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Band energies in tow-band model for FeSCs in the coexistence state

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Abstract. The gap structure and pairing mechanism for iron based superconductors is hotly discussed as a central issue since their discovery. The energy band structure of iron based superconductors is calculated by a tight-binding two band model with the coexistence of superconductivity and Jahn-Teller distortion. We have proposed here a $s^{\pm}$-wave pairing symmetry of the form $cosk_x \times cosk_y$ in a two-band model for the coexistence of the two order parameters in the mean field approximation. The model is solved by Zubarev's double-time Green's function technique to find their selfconsistent gap equations and are solved self-consistently numerically. The band energies are discussed.

Keywords: Iron based superconductors; Superconducting gap; Jahn-Teller effect; Band energies.

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1 Introduction

The discovery of iron-based superconductors (FeSCs) with different chemical compositions [1], such as 1111-material (*LaFeAsO*), 122-material ($BaFe_2As_2$), 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 interband electronelectron repulsion [2, 3]. The pairing in the FeSCs is a strong coupling phenomenon and the pairing gap is not confined to the Fermi surface. This phenomenon was interpreted [4] on the observation of a sizeable superconducting gap on a band which does not cross the Fermi level. For the

FeSCs, different materials have different structures of the superconducting (SC) gap which may indicate that the gap symmetry in FeSCs is material dependent [2, 5, 6]. Both hole and electron pockets are observed in doped FeSCs and the gap symmetry there is like the $s^{\pm}$-wave state [3]. The theoretical model is described in section 2, the calculation of electron Green's functions which relate the order parameters of the SC and the Jahn-Teller(JT) distortion are in section 3. The discussions of the results obtained are described in section 4 and concluded in section 5.

2 Theoretical Model

The assumption of the crystal field splitting and the orbital hopping effect considers the $3d_{xz}$ and $3d_{yz}$ orbitals of Fe for low energy physics discussions [7]. Here we have considered a model Hamiltonian for the coexistence of SC and JT interactions in the $s^{\pm}$-wave symmetry and solved selfconsistently. The hopping of the conduction electrons between the neighbouring sites of the two degenerate orbits of Fe^{2+} is described by the Hamiltonian H_0 as

$$H_0 = \sum_{\alpha,k,\sigma} \varepsilon_k \left[(c^{\dagger}_{i,\alpha,k,\sigma} c^{\dagger}_{j,\alpha,k,\sigma} + c^{\dagger}_{i,\alpha,k,\sigma} c_{j,\alpha',k,\sigma}) + H.c. \right]. \quad (1)$$

Here, $c^{\dagger}_{i,\alpha,k,\sigma}(c_{i,\alpha,k,\sigma})$ and $c^{\dagger}_{j,\alpha,k,\sigma}(c_{j,\alpha,k,\sigma})$ are creation (annihilation) operators of the conduction electrons of iron ions at two neighbouring sites *i* and *j* and two JT distorted orbitals α = 1 and 2 respectively, with momentum *k* and spin σ. We assume a simple nearest-neighbour hopping tight-binding form $\varepsilon_k = -2t_0(\cos k_x + \cos k_y)$ on a square lattice, where t0 is the hopping integral.

The lattice distortion via JT effect [8, 9] may be from the degeneracy of $3d_{xz}$ and $3d_{yz}$. The structural transition from tetragonal to orthorhombic distortion is exhibited by the iron pnictide superconductors. This is described by a two level configurational distortion at each distorted tetrahedron where the Fe ion exists. The population difference between the two bands is observed in the degenerate conduction band due to the presence of the tetragonal distortion. The lattice strain splits the single degenerate band into two band energies $\varepsilon_{1,2}(k) = \varepsilon_k \pm Ge$ with the increase of the population difference. Here, the strength of the electron-lattice interaction is denoted by *G* and the strength of the static lattice strain by *e*. Now the JT Hamiltonian is described as

$$H_{JT} = -Ge\sum_{\alpha,k,\sigma}(-1)^{\alpha}\left[(c^{\dagger}_{i,\alpha,k,\sigma}c_{j,\alpha,k,\sigma}) + H.c. + \frac{1}{2}C_0e^2\right], \quad (2)$$

where the lattice strain *e* is defined as

$$e = \left(\frac{G}{C_0}\right)\sum_{\alpha,k,\sigma}(-1)^{\alpha}\left[\langle c^{\dagger}_{i,\alpha,k,\sigma}c_{j,\alpha,k,\sigma}\rangle + \langle c^{\dagger}_{j,\alpha,k,\sigma}c_{i,\alpha,k,\sigma}\rangle\right]. \quad (3)$$

Here, $\frac{1}{2}C_0e^2$ represents the elastic energy of the system with C_0 being the elastic constant. Under the condition that the gain in electronic energy is more than the elastic energy $\frac{1}{2}C_0e^2$ then the strain is stabilised.

