

Multiband $s\pm$ Eliashberg theory and temperature-dependent spin-resonance energy in iron pnictide superconductors

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(Received 12 November 2010; revised manuscript received 26 January 2011; published 30 March 2011)

The phenomenology of iron pnictide superconductors can be explained in the framework of a three-band $s\pm$ wave Eliashberg theory with only two free parameters plus a *feedback effect*, i.e., the effect of the condensate on the antiferromagnetic spin fluctuations responsible for the superconductivity in these compounds. I have examined the experimental data of four materials, $\text{LaFeAsO}_{1-x}\text{F}_x$, $\text{SmFeAsO}_{1-x}\text{F}_x$, $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, and $\text{Ba}(\text{Fe}_x\text{Co}_{1-x})_2\text{As}_2$, and I have found that it is possible to reproduce the experimental critical temperature and gap values in a moderate strong-coupling regime, $\lambda_{\text{tot}} \approx 1.7 - 2.0$.

DOI: [10.1103/PhysRevB.83.092508](https://doi.org/10.1103/PhysRevB.83.092508)

PACS number(s): 74.70.Xa, 74.20.Fg, 74.20.Mn

The new class of Fe-based compounds,¹⁻³ just like the cuprates⁴ and the heavy fermions,⁵ all have some similar characteristics. Two examples are the high values of rate $2\Delta/T_c$ and the presence of the pseudogap.^{4,6,7} For all three classes of material, it is proposed that the superconductivity will be mediated by antiferromagnetic spin fluctuations.^{4,8,9} The most obvious difference is that almost all of the iron compounds present a multiband behavior, while for high- T_c cuprate superconductors (HTCS) and heavy fermions, this is detected only in some particular cases. The multiband nature of Fe-based superconductors may give rise to a multigap scenario,¹⁰ and this is indeed emerging from many different experimental data showing evidence for rather high gap ratios of $\approx 2-3$.¹¹ In this regard, neither a three-band BCS model^{9,12,13} nor a four-band Eliashberg model¹⁴ with small values of the coupling constants and large boson energies are adequate: the former can only account for the gap ratio and T_c , but not for the exact experimental gap values, and the latter provides a calculated critical temperature larger than the experimental one. The high experimental value of the larger gap suggests that high values of the coupling constants might be necessary to explain the experimental data within a three-band model;^{15,16} one has therefore to employ the Eliashberg theory for strong-coupling superconductors.^{15,16} In my early works,^{15,16} I found that a three-band Eliashberg model allows one to reproduce various experimental data. This suggests that these compounds can represent a case of dominant negative interband-channel superconductivity ($s\pm$ wave symmetry) with small typical boson energies (≈ 10 meV) but too-high values of the electron-boson coupling constants ($1.9 \leq \lambda_{\text{tot}} \leq 5.9$). The way to solve this problem is suggested by the experimental measurements of Inosov and coworkers.¹⁷ They found that the temperature evolution of the spin-resonance energy follows the superconducting energy gap, and this should indicate a *feedback effect*^{4,18,19} of the condensate on the spin fluctuations. This assumption is the starting point of my argument. The procedure is as follows: First, I choose the experimental low-temperature spin resonance as representative of the boson energy, and I fix the two remaining free parameters to reproduce the exact experimental gap values; then, with the same parameters, I calculate the critical temperature T_c^* . I find $T_c^* \gg T_c^{\text{exp}}$ in all cases where T_c^{exp} is the experimental critical temperature. In

the successive step, I use the same input parameters utilized before except for the electron-boson spectral functions that have an energy peak with the same temperature dependence of the superconductive gap. Of course, at $T = T_c^*$, the energy peak is equal to zero, while at $T = 0$ K, the new spectral functions are equal to the old ones. In this way, taking into account the feedback effect of the condensate^{4,18,19} on the antiferromagnetic spin fluctuations, I explain the experimental data (the gap values and the critical temperature) in a model that has only two free parameters in a moderate strong-coupling regime ($\lambda_{\text{tot}} \approx 1.7 - 2$).

