A multiband model for $SmFeAsO_{1−x}F_x$

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Abstract. A multi-band model within the BCS framework is proposed for the description of iron-based oxypnictide superconductors. A $s$-wave pairing symmetry and different doping values are considered. This model is used to describe some properties of the oxypnictide $SmFeAsO_{1−x}F_x$ superconductor. The electron-phonon coupling of the corresponding Fe in-plane breathing mode is considered. The Fe isotope effect is evaluated as function of the coupling parameter as well as other relevant parameters of the model.

1. Introduction
The discovery of high transition temperature superconductivity (HTSC) in $LaO_{1−x}F_xFeAs$ [1] has triggered interest in the development of transition-metal superconductors. F doping strongly affects the electronic properties of iron-based oxypnictide superconductors[2], the replacement of $O^2−$ by $F^−$ in the layered iron-based $LaOFeAs$ originates a superconducting transition. In fact it was found that the $Fe−As$ based compounds become superconductors by electron doping. Some of these materials have transition temperatures up to $54K$, as in $SmFeAsO_{1−x}F_x$. In the oxypnictides as in the cuprate superconductors the conduction is also two dimensionally confined, in the oxypnictides the conduction occurs in the $Fe−As$ layers.

The fact that the critical temperature varies with the isotopic mass was an evidence for the interaction between the electrons and the lattice vibrations (phonons). In the iron oxypnictides strong iron isotope effect on $T_c$ has been reported[3], however a very small oxygen isotope effect on $T_c$ has been found. It could be because the iron-arsenide plane is the conducting layer in these materials. These results are a proof that the electron-phonon interaction is an important mechanism in the iron oxypnictides. The fact that the superconductivity in oxypnictide superconductors shows a strong sensitivity to the crystal lattice suggest the possibility of electron-phonon coupling [4]. Pairing symmetry is an important element toward understanding the mechanism of high-$T_c$ superconductivity. From optical measurements it was found that $Fe$-based superconductors have $s$-wave symmetry superconductivity[4].

Understanding of the electronic structure at the Fermi level can give some useful clues to unravel the fundamental ingredients responsible for the high transition temperature $T_c$[5]. However, to present the underlying physical process remains unknown. In this context, it seems crucial to study new ideas that use simplified schematic models to isolate the mechanism(s) that generate HTSC. Electronic structure calculations for the iron oxypnictides show overlapping energy bands at the Fermi level. Numerous indications point to the multiband nature of the
superconductivity in these materials. The agreement of the multiband model with experimental findings, suggests that Fe-based superconductors are multiband systems[4].

A two-dimensional (2D) multi-band model within the BCS framework is proposed in this work. As a prototype of multiband superconductors, a two overlapping band model is considered. This model, which can be taken as a minimal singularity in the density of states (DOS), and the BCS framework, can lead to higher $T_c$ values than those expected from the traditional phonon barrier. The energy band overlapping, modifies the DOS near the Fermi level allowing the high $T_c$ values observed. For physical consistency, an important requirement of the proposed model is that the band overlapping parameter is not larger than the phonons energy, $E_{ph}$. The model here proposed will be used to describe some properties of iron-based oxypnictide superconductors, in particular $SmFeAsO_{1-x}F_x$, in terms of the doping and the parameters of the model.

2. The model

We begin with the famous gap equation

$$\Delta(k) = \sum_k V(k, k') \Delta(k) \tanh(E_k/2k_B T_k)$$

in the weak coupling limit, with $V(k, k')$ the pairing interaction, $k_B$ is the Boltzmann constant, and $E_k^2 = \epsilon_k^2 + \Delta_k^2$, where $\epsilon_k = \hbar^2 k^2/2m$ are the self-consistent single-particle energies.

For the electron-phonon interaction, we have considered $V(k, k') = V_0$, with $V_0$ a constant, when $|\epsilon_k|$ and $|\epsilon_{k'}|$ $\leq E_{ph}$ and 0 elsewhere. As usual the attractive BCS interaction is nonzero only for unoccupied orbitals in the neighborhood of the Fermi level $E_F$. The superconducting order parameter, $\Delta(k) = \Delta(T)$ if $|\epsilon_k| \leq E_{ph}$ and 0 elsewhere.

With these considerations we propose a two overlapping bands model. As a particular distribution in momentum space the following form has been considered

$$n_k = \Theta(\gamma k_F - k) + \Theta(\gamma k_F - k) \Theta(k - \beta k_F),$$

with $k_F$ the Fermi momentum and $0 < \beta < \gamma < 1$. In order to keep the average number of electron states constant, the parameters are related in the 2D system by the equation $2\gamma^2 - \beta^2 = 1$, then only one of the relevant parameters is independent. The distribution in momentum induces one in energy, $E_\beta < E_\gamma$ where $E_\beta = \beta^2 E_F$ and $E_\gamma = \gamma^2 E_F$. The phonon available energy provided by the material itself is introduced by the Fe in-plane breathing mode, which can be associated to a large electron-phonon coupling constant. Then it is required that the band overlapping be of the order or smaller than the cutoff energy $E_{ph}$. That means $(1 - \gamma^2)E_F \leq E_{ph}$. The minimum $\gamma^2$ value consistent with our model is $\gamma_{ph}^2 = 1 - E_{ph}/E_F$. While $E_F - E_\gamma \leq E_{ph}$, implies that the energy difference between the anomalously occupied states must be provided by the material itself.

