	-, -		8.3, 38	34.16, -31.74	-, -
326.21	399.43	375.92	(1, 3)	6.4, 38	0.311, 0.118	2.35, 1.40×10^{-2}	(1, 5)	6.4, 38	0.265, 0.164	1.33, 0.144
(1)	(3)	(5)		8.3, 48	0.303, 0.169	2.15, 0.192		8.3, 48	0.236, 0.236	0.835, 0.958
				8.3, 38	-1.245, 2.337	-, -		8.3, 38	-0.684, 1.704	-, -
124.58	172.08	148.57	(1, 4)	7.1, 38	0.028, 0.571	1.25×10^{-14} , 6.23	(1, 6)	7.1, 38	0.151, 0.439	7.49×10^{-2} , 2.92
(2)	(4)	(6)		8.3, 44	0.136, 0.474	3.60×10^{-2} , 4.10		8.3, 44	0.232, 0.372	0.766, 1.87
				8.3, 38	1.257, -0.271	-, -		8.3, 38	1.259, -0.279	-, -
			(2, 3)	7.5, 38	0.480, 0.146	$3.05, 7.31 \times 10^{-2}$	(2, 5)	7.3, 38	0.476, 0.151	$2.99, 8.63 \times 10^{-2}$
				8.3, 43	0.429, 0.203	2.31, 0.497		8.3, 43	0.423, 0.211	2.23, 0.572
				8.3, 38	1.679, -0.753	-, -		8.3, 38	2.28, -1.35	-, -
			(2, 4)	7.5, 38	0.460, 0.236	2.76, 0.436	(2, 6)	7.6, 38	0.494, 0.228	3.26, 0.327
				8.3, 42	0.259, 0.439	0.469, 3.41		8.3, 41	0.390, 0.356	1.79, 1.64

Notes on tables: Atomic masses used in the calculation of Debye temperatures are: 137.33 K (Ba), 39.098 K (K), 74.92 K (As), 55.847 K (Fe). *Entry marked (1) is obtained when Ba is the upper bob (and K the lower one); θ_k^c are not given as they are not used as shown) in the double pendulum; the one marked (2) is obtained with bobs interchanged. *The θ_i^c in next two columns are to be similarly interpreted. *Note, however, that a pair of θ_i^c s that satisfies Equation (1) is (3) and (6), not (3) and (5).

3), then, while invoking (3), a guess is required about the ion species (Ba, or Fe, or As) that is responsible for $W_1(0)$. This issue is circumvented in approach c), which is also the approach one must follow if $\Delta_1(0)$ is the parameter known with the least accuracy—as is generally the case. Therefore, we first give below an account of approach c).

6) Let the Ba and Fe ion species be invoked to determine the two λ s via (4) and (5). Note that one cannot assume that $\theta_{Fe}^c = \theta_{As}^c = \theta(x)$ because it causes the characteristic determinant of the equations to vanish whence the λ 's become indeterminate. The combinations of θ s (**Table 1**) that we need to consider are: (1, 3), (1, 4), (2, 3) and (2, 4). Further, we require as input the values of T_c and $W_2(0)$; guided by [7], we adopt $T_c = 38$ K and $W_2 = 8.3$ MeV to solve for the λ s. We remark that if among the four pairs of λ values that are thus obtained there is a pair that automatically satisfies constraint (6), then (3) enables one to straightaway calculate two possible values for $W_1(0)$, one for each λ together with the associated θ . If one or both of these are in accord with experiment, then one is also led to the identification of the ion species

responsible for it. This will happen only if the input values for the T_c and $W_2(0)$ are accurately known. Generally, the latter of these is known with greater uncertainty, an uncertainty that GBCSEs can help to resolve.