I choose four representative cases (three hole type and one electron type): $\text{LaFeAsO}_{1-x}\text{F}_x$, $\text{SmFeAsO}_{1-x}\text{F}_x$, $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, and $\text{Ba}(\text{Fe}_x\text{Co}_{1-x})_2\text{As}_2$. The electronic structure of the hole-type compounds can be approximately described by a three-band model⁹ with two hole bands (indicated in the following as bands 1 and 2) and one equivalent electron band (indicated as band 3),^{15,16} while the electron type has one hole band (indicated in the following as band 1) and two equivalent electron bands (indicated as bands 2 and 3).²¹ In the hole-type case, the s -wave order parameters of the hole bands Δ_1 and Δ_2 have the opposite sign compared to the electron band Δ_3 ,²⁰ while in the electron-type case, Δ_1 has the opposite sign compared to the two electron bands Δ_2 and Δ_3 .²¹ In such systems, intraband coupling could be provided by phonons (ph), and interband coupling by antiferromagnetic spin fluctuations (sf).²⁰ I summarize the experimental data relative to the following four considered cases:

1) the compound $\text{LaFeAsO}_{0.9}\text{F}_{0.1}$ (LaFeAsOF) with $T_c^A = 28.6$ K where point-contact spectroscopy measurements gave $\Delta_1(0) \approx 8.0$ and $\Delta_2(0) \approx 2.8$ meV;⁷

2) $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$ (BaKFeAs) with $T_c = 37$ K where angle-resolved photoelectron spectroscopy (ARPES) measurements gave $\Delta_1(0) = 12.1 \pm 1.5$, $\Delta_2(0) = 5.2 \pm 1.0$, and $\Delta_3(0) = 12.8 \pm 1.4$ meV;²²

3) the compound $\text{SmFeAsO}_{0.8}\text{F}_{0.2}$ (SmFeAsOF) with $T_c^A = 52$ K ($T_c^{\text{bulk}} = 53$ K) where, according to point-contact spectroscopy measurements, $\Delta_1(0) = 18 \pm 3$ and $\Delta_2(0) = 6.2 \pm 0.5$ meV;²³ and

4) the compound $\text{Ba}(\text{Fe}_x\text{Co}_{1-x})_2\text{As}_2$ (BaFeCoAs) with $T_c^A = 22.6$ K ($T_c^{\text{bulk}} = 24.5$ K) where, according to point-contact spectroscopy measurements, $\Delta_1(0) = 4.1 \pm 0.4$ and $\Delta_2(0) = 9.2 \pm 1.0$ meV.²¹

T_c^A is the critical temperature obtained by Andreev reflection measurements and T_c^{bulk} is the critical temperature extracted by transport measurements. Note that, only in the case of ARPES, the gaps are associated to the relevant band. Since point-contact spectroscopy measurements generally give only two gaps, the larger one has been arbitrarily indicated as Δ_1 , supposing that $\Delta_1 \sim |\Delta_3|$.

To obtain the gaps and the critical temperatures within the $s \pm$ wave, three-band Eliashberg equations,²⁴ one has to solve six coupled equations for the gaps $\Delta_i(i\omega_n)$ and the renormalization functions $Z_i(i\omega_n)$, where i is a band index (that ranges between 1 and 3) and ω_n are the Matsubara frequencies. If one neglects, for simplicity, the effect of magnetic and nonmagnetic impurities, the imaginary-axis equations^{15,16} are

$$\omega_n Z_i(i\omega_n) = \omega_n + \pi T \sum_{m,j} \Lambda_{ij}^Z(i\omega_n, i\omega_m) N_j^Z(i\omega_m), \quad (1)$$

$$Z_i(i\omega_n) \Delta_i(i\omega_n) = \pi T \sum_{m,j} [\Lambda_{ij}^\Delta(i\omega_n, i\omega_m) - \mu_{ij}^*(\omega_c)] \Theta(\omega_c - |\omega_m|) N_j^\Delta(i\omega_m), \quad (2)$$

