Spin-fluctuation mechanism of superconductivity in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ ferropnictides

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Abstract. Gap structure and spin-fluctuation pairing mechanism in the iron-based superconductors Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ is studied. We demonstrate that the overdoped compounds Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ have a three-gap structure with substantially different order parameters and a weak interband spin-fluctuation coupling. In the three-gap state of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, the anisotropic electronic gap has an intermediate value between two isotropic hole gaps. During transition to the optimal regime, the electron gap strongly increases (by a factor of two) and gets close to the largest hole gap value, while the electron gap anisotropy sharply decreases pointing to a strong increase in the interband interaction, with spin fluctuations accompanying the antiferromagnetic transition. The same two-gap state with close values of the electron and largest hole gaps is preserved even with further decrease in doping. The performed study shows that the spin-fluctuation pairing mechanism has a significant effect on doping evolution of the electron gap only. The doping evolution of the dominant hole gap in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ is not directly related to the evolution of the spin fluctuations.

The iron-based superconductors (FeSCs) with a highly anisotropic quasi-two-dimensional Fermi surface (FS) and low carrier density in hole (centered at $\Gamma$ point) and electronic (centered at points X = ($\pi$, 0) and Y = (0, $\pi$)) bands (figure 1) are potentially related to systems with correlated electrons. Electron-electron correlations in FeSCs are relatively small compared with HTSC cuprates. The parent iron-based compounds, in contrast to HTSC cuprates, are antiferromagnetic (AFM) metals that have not associated with magnetism electronic states on the Fermi surface that are available for superconducting pairing. Electronic doping increases electron X/Y pockets and reduces hole $\Gamma$ pockets, and hole vice versa. With an increase in doping, the suppression of antiferromagnetism leads to the appearance of superconductivity (SC). In this region, the AFM and the SC gaps coexist on the FS. Experimentally, in different FeSCs, order parameters are observed with both s and d (with nodes in some parts of the FS) symmetry. The strong anisotropy of the order parameter is usually associated with the non-phonon (electron-electron) superconductivity mechanism. Indirectly, the non-phonon superconductivity nature of FeSCs can be indicated by experimentally observed in FeSCs on large (on the order of AFM vectors $Q = (\pi, 0)$, $(0, \pi)$ wave vectors $q$ (interband) isotropic spin and on small $q$ (intra-band) quadrupole $d_{x^2-y^2}$ charge (orbital) electron fluctuations. A non-phonon (with repulsive interelectron interaction) SC in such systems is possible only with the dominance of the interband...
interaction [1], which always increases the SC gaps and $T_c$. According to the spin-fluctuation theory [2, 3], in FeSCs with hole (h) and electronic (e) pockets, there is always a non-phonon superconductivity channel, since in these superconductors the interband e-h interaction $V_{eh}(Q)$ exceeds the intraband Coulomb repulsion of $U_C$ for small $q$. Depending on the sign of $V_{eh}$, either gaps with opposite signs of the e and h pockets of the FS are formed in the system (the so-called s$_{±}$ pairing: $V_{eh} > 0$, figure 2) or the traditional s$_{++}$ pairing ($V_{eh} < 0$). The intensity of $V_{eh}$ spin fluctuations is determined by the proximity to the AFM transition and is highly dependent on doping. Figure 2 shows the dominant mechanisms of the non-phonon superconductivity near (left) and far from (right) the AFM transition.

The electron-phonon attraction $U_{EP}$ reduces the electron-electron repulsion in all non-phonon channels and can transform the sign-reversed gap with nodes (figure 2, right) into a sign-preserved gap with minima. Taking into account the electron-phonon interaction (EPI), the influence of the spin-fluctuation mechanism on the superconductivity in the e and h bands becomes unequal due to the different density of states $\gamma_n$ (and EPI) and the dominant SC mechanisms in the e and h bands can vary and also change when changes in doping $x$ depending on the values of $\gamma_n(x)$ and $V_{eh}(x)$ in the bands.

Direct comparison of the spin-fluctuation theory with experimental data is complicated by the fact that in the most fully studied optimally doped FeSCs due to strong $V_{eh}$ interactions ($V_{eh} \geq U_{EP}$), the maximal h-gap and e-gap converge (unite in a e-h cluster) and coincide within the experimental error. In this region of $V_{eh} \geq U_{EP}$, the two-band superconductivity equations are linearly dependent and allow ambiguous interpretation of the mechanism of superconductivity. In particular, within experimental error, the properties of FeSCs with close h and e gaps can always be explained by a strong interband e-h interaction (spin-fluctuation theory), which, however, is not convincing evidence. It is more reliable to estimate the interband e-h interaction in the overdoped FeSCs far from the AFM transition with relatively weak $V_{eh}$ and substantially different e and two h gaps – “three-gap” FeSCs. A further study of the doping evolution of the three-gap state with a decrease in doping in comparison with the results of the spin-fluctuation theory allows us to clarify the role of non-phonon mechanisms in FeSCs.