The superconductivity comes from Cooper pairs in the Fe-Fe plane. Here, the superconductivity is introduced to the system through the BCS pairing interaction, which is assumed to be existing only within the same orbitals and the same strength of the interactions. So the mean-field pairing Hamiltonian is written as

$$H_{SC} = -\sum_{\alpha,k}\Delta_k\left[(c^{\dagger}_{i,\alpha,k,\uparrow}c^{\dagger}_{i,\alpha,-k,\downarrow} + c^{\dagger}_{j,\alpha,k,\uparrow}c^{\dagger}_{j,\alpha,k,\uparrow}c^{\dagger}_{j,\alpha,-k,\downarrow}) + H.c.\right], \quad (4)$$

where α=1, 2. For $s^{\pm}$-wave symmetry the SC gap parameter will be $\Delta_k = \Delta(T)\cos k_x \times \cos k_y$. Now, the momentum dependent superconducting gap parameter Δ_k is defined as

$$\Delta_k = -\sum_{\alpha,k,k'}\tilde{V}(k-k')(\langle c^{\dagger}_{i,\alpha,k',\uparrow}c^{\dagger}_{i,\alpha,-k',\downarrow}\rangle + \langle c^{\dagger}_{j,\alpha,k',\uparrow}c^{\dagger}_{j,\alpha,-k',\downarrow}\rangle), \quad (5)$$

here $\tilde{V}$ is the effective exchange interactions [10] of the SC order parameter and is expressed as $\tilde{V}\ (k-k') = -V_0f_kf_{k'}$ with $(cosk_x \times cosk_y)$. Here, we consider the $s^{\pm}$-wave pairing form factor as $cosk_x \times cosk_y$. Now, the total Hamiltonian describing the system is given by

$$H = H_0 + H_{JT} + H_{SC}. \quad (6)$$

3. Calculation of order parameters

The Zubarev's single particle double-time Green's function technique [11] is being used to calculate the Green's functions for the Hamiltonian in eqn.(6). For site *i* the Green's functions are defined as

$$A_1(k,\omega)=\langle\langle c_{i,\alpha,k,\sigma}; c^{\dagger}_{i,\alpha,k,\sigma}\rangle\rangle_{\omega}\ ;\ A_2(k,\omega)=\langle\langle c^{\dagger}_{i,\alpha,-k,\sigma'}; c^{\dagger}_{i,\alpha,k,\sigma}\rangle\rangle_{\omega}$$

$$A_3(k,\omega)=\langle\langle c_{j,\alpha,k,\sigma}; c^{\dagger}_{i,\alpha,k,\sigma}\rangle\rangle_{\omega}\ ;\ A_4(k,\omega)=\langle\langle c^{\dagger}_{j,\alpha,-k,\sigma'}; c^{\dagger}_{i,\alpha,k,\sigma}\rangle\rangle_{\omega}.$$

The Green's functions for site *j* are defined as

$$B_1(k,\omega)=\langle\langle c_{j,\alpha,k,\sigma}; c^{\dagger}_{j,\alpha,k,\sigma}\rangle\rangle_{\omega}\ ;\ B_2(k,\omega)=\langle\langle c^{\dagger}_{j,\alpha,-k,\sigma'}; c^{\dagger}_{j,\alpha,k,\sigma}\rangle\rangle_{\omega}$$

$$B_3(k,\omega)=\langle\langle c_{i,\alpha,k,\sigma}; c^{\dagger}_{j,\alpha,k,\sigma}\rangle\rangle_{\omega}\ ;\ B_4(k,\omega)=\langle\langle c^{\dagger}_{i,\alpha,-k,\sigma'}; c^{\dagger}_{j,\alpha,k,\sigma}\rangle\rangle_{\omega}.$$