where $\Lambda_{ij}^Z(i\omega_n, i\omega_m) = \Lambda_{ij}^{\text{ph}}(i\omega_n, i\omega_m) + \Lambda_{ij}^{\text{sf}}(i\omega_n, i\omega_m)$, and $\Lambda_{ij}^\Delta(i\omega_n, i\omega_m) = \Lambda_{ij}^{\text{ph}}(i\omega_n, i\omega_m) - \Lambda_{ij}^{\text{sf}}(i\omega_n, i\omega_m)$. Θ is the Heaviside function and ω_c is a cutoff energy. In particular, $\Lambda_{ij}^{\text{ph},\text{sf}}(i\omega_n, i\omega_m) = 2 \int_0^{+\infty} d\Omega \Omega \alpha_{ij}^2 F^{\text{ph},\text{sf}}(\Omega) / [(\omega_n - \omega_m)^2 + \Omega^2]$. $\mu_{ij}^*(\omega_c)$ are the elements of the 3×3 Coulomb pseudopotential matrix. Finally, $N_j^\Delta(i\omega_m) = \Delta_j(i\omega_m) / \sqrt{\omega_m^2 + \Delta_j^2(i\omega_m)}$ and $N_j^Z(i\omega_m) = \omega_m / \sqrt{\omega_m^2 + \Delta_j^2(i\omega_m)}$. The electron-boson coupling constants are defined as $\lambda_{ij}^{\text{ph},\text{sf}} = 2 \int_0^{+\infty} d\Omega \frac{\alpha_{ij}^2 F^{\text{ph},\text{sf}}(\Omega)}{\Omega}$.

The solution for Eqs. (1) and (2) requires a huge number of input parameters (18 functions and 9 constants); however, some of these parameters are related to each other, some can be extracted from experiments, and some can be fixed by suitable approximations. As shown in Ref. 20, in the case of pnictides, we can assume that: (i) the total electron-phonon coupling constant is small,²⁵ (ii) phonons mainly provide intraband coupling; and (iii) spin fluctuations mainly provide interband coupling. To account for these assumptions in the simplest way, I will take $\lambda_{ii}^{\text{ph}} = \lambda_{ij}^{\text{ph}} = 0$ (upper limit of the phonon coupling²⁵ ≈ 0.35), $\lambda_{ii}^{\text{sf}} = 0$ (only interband

sf coupling), and $\mu_{ii}^*(\omega_c) = \mu_{ij}^*(\omega_c) = 0$.¹⁵ Within these approximations, the electron-boson coupling-constant matrix λ_{ij} becomes^{9,15,21}

$$\lambda_{ij} = \begin{pmatrix} 0 & \lambda_{12} & \lambda_{13} \\ \lambda_{21} = \lambda_{12} \nu_{12} & 0 & \lambda_{23} \\ \lambda_{31} = \lambda_{13} \nu_{13} & \lambda_{32} = \lambda_{23} \nu_{23} & 0 \end{pmatrix}, \quad (3)$$

where $\nu_{ij} = N_i(0)/N_j(0)$, and $N_i(0)$ is the normal density of states at the Fermi level for the i th band. In the hole case, it is $\lambda_{21} = \lambda_{12} = 0$, while in the electron case, it is $\lambda_{23} = \lambda_{32} = 0$. In the numerical simulations, I used the standard form for the antiferromagnetic spin fluctuation:²⁶ $\alpha_{ij}^2 F^{\text{sf}}(\Omega) = B_{ij} \Omega \Omega_{ij} \Theta(\Omega_{\text{max}} - \Omega) / (\Omega^2 + \Omega_{ij}^2)$, where B_{ij} are the normalization constants necessary to obtain the proper values of λ_{ij} while Ω_{ij} are the peak energies. In all the calculations, $\Omega_{ij} = \Omega_0$. The maximum sf energy is $\Omega_{\text{max}} = 10\Omega_0$, the cutoff energy is $\omega_c = 30\Omega_0$, and the maximum quasiparticle energy is $\omega_{\text{max}} = 40\Omega_0$. For the typical sf energy Ω_0 , I use the spin-resonance energy that has been measured, and for all compounds examined, I assume the relation $\Omega_0 = (2/5)T_c$ that is available in the literature is correct.²⁷ Band structure calculations provide information about the factors ν_{ij} that enter into the definition of λ_{ij} [Eq. (3)]. In the case of LaFeAsO_{0.9}F_{0.1}, I know that $\nu_{13} = 0.91$ and $\nu_{23} = 0.53$;²⁸ in Ba_{0.6}K_{0.4}Fe₂As₂, $\nu_{13} = 1$ and $\nu_{23} = 2$;⁹ in SmFeAsO_{0.8}F_{0.2}, $\nu_{13} = 0.4$ and $\nu_{23} = 0.5$;²⁸ and in Ba(Fe_xCo_{1-x})₂As₂, $\nu_{12} = 1.12$ and $\nu_{13} = 4.50$.²⁸ I initially solve the imaginary-axis Eliashberg equations [Eqs. (1) and (2)] to calculate the low-temperature value of the gaps (which are actually obtained by analytical continuation to the real axis by using the technique of the Padé approximants) and so I fix the two free parameters of the model, λ_{13} and λ_{23} (λ_{12}). By properly selecting the values of λ_{13} and λ_{23} (λ_{12}), it is relatively easy to obtain the experimental values of the gaps with reasonable values of $\lambda_{\text{tot}} = \frac{\sum_{ij} N_i(0) \lambda_{ij}}{\sum_{ij} N_i(0)}$ (between 1.72 and 2.04).