7) Returning to the Ba + Fe scenario under consideration, among the four pairs of λ values that are obtained (**Table 1**), the pair corresponding to Debye temperatures (1, 3) is in gross disagreement with criterion (6). Of the remaining three, all of which also violate (6), let us first consider the one that is closest to satisfying it:

$$\lambda_{Ba}^c = 1.257, \lambda_{Fe}^c = -0.271.$$

Now if T_c is accurately known, then vary the value of $W_2(0)$ gradually till both the λ s satisfy (6). Once this is achieved, calculate $\Delta_1(0)$ via (3)—with $(\lambda_{Ba}^c, \theta_{Ba}^c)$ and $(\lambda_{Fe}^c, \theta_{Fe}^c)$. Following this procedure we find that $W_2 = 7.3$ MeV leads to $W_{Ba} = 3.05$ MeV (the experimental value is $\Delta_1(0) = 3.6(0.5)$ MeV [7] and $W_{2(Fe)} = 0.04$ MeV—via λ s given in **Table 1**. Pertinent questions at this point are: why stop after a pair of λ values satisfying constraint (6) is found? Why not seek to find even lower λ values? One can do so, of course. However, this leads

one farther away from the starting point of $W_2(0) = 8.3$ MeV. If $W_2(0)$ is believed to be accurately known, then apply the same procedure by varying T_c . In this case T_c has to be increased in order to obtain the λ s that satisfy constraint (6). Thus, $T_c = 43$ K yields $\lambda_{\text{Ba}}^c = 0.429$, $\lambda_{\text{Fe}}^c = 0.203$, which lead to $\Delta_1(0)_{\text{Ba}} = 2.31$ MeV, $\Delta_1(0)_{\text{Fe}} = 0.5$ MeV. Also given in **Table 1** are the results of a similar exercise for all the other pairs of λ values not only in the Ba + Fe scenario, but also in the Ba + As scenario. We are thus led to the results: a) In the Ba + Fe scenario, the *only* combination of Debye temperatures that can account for the experimental features of BaAs is (2, 3) since this leads to set {3.05 MeV, 7.3 MeV, 38 K}, the experimental range of the values of the gaps being: $\Delta_1(0) = 3.6(0.5)$ MeV and $\Delta_2(0) = 8.3(0.9)$ MeV; b) Similarly, in the Ba + As scenario the only acceptable combination of Debye temperatures is (2, 6) which leads to the set {3.27 MeV, 7.6 MeV, 38 K}; c) In both cases the smaller gap is due to Ba and the theory has led to it *per se*; d) It seems interesting to note that if both the Ba + Fe and the Ba + As scenarios are invoked for the formation of CPs then, *in principle*, one can account for the four gaps that have recently been reported from an ARPES experiment [11].

8) We now deal with approach a), paragraph c). Assuming that $\Delta_1(0) = 3.6$ MeV and $\Delta_2(0) = 8.3$ MeV [7], we seek to calculate the T_c of the CS via (4) “after the λ s are determined via (3) and (5) by invoking both the (Ba, Fe) and the (Ba, As) pairs. The combinations of Debye temperatures that we now have to deal with, together with the results that they lead to, have been given in **Table 2**. This table also provides a guide, should it be

needed, about employing approach b), paragraph c). The results in this table are not conclusive because of the uncertainties in *both*—the input values of $\Delta_1(0)$ and $\Delta_2(0)$. Nevertheless, it seems significant that the lowest best result for T_c , *i.e.* 40.7 K, should have been led to by the (2, 6) combination of Debye temperatures as was the case above.

4.2. Three-Gap Scenario

The equality between $|W|$ (which is defined via the relation $2E_F + W$ for the total energy of a CP where E_F is the Fermi energy) and Δ [5] implies that there must be three $|W|$ s if there are three gaps. We now take into account CPs bound via *three*-phonon exchanges in addition to those that are bound via one- and two-phonon exchanges. Equations (3) and (5) are therefore supplemented [14,15] by

$$1 = \lambda_1^c \ln \left[1 + \frac{2\hbar(\omega_D)_1^c}{|W_3(0)|} \right] + \lambda_2^c \ln \left[1 + \frac{2\hbar(\omega_D)_2^c}{|W_3(0)|} \right] + \lambda_3^c \ln \left[1 + \frac{2\hbar(\omega_D)_3^c}{|W_3(0)|} \right] \quad (7)$$

Further, (4) now goes over to

$$1 = \lambda_1^c \int_0^{\theta_1^c/2T_c} \frac{\tanh(x)}{x} dx + \lambda_2^c \int_0^{\theta_2^c/2T_c} \frac{\tanh(x)}{x} dx + \lambda_3^c \int_0^{\theta_3^c/2T_c} \frac{\tanh(x)}{x} dx \quad (8)$$

Table 2. Values of λ s calculated via Equations (3) and (5) for different pairs of Debye temperatures given in Table 1, and the T_c -values that they lead to via Equation (4). With the exception of two of these which are only *marginally* greater than 0.5 (e.g., 0.515 in both the Ba + Fe and the Ba + As scenarios), all the λ s satisfy constraint (6).

