Hybridization of three-band structure in Fe-based superconductors

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We study the superconducting gap structure of multi-band systems by a self-consistent numerical method using Bogoliubov-deGennes equations. The main result shows that hybridization between the bands causes the superconducting critical temperature ($T_c$) of each band to converge to a single value. We show that this approach reproduces the observed three gaps and single $T_c$ in different compounds of Ba$_{1-x}$K$_x$Fe$_2$As$_2$.

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I. INTRODUCTION

The Fe-based superconductors (FeSCs) revealed to be the first class of high-$T_c$ superconducting materials with multi-band and multi-gap structure [1]. Unlike MgB$_2$ with two bands and two BCS-like superconducting gaps [2] – multi-bands and multi-gaps in the FeSCs appear to be more complicated. Experiments such as angle-resolved photoemission spectroscopy (ARPES) [1, 3, 4], point-contact Andreev reflection spectroscopy (PCAR) [5–7] and muon-spin rotation ($\mu$SR) [8] identify at least two nodeless $s$-wave like superconducting gaps. As a typical example, ARPES identifies nearly two coinciding gap structures in the $\alpha(\gamma)$ bands with $\Delta_{\alpha(\gamma)}(0) \approx 13$ meV, and another one in the large $\beta$ pocket with $\Delta_\beta(0) \approx 6$ meV for Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ with $T_c = 38$ K [1]. Still, a concordant theoretical approach on the temperature dependence of the multi-gap structure of FeSCs is an ongoing discussion [9].

In this paper, we investigate the temperature dependence of the three-gap structure of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ with $T_c = 23$, 32 and 38 K as observed by ARPES [1, 4, 10, 11] and PCAR [5–7] by a multi-band Bogoliubov-deGennes (BdG) method with intra and inter-band hoppings and a two-body attractive potential induced by charge disorder [12, 13]. In a charge inhomogeneous system [14, 15] an attractive interaction may arise favouring pairing; and the pairing amplitude depends on the free-energy domain walls arising from the charge segregation process. Reference [16] showed that the interface free-energy between low and high density phases varies with temperature. Mounting evidence indicates that encountered electronic inhomogeneities may not be due to disorder induced by chemical doping, but may represent a universal intrinsic feature of high-temperature FeSCs [12, 17–20]; a common feature to cuprates. Until now, there has been little theoretical effort to address intrinsic electronic inhomogeneities in FeSCs that break translational symmetry of the charge distribution (not the crystal lattice).

Fe-based superconductors are usually described in terms of minimal multi-orbital models to address the five 3$d$ orbitals of Fe and its interactions [21–23]. However, since ARPES data [10] fits to a model [24] where each Fermi pocket can be modelled by a single band, we are motivated to use multi-band (BdG) theory instead. This enables us to study the temperature dependence of the multi-band gap structure $\Delta_\nu(T)$, where $\nu$ refers to the $\alpha$, $\beta$ and $\gamma$ band. The mean-field Hamiltonian is thus given by

\begin{equation}
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\[ H_{\text{MF}} = \sum_{i \neq j, \mu, \nu, \sigma} t_{\mu \nu}(i,j)c_{\mu \sigma}^\dagger(i)c_{\nu \sigma}(j) - \sum_{i, \mu, \sigma} \tilde{\mu}_\nu(i)c_{\mu \sigma}^\dagger(i)c_{\nu \sigma}(i) + \sum_{i, \mu, \nu} \left[ \Delta_\nu(i,j)c_{\mu \uparrow}^\dagger(i)c_{\nu \downarrow}(i) + \text{h.c.} \right], \tag{1} \]

where \( \mu \) and \( \nu \) are band indices that run over the \( \alpha \), \( \beta \) and \( \gamma \) pockets, each with its respective dominating band as identified by ARPES [10]. The spin index \( \sigma \) assumes either \( \uparrow \) or \( \downarrow \), and the creation and annihilation operators obey the Fermi anti-commutation relation \{\( c_{\mu \sigma}(i), c_{\nu \sigma}^\dagger(j) \}\} = \delta_{ij} \delta_{\mu \nu} \delta_{\sigma \sigma'}.

