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Co-existence of Spin Density Wave and Jahn-Teller Distortion in Iron Oxypinctide Superconductors : A Two Band Tight-Binding Model Approach

R MOHAPATRA[1] and G C ROUT[2†]

[1]Dept. of Physics, Jhadeswar +3 Science Degree College, Balasore, Odisha , India
[2†]Physics Enclave, 2H-Block-2, Krishna Garden Apartment,Jagamara,Khandagiri,Bhubaneswar, Odisha,751030
†Corresponding author: mail id- gcr@iopb.res.in,

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Abstract: The recently discovered iron based oxypinctide superconductors exhibit an interesting interplay of spin ordering, orbital ordering, superconducting ordering beside stripe phases. These superconductors are bad metals and poor insulators. All the five 3d-electrons of the iron ion contribute substantially to display the physical parameter. We propose here a two band model consisting of the contributions of d_{xz} and d_{yz} orbitals, which lie near the Fermi surface. The model consists of two degenerate bands due to d_{xz} and d_{yz} electronic states with same kinetic energy ε_k , which consists of the contributions up to fourth nearest neighbor. The Jahn-Teller(JT) distortion removes the degeneracy of the conduction band by introducing JT gap of magnitude 2Ge in both the bands. The two orbitals are hybridized with a weak electron momentum dependent energy $\varepsilon_{xy}(\mathbf{k})$. We introduced the mean-field level spin density wave(SDW) gap with same spin gap parameter (Δ_s) , with same nesting wave vector 'Q' in both the orbitals. The four coupled electron Green's functions are derived by using Zubarev's Green's function technique and the quasi-particle bands are calculated. The gap equations for SDW and lattice distortion are calculated from these Green's functions and are solved self consistently. Similarly electron density of states, which is proportional to the tunneling conductance measured by scanning tunneling measurements (STM) is calculated and compared with the experimental data. The gap equations are studying by varying different physical parameters of the system.

Keywords : Iron oxypinctide superconductors, spin density wave interactions, Jahn-Teller distortion.

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1. Introduction

The discovery of superconductivity in Fe-based material initiated enormous research interest in the field of high temperature superconductivity. So far, many families of iron-based superconductors have been discovered [1, 2, 3, 4] with critical temperature 55K in $SmO_{1-x}F_xFeAs$ [5] and 56K in $Gd_{1-x}Th_xFeAsO$[6]. It is widely believed that the superconductivity in these materials based on common planer layers of iron atoms joined by chalcogen and pnictogen anions. The undoped parent compound LaFeAsO shows antiferromagnetic spin density wave(SDW) at T_{SDW} = 137K preceded by a structural distortion from tetragonal to orthorhombic at T_S=155K [7]. Also the other parent oxypnictides like PrFeAsO with T_{SDW} = 135K and T_S=154K[8], CeFeAsO with T_{SDW} = 140K and T_S=155K [9], SmFeAsO with T_{SDW} = 135K and T_S=155K [10] etc. are reported. After doping superconductivity appear with suppression of both transition temperatures. So all these phenomena are closely related to each other and thought to arise from common origin.

The band structure calculations [11,12] have shown that the density of states(DOS) near Fermi level gets its maximum contribution from the Fe-3d orbitals. These 3d orbitals appear to play an essential role in determining the momentum dependence of the spin and orbital fluctuations which appear to mediate an electronic pairing mechanism. Kriiger et al. [13] have emphasized that out of the five 3d orbitals of iron, the d_{xz} and d_{yz} are possible candidates for structural phase transition (SPT). At low temperatures, the degenerate d_{xz} or d_{yz} orbitals splits into two due to lattice strain producing Jahn-Teller (JT) distortion and thereby giving rise to an insulating state in the system.

In this present communication, we consider a minimal two band model (d_{xz}, d_{yz} bands) approach in the presence of next-nearest-neighbor hybridization between d_{xz} and d_{yz} orbitals. Further we have considered similar SDW instabilities in both the bands satisfying the nesting property $\varepsilon(k+Q) = -\varepsilon(k)$ with Jahn-Teller(JT) distortion in both the bands. We attempt to study the interplay of SDW gap, JT energy gap through electron density of states of the system. We present the formalism in section-2, calculation of gap equation and the DOS from electron Green's function in section-3, results and discussion in section-4 and finally conclusion in section-5.