Ba + Fe scenario			Ba + As scenario				
Debye temps	$\lambda_{\text{Ba}}, \lambda_{\text{Fe}}$	T_c	Debye temps	$\lambda_{\text{Ba}}, \lambda_{\text{As}}$	T_c		
(1, 3)	0.355	0.121	47.9	(1, 5)	0.355	0.124	47.8
(1, 4)	0.355	0.177	46	(1, 6)	0.355	0.192	45.5
(2, 3)	0.515	0.153	42.2	(2, 5)	0.515	0.157	42.2
(2, 4)	0.515	0.224	41.1	(2, 6)	0.515	0.242	40.7
(3, 1)	0.333	0.125	48.4	(5, 1)	0.339	0.127	48.2
(3, 2)	0.333	0.201	45.6	(5, 2)	0.339	0.204	45.4
(4, 1)	0.449	0.154	44.1	(6, 1)	0.477	0.159	43.2
(4, 2)	0.449	0.242	42	(6, 2)	0.477	0.256	41.2

Notes on tables: Atomic masses used in the calculation of Debye temperatures are: 137.33 K (Ba), 39.098 K (K), 74.92 K (As), 55.847 K (Fe). *Entry marked (1) is obtained when Ba is the upper bob (and K the lower one); θ_x^c are not given as they are not used as shown in the double pendulum; the one marked (2) is obtained with bobs interchanged. *The θ_i^c in next two columns are to be similarly interpreted. *Note, however, that a pair of θ_i^c s that satisfies Equation (1) is (3) and (6), not (3) and (5).

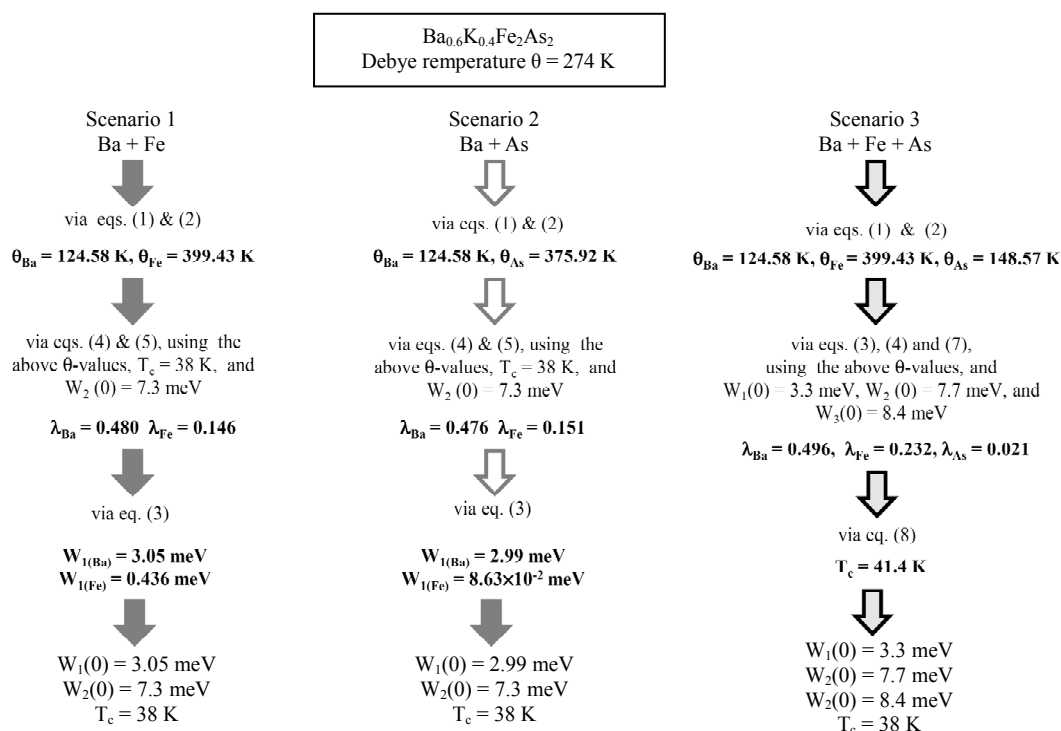


Figure 1. Schematic diagram giving the best-case values for the T_c and the gap-values led to by GBCSEs for $Ba_{0.6}K_{0.4}Fe_2As_2$ based on its characterization via 2- and 3-gap scenarios.