The solution of these Green's functions gives us two quasi particle energy bands $\omega_i(i=1,2)$ calculated to be

$$\omega_1=\pm\sqrt{E_{1k}^2+\Delta_k^2}\ ;\ \omega_2=\pm\sqrt{E_{2k}^2+\Delta_k^2}\,. \tag{7}$$

Here, $E_{1,2k}=\varepsilon_k\pm Ge$ and we have $\omega_i=\omega_i(Ge,\Delta_k)$ i.e., there is the interference of the two gap parameters. The expression for free energy is the standard for the coexistence state of SC and JT phase which is written as $F=-k_BT\sum_{k,i}\ln[1+\exp\{-\beta\omega_i(k)\}]$, with $\beta=\frac{1}{K_BT}$, k_B and T are the Boltzmann constant and the absolute temperature respectively. Here, throughout the calculations, we have considered $\hbar=k_B=1$.. The minimisation of the above equation with respect to $\frac{\partial F}{\partial e}=0$ e i.e, gives the selfconsistent gap equation for strain e. The eqn.(3) comes from such kind of minimisation which is written as

$$e=-\frac{Ge}{2C_0}\sum_k\left[\frac{1}{\omega_1^2-\omega_2^2}\{F_1(k,T)-F_2(k,T)\}\right] \tag{8}$$

where

$$F_{1,2}(k,T)=\frac{1}{\omega_{1,2}}\left(\omega_{1,2}^2-E_{1,2}^2\right)\tan h\frac{\beta\omega_{1,2}}{2}.$$

The Green's functions $A_2(k,\omega)$ and $B_2(k,\omega)$ define the SC gap parameter of eqn.(5) as

$$\Delta_k=-\frac{1}{2}\sum_k\left[\tilde{V}(k,k')\frac{1}{\omega_1^2-\omega_2^2}\left\{F_3(k,T)-F_4(k,T)\right\}\right] \tag{9}$$

where

$$F_{3,4}(k,T)=\frac{1}{\omega_{1,2}}\left(h/2+\Delta\right)\left(\omega_{1,2}^2-E_{1,2}^2-2\varepsilon_0^2\right)\tan h\frac{\beta\omega_{1,2}}{2}\,.$$

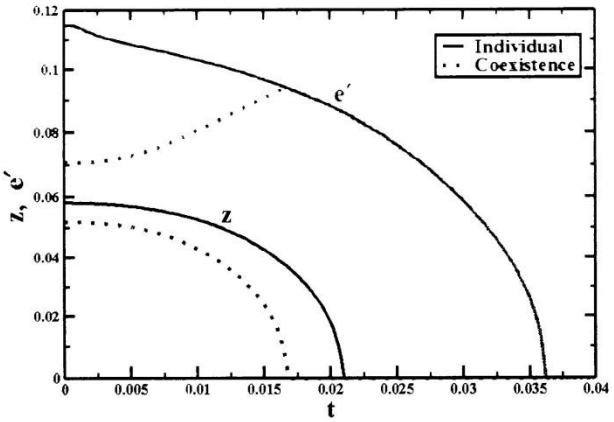

Fig. 1: The individual and selfconsistent plots of the SC gap z and lattice strain energy e′ *v*s reduced temperature *t* for fixed values of SC coupling g = 0.32 and the JT coupling g_1 = 1.42.

The *k*-sum involved in eqns.(8) and (9) is converted into integral form which leads to double integrals for k_x and k_y variables in $a-b$ plane. The summation $\sum_k = N(0)\frac{S}{(2\pi)^2}\int\int dk_x dk_y$ in *FeAs* plane with appropriate limits of integration and *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

The coupled equations (8) and (9) for the 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 to be lying at the middle of the band gap and the width of the conduction band $W = 8t_0 (\simeq 1eV)$. All the parameters involved in the gap equations are scaled by the conduction band width *W*. So, the dimensionless parameters are the SC gap $z = \frac{\Delta(T)}{2t_0}$, the lattice strain $e = \frac{e}{e_0}$, the reduced temperature $t = \frac{k_B T}{2t_0}$, the SC coupling constant $g = N(0)\,V_0$

and the JT coupling constant $g_1 = \frac{GN(0)}{2t_0}$. Figure 1 shows the plots of the two order parameters in the independent and coexistence states. In the independent state both the order parameters show mean-field behaviour and the reduced SC gap is calculated to be $\frac{2\Delta(0)}{k_B T_c} = 5.52,$ which very high as compared to BCS universal value of 3.52. For the multi-orbital FeSCs the reduced SC gap value $\frac{2\Delta(0)}{k_B T_c}$ is very high as compared to the universal BCS value of 3.52 [12, 13] which is an essential property of the FeSCs. In the coexistence state the JT order parameter is suppressed within the SC critical temperature t_c and shows mean-field behaviour beyond that without changing its distortion temperature t_d. The SC order is suppressed throughout the temperature range with the decrease of t_c. The reduced SC gap value $\frac{2\Delta(0)}{k_B T_c}$ is enhanced to 6.11, because of the more decrease of t_c.

