PHYSICAL REVIEW B **79**, 060502(R) (2009)

Interband superconductivity: Contrasts between Bardeen-Cooper-Schrieffer and Eliashberg theories

Oleg V. Dolgov
Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

Igor I. Mazin and David Parker
Naval Research Laboratory, 4555 Overlook Avenue SW, Washington, DC 20375, USA

Alexander A. Golubov
Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands
(Received 7 October 2008; revised manuscript received 25 November 2008; published 4 February 2009)

The recently discovered iron pnictide superconductors apparently present an unusual case of interband-channel pairing superconductivity. Here we show that in the limit where the pairing occurs within the interband channel, several surprising effects occur quite naturally and generally: different density of states on the two bands leads to several unusual properties, including a gap ratio which behaves inversely to the ratio of density of states; the weak-coupling limits of the Eliashberg and the BCS theories, commonly taken as equivalent, in fact predict qualitatively different dependence of the Δ_1/Δ_2 and Δ/T_c ratios on coupling constants. We show analytically that these effects follow directly from the interband character of superconductivity. Our results show that in the interband-only pairing model the maximal gap ratio is $\sqrt{N_2/N_1}$ as strong-coupling effects act only to reduce this ratio. Our results show that pnictide BCS calculations must use renormalized coupling constants to get accurate results. Our results also suggest that if the large experimentally reported gap ratios (up to a factor 2) are correct, the pairing mechanism must include more intraband interaction than what is usually assumed.

DOI: 10.1103/PhysRevB.79.060502 PACS number(s): 74.20.Rp, 76.60.−k, 74.25.Nf, 71.55.−i

Although first proposed 50 years ago, multiband superconductivity where the order parameter is different in different bands had not attracted much interest until 2001 when MgB_2 was found to be a two-band superconductor. MgB_2 represents a particular case where one "leading" band enjoys the strongest pairing interactions, while the interband-pairing interaction, as well as the intraband pairing in the other band, is weak. There is growing evidence that the recently discovered superconducting ferropnictides represent another limiting case: the pairing interaction is predominantly interband, while the intraband pairing in both bands is weak. This leads to a number of interesting and unexpected effects, including the fact that a repulsive interband interaction may be nearly as effective in creating superconductivity as an attractive one.

In this Rapid Communication we will show another unusual feature of the two-band "interband" superconductivity (meaning superconductivity induced predominantly by interband interactions): entirely counterintuitively, *the BCS theory for such superconductors is not the weak-coupling limit of the Eliashberg theory*, and the difference is not only quantitative but qualitative. This fact holds for either repulsive (as, presumably, in pnictides) or attractive interactions.

Specifically, we will concentrate on the dependence of the superconducting gaps in the two bands on the ratio of the densities of states and the magnitude of the superconducting coupling. We will show that the gap ratio is always smaller in the Eliashberg theory than in the BCS theory, the deviation grows with coupling strength and with temperature, and it is largest just below T_c.

Let us start with the BCS equations[1] and their multiband generalization as proposed by Suhl *et al.*[2] For a two-band interband-only case, with gap parameters given on the two bands as Δ_1 and Δ_2, the BCS gap equations take the form

$$\Delta_1 = \sum_k \frac{V\Delta_2 \tanh(E_{2,k}/2k_BT)}{2E_{2,k}},$$

$$\Delta_2 = \sum_k \frac{V\Delta_1 \tanh(E_{1,k}/2k_BT)}{2E_{1,k}}, \qquad (1)$$

where $E_{i,k}$ is the usual quasiparticle energy in band i given by $\sqrt{(\varepsilon_{i,k}-\mu)^2+\Delta_i^2}$, the normal-state electron energy is $\varepsilon_{i,k}$, μ is the chemical potential, and V is the interband interaction causing the superconductivity. V can be either attractive (>0 in this convention) or repulsive (as presumably in the pnictides[3,4]). In the case of an attractive interband interaction the gap will have the same sign on both Fermi surfaces, while for a repulsive interaction the signs will be opposite. Otherwise all equations are exactly the same. For simplicity, in the rest of this Rapid Communication, whenever V, λ, Δ_1, or Δ_2 is used, these should be understood as absolute values: $|V|$, $|\Delta|$, and so on.