Thus we have four Equations (3), (5), (7) and (8), involving the three interaction constants λ_1^c , λ_2^c and λ_3^c and which can be determined with the input of any three quantities from the set $\{\Delta_1(0), \Delta_2(0), \Delta_3(0), T_c\}$. Since the greatest uncertainty among these pertains to $\Delta_3(0)$, we first seek to calculate it by determining the three λ s via (3), (5) and (8). Guided by the findings of Section 4.1, we invoke Debye temperature (2), see **Table 1**, for pairs bound via one-phonon exchanges, the combination of Debye temperatures (2, 6) for pairs bound via two-phonon exchanges, and the combination (2, 6, 3) in the equation for T_c .

As our starting point for the inputs, we use the set: $\{\Delta_1(0) = 3.6$ MeV, $\Delta_2(0) = 8.3$ MeV, 38 K $\}$. This leads to values of the three λ s as $\{0.515, 0.243, -0.02\}$. Since these values are in conflict with constraint (6), we first vary $\Delta_1(0)$: lowering its value to 3.3 MeV reduces the first two values to 0.496 and 0.26, but the third value (-0.02) remains unchanged. Keeping $\Delta_1(0) = 3.3$ MeV, we now reduce the value of $\Delta_2(0)$ whence, at 7.6 MeV, we find $\lambda_2^c = 0.227$ and $\lambda_3^c = 2.871 \times 10^{-5}$ while λ_1^c remains unchanged at 0.496. This set of λ s leads to $|\Delta_3(0)| = 7.6$ MeV via (7), which is not surprising because λ_3^c is negligible. In a heuristic spirit, if we keep $\Delta_1(0)$ and $\Delta_2(0)$ fixed at 3.3 and 7.3 MeV respectively, and increase T_c from 38 to 42 K, $|\Delta_3(0)|$ attains a value of 8.5 MeV.

As further illustrations of how the GBCSEs may be

used, we draw attention to the gap values determined via the specific heat data [10]: 3.6, 8.5, and 9.2 MeV. One can determine the three λ s by using these as input into (3), (5) and (7), and then calculate T_c via (8). Using the (2, 6, 3) combination of temperatures, the values of λ s so found are: 0.515, 0.232 and 0.021. Since the first of these violates constraint (6), we need to vary $\Delta_1(0)$; changing its value from 3.6 to 3.3 MeV without changing the values of $\Delta_2(0)$ and $\Delta_3(0)$, we find the λ -values to be: 0.496, 0.27 and 0.02. Equation (8) now yields $T_c = 44.5$ K. We note that the input of 3.3, 7.7, and 8.4 MeV for the gap values leads to 0.496, 0.232, and 0.021 for the three λ s, which lead to $T_c = 41.4$ K. We finally note that, of course, one can also seek to determine $\Delta_1(0)$ or $\Delta_2(0)$ with the input of $\{\Delta_2(0)$ or $\Delta_1(0), \Delta_3(0), T_c\}$. These lead to results similar to those already quoted. The best scenarios are illustrated in **Figure 1**.

As just shown, two gaps and the T_c of the iron-pnictide CS dealt with here are calculated by determining the sets $\{\lambda_1, \theta_1\}$ and $\{\lambda_2, \theta_2\}$. The use of both of these in (5) yields the larger gap, Δ_2 , while use of *one* of these in (3) yields the smaller gap, Δ_1 . Hence the question: what about the gap yielded by the other set via (3)? Not only in the present instance (see **Table 1**) but quite generally, the value of this gap is much smaller than Δ_1 and often approaches zero [14,15]. Such gaps show up as nodes or lines of nodes on the Fermi surface and while for Ba-As they were reported by, among others [8], and have of late

been studied with avid interest as evidenced by [17-19]. Note also that we found above a value of 2.871×10^{-5} for λ_3 in the three-gap scenario, which leads to a vanishing value for gap. Based on [14,15] and the present work, we conjecture that the almost-vanishing gaps, such as that for λ_3 , should be a feature of most (if not all) CSs. We note that this feature, as also reported in [17-19], appears to support the scenario in which CPs are formed via more than one phonon exchanges.

