Band energies in two-band model for Fe based superconductors in the coexistence state

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Abstract. The superconductivity in iron based superconductors is hotly discussed since its discovery. The pairing mechanism and the gap structures for such superconductors are the core of attraction for debate. The superconductivity exists on the suppression of the pseudo gaps like antiferromagnetism and structural distortion. The Fermi surface band structure is studied by proposing a tight binding two-orbital model in $s\pm$-wave pairing symmetry for the coexistence of Jahn-Teller distortion and antiferromagnetism with superconductivity.

1. Introduction

The iron-based superconductors (FeSCs) were discovered with chemical compositions [1, 2], such as 1111-material (LaFeAsO), 122-material (BaFe$_2$As$_2$), 111-material (NaFeAs) and 11-material (FeSe) have opened a new field to study the high temperature superconductivity. These superconductors motivated research on two-band superconductors where the pairing between electrons is produced by inter band electron-electron repulsion [3–6]. The development of sensible microscopic models is the first step towards the elucidation of the normal state and superconducting properties of the FeSCs. The effective low-energy model may be the starting point to study the main properties of the electronic states near the Fermi level as well as their interactions[7]. The models defined in the orbital basis provide qualitative insight into the role of the orbital degrees of freedom which analyse superconductivity and other instabilities without restricting to the Fermi surfaces. These models do not go beyond mean-field and do not distinguish between high and low energies. The models which are defined in the basis of bands, they use geometry of Fermi surfaces to capture low energy physics and allow one to go beyond mean-field and investigate the interplay between magnetism and superconductivity. The drawback of these models is that, they cannot capture orbital dependent features like spontaneous orbital order.

The Fermi surface is not confined to the gaps of different pairings though the pairing in the FeSCs is a strong coupling phenomenon [8]. The observed superconducting (SC) gap in any band is not able to pass through the Fermi surface which is being interpreted by the pairing mechanism. In the Fermi surface the SC gap for FeSCs may indicate the gap symmetry for different materials [3, 9–13]. The gap symmetry in FeSCs is like $s\pm$-wave which have both electron and hole pockets [4, 5, 14]. The long range antiferromagnetic order has been observed along with the tetragonal to orthorhombic lattice distortion in the parent compounds of FeSCs [1, 15, 16]. This phenomenon prompted us to propose
such a model for the coexistence of the SC, AFM and Jahn-Teller (JT) distortion. The rest of the paper is presented as the theoretical model in section 2, section 3 contains the necessary calculations for the three order parameters, the results so obtained are discussed in section 4 and finally concluded in section 5.

2. Theoretical Model

A tight-binding model Hamiltonian is considered for the coexistence of the SC, AFM and JT distortion with nearest neighbour hopping in the $s^\pm$-wave symmetry. The Fe lattice is divided into two sub-lattices due to AFM spin alignment and the hopping of conduction electrons takes place between two degenerate Fe$^\pm$-orbitals. This is described by the Hamiltonian $H_0$ as

$$H_0 = \sum_{\alpha} \epsilon_{\alpha, i, k, \sigma} c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} + H.c.$$  

where $\alpha$ represents $1$ and $2$ are the two JT distorted orbitals with momentum $k$ and spin $\sigma$. The conduction electron creation (annihilation) operators are $c_{i,\alpha, k, \sigma}^\dagger$ and $c_{i,\alpha, k, \sigma}$ with the square lattice nearest neighbour tight-binding hopping in the form $\epsilon_{\alpha, i, k} = -t_0 (\cos k_x + \cos k_y)$ where $t_0$ is the hopping integral.

The sub-lattice magnetisation is produced in the neighbouring sites due to the Heisenberg exchange interaction between the magnetic moments. In this scenario the mean field AFM Hamiltonian for the sub-lattice magnetisation can be written as

$$H_{AFM} = \frac{h}{2} \sum_{\alpha, \sigma} \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} - c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right]$$

Here, $s = \pm 1$ is the spin index and it is $+1$ for up and $-1$ for down spins respectively. The AFM order parameter $h$ is described as

$$h = \frac{1}{2} g_L \mu_B \sum_{\alpha, \sigma} \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} - c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right]$$

The $t_2g$ degenerate orbitals $3d_{xz}$ and $3d_{yz}$ are responsible for the JT distortion in the lattice. The single degenerate band splits into two bands as $\epsilon_{\alpha, i, j}(k) = \epsilon(k) + Ge$. We have considered here the static lattice strain by $e$ and the electron-lattice interaction strength as $G$. The mean field JT Hamiltonian is defined as

$$H_{JT} = -Ge \sum_{\alpha} \frac{(-1)^{\alpha}}{2} \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} + c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right] + H.c.$$

and the corresponding lattice strain $e$ is defined as

$$e = \left( \frac{G}{C_0} \right) \sum_{\alpha} \frac{(-1)^{\alpha}}{2} \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} + c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right].$$

In this expression the elastic energy is represented as $1/2C_0e^2$ with the elastic constant $C_0$.