The BCS theory assumes V to be constant up to the cutoff energy ω_c. Following the BCS prescription, we can convert the momentum sums to energy integrals up to a cutoff energy ω_c and assume Fermi-level density of states (DOS) N_1 and N_2. Near T_c these equations can be linearized giving

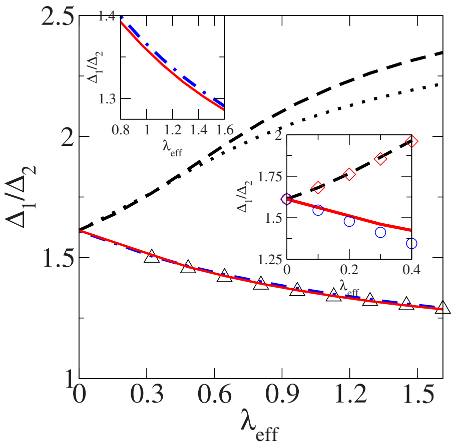

FIG. 1. (Color online) The ratio of the gap functions in an interband-pairing case, as a function of λ_{eff}, for the BCS (dashed line) and Eliashberg-Einstein (line) spectrum and spin-fluctuation (triangle) spectrum cases. The dotted line represents numerical Eliashberg-Einstein spectrum results in which the mass-renormalization parameter has been artificially taken as 1, showing that the difference between BCS and Eliashberg is mainly a mass-renormalization effect. The dashed-dotted line (lower part, main panel, and upper inset) is the renormalized BCS (RBCS) (Ref. 8) approximation to the Eliashberg numerical results. Inset: analytic approximations to numerical results; diamonds are BCS, Eq. (5), and circles are Eliashberg, Eq. (15).

$$\Delta_1 = \Delta_2 \lambda_{12} \ln(1.136\omega_c/T_c),$$

$$\Delta_2 = \Delta_1 \lambda_{21} \ln(1.136\omega_c/T_c), \tag{2}$$

where $\lambda_{12}=N_2V$—the dimensionless coupling constant with a similar expression for λ_{21}. These equations readily yield $\lambda_{\text{eff}}=\sqrt{\lambda_{12}\lambda_{21}}$ and $\Delta_2/\Delta_1=\sqrt{N_1/N_2}\equiv\alpha_0$. This result has been obtained before.[5,6] Similarly, at $T=0$ in the weak-coupling limit,

$$\Delta_1 = \Delta_2 \lambda_{12} \sinh^{-1}(\omega_c/\Delta_2),$$

$$\Delta_2 = \Delta_1 \lambda_{21} \sinh^{-1}(\omega_c/\Delta_1). \tag{3}$$

Obviously, for $\lambda_{\text{eff}}\to 0$ we have $T_c\to 0$ and the relation $\Delta_2/\Delta_1=\sqrt{N_1/N_2}$ should hold. The same is not true for $\lambda_{\text{eff}}>0$. For clarity in all of the following we assume that $N_1>N_2$ so that $\Delta_2>\Delta_1$. We denote N_1/N_2 as β so that $\alpha_0=\sqrt{\beta}$.

Our first-principles calculations[4] suggest for the pnictides $\beta\equiv N_1/N_2\lesssim 1.4$, corresponding to the gap ratio $\alpha\lesssim 1.2$. Experimental estimates for the gaps differ wildly, yielding gap ratios α ranging from 1.3 to 3.4. Since the goal of this Rapid Communication is to address the effect of the density-of-states difference on the gap ratio, we will use an intermediate number[7] $\beta=2.6(\alpha_0=1.6)$.

The fact that the band with the *larger* DOS ends up with a *smaller* gap is somewhat counterintuitive. This is a direct result of the interband-only pairing—the pairing amplitude on one band is generated by the DOS on the *other*. The numerical solution of Eq. (2) at $T=0$ (Fig. 1) gives, as expected, $\alpha=\sqrt{\beta}=1.6$ at $\lambda_{\text{eff}}\to 0$. As a function of λ_{eff} it increases linearly, reaching ≈ 2.3 at $\lambda_{\text{eff}}\approx 1.6$ (note that as discussed below, it will ultimately saturate at $\beta=2.6$ in the superstrong limit). This increase can be easily explained.