In the last framework the summation in Eq.(1) is changed to an integration which is done over the (symmetric) generalized Fermi surface defined above. One gets

$$1 = \lambda \int_{E_\gamma - E_{ph}}^{E_\gamma + E_{ph}} \frac{\sqrt{\Xi_k}}{2k_B \bar{T}} \tanh\left(\frac{\Xi_k}{2k_B \bar{T}}\right) \frac{d\epsilon_k}{\sqrt{\Xi_k}} + \frac{\lambda}{2} \int_{E_\beta}^{E_F} \frac{\sqrt{\Xi_k}}{2k_B \bar{T}} \tanh\left(\frac{\Xi_k}{2k_B \bar{T}}\right) \frac{d\epsilon_k}{\sqrt{\Xi_k}}$$

In this equation $\Xi_k = (\epsilon_k - E_F)^2 + \Delta(T)^2$, the coupling parameter is $\lambda = V_0 D(E)$, with $D(E)$ the electronic density of states, which is a constant for the 2D system in the integration range.
Notice that there is an anomalous occupancy at each $\gamma^2$ value, then the electronic density of states depends on $\gamma^2$. $E_F = \frac{h^2 \pi}{m} n_{2D}$, with $n_{2D}$ the carriers density per FeAs layer, this value can be calculated from Hall coefficient data and lattice parameters for different doping [6].

The two integrals correspond to the bands proposed by Eq. (2). The integration over the surface at $E_\gamma$ in the first band, is restricted to states in the interval $E_\gamma - E_{ph} \leq E_k \leq E_\gamma + E_{ph}$. In the second band, in order to conserve the particle number, the integration is restricted to the interval $E_\beta \leq E_k \leq E_F$, if $E_\gamma + E_{ph} > E_F$, with $E_\beta = (2 \gamma^2 - 1)E_F$, in terms of the parameter $\gamma^2$ in our model.

The critical temperature is introduced via the Eq. (3) at $T = T_c$, where the gap becomes $\Delta(T_c) = 0$. At this temperature this equation relates $T_c$ to the coupling constant $\lambda$ and to the anomalous occupancy parameter $\gamma^2$. This relationship determines the $\gamma^2$ values which reproduce the critical temperature of several high-$T_c$ superconductors in the weak coupling region.

The model presented in this section can be used to describe high-$T_c$ iron oxypnictide superconductors [8]. In any case a specific material must be selected to introduce the available experimental data. Ranges for the coupling parameter $\lambda$ in the weak coupling region, and the overlapping parameter $\gamma^2$, consistent with the model can be obtained for each material. The relationship between the characteristic parameters will be obtained for Fe – As based compounds at several doping concentrations $x$ localized only in the superconducting region of phase diagram of the system. The iron isotope exponent $\alpha_I$ for the superconducting transition $\alpha_I = \frac{d\ln T_c}{d\ln M}$, is also evaluated. In order to get numerical results the model will be used to describe the iron oxypnictide $SmFeAsO_{1-x}F_x$. Experimental results reported for this material [6], and optical modes of Fe-As based superconductors [7] were used in our calculations.

3. Results and discussion
In Fig.1 the coupling parameter $\lambda$ as a function of the band overlapping is shown for the iron oxypnictide $SmFeAsO_{1-x}F_x$ in the range $\gamma_{ph}^2 \leq \gamma^2 < 1$ with the minimum value of the overlapping constant $\gamma_{ph}^2 = 0.85$ for $x = 0.2$. The results are obtained for the material with the optimal doping, $x = 0.2$ and for $x = 0.15$. The values of $\lambda$ obtained with our model are in the weak coupling region. 

In Fig.2 the Fe isotope exponent as a function of $\gamma^2$ obtained with our model is shown for $SmFeAsO_{1-x}F_x$ at doping $x = 0.15$, in which the experimental result of Ref.([3]) is also shown. The exponent $\alpha_I$ is calculated using Eq. (3) at $T = T_c$. The dependence of the mass $M$
Figure 2. The Fe isotope exponent for $\text{SmFeAsO}_{1-x}F_x$ at $x = 0.15$. The horizontal line corresponds to the experimental result of Ref.([3]).

was introduced via $dT_c/T_c = -\alpha_I dM/M$ and $E_{ph} \propto (M)^{-1/2}$. The $\alpha_I$ curve has a minimum value $\alpha_I = 0.35$ at $\gamma^2 = 0.95$. This minimum value of the isotopic effect is very near to the experimental value $\alpha_I = 0.34$ and agrees with theoretical calculations [9]. The previous result and the calculated electron-phonon coupling $\lambda = 0.33$ obtained from the Fig.1 for an overlapping parameter $\gamma^2 = 0.95$ are consistent with a phonon mediated superconductivity on Fe−As in the weak coupling regime.

Based on band structure calculations for Fe−As superconductors, we presented an overlapping band model with s-wave symmetry, to describe high-$T_c$ oxynitride superconductors, within the BCS framework. We have used a model with two overlapping bands at the Fermi level in the 2D fermion gas. We report the behavior of the coupling parameter $\lambda$ as function of the overlapping parameter $\gamma^2$, for different doping samples. The $\lambda$ values consistent with the model are in the weak coupling region. The electron-phonon coupling of the corresponding Fe in-plane breathing mode is considered and the minimum band overlapping parameter is consistent with this value. The band overlapping allows the improvement of the results obtained with a s-wave mean-field approximation, in a scheme in which the electron-phonon interaction is the relevant one for high-$T_c$ mechanism i.e., the energy scale of the band overlapping $(1 - \gamma^2)E_F$, is of the order of the phonon energy. This energy is then the overall scale that determines the highest $T_c$ and gives credibility to the model because it requires an energy scale accessible to the lattice. The Fe isotope exponent is evaluated and it agrees with experimental values reported.

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