The mean-field SC pairing Hamiltonian is written as

$$H_{SC} = -\sum_{\alpha} \Delta_k \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} + c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right] + H.c.$$

The SC gap parameter for $s^\pm$-wave symmetry will be $\Delta_k = \Delta(T)\cos k_x \times \cos k_y$. This SC gap parameter $\Delta_k$ is momentum dependent and is defined as

$$\Delta_k = -\sum_{\alpha, \sigma} \tilde{V}(k-k') \left[ c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} + c_{i,\alpha, k, \sigma}^\dagger c_{i,\alpha, k, \sigma} \right] + H.c.$$

here the SC exchange interaction is $\tilde{V}$ and is expressed as $\tilde{V}(k-k') = -V_{eff}f_k$ with $f_k = \cos k_x \times \cos k_y$. The pairing form factor for $s^\pm$-wave symmetry is considered as $\cos k_x \times \cos k_y$. However, it is important...
to realize that the s±-wave gap function is not synonymous to cosk_x.cosk_y. The system is described by the total Hamiltonian as

\[ H = H_0 + H_{\text{AFM}} + H_{J'F} + H_{SC}. \]  

\( \cdots (8) \)

3. Calculation of order parameters

We have adopted the double-time single particle Green’s function method for the calculation of order parameters [17] involved in the Hamiltonian in eqn.(8). The Green’s functions are defined separately for \( i \) and \( j \) sites as follows:

\[ \omega_{i}^{\sigma \alpha, \sigma \alpha} = \begin{cases} \omega_{i}^{\sigma \alpha, \sigma \alpha} & \text{for } i = 1, 2, 3, 4; \\ \omega_{i}^{\sigma \alpha, \sigma \alpha} & \text{for } j = 1, 2, 3, 4. \end{cases} \]

These coupled Green’s functions are solved for quasi particle energy bands \( \omega_i \) (\( i = 1 \sim 4 \)) given by

\[ \frac{\omega_1}{2} = -\frac{S_1 + \sqrt{S_1^2 - 4T_1}}{2} \quad ; \quad \frac{\omega_2}{2} = -\frac{S_1 - \sqrt{S_1^2 - 4T_1}}{2} \]

\[ \frac{\omega_3}{2} = -\frac{S_2 + \sqrt{S_2^2 - 4T_2}}{2} \quad ; \quad \frac{\omega_4}{2} = -\frac{S_2 - \sqrt{S_2^2 - 4T_2}}{2} \]  

\( \cdots (9) \)

with \( S_1 = 2(E_1^2 + 2\epsilon_k^2), \quad S_2 = 2(E_2^2 + 2\epsilon_k^2), \quad T_1 = E_1^2 + 4\epsilon_k^2(h/2 + \Delta_k) \) and \( T_2 = E_2^2 + 4\epsilon_k^2(h/2 - \Delta_k) \). Here, \( E_1^2 = (h/2 \pm \Delta_k)^2 + (Ge)^2 \) with \( \omega_i = \omega_i(Ge, h, \Delta_k) \), which shows that all the gap parameters interfere with each other.

The antiferromagnetic gap parameter defined in eqn.(3) is calculated to be

\[ \hbar = \frac{8\Delta H_B}{4} \sum_k [\frac{1}{\omega_1^2 - \omega_2^2} \{F_1(k, T) - F_2(k, T)\} + \frac{1}{\omega_3^2 - \omega_4^2} \{F_3(k, T) - F_4(k, T)\}] \]  

\( \cdots (10) \)

Where

\[ F_{1,2}(k, T) = \frac{h}{\omega_{1,2}} + \Delta_k \left[ \omega_{1,2}^2 - E_1^2 - 2\epsilon_k^2 \right] \tanh \left( \frac{\beta \omega_{1,2}}{2} \right) \]

\[ F_{3,4}(k, T) = \frac{h}{\omega_{3,4}} - \Delta_k \left[ \omega_{3,4}^2 - E_2^2 - 2\epsilon_k^2 \right] \tanh \left( \frac{\beta \omega_{3,4}}{2} \right) \]