Let us define x such that $\alpha=\beta^{1/2}(1+x)=\alpha_0(1+x)$, so that $x\ll 1$ at $\lambda_{\text{eff}}\ll 1$, and substitute $\sinh^{-1}(\omega_c/\Delta)\to\ln(2\omega_c/\Delta)$. A few lines of algebra then lead to

$$x = \frac{\ln\beta}{2(1+2/\sqrt{\lambda_{12}\lambda_{21}})} \simeq \frac{\lambda_{\text{eff}}\ln\beta}{4}. \tag{4}$$

This result was also obtained by Bang and Choi.[6] The quadratic in λ term can also be worked out and reads

$$\frac{\Delta_2}{\Delta_1} = \sqrt{\beta}\left[1 + \frac{\lambda_{\text{eff}}\ln\beta}{4} + \frac{\lambda_{\text{eff}}^2(4\ln\beta + \ln^2\beta)}{32}\right]. \tag{5}$$

As Fig. 1 shows, this expression describes the numerical solution at small λ very well. Although not apparent from the plots, the Δ_2/Δ_1 ratio will saturate at large λ, as shown by Bang and Choi,[6] and can also be seen from Eq. (3) since

$$\Delta_1 = \Delta_2\lambda_{12}\sinh^{-1}(\omega_c/\Delta_2) \to \lambda_{12}\omega_c \quad \text{for } \Delta_2 \gg \omega_c.$$

Similarly, in this limit $\Delta_2=\lambda_{21}\omega_c$ so that $\Delta_2/\Delta_1=\lambda_{21}/\lambda_{12}=N_1/N_2$. All these BCS results, however, are inconsistent with a known analytical result[9] that in the superstrong (Eliashberg) limit $\lambda_{\text{eff}}\gg 1$, the gap ratio $\alpha\to 1$ is independent of β. Let us now move to Eliashberg[10] theory.

In this theory, the BCS gap function Δ_0 is replaced by a complex energy-dependent quantity $\Delta_0(\omega)$, which must be determined along with a mass-renormalization parameter $Z(\omega)$. One commonly formulates the equations in terms of $\phi(\omega)=Z(\omega)\Delta(\omega)$, and these equations can be solved either on the real frequency axis or on the imaginary axis (using Matsubara frequencies). These equations are formulated in a two-band interband-pairing case on the imaginary axis as follows (some of the notations are repeated from Ref. 8):

$$\Delta_1(i\omega_n)Z_1(i\omega_n) = \pi T\sum_m K_{12}(i\omega_m - i\omega_n)\frac{\Delta_2(i\omega_m)}{\sqrt{\omega_m^2+\Delta_2^2(i\omega_m)}}, \tag{6}$$

$$Z_1(i\omega_n) = 1 + \frac{\pi T}{\omega_n}\sum_m K_{12}(i\omega_m - i\omega_n)\frac{\omega_m}{\sqrt{\omega_m^2+\Delta_2^2(i\omega_m)}}. \tag{7}$$

Here the kernel K_{12} is given by

$$K_{12}(i\omega_m - i\omega_n) = 2\int_0^\infty \frac{\Omega B_{12}(\Omega)d\Omega}{\Omega^2+(\omega_m-\omega_n)^2}.$$

This B_{12} represents the electron-boson coupling function which supplants the pairing potential used in the BCS theory, and there is an exactly analogous equation for band 2. Here $B_{12}(\Omega)/B_{21}(\Omega)=N_2/N_1=1/\beta$.

First we assume a simple Einstein-type electron-boson coupling function. The numerical solution of the Eliashberg equation (7) finds that the ratio of the gaps *decreases* with λ, which is opposite to the BCS prediction that the ratio of the gaps *increases* with increasing coupling. This can be understood analytically as well.