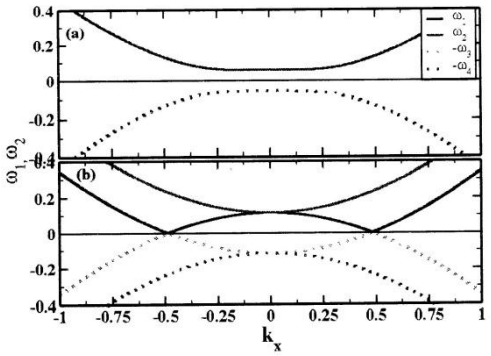

Fig. 2: Plots of energy bands and the bare dispersion ε_k vs k_x for $k_y = \pi$ in the independent state using parameters from figure 1 for (a) z = 0.058, e' = 0 and (b) z = 0, e′ = 0.115.

The electronic structure and the high transition temperatures of the FeSCs suggest that the pairing interaction is of electronic origin. The band structure calculations have shown that, superconductivity in FeSCs is associated with the *Fe* layer [14, 15] and that the density of states near the Fermi level gets its maximum contribution from the *Fe*-3*d* orbitals. Equation (7) describes the two energy bands for the system. Figure 2 show the plots of energy bands and bare dispersion in the independent states. In figure 2(a) the energy bands show a gap equivalent to the SC gap (z = 0.058) and in figure 2(b) the same gap is equivalent to the JT gap (e' = 0.115) at the Fermi surface. Figure 3 shows the plots of energy bands and bare dispersion in the coexistence state. In this plot we have two gaps

identified as I and II. The gap I at the k_x = 0 is equivalent to 0.088, which corresponds to the value of $\sqrt{z^2+e'^2}$ and the gap II is equivalent to 0.048, which corresponds to the value of $\sqrt{z^2+e'^2}$, which means that there is the interference of the two order parameters in the coexistence state.

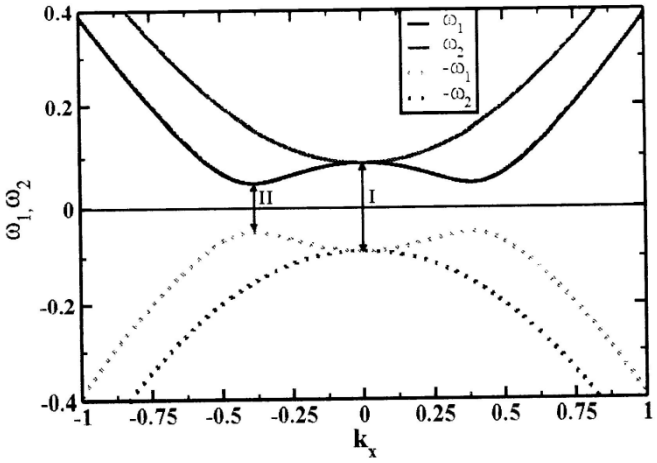

Fig. 3: Plots of energy bands and the bare dispersion ε_k vs k_x for $k_y = \pi$ in the coexistence state using parameters from figure 1 for z = 0.052 and e' = 0.071.

5 Conclusion

In this communication, we have discussed the interplay of two orders parameters i.e., SC and JT orders present in the iron pnictide systems. The interplay shows that there is a strong dependence of one another in the coexistence phase. The SC order parameter (z) is suppressed throughout the temperature range in the interplay region. As shown in different high-T_c superconductors, it is observed that the growth of lattice strain energy is arrested at t_c. The superconducting transition is decreased more compared to the suppression of the SC gap at the zero temperature, resulting in the increase of the reduced SC gap parameter $\frac{2\Delta(0)}{k_B T_c}$. The band energy plots shows the clear existence of the SC gap the JT gap in the independent state and the interference of the two in the coexistence state.

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