The free energy expression in its standard form is written as

\[ F = -k_B T \sum_{k,i} \ln[1 + \exp(-\beta \omega_i(k))], \]  

\( \cdots (11) \)

with \( \beta = 1/k_BT, \ k_B \) and \( T \) mentioned in the above expression are the Boltzmann constant and the absolute temperature respectively. We have considered \( \hbar = k_B = \hbar \) throughout the calculation. The self-consistent expression for lattice strain \( e \) can be obtained from the minimisation of the above equation. Hence the eqn.(5) now can written as

\[ e = -\frac{Ge}{2C_0} \sum_k \left[ -\frac{1}{\omega_1^2 - \omega_2^2} \{F_1(k, T) - F_2(k, T)\} + \frac{1}{\omega_3^2 - \omega_4^2} \{F_3(k, T) - F_4(k, T)\} \right] \]  

\( \cdots (12) \)

Where

\[ F_{5,6}(k, T) = \frac{1}{\omega_{1,2}} \left( \omega_{1,2}^2 - E_1^2 \right) \tanh \left( \frac{\beta \omega_{1,2}}{2} \right) \]

\[ \cdots \]
The SC gap parameter defined in eqn.(7) can be obtained from the Green’s functions $A_2(k, \omega)$ and $B_2(k, \omega)$ as

$$
\Delta_k = -\frac{1}{2} \sum \left[ \tilde{V}(k-k') \left\{ \frac{1}{\omega_1^2 - \omega_2^2} \left[ F_9(k, T) - F_{10}(k, T) \right] - \frac{1}{\omega_3^2 - \omega_4^2} \left[ F_{11}(k, T) - F_{12}(k, T) \right] \right\} \right] \ldots(13)
$$

where

$$F_{9,10}(k, T) = \frac{1}{\omega_{1,2}} \left( \frac{\hbar}{2} + \Delta_k \right) \left( \omega_{1,2}^2 - E_i^2 - 2\epsilon_i^2 \right) \tanh \left( \frac{\beta \omega_{1,2}}{2} \right),$$

$$F_{11,12}(k, T) = \frac{1}{\omega_{3,4}} \left( \frac{\hbar}{2} - \Delta_k \right) \left( \omega_{3,4}^2 - E_i^2 - 2\epsilon_i^2 \right) \tanh \left( \frac{\beta \omega_{3,4}}{2} \right).$$

In the above eqns.(10), (12) and (13) the $k$-sum takes the form of double integration in the $a-b$ plane for the variables $k_x$ and $k_y$. The summation $\int \int dk_x dk_y$ is FeAs plane where $S$ is the area of the square lattice and $N(0)$ is the conduction electron density of states around Fermi surface.

4. Results and Discussion

4.1. Coexistence of order parameters

The coupled equations (10), (12) and (13) for the AFM gap ($h$), the JT gap ($e'=g_1\times e$) and the SC gap ($z$) respectively are solved self-consistently numerically. We have considered the half-filling band situation with the Fermi level as zero ($\epsilon_F = 0$) to be lying at the middle of the AFM band gap and the width of the conduction band $W=t_0$ ($\sim$1eV). All the parameters involved in the gap equations are scaled by the conduction band width $W$. So, the dimensionless parameters are the SC gap $z=\Delta(T)/W$, the AFM gap $h_1=h/W$, the lattice strain $e=e/W$, the reduced temperature $t=k_BT/W$, the SC coupling constant $g=N(0)V_0$, the JT coupling constant $g_1=GN(0)/W$ and the AFM coupling constant $g_2=g_2\mu_B N(0)/W$. Figure 1 shows the plots of the three order parameters in the independent and coexistence states. In the coexistence state the critical temperatures of the order parameters are in the order of $t_d>t_N>t_c$, where $t_d$ is the JT distortion temperature, $t_N$ is the Ne’el temperature and $t_c$ is the SC transition temperature. In the coexistence state the SC order parameter is suppressed throughout the temperature range with respect to its independent state with the decrease of the transition temperature $t_c$ from 0.0195 to 0.0125. Due to this the reduced SC gap value $2\Delta(0)/k_BT_c = 5.53$ in the independent state is decreased to 2.72 in the coexistence state. For the multi-orbital FeSCs the reduced SC gap value $2\Delta(0)/k_BT_c$ is very high as compared to the universal BCS value of 3.52 which is an essential property of the FeSCs. The AFM order parameter is suppressed in the coexistence of the order parameters with enhancement of its Ne’el temperature $t_N$. But the JT transition temperature $t_d$ is not changed due to coexistence; however, the gap value is suppressed for the temperature range less than $t_c$ and shows mean-field behavior beyond $t_c$.  