First of all, we observe that neglecting the mass renormalization by setting $Z=1$ in Eq. (6) yields results very close to the BCS solution [in fact, the deviation from the lowest-order approximation of Eq. (4) is mainly due to the increasing difference between $\sinh^{-1}(\omega_c/\Delta)$ and $\ln(2\omega_c/\Delta)$]. Let us now work out the effect of the mass renormalization.

Assuming an Einstein spectrum with the frequency Ω, at $T=0$ Eqs. (6) and (7) reduce to

$$\Delta_1(\omega)Z_1(\omega) = \frac{\lambda_{12}\Omega^2}{2}\int_{-\infty}^{\infty}\frac{d\omega'\Delta_2(\omega')}{[\Omega^2+(\omega-\omega')^2][\sqrt{\omega'^2+\Delta_2^2(\omega)}]}$$

and

$$Z_1(\omega) = 1+\frac{1}{2\omega}\lambda_{12}\Omega^2\int_{-\infty}^{\infty}d\omega' \times\frac{\omega'}{[\Omega^2+(\omega-\omega')^2][\sqrt{\omega'^2+\Delta_2^2(\omega)}]}$$

with a similar equation for Δ_2 and Z_2. In the popular "square-well" approximation[11,12] the equations become

$$\Delta_1(\omega)Z_1(\omega) = \frac{\lambda_{12}\theta(\Omega-|\omega|)}{2}\int_{-\infty}^{\infty}d\omega'\,\theta(\Omega-|\ \omega')| \times\frac{\Delta_2(\omega')}{[\Omega^2+(\omega-\omega')^2](\sqrt{\omega'^2+\Delta_2^2})}, \tag{8}$$

$$Z_1(\omega) = 1+\frac{1}{2\omega}\lambda_{12}\int_{-\infty}^{\infty}d\omega'\,\theta(\Omega-|\omega-\omega'|) \times\frac{\Delta_2(\omega')}{[\Omega^2+(\omega-\omega')^2](\sqrt{\omega'^2+\Delta_2^2})}, \tag{9}$$

which may be readily integrated to yield the following renormalization behavior for $Z(\omega)$:

$$Z_1(\omega) = 1+\lambda_{12} \quad \text{for} \quad \omega<\Omega \tag{10}$$

$$=1+\lambda_{12}\Omega/\omega \quad \text{for} \quad \Omega<\omega<2\Omega \tag{11}$$

$$=1+\lambda_{12}/2 \quad \text{for} \quad \omega>2\Omega. \tag{12}$$

This mass-renormalization behavior can then be incorporated in the previous BCS equations yielding a natural result,

$$\Delta_1(1+\lambda_{12}) = \Delta_2\lambda_{12}\sinh^{-1}(\omega_c/\Delta_2), \tag{13}$$

$$\Delta_2(1+\lambda_{21}) = \Delta_1\lambda_{21}\sinh^{-1}(\omega_c/\Delta_1), \tag{14}$$

reducing to Eq. (3) if λ_{12} in Eq. (3) would be substituted by $\lambda_{12}/(1+\lambda_{12})$, and similarly for λ_{21}. In Ref. 8 this approximation (termed "RBCS") has been used, and we will see that this approximation captures the full Eliashberg results extremely well.

In the linear order in λ, we have

$$\frac{\Delta_2}{\Delta_1} = \sqrt{\beta}\left(1+\frac{\lambda_{\rm eff}\ln\beta}{4}+\frac{\lambda_{12}-\lambda_{21}}{2}\right). \tag{15}$$

The last term is negative and always larger than the previous one (independent of β). Thus, the net effect is always opposite to what the unrenormalized BCS theory predicts. We have plotted up the above analytic approximation in Fig. 1 (solid line in the inset) and find good agreement for $\lambda_{\rm eff}<0.4$, showing that the mass renormalization is responsible for the lessening of the gap ratios with increasing coupling in Eliashberg theory. Also contained in Fig. 1, main panel and upper inset, is a comparison of the results of the RBCS approximation with the Eliashberg numerical results, which agree nearly perfectly.