However, in all the materials examined, the high $2\Delta_{1,3}/k_B T_c$ ratio (of the order of 8–9) makes it possible to reproduce *also* the values of the large gap(s) only if the calculated critical temperature T_c^* is considerably higher than the experimental one. To solve this problem, which is also present in the HTCS, I assume there exists an effect of feedback^{4,18,19} of the condensate and, in a phenomenological way, I introduce in the Eliashberg equation a temperature

TABLE I. The values of Ω_0 and λ_{ij} that allow reproduction of the experimental gap values. λ_{tot} is compared with $\lambda_{\text{tot}}^{\text{old}}$, which is the value determined in the previous works.^{15,16,21} In the first rows, the sf spectral functions used have the usual shape, while those in the second rows have the Lorentzian shape.

	λ_{tot}	$\lambda_{\text{tot}}^{\text{old}}$	$\lambda_{12/21}$	$\lambda_{13/31}$	$\lambda_{23/32}$	Ω_0 (meV)
BaFeCoAs	1.87		0.76/0.85	1.21/5.44	0.00/0.00	9.04
	2.83	1.93	0.91/1.02	2.08/9.35	0.00/0.00	9.04
LaFeAsOF	1.75		0.00/0.00	2.11/1.91	0.40/0.21	11.44
	2.38	2.53	0.00/0.00	2.93/2.66	0.46/0.24	11.44
BaKFeAs	2.04		0.00/0.00	2.27/2.27	0.56/0.28	14.80
	2.84	3.87	0.00/0.00	3.21/3.21	0.67/0.34	14.80
SmFeAsOF	1.72		0.00/0.00	1.55/3.88	0.42/0.84	20.80
	2.39	5.90	0.00/0.00	2.23/5.58	0.49/0.98	20.80

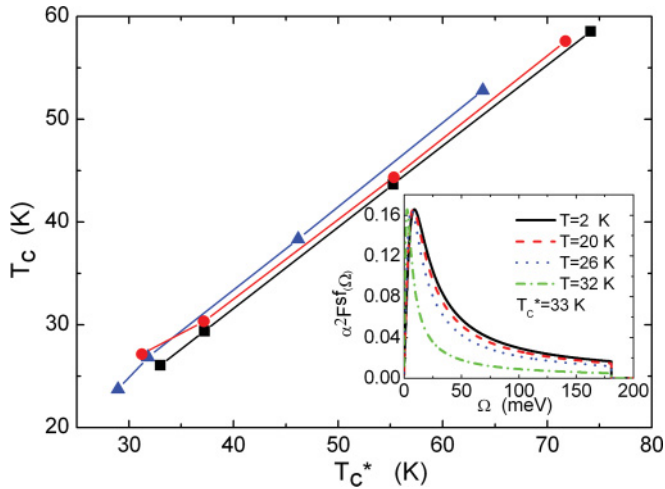


FIG. 1. (Color online) The calculated critical temperature T_c with the feedback effect vs standard critical temperature T_c^* in three different situations: only interband sf coupling with standard spectral functions (black squares), interband sf coupling with standard spectral functions and small intraband ph coupling (red circles), and only interband sf coupling with Lorentzian spectral functions (blue triangles). The inset is the sf spectral function for the $\text{Ba}(\text{Fe}_x\text{Co}_{1-x})_2\text{As}_2$ at different temperatures ($T < T_c^*$) with the feedback effect.