5. Conclusions

1) We first note that if the drop in the property (e.g., resistivity) of a CS is *sharp*, then there is no ambiguity in defining its T_c . If not, the mid-point of the temperature-range over which the drop takes place is sometimes quoted as the T_c . The present study and also earlier work [14,15] suggests that in applying GBCSEs, T_c should be taken as the temperature which marks the onset of the said drop.

2) It was noted that the Debye temperature of the CS to which GBCSEs are applied is an important parameter. The value of this parameter used by us is the one quoted in [6] which need not necessarily be the value characterizing different samples of Ba-As for which the T_c and the gap values have been quoted in the literature. The significance of the detailed *quantitative* results presented here needs to be assessed in light of this limitation.

3) Given the current experimental situation, we have shown that the GBCSEs can achieve for the iron pnictide SC Ba-As, which is a CS, what the usual BCS equations do for simple SCs. Hence they may be of value in the ongoing work concerned with the other iron-pnictide SCs. Extension of our approach to deal with CSs that may be characterized by four gaps is straightforward. A *tangible* treatment for such an SC will, however, require precise experimental values of its T_c and at least *some* of its gaps.

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REFERENCES

- [1] Y. Kamihara, T. Watanabe, M. Hirano and H. Hosono, "Iron-Based Layered Superconductor $\text{La}[\text{O}_{1-x}\text{Fe}_x]\text{FeAs}$ ($x = 0.05 - 0.12$) with $T_c = 26$ K," *Journal of the American Chemical Society*, Vol. 130, No. 11, 2008, pp. 3296-3297. [doi:10.1021/ja800073m](https://doi.org/10.1021/ja800073m)
- [2] H. Takahashi, K. Igawa, K. Arii, Y. Kamihara, M. Hirano and H. Hosono, "Superconductivity at 43 K in an Iron-Based Layered Compound $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$," *Nature*, Vol. 453, No. 7193, 2008, pp. 376-378. [doi:10.10/nature06972](https://doi.org/10.10/nature06972)
- [3] K. Ishida, Y. Nakai and H. J. Hosono, "To What Extent Iron-Pnictide New Superconductors Have Been Clarified: A Progress Report," *Journal of the Physical Society of Japan*, Vol. 78, 2009, Article ID: 062001. [doi:10.1143/JPSJ.78.062001](https://doi.org/10.1143/JPSJ.78.062001)
- [4] P. M. Aswathy, J. B. Anooja, P. M. Sarun and U. Syamaprasad, "An Overview on Iron Based Superconductors," *Superconductor Science and Technology*, Vol. 23, No. 7, 2010, Article ID: 073001. [doi:10.1088/0953-2048/23/7/073001](https://doi.org/10.1088/0953-2048/23/7/073001)
- [5] G. P. Malik, "On the Equivalence of Binding Energy of a Cooper Pair and the BCS Energy Gap: A Framework for Dealing with Composite Superconductors," *International Journal of Modern Physics B*, Vol. 24, No. 9, 2010, p. 1159. [doi:10.1142/S0217979210055408](https://doi.org/10.1142/S0217979210055408)
- [6] G. Mu, H. Luo, Z. Wang, L. Shan, C. Ren and W. Wen, "Low Temperature Specific Heat of the Hole-Doped $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ Single Crystals," *Physical Review B*, Vol. 79, No. 17, 2009, Article ID: 174501. [doi:10.1103/PhysRevB.79.174501](https://doi.org/10.1103/PhysRevB.79.174501)
- [7] L. Shan, Y. Wang, B. Shen, B. Zeng, Y. Huang, A. Li, et al., "Observation of Ordered Vortices with Andreev Bound States in $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$," *Nature Physics*, Vol. 7, 2011, pp. 325-331. [doi:10.1038/nphys1908](https://doi.org/10.1038/nphys1908)