The lessening of the gap ratios with increasing coupling might in hindsight have been expected given that the Fermi surface with the larger gap at weak coupling can be expected to have larger self-energy interactions in Eliashberg theory, reducing the gap anisotropy. This trend is also consistent with the superstrong-coupling limit of equal gaps, as mentioned previously. Of course, the effect of mass renormalization on the superconductivity in the sense of a coupling-constant renormalization by a factor of $1/(1+\lambda)$ is well known (see, e.g., Ref. 13), as well as the fact that this renormalization can be different for different bands in a multiband superconductor (see, e.g., Ref. 14). It is interesting, however, that this fact leads to unexpected effects in the case of interband superconductivity.

The above suggests that BCS-type analyses of the pnictides in an interband-pairing limit *must* use the Eliashberg/renormalized BCS approximation (i.e., letting $\lambda_i\rightarrow\frac{\lambda_i}{1+\lambda_i}$) in order to get even qualitatively correct answers. In particular, omitting this renormalization has led to a belief that Eliashberg theory predicts an enhancement of gap ratios relative to BCS when in fact the opposite is true.

As we mentioned in the beginning, Eq. (15) remains exactly the same whether the interband interaction is repulsive or attractive as long as all Δ's and λ's are understood as absolute values. The reason is, of course, that the mass renormalization is always positive, independent of the sign of the interaction.[15] One may ask another question, whether the mass-renormalization constants are the same as the pairing coupling constants. Generally speaking, for unconventional superconductivity where $\Delta(\mathbf{k})\neq\text{const}$, this is not true (cf. Ref. 16). In the case of purely interband interaction, though, these constants only differ in sign.

Interestingly, this strong-coupling renormalization effect remains operative at all temperatures up to T_c, while the previous term in Eq. (15) vanishes at T_c. Therefore (cf. Fig. 2) the actual gap ratio is even closer to 1 near T_c than at $T=0$.

Finally, we note that the above Eliashberg results were obtained using an Einstein spectral function for simplicity, but as indicated on the plot the use of a typical spin-fluctuation spectrum $[\sim\omega\Omega/(\omega^2+\Omega^2)]$ does not alter the results.

Another interesting observation to be made concerns the $\Delta(0)/T_c$ ratios predicted by BCS and Eliashberg theories. In the conventional weak-coupling one-band BCS theory this ratio does not depend on λ. This is no longer the case in the two-band BCS with the interband coupling only. In the lowest order the reduced gaps are simply $\Delta_2(0)/T_c=1.76\beta^{1/4}$ and $\Delta_1(0)/T_c=1.76\beta^{-1/4}$. The next order can be worked out using Eq. (5),

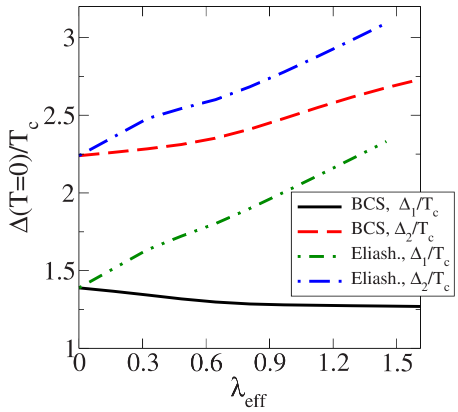

FIG. 2. (Color online) $\Delta(T=0)/T_c$ ratios are shown as a function of the overall coupling constant.

$$\frac{\Delta_2(0)}{T_c} = 1.76\beta^{1/4}\left(1 + \lambda_{\text{eff}}\frac{4\ln\beta - \ln^2\beta}{32}\right), \tag{16}$$

$$\frac{\Delta_1(0)}{T_c} = 1.76\beta^{-1/4}\left(1 - \lambda_{\text{eff}}\frac{4\ln\beta + \ln^2\beta}{32}\right). \tag{17}$$

This is confirmed by numerical calculations (Fig. 2): the smaller gap ratio decreases with λ_{eff}, while the other gap increases. Since the Eliashberg equation makes the gaps closer with increased coupling, this odd behavior does not show up; both reduced gaps grow with λ.