2. Formalism

We have considered here the simple tight-binding two band model proposed by Raghu et. al [14]. To account for Jahn-Teller distortion in the system, for degenerate d_{xz} and d_{yz} orbitals with orbital index α=1, 2, the Hamiltonian appears as

$$H_1 = \sum_{\alpha,k,\sigma} (\varepsilon_{kx} - \mu)^{\alpha} d^{\dagger}_{\alpha,kx,\sigma} d_{\alpha,kx,\sigma} + \sum_{\alpha,k,\sigma} (\varepsilon_{ky} - \mu) d^{\dagger}_{\alpha,ky,\sigma} + d_{\alpha,ky,\sigma}$$

$$+ \sum_{\alpha,k,\sigma} \varepsilon_{kxy} \left(d^{\dagger}_{\alpha,kx,\sigma} d_{\alpha,ky,\sigma} + d^{\dagger}_{\alpha,ky,\sigma} d_{\alpha,kx,\sigma} \right) \quad (1)$$

The first and second term in eq.(1) represents the hopping of the electrons with creation operator $d^{\dagger}_{\alpha kx\sigma}$ ($d^{\dagger}_{\alpha ky\sigma}$) for the d_{xz} and d_{yz} orbitals with electron momentum vector **k** and spin σ and the corresponding band energies ε_{kx} (ε_{ky}). Here μ is chemical potential. The third term represents the hybridization between the d_{xz} and d_{yz} orbitals via the As-p orbitals with the momentum dependent hybridization strength ε_{kxy}. The orbital band dispersions are written as

$$\varepsilon_{kx} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y,$$
$$\varepsilon_{ky} = -2t_2 \cos k_x - 2t_1 \cos k_y - 4t_3 \cos k_x \cos k_y,$$
$$\varepsilon_{kxy} = -4t_4 \sin k_x \sin k_y$$

where, the tight binding parameters, i.e. t_1, t_2, t_3 and t_4 are the respective nearest-neighbor hopping integrals. Here t_1 is the nearest-neighbor hopping integral between σ - orbitals and t_2 is the nearest-neighbor hopping integral between π-orbitals. Further, t_3 represents the second neighbor hopping integral between similar orbitals, while t_4 represents the second neighbor hopping integral between different orbitals. The static JT interaction and the SDW interactions are written as

$$H_2 = -Ge \sum_{\alpha,k,\sigma} (-1)^{\alpha} \left(d^{\dagger}_{\alpha,kx,\sigma} + d_{\alpha,kx,\sigma} + d^{\dagger}_{\alpha,ky,\sigma} + d_{\alpha,ky,\sigma} \right)$$

$$+ \sum_{\alpha,k,\sigma} \Delta_s(k) \left(d^{\dagger}_{\alpha,kx,\sigma} + d_{\alpha,k+Q.x,-\sigma} + d^{\dagger}_{\alpha,ky,\sigma} + d_{\alpha,k+Q.y,-\sigma} \right) + \frac{1}{2} Ce^2 \quad (2)$$

The first term in eq (2) represents the static JT interaction in both the d_{xz} and d_{yz} orbitals. Due to JT distortion the two bands become non-degenerate separated by JT band gap of 2Ge, where G is the isotropic JT coupling constant and e is the temperature dependent lattice strain. The second term represents the spin density wave (SDW) interaction in both the orbitals d_{xz} and d_{yz} with same momentum dependent SDW gap $\Delta_s(\mathbf{k})$. The last term represents the lattice energy with elastic constant C. The total Hamiltonian given in eq(1) and eq(2) is considered for calculation of SDW gap and JT gap.

3. Calculation of gap equation

In order to solve the SDW gap and JT gap, we derive four coupled electron Green's functions for the Hamiltonian given in eqs.(1) and (2) by Zubarev's Green's function technique. The d_{xz} band electron Green's function is found to be

$$A_{1\alpha}(k,\omega) = \langle\langle d_{\alpha,kx,\sigma}, d^{\dagger}_{\alpha,kx,\sigma}\rangle\rangle_{\omega} = \frac{1}{2\pi}\frac{k_{\alpha 1}(\omega)}{|D_{\alpha}(\omega)|} \tag{3}$$

where,

$$k_{\alpha 1}(\omega) = \left(\omega_{\alpha k}^2 - E_{\alpha ky}^2\right)\left(\omega_{\alpha k} + \varepsilon_{\alpha kx}\right) - (\omega_{\alpha k} - \varepsilon_{\alpha ky})\varepsilon_{kxy}^2, E_{\alpha ky}^2 = \varepsilon_{\alpha ky}^2 + \Delta_s^2$$

