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# A Tight Binding two Band Study of Tunneling Conductance in Jahn-Teller Distorted iron based Superconductors

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**Abstract.** All the five d-electrons of iron based oxypnictide superconductor of compound MFeAsO (M = La, Ce, Sm, Nd) play an important role in the density of states (DOS) of the system. However the $d_{xz}$ and $d_{yz}$ orbitals contribute significantly to the electron density of the system near the Fermi level. Hence, a two band model is expected to explain correctly the electron properties of the system. We have adopted this two band model to investigate the tunneling conductance of the iron based system. Apart from nearest and next-nearest-neighbor electron hopping integrals, the model includes the Jahn- Teller (JT) type isotropic strain. The Hamiltonian is solved by using Zubarev's Green's function technique. Finally the tunneling conductance which is proportional to the electron density of states is calculated from the imaginary part of the electron Green's functions. The DOS is computed numerically by varying the physical parameters like JT coupling, elastic constant, temperature and chemical potential. The results are discussed in the paper.

**Keywords:** Iron-based superconductors, Jahn-Teller effect, scanning tunneling microscopy.

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## 1. Introduction

The discovery of high $T_C$ superconductivity in iron-based compounds has marked a turning point in the study of non-copper based superconductors [1]. The 1111 class (RFeAsO, R = La, Nd, Gd, Sm) and the 122 class ($AFe_2X_2$, with A = K, Na and X = As, P, Te, Se, S) of iron-based superconductors have attracted

immensely for the experimental and theoretical investigations. The scanning tunneling microscopy (STM) measurements on $SmEeAsO_{1-x}F_x$ shows single and double gapped spectra displaying the superconducting pairing symmetry as well as the presence of superconductivity spin density wave (SDW) and lattice distortion [2]. Several reviews report the STM results of Fe–based superconductors [3, 4, 5]. Mohapatra et. al. [6] have reported a tight-binding two band model with Jahn-Teller (JT) distortion in both the bands as well as SDW in both bands to explain the multiple gaps in STM spectra [7, 8, 9]. In the present communications, we propose the same two band model with Jahn-Teller (JT) distortion separating the $d_{xz}$ and $d_{yz}$ bands of iron based oxypnictide superconductors in the normal state of the system and investigate the tunneling conductance by varying the physical parameters of the system.

## 2. Formalism and calculation of Density of states (DOS)

The two band model with the hybridization between the two bands conveniently explains the electron properties of 1111 type like iron based oxypnictide superconductors (for example LaFeAsO). Raghu et. al. and Mohapatra et. al. [10, 6] had used this model to explain the electronic, magnetic and elastic properties of these systems. In the present work, we have proposed a JT type structural distortion in this system where $d_{xz}$ band is raised by the energy, Ge and $d_{yz}$ band is suppressed by the energy, -Ge where G and e are respectively the JT coupling and isotropic lattice strain. The Hamiltonian is written as,

$$H = \sum_{k,\sigma} E_{kx} d^{+}_{kx\sigma} d_{kx\sigma} + \sum_{k,\sigma} E_{ky} d^{+}_{ky\sigma} d_{ky\sigma} + \sum_{k,\sigma} E_{kxy} (d^{+}_{kx\sigma} d_{ky\sigma} + d^{+}_{ky\sigma} d_{kx\sigma}) \quad (1)$$

where $E_{kx}$ and $E_{ky}$ are the modified dispersion energies of these $d_{xz}$ and $d_y$ bands of the iron ion of this system. These dispersions are given by,

$$\begin{aligned} E_{kx} &= -2t1\cos kx - 2t2\cos ky - 4t3(\cos kx \times \cos ky) \\ E_{ky} &= -2t2\cos kx - 2t1\cos ky - 4t3(\cos kx \times \cos ky) \\ E_{kxy} &= -4t4(\sin kx \ \sin ky) \end{aligned} \quad (2)$$

Here t1, t2, t3 and t4 are electron hoppings of nearest and next-nearest neighbors, next nearest neighbor hopping between similar d – orbitals and next-nearest neighbor hopping between dissimilar d – orbitals of iron ion with μ as the chemical potential.