For completeness, we also show in Fig. 3 the behavior (in Eliashberg theory) of the reduced gaps as a function of the DOS ratio $N_1/N_2=\lambda_{21}/\lambda_{12}$. As might be expected, as the DOS ratio becomes very small the gap ratios move apart appreciably. Interestingly, T_c (shown in the right panel) is not constant as it would be in a weak-coupling regime but varies significantly for coupling-constant ratios far from 1. This is a result of the use of comparatively large coupling constants on one band when the other coupling constant is small, so that T_c suppression due to thermal excitation of real phonons (an effect not present in the BCS formalism) is stronger.

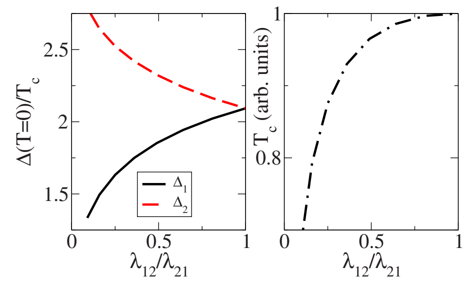

FIG. 3. (Color online). (Left) The behavior of the Eliashberg $\Delta(0)/T_c$ ratios as a function of the ratio of coupling constants. (Right) The behavior of T_c in this case. For both cases λ_{eff} is fixed at 1.

To conclude, in this work we have shown for the interband-only pairing that the two-band superconductivity is qualitatively incorrectly described by the BCS formalism even for the weak-coupling limit. BCS and Eliashberg theories predict qualitatively different behavior (as a function of coupling constant) for such basic characteristics as the gap ratio $\alpha=\Delta_2/\Delta_1$ as well as for the reduced gaps Δ/T_c. In particular, the *sign* of $d\alpha/d\lambda$ changes from BCS to Eliashberg theory. We have found this result analytically and numerically by solving Eliashberg equations for the model spectra. This finding is relevant to the superconducting pnictides where the interband-pairing regime is believed to be realized.

[1] J. R. Schrieffer, *Theory of Superconductivity* (Perseus, Reading, MA, 1999).
[2] H. Suhl, B. T. Matthias, and L. R. Walker, Phys. Rev. Lett. **3**, 552 (1959).
[3] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, Phys. Rev. Lett. **101**, 087004 (2008).
[4] I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du, Phys. Rev. Lett. **101**, 057003 (2008).
[5] D. Parker, O. V. Dolgov, M. M. Korshunov, A. A. Golubov, and I. I. Mazin, Phys. Rev. B **78**, 134524 (2008).
[6] Y. Bang and H.-Y. Choi, Phys. Rev. B **78**, 134523 (2008).
[7] Ł. Malone, J. D. Fletcher, A. Serafin, A. Carrington, N. D. Zhigadlo, Z. Bukowksi, S. Katrych, and J. Karpinski, arXiv:0806.3908 (unpublished).
[8] E. J. Nicol and J. P. Carbotte, Phys. Rev. B **71**, 054501 (2005).
[9] O. V. Dolgov and A. A. Golubov, Phys. Rev. B **77**, 214526 (2008).
[10] G. M. Eliashberg, Sov. Phys. JETP **11**, 696 (1960).
[11] P. B. Allen and B. Mitrovic, Solid State Phys. **37**, 1 (1982).
[12] The square-well model is not a consistent approximation as different functional forms are assumed for Δ in the first and in the second Eliashberg equations. Sometimes this may lead to qualitative errors [e.g., O. V. Dolgov, I. I. Mazin, A. A. Golubov, S. Y. Savrasov, and E. G. Maksimov, Phys. Rev. Lett. **95**, 257003 (2005)]. In this particular case, however, it can be shown that using more accurate and consistent functional forms, $\Delta_1(\omega) = \Delta_1(0)\Omega^2/(\omega^2+\Omega^2)$ and $Z_1(\omega)=1+(\lambda_{12}\Omega/\omega)\tan^{-1}(\omega/\Omega)$, leads to essentially the same result.
[13] J. P. Carbotte, Rev. Mod. Phys. **62**, 1027 (1990).
[14] I. I. Mazin and V. P. Antropov, Physica C **385**, 49 (2003).
[15] P. Monthoux and G. G. Lonzarich, Phys. Rev. B **63**, 054529 (2001).
[16] D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B **34**, 8190 (1986).