$$F_{3,8}(k, T) = \frac{1}{\omega_{3,4}} \left( \omega_{3,4}^2 - E_i^2 \right) \tanh \left( \frac{\beta \omega_{3,4}}{2} \right).$$
Figure 1: (Colour online) The plots of SC gap $z$, the JT gap $e'$ and the AFM gap $h$ in the independent and coexistence states vs reduced temperature $t$ for fixed values of SC coupling $g=0.3$, the JT coupling $g_1=1.2$ and the AFM coupling $g_2=1.0$.

Figure 2: (Colour online) The plots of SC gap $z$, the JT gap $e'$ and the AFM gap $h$ in the independent and coexistence states vs reduced temperature $t$ for fixed values of SC coupling $g=0.32$, the JT coupling $g_1=1.4$ and the AFM coupling $g_2=2.2$.

Figure 2 shows the plots of the three order parameters for the situation in which their critical temperatures are in the order of $t_N>t_d>t_c$ in the independent state. Both the AFM and JT order parameters suppressed throughout the temperature range in the coexistence state. The rate of suppression of the AFM order parameter is so high that, the Ne‘el temperature $t_N$ goes so smaller to the JT transition temperature $t_d$. The SC gap parameter is suppressed towards the lower temperatures with an enhancement of the $t_c$ from 0.021 to 0.038. So, the reduced SC gap value $2\Delta(0)/k_BT_c=5.52$ in the independent state is also decreased in the coexistence state to 1.59.

4.2. Energy bands

The electronic origin of pairing interaction in FeSCs are suggested by their electronic structure and high transition temperature properties. The superconductivity in iron based superconductors is associated with the density of states near Fermi level which gets its maximum contribution from Fe3d-orbitals and Fe layers. The energy bands for the system in the proposed model is described in equation (9). Figures 3 and 4 shows the plots these energy bands and the dispersion $\varepsilon_k$ vs $k_x$ for $k_y=\pi$ in both the cases $t_d>t_c>t_N$ and $t_c>t_d>t_N$ respectively for the coexistence state with the corresponding SC gap, JT gap and the AFM gap values at the zero temperature i.e., $t=0$. These figures show that there is a strong interference of all the three gap parameters. At the saddle point ($k_x=0$) the energy bands are pushed away from it and the gap value from the Fermi level is equivalent to the interference value of these gap parameters.
Figure 3: (Colour online) Plots of $\omega_i$ vs $k_x$ for $k_y = \pi$ using parameters from figure 1 for $z = 0.017$, $e' = 0.040$ and $h_1 = 0.028$.

Figure 4: (Colour online) Plots of $\omega_i$ vs $k_x$ for $k_y = \pi$ using parameters from figure 2 for $z = 0.030$, $e' = 0.092$ and $h_1 = 0.036$.

5. Conclusions

The interplay of three long range orders i.e., superconductivity, Jahn-Teller distortion and antiferromagnetic orders, present in FeSCs are discussed in this communication. In the phase diagram of iron pnictide superconductors display the coexistence of the interplay of SC, AFM and structural orders. Many people have been studied the coexistence of other order parameters with superconductivity for these materials. In the coexistence phase the interplay shows strong dependence of one another in this study. The superconductivity along with its transition temperature is suppressed in the interplay region for the case of $t_d > t_N > t_c$ and the transition temperature for superconductivity is enhanced with a suppression of the SC gap value for the case of $t_c > t_N > t_d$. The AFM order ($h$) is suppressed in the first case with increase of the $t_N$ and in the second case it is suppressed throughout the temperature region. The distortion temperature $t_d$ is not changed for its higher value than the others with a suppression in the coexistence region, however it is suppressed throughout the temperature range for the second case. The lattice strain energy is being arrested at $t_c$, as observed for different high-Tc superconductors, which can be observed here in presence of the AFM order. The coexistence of superconductivity with JT distortion and AFM order has been studies separately for FeSCs in presence of external magnetic field and reported [18, 19].

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