The tight-binding Hamiltonian given in equation (1) is solved by the Zubarev's Green's function technique [3].The Green's functions A (k, ω) and B (k, ω) associated with the electrons of $d_{xz}$ and $d_{yz}$ orbitals are found to be,

$$\boldsymbol{A(k,\omega) = \langle\langle d_{kx\sigma}\,;\, d^{+}_{kx\sigma}\rangle\rangle_{\omega} = \frac{1}{2\pi}\frac{(\omega - E_{ky})}{|D(\omega)|}}$$

$$\boldsymbol{B(k,\omega) = \langle\langle d_{ky\sigma}\,;\, d^{+}_{ky\sigma}\rangle\rangle_{\omega} = \frac{1}{2\pi}\frac{(\omega - E_{kx})}{|D(\omega)|}} \quad (3)$$

where $\boldsymbol{|D(\omega)| = (\omega - \omega_{1k})(\omega - \omega_{2k})}$ with quasi-particle band energies $\boldsymbol{\omega_{1k}}$ and $\boldsymbol{\omega_{2k}}$ are,

$$\boldsymbol{\omega_{1k}\,,\omega_{2k} = \frac{E_{kx}+E_{ky}}{2} - \mu \pm \sqrt{\left[\left(\frac{E_{kx}-E_{ky}}{2}\right)^{2} + E^{2}_{kxy}\right]}} \quad (4)$$

The lattice strain (e) is calculated by minimizing the electron free energy of this system and is computed self-consistently. Since the electron density of states (DOS) is directly proportional to the conducting spectra observed by the scanning tunneling microscopy (STM), the density of states is calculated from the imaginary part of the Green's function using the formula, $\boldsymbol{DOS = \sum_{k,\sigma}\rho_{k\sigma}(\omega)}$. The spectral density function $\boldsymbol{\rho_{k\sigma}(\omega)}$ is defined as, $\boldsymbol{\rho_{k\sigma}(\omega) = -2\pi\, Im[A(k,\omega) + B(k,\omega)]}$. Finally the spectral density function appears as,

$$\boldsymbol{\rho_{k\sigma}(\omega) = \frac{(2\omega - E_{kx} - E_{ky})Q}{P^{2}+Q^{2}}} \quad (5)$$

where $\boldsymbol{P = (\omega - \omega_{1k})(\omega - \omega_{2k}) - \eta^{2}}$, $\boldsymbol{Q = (2\omega - \omega_{1k} - \omega_{2k})}$ and η is the small spectral width applied to the frequency ω. The dimensionless parameters are the hopping integrals t1 = 1, t2 = 1.3, t3 = -0.85, t4 = -0.85. The conduction band energy c = ω/t1, JT coupling g = G/t1, elastic constant c1= C/t1, chemical potential um = μ/t1, temperature t = $k_B$T/t1 and spectral width e = η/t1.

## 3. Results and Discussion

The temperature dependent Jahn-Teller (JT) gap is computed self-consistently by taking 95×95 grid points of the electron momentum as shown in figure 1. The JT gap is varied by taking different JT couplings i.e, g = 1.38, 1.40, 1.42. For a given JT coupling g = 1.38, the JT gap exhibits mean-field-behavior at low temperatures and gradually decreases towards higher temperatures without showing a sharp structural phase transition due to the effect of hybridization between the two bands. However, the structural transition occurs at the temperature $t_S \approx 0.12$ ($T_S \approx 150$ K for t1≈ 0.125 eV ≈ 1250 K). The JT gap

increases throughout the temperature with the increase of JT coupling. This shows that the separation between the $d_{xz}$ and $d_{yz}$ bands increases with JT coupling resulting in the onset of higher insulating phase due to the presence of JT coupling. The oxypnictide superconductors are bad conductors and bad insulators [15]. The structural transition temperatures for different iron based superconductors are 158 K for LaFeAsO [4], $T_S$ = 175 K for SmFeAsO [5] and $T_S$ = 135 K for GdFeAsO [6]. All the structural transition temperatures lying in the range of 135 K to 175 K can be explained by changing the JT couplings from 1.38 to 1.42.

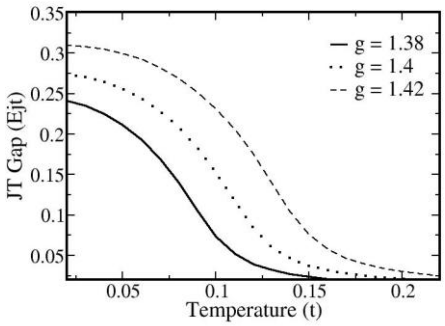


**Figure-1**

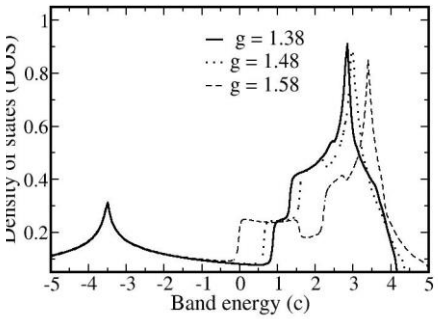


**Figure-2**

**Fig. 1** shows the plot of JT gap (Ejt) vs. temperature (t) for different values of JT couplings g = 1.38, 1.4, 1.42 for fixed values of elastic constant c1 = 1.3 and chemical potential um = 1.4. **Fig. 2** shows the plot of density of states (DOS) vs. band energy (c) for different values of JT couplings g = 1.38, 1.48, 1.58 for fixed values of elastic constant c1 = 1.3, chemical potential um = 1.4 and temperature t = 0.025.