dependence of the representative boson energy $\Omega_0(T) = \Omega_0 \tanh(1.76\sqrt{T_c^*/T - 1})$ that reproduces both the approximate gap temperature dependence in the strong-coupling case¹⁹ and the experimental spin-resonance one.¹⁷ The primary effect of this assumption is the lowering of the critical temperature, leaving unchanged the gap values at $T \ll T_c^*$, because the critical temperature is roughly proportional to the electron-

boson coupling constant and to the representative boson energy $\Omega_0(T)$ of the material: in this case, $\Omega_0(T)$ decreases and so T_c . For a completely consistent procedure, $\Omega_0(T) = \Omega_0\eta(T)$ should be used, where $\eta(T)$ is the temperature-dependence part of the superfluid density $\rho(T) = \rho(0)\eta(T)$, and $\rho(0)$ is the superfluid density at $T = 0$ K. $\eta(T)$ is a function of $\Delta_i(i\omega_n)$ and so, in this way, the numerical solution of the Eliashberg equations becomes remarkably more complex and time consuming.

I am aware that the temperature dependence of $\Omega_0(T)$ is added *ad hoc* and is not obtained self-consistently, but this is an attempt to determine if the chosen path can lead to interesting results. What is important is that this mechanism of feedback can justify the experimental values for the gaps, their dependence on temperature, and the critical temperature with a model that has only two free parameters. Moreover, the parameters determined are reasonable, and λ_{tot} is very similar for all four materials examined and in agreement with the values proposed by other authors.²⁶ I solve the Eliashberg equations in three different situations: (1) where only sf interband coupling is present and the sf spectral functions have the usual shape, (2) where sf interband coupling with a small ph intraband contribution are present and sf spectral functions have the usual shape, and (3) where only sf interband coupling is present and the sf spectral functions have the Lorentzian shape. In the first case, the coupling constant λ_{tot} is in the range 1.72–2.04. The results are almost independent from Ω_{max} because, for example, in the case of BaFeCoAs , multiplying Ω_{max} by a factor of two, I obtain the same values of the gaps and T_c with $\lambda_{\text{tot}} = 1.68$, i.e., with a reduction of 0.18 which is very small. The agreement with the experimental critical temperature is good. The small variation of the total