The \( t_{\mu \nu}(i,j) \) are intra-band \( (\mu = \nu) \) and inter-band \( (\mu \neq \nu) \) hopping amplitudes between lattice sites \( i \) and \( j \), which we include up to second nearest neighbours to fit ARPES band dispersion [10]. We introduced a short-hand notation for the shifted chemical potential \( \tilde{\mu}_\nu(i) = \mu_\nu(i) - U_\nu(i)\rho_\nu(i)/2 \), which includes: the local chemical potential \( \mu_\nu(i) \), the on-site Coulomb repulsion \( U_\nu(i) \) that due to the mean-field treatment just enters as a rescaling factor, and the band charge density \( \rho_\nu(i) \). The band density \( \rho_\nu(i) \) is self-consistently regulated by adjusting \( \mu_\nu(i) \) until \( \rho_\nu(i) \) converges to some fixed value. The local BdG superconducting gap is \( \Delta_\nu(i,j) = -V(T)(c_{\nu \uparrow}(i)c_{\nu \downarrow}(j)) \), from which we construct the full BdG matrix that has dimension \( 6N^2 \times 6N^2 \) in the three-band case, where \( N \times N \) is the lattice’s dimension. The symmetric positive quasi-particle excitations \( \{E_n\} \) are used to calculate the local s-wave gap at a temperature \( T \) for each band

\[ \Delta_\nu(i) = -V_\nu(i) \sum_n u_{\nu \nu}(i) v_{\nu \nu}(i) \tanh \left( \frac{E_n}{2k_BT} \right), \tag{5} \]

and the band density \( \rho_\nu(i) = \sum_\sigma \langle c_{\nu \sigma}^\dagger(i)c_{\nu \sigma}(i) \rangle \) as

\[ \rho_\nu(i) = 2 \sum_n \left( |u_{\nu \nu}(i)|^2 f_n + |v_{\nu \nu}(i)|^2 (1 - f_n) \right), \tag{6} \]

where \( f_n \) is the Fermi distribution of quasi-particles. Equations (5) and (6) are self-consistently solved in conjunction with equation (4). Equation (5) allows for the simultaneous determination of \( \Delta_\alpha(T) \), \( \Delta_\beta(T) \), and \( \Delta_\gamma(T) \).

A typical solution of equation (5) with a single constant attractive potential for all three bands for independent band dynamics (no inter-band hopping) is shown on the left panel of figure 1. Hoppings are the same as in table I. In this case, lower intra-band hoppings that yield lower kinetic energies generate bigger gaps and consequently different \( T_c \)'s. However, by allowing hybridization of charge carriers between bands, that is, non-zero inter-band hoppings, the character of the three-gap structure changes drastically as shown on the right panel of figure 1. The crucial difference in the hybridized case is a single value for \( T_c \) for all three bands, in accordance with experimental observations [1, 3–7]. The experimental detection of many multi-band and multi-gap systems with a single superconducting \( T_c \) is the main motivation to study inter-band dynamics of Fe-based superconductors by a BdG system with hybridized bands.

**III. TEMPERATURE DEPENDENCE OF THE THREE-GAP STRUCTURE**

In this section we apply multi-band BdG theory to model Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) with \( T_c = 23, 32 \) and 38 K. For all three compounds we solved a three-band \( N \times N \) periodic square lattice with first and second nearest neighbour intra-band hopping parameters extracted from ARPES tight-binding fitting [10] shown in the first three columns of table I. Following ARPES results, we choose inter-band hoppings to reflect band intersections between the \( \alpha/\beta \) and \( \beta/\gamma \) pockets [10, 26], which are shown in the last three columns of table I. There is no intersection between \( \alpha/\gamma \) [10].

In the BdG procedure the temperature dependent s-wave gaps \( \Delta_\alpha(T) \), \( \Delta_\beta(T) \), and \( \Delta_\gamma(T) \) are self-consistently determined by equation (5). PCAR techniques [6, 7] find two superconducting bands, whereas...
We performed the calculations assuming a homogeneous charge distribution with \((\rho_\alpha, \rho_\beta, \rho_\gamma) = (0.192, 0.084, 0.12)\) that are proportional to Fermi pocket areas [26], and Fermi velocities [1, 8]. The calculations with constant densities is justified because the average gap of a disordered density system is the same of that of a homogeneous one, provided the average density equals the homogeneous one. The hoppings in table I and the above densities are used for all three compounds discussed in this paper.