The electron density of states (DOS) or tunneling conductance is computed for the range of band energy (c) by varying JT couplings as shown in figure 2. The DOS exhibits two van – Hove singularities corresponding to the two bands. In other words, the low energy singularity occurs at energy c = -3.5 at the middle of the valence band lying below the Fermi level (c < 0) and the sharply peaked singularity occurring at band energy c = 3 is associated with the conduction band. However, the electron density of states is lower at the Fermi level (c = 0) exhibiting that the iron based oxypnictide systems are bad metals and bad insulators [15]. Further, the DOS in the conduction band shows a sharp jump at the chemical potential um = 1.4 corresponding to electron doping in the system [7]. The increase of JT coupling modifies the DOS in the conduction band rather than the valence band. The van – Hove singularity in the conduction band shifts

to the higher energies with the energy equivalent to JT gap energy i.e, $E_{JT} = 2Ge$. Further, the JT coupling also enhances the electron density of state near the Fermi level. It is to note further that, the sharp jump in DOS at chemical potential shifts to higher energies with the increase of JT coupling indicating that the chemical potential shifts to higher energies showing that the electron doping behavior is enhanced with the increase of JT coupling.

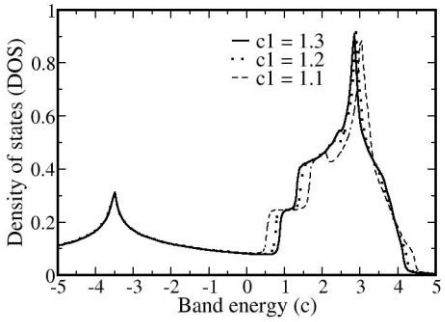


**Figure-3**

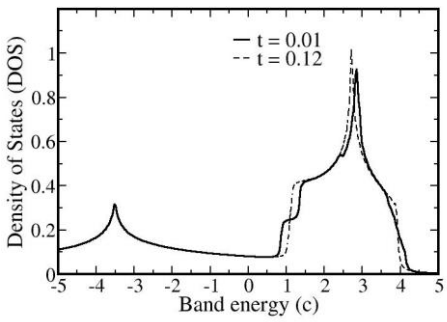


**Figure-4**

**Fig. 3** shows the plot of density of states (DOS) vs. band energy (c) for different elastic constants c1 = 1.3, 1.2, 1.1 for fixed JT couplings g = 1.38, chemical potential um = 1.4 and temperature t = 0.025. **Fig. 4** shows the plot of density of states (DOS) vs. band energy (c) for different temperatures t = 0.01, 0.12 for fixed JT couplings g = 1.38, elastic constant c1 = 1.3, chemical potential um = 1.4.

The effect of elastic constant of this system on tunneling conductance is shown in figure 3. The increase of elastic constant means increase of elastic energy of the system. The increase in elastic energy is compensated by decrease in the electronic energy of the system. It is observed that the elastic constant has no effect on the DOS in the valence band ($c < 0$) which is completely filled with the electrons. However, the elastic constant appreciably modifies the electron density of states in the partially filled conduction band. The van – Hove singularity in the conduction band shifts to higher energies with the decrease of elastic constant equivalent to the elastic energy i.e, $1/2c1e^2$. However, the elastic constant has very small effect on DOS near the Fermi level ($c = 0$).

The effect of temperature on the DOS is shown in figure 4. The DOS plotted at two different temperatures i.e, at lower temperature t = 0.01 and at higher temperature t = 0.12 near structural phase transition temperature. The temperature has no effect on the DOS in the filled valence band. However, the temperature modifies the DOS of the partially filled conduction band laying the above Fermi level ($c > 0$). The van – Hove singularity in the conduction band shifts to lower energies with increase of temperature. There are several experimental reports on

tunneling conductance or DOS on oxypnictide superconductors in superconducting phases only. However, there are a few experimental reports on the tunneling conductance on structurally distorted normal phase of oxypnictide superconductors. It is to note further that Mohapatra et. al. [7, 8] have reported the tight-binding study of the tunneling conductance of 1111 iron based systems taking JT distortion in both the bands and the SDW interactions. More recently, Jena. et. al. have reported role of JT distortion [16] and interplay of JT effect and superconductivity in Fe-based superconductors within one band model approach [17].

## 4. Conclusions

We have reported here a tight-binding two band model with orbitally ordered structural distortion in iron based oxypnictide superconductors. We have calculated tunneling conductance by Green's function technique and computed numerically. The elastic constant and the JT coupling modify the density of states of the partially filled conduction band, while they do not affect the density of states of the completely filled valence band. The van – Hove singularity of the conduction band shifts to higher energies with the increase of the JT coupling and with the decrease of elastic constant.

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