- [8] H. Ding, P. Richard, K. Nakayama, K. Sugawara, T. Arakane, Y. Sekiba, et al., "Observation of Fermi-Surface-Dependent Nodeless Superconducting Gaps in $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$," *Europhysics Letters*, Vol. 83, No. 4, 2008, Article ID: 47001. [doi:10.1209/0295-5075/83/47001](https://doi.org/10.1209/0295-5075/83/47001)
- [9] C. Ren, Z. Wang, H. Luo, H. Yang, L. Shan and W. Hai-Hu, "Evidence for Two Energy Gaps in Superconducting $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ Single Crystals and the Breakdown of the Uemura Plot," *Physical Review Letters*, Vol. 101, No. 25, 2008, Article ID: 257006. [doi:10.1103/PhysRevLett.101.257006](https://doi.org/10.1103/PhysRevLett.101.257006)
- [10] P. Popovich, A. V. Boris, O. V. Dolgov, A. A. Golubov, D. L. Sun, C. T. Lin, et al., "Specific Heat Measurements of $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ Single Crystals: Evidence for a Multi-band Strong-Coupling Superconducting State," *Physical Review Letters*, Vol. 105, No. 2, 2010, Article ID: 027003. [doi:10.1103/PhysRevLett.105.027003](https://doi.org/10.1103/PhysRevLett.105.027003)
- [11] Y. Zhang, L. X. Yang, F. Chen, B. Zhou, X. F. Wang, X. H. Chen, X. H., et al., "Out-of-Plane Momentum and Symmetry-Dependent Energy Gap of the Pnictide $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ Superconductor Revealed by Angle-Resolved Photoemission Spectroscopy," *Physical Review Letters*, Vol. 105, No. 11, 2010, Article ID: 117003. [doi:10.1103/PhysRevLett.105.027003](https://doi.org/10.1103/PhysRevLett.105.027003)
- [12] F. Seitz, "The Modern Theory of Solids," McGraw Hill, New York, 1940.
- [13] G. P. Malik and U. Malik, "On the Calculation of T_c 's of Superconducting Binary Alloys Based on Two-Phonon Exchange Mechanism," *Physica B*, Vol. 348, No. 1-4, 2004, pp. 341-346. [doi:10.1016/j.physb.2003.12.009](https://doi.org/10.1016/j.physb.2003.12.009)
- [14] G. P. Malik, "Generalized BCS Equations: Applications," *International Journal of Modern Physics B*, Vol. 24, No. 19, 2010, p. 3701. [doi:10.1142/S0217979210055858](https://doi.org/10.1142/S0217979210055858)
- [15] G. P. Malik and U. Malik, "A Study of the Thallium- and Bismuth-Based High-Temperature Superconductors in the

- Framework of the Generalized BCS Equations,” *Journal of Superconductivity and Novel Magnetism*, Vol. 24, No. 1-2, 2011, pp. 255-260. [doi:10.1007/s10948-010-1009-0](https://doi.org/10.1007/s10948-010-1009-0)
- [16] J. M. Blatt, “Theory of Superconductivity,” Academic Press, New York, 1964, p. 206.
- [17] D. Lee, “Iron-Based Superconductors: Nodal Rings,” *Nature Physics*, Vol. 8, 2012, pp. 364-365. [doi:10.1038/nphys2301](https://doi.org/10.1038/nphys2301)
- [18] Y. Zhang, Z. R. Ye, Q. Q. Ge, F. Chen, J. Jiang, M. Xu, B. P. Xie, *et al.*, “Nodal Superconducting-Gap Structure in Ferropnictide Superconductor $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$,” *Nature Physics*, Vol. 8, 2012, pp. 371-375. [doi:10.1038/nphys2248](https://doi.org/10.1038/nphys2248)
- [19] M. P. Allan, A. W. Rost, A. P. Mackenzie, Y. Xie, J. C. Davis, K. Klhou, *et al.*, “Anisotropic Energy Gaps of Iron-Based Superconductivity from Intraband Quasiparticle Interference in LiFeAs ,” *Science*, Vol. 336, No. 6081, 2012, pp. 563-567. [doi:10.1126/science.1218726](https://doi.org/10.1126/science.1218726)