and $|D_{\alpha}(\omega)|$ appearing in the denominator is a function of dispersions in both bands, JT energy gap and SDW gap and hopping integrals (not given in details). Similar expressions for Green's function ($B_{1\square}(\mathbf{k},\omega)$) are found for d_{yz} band. Equating $|D_{\alpha}(\omega)|=0$, we find the quasi-particle dispersion bands, which are given by

$$\pm\omega_{\alpha 1\mathbf{k}}, \pm\omega_{\alpha 2\mathbf{k}} = \pm\left[\varepsilon_{\alpha}^{2+} + \Delta_s^2 + \varepsilon_{kxy}^2 + \left(\left(\varepsilon_{\alpha}^{2-}\right)^2 + 4\left(E_{\alpha+}\right)^2\varepsilon_{kxy}^2\right)^{1/2}\right]^{1/2}$$

where,

$$E_{\alpha+}^2 = (\varepsilon_{\alpha}^{+})^2 + \Delta_s^2,\ \varepsilon_{\alpha}^{\pm} = 0.5\left(\varepsilon_{\alpha kx} \pm \varepsilon_{\alpha ky}\right),\ \varepsilon_{\alpha}^{2\pm} = 0.5\left(\varepsilon_{\alpha kx}^2 \pm \varepsilon_{\alpha ky}^2\right)$$

$$\varepsilon_{akx} = \varepsilon_{kx} - \mu - (-1)^{\alpha} Ge,\ \varepsilon_{\alpha ky} = \varepsilon_{ky} - \mu - (-1)^{\alpha} Ge$$

Minimizing the free energy of the system, we calculate the lattice strain '*e*' in terms of correlation functions, which is written as

$$e = \frac{G}{2C}\sum_{\alpha,k,\sigma}(-1)^{\alpha}\left[\left\langle d_{\alpha,kx,\sigma}^{\dagger} d_{a,kx,\sigma}\right\rangle + \left\langle d_{\alpha,ky,\sigma}^{\dagger} d_{\alpha,ky,\sigma}\right\rangle\right] \tag{4}$$

The SDW gap parameter is defined as

$$\Delta_s(\boldsymbol{k}) = \sum_{\boldsymbol{k},\sigma} V(\boldsymbol{k})[< d^{\dagger}_{\alpha,kx,\sigma} d_{\alpha,k+Q,x,-\sigma} > + < d^{\dagger}_{\alpha,ky,\sigma} d_{\alpha,k+Q,y,-\sigma} > \tag{5}$$

The electron density of states (DOS), which is proportional to tunneling conductance spectra measured by scanning tunneling microscopy (STM), is found from the imaginary part of the electron Green's functions. The DOS for the system is defined as

$$DOS = -2\pi \sum_{\alpha} \sum_{k,\sigma} \mathrm{Im}\left[A_{1\alpha}(\mathbf{k},\omega) + B_{1\alpha}(\mathbf{k},\omega)\right] \tag{6}$$

The lattice strain and SDW gap are solved self-consistently and numerically and hence DOS is computed. The dimensionless parameters involved in the calculation are made dimensionless with respect to nearest neighbour hopping integral parameter t_1. The tight-binding parameters are $t_1 = -1$, $t_2 = 1.3$, $t_3 = -0.85$, $t_4 = -0.85$. Here hopping integral t_1 is taken as 0.125eV≃1250K. The scaled parameters are SDW coupling $g_1 = g_1\mu_B/t_1$, the SDW gap $z_1 = \Delta_S/t_1$, JT coupling $g_2 = G/t_1$, the spectral width $e_1=\eta/t_1$, elastic constant $c_1 = C/t_1$, reduced band energy $c = \omega/t_1$ and reduced temperature $t = k_BT/t_1$.

4. Result and Discussion

These JT energy gap and the SDW gap equations given in the eqs.(4) and (5) are computed self-consistently and their temperature dependence is shown in Fig.-1(a). The SDW gap shows mean-field temperature dependence with SDW transition temperature $t_{SDW} \simeq 0.072$ ($T_{SDW} \simeq$ 90K) for the SDW coupling $g_1 =$ 1.9945. Due to the interplay of SDW interaction and JT distortion the JT gap is suppressed in the interplay region at low temperatures. The JT gap gradually increases near t_{SDW}, where SDW gap decreases. Finally the JT gap increase to its maximum gap values and then exhibits a mean field behavior with JT transition temperature $t_s \simeq 0.265$($T_s \simeq$ 325K) corresponding to