The experimental data suitable for such a study are few and are associated with the study of the doping dependence of the electronic heat capacity of FeSCs. Figure 3 shows examples of the evolution of the electron heat capacity $c_e(x,t)$ of the overdoped “three-gap” FeSCs to the AFM transition region and the optimal (with maximum $T_c$) doping concentrations. Reduction of $c_e(x,t)$ at intermediate temperatures and an increase in $c_e(x,t)$ near $T_c$, in accordance with the entropy conservation law $\int_0^1 c_s(x,t) dt = 1$ indicates a convergence of electron $\Delta_e(x,t)$ and maximum hole $\Delta_{2h}(x,t)$ gaps as the AFM transition approaches and $V_{eh}(x)$ increases, as is assumed by the spin-fluctuation theory. However, according to [4, 5], the density of states $\gamma_n(x)$ (and EPI) also increases with decreasing doping, reaching a maximum at optimal concentrations, and the role of the phonon and non-phonon mechanisms in increasing $T_c$ remains unclear.

The proposed [6, 7] BCS-like (taking into account the effects of strong coupling) analysis of experimental data from FeSCs allows determining the magnitude and symmetry of the SC gaps, as
Figure 3. Temperature dependence of the electron heat capacity. Experimental data for Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) (a) and NaFe\(_{1-x}\)Co\(_x\)As (b) in underdoped and overdoped regimes taken from Refs. [4] and [5], correspondingly.

well as the effective interband interaction constants and studying the contribution of electron-electron correlations to the superconductivity of FeSCs. Due to the large number of fitting parameters in the three-band equations, it is possible to reliably investigate \(c_s(x,t)\) only for the most thoroughly studied family of Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) with the use of available results of studies of terahertz and infrared optical spectra, reflection coefficient and photoemission spectra (ARPES) (see [6]).

The doping dependence of the SC gaps \(\Delta(x)\) and \(T_c(x)\) is associated with a change in the intraband pairing constants \(\lambda_{ii}^0 \approx U(q \rightarrow 0)\gamma_i(x)\) and interband interaction \(\lambda_{ij}^0 \approx V_{ij}\gamma_i(x)\gamma_j(x)\). The interaction \(V(Q, x)\), determined by the doping dependence of the intensity of spin fluctuations, increases with decreasing electron doping, reaching a maximum near the AFM transition. Examples of the three-band approximation of the electron heat capacity \(c_s(x,t)\) Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) [4] for some doping concentrations are shown in figure 4. Analysis of the dependence of \(c_s(x,t)\) Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) shows that, in the overdoped regime, the interband spin-fluctuation interaction \(V_{eh}(x)\) far from the AFM transition is small compared to the intraband \(U\). The superconducting state has a three-gap structure in which the anisotropic (without nodes) electron \(\Delta_e(x,\phi)\) gap occupies an intermediate position between the dominant inner \(\Delta_2h(x, \phi)\) and outer \(\Delta_1h(x, \phi)\) isotropic hole gaps. Superconductivity of overdoped Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) compounds with dominant intraband pairing and weak spin-fluctuation \(2h-e\) interaction cannot be explained only by spin-fluctuation theory with repulsive \(U_C\) intraband interaction for small \(q\) without taking into account the strong EPI, \(U_{EF}\). Correlation effects in overdoped compounds appear only in the \(e\)-band with a low density of states \(\gamma_e(x)\), in which the intraband EPI is enhanced by the interaction with \(d_{x^2-y^2}\) charge (orbital) fluctuations with small wave vectors. The doping dependence of the critical temperature of overdoped Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) can be explained by an increase in intraband EPI pairing in the \(2h\)-band due to an increase in the density of states with a decrease in doping.

Near the AFM transition, the electron \(e\)-gap increases sharply, approaching the dominant \(2h\) gap. The analysis of \(c_s(x,t)\) shows that the increase in the \(e\)-gap is due to the doping increase in the interband \(e-2h\) interaction and can be explained by the strong doping dependence of the intensity of spin fluctuations in the AFM transition region observed in Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\). The same two-gap state with close electron and inner hole gaps \(\Delta_2h(x, \phi) \approx \Delta_e(x,\phi)\) is also preserved in the AFM-SC coexistence phase. In this phase, the hole gaps and the \(e\)-gap coupled with the \(2h\) band by the strong \(e-2h\) interaction decrease with decreasing doping, as well as the density of states available for superconducting pairing due to competition with the opening AFM gap.

The doping dependence of \(e\) and \(h\) gaps is schematically shown in figure 5. It also shows the dependence of the density of states \(\gamma_e(x)\) [4] in arbitrary units (solid squares). The results of our analysis show that the density of states \(\gamma_e(x)\) (and the intraband EPI) in the \(e\)-band is substantially less
than in the h-band. As a result, the correlation effects appear in the e-band most strongly and the doping dependence of the e-gap is determined mainly by the strong doping dependence of the intensity of spin fluctuations in the AFM transition region. In contrast to the correlated e-band in h-band with a significantly higher density of states and EPI, the interband h-e spin-fluctuation interaction is small compared to the intraband EPI. Doping dependence of 1,2h-gaps and critical temperature $T_c(x) = 2\Delta_{1h}(x)/T_c(x) = 5$, both before and after the AFM transition is associated with a change in the density of states in the h-bands and is explained by the doping dependence of the intraband EPI.

This study demonstrates that the non-phonon spin-fluctuation mechanism has a strong effect on superconductivity in the e-band with an anisotropic Fermi surface and low density of states and is the cause of the experimentally observed order parameter anisotropy, but the doping evolution of the dominant 2h gap in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ is not directly related to the evolution of the spin fluctuations.

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