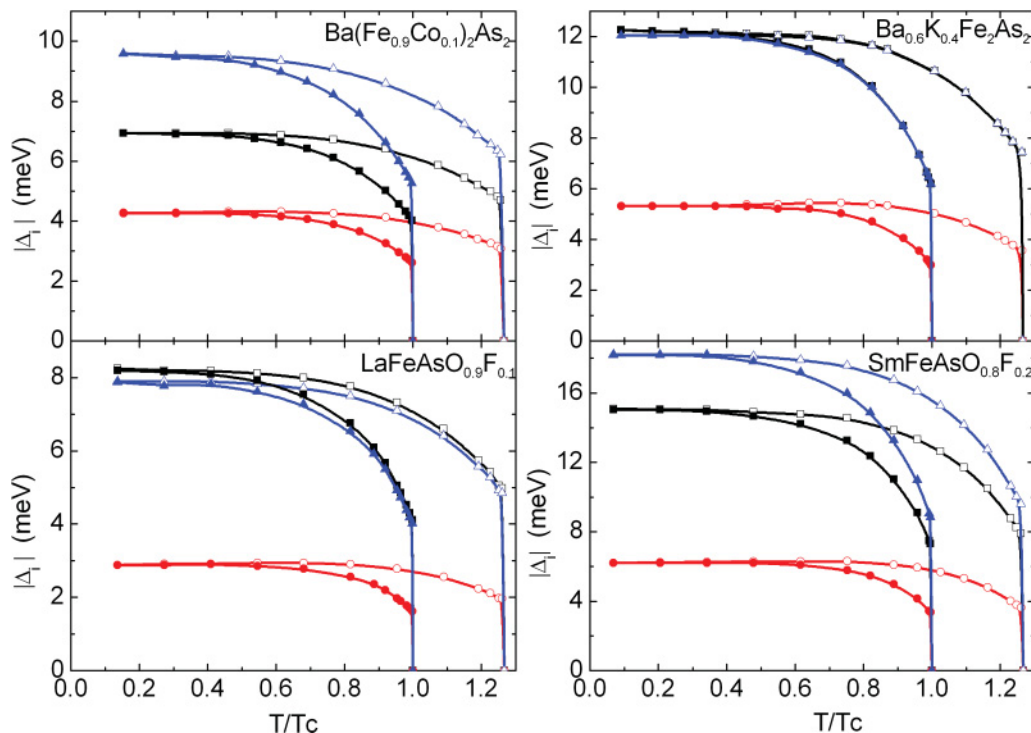


FIG. 2. (Color online) The calculated temperature dependence of $|\Delta_i|$ from the solution of real-axis Eliashberg equations in the standard case (open symbol) and when the feedback effect is present (solid symbol): $|\Delta_1|$ black squares, $|\Delta_2|$ red circles, and $|\Delta_3|$ blue triangles.

TABLE II. The calculated values of the gaps and of the two critical temperatures with and without the feedback effect. In the first rows, the sf spectral functions used have the usual shape, while those in the second rows have the Lorentzian shape.

	Δ_1 (meV)	Δ_2 (meV)	Δ_3 (meV)	T_c (K)	T_c^* (K)
BaFeCoAs	6.63	-4.07	-9.18	26.07	33.00
	7.02	-4.12	-9.18	23.73	28.95
LaFeAsOF	8.01	2.82	-7.75	29.37	37.22
	8.01	2.77	-7.71	26.86	31.81
BaKFeAs	12.04	5.20	-12.00	43.66	55.26
	12.04	5.24	-11.91	38.33	46.18
SmFeAsOF	14.86	6.15	-18.11	58.53	74.13
	15.51	6.15	-18.00	52.80	63.82

coupling in the four compounds considered is noticeable. In the second case, there is also an intraband phonon contribution, equal in any band and in any compound, for simplicity, with $\lambda_{ij}^{\text{ph}} = 0.35$ and $\Omega_0^{\text{ph}} = 18$ meV, which are the upper limits for the ph coupling constants and the representative ph energies.²⁵ The ph spectral functions have the Lorentzian shape,¹⁵ with the peaks at the same energy, $\Omega_{ij} = \Omega_0^{\text{ph}}$, and with half width always equal to 2 meV ($\omega_c = 12\Omega_0^{\text{ph}}$). λ_{tot} and T_c are practically the same as the previous case. This last fact indicates that the effect of intraband phonon contribution is negligible. In the third case (the Lorentzian shape of sf spectral functions), the agreement with the experimental critical temperatures is

very good in all compounds, but the total coupling is larger ($2.38 \leq \lambda_{\text{tot}} \leq 2.84$).

In Fig. 1 it is possible to see the linear relation between T_c and T_c^* in all three examined cases. Table I shows the input parameters of the Eliashberg equations in the first and third case examined for the four compounds. Table II shows the calculated values of the gaps and the critical temperatures T_c and T_c^* obtained by numerical solution of the Eliashberg equations. Once the values of the low-temperature gaps were obtained, I calculated their temperature dependence by directly solving the three-band Eliashberg equations in the real-axis formulation, instead of using the analytical continuation to the real axis of the imaginary-axis solution. Of course, the results of the two procedures are virtually identical at low temperature. In all cases, their behavior is rather unusual and completely different from the BCS one, since the gaps slightly decrease with increasing temperature until they suddenly drop close to T_c as it is shown in Fig. 2. This arises from a complex nonlinear dependence of the Δ vs T curves on λ_{ij} , and is possible only in a strong-coupling regime.²⁹ Curiously, in all four compounds, the rate T_c^*/T_c is 1.27. In conclusion, I have shown that a simple Eliashberg three-band model, with antiferromagnetic spin-fluctuation electron coupling in a moderate strong-coupling regime with only two free parameters and a feedback effect, can reproduce, in a *quantitative* way, the experimental critical temperature and the amplitude of the energy gaps.

I thank R.S. Gonnelli, E. Cappelluti, L. Benfatto, and S. Galasso for the useful and clarifying discussions.

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