To model Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) compounds with different \(T_c\)'s we use different phenomenological parameters appearing in equation (2) as summarized in table II. The results for the compound with \(T_c = 23\) K is depicted on the left panel of figure 2. The coloured solid lines are the theoretical BdG curves obtained from (5). We observe that PCAR [6, 7] (black triangles) scales with the BdG \(\alpha/\gamma\) bands. In the case of the compound with \(T_c = 32\) K we show experimental points from ARPES [3] in comparison to the theoretical BdG curves on the right panel of figure 2. Experimental points for the \(\beta\) bands were unavailable and estimated under 4 meV [3], consistent with the blue \(\beta\) BdG curve. The results for Ba\(_{0.6}\)K\(_{0.4}\)Fe\(_2\)As\(_2\) with \(T_c = 38\) K are shown in figure 3, where each band is shown separately for clarity. Two different sets of ARPES points are displayed denoted by ARPES1 referring to [1] and ARPES2 according to [11].

Despite of the size of the small lattice used in our multi-band calculations, we obtain a reasonable agreement with the experimental values, using a single attractive potential (equation (2)) for the three bands for each compound. The misfit of the experimental points with respect to the theoretical BdG curves may be due to differences in the tight binding hoppings, whose base model [24] did not include inter-band hoppings; and limitations of the lattice size due to the disadvantage of using an exact diagonalization technique on multi-bands. New calculations using a more powerful method that allows investigation of much larger arrays are being presently considered. However, we believe that the essential properties of these compounds are captured by the present calculations.

Both figures 2 and 3 show how the two similar \(\alpha\) and \(\gamma\) gap structures drop coincidently with \(\beta\) at a single \(T_c\). This is only achieved through non-zero inter-band hoppings – hybridization between the bands within multi-band BdG theory. The radical change of the \(\beta\) band with respect to the band independent case (figure 1) band can be understood from the fact the its intra-band hopping is substantially lower as compared to the two other bands as shown in table I, which causes a bigger gap if bands do not communicate. By turning inter-band hybridization on, the behaviour of the bands is changed (especially for \(\beta\), and band inter-dependence causes the system to have a single \(T_c\).

### IV. Conclusion

The multi-gap \(\Delta_v(T)\) as a function of temperature measured in many experiments [1, 3, 6, 7, 11] were closely reproduced by a multi-band BdG model, where the inter-band hoppings are the essential ingredient to obtain a single \(T_c\) for all three bands. We used band representation instead of orbital representation to address gaps ob-

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**TABLE I**: First and second nearest neighbour intra and inter-band hoppings \(t_{\mu\nu}\) in meV used in the present calculations. Intra-band hoppings were extracted from ARPES and inter-band hoppings closely agree with band dispersion [10]. The parameters of this table are used for all three compound discussed in this paper.

| Hoppings (meV) | \(t_{\alpha\alpha}\) | \(t_{\alpha\beta}\) | \(t_{\alpha\gamma}\) | \(t_{\beta\gamma}\) | \(t_{\alpha\gamma}\) |
|---------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \(T^1\)       | 160             | 13              | 380             | 165             | 0               |
| \(T^2\)       | -52             | 42              | 80              | 0               | 0               |

**TABLE II**: Phenomenological values of the electronic phase transition temperature \(T_{PS}\) and potential \(|V_0|\) in equation (2) used to model Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) with different \(T_c\)’s.

| Compound       | \(T_c\) (K) | \(T_{PS}\) (K) | \(|V_0|\) (meV) |
|----------------|-------------|----------------|----------------|
| Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) | 23          | 80             | -300           |
| Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) | 32          | 130            | -360           |
| Ba\(_{0.6}\)K\(_{0.4}\)Fe\(_2\)As\(_2\) | 38          | 165            | -400           |
FIG. 3: Temperature dependence of (a) the jointly obtained superconducting gaps $\Delta_\nu(T)$ from multi-band BdG theory (solid lines) in comparison to references [1] (empty points) and [11] (solid points) for Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$ with $T_c = 38$ K and $N = 8$. We show the three sets of data corresponding to (b) $\nu = \alpha$, (c) $\nu = \beta$, and (d) $\nu = \gamma$ separately for clarity.

served in the $\alpha$, $\beta$ and $\gamma$ pockets of three Ba$_{1-x}$K$_x$Fe$_2$As$_2$ compounds. Even though each band or Fermi pocket is determined by modelling the hybridizing 3d orbitals of Fe [27–29], we captured the dominant bands relevant to each pocket. The main conclusion is that the multi-band hybridizations are crucial ingredients to the Ba$_{1-x}$K$_x$Fe$_2$As$_2$ system and this is revealed by the single value of $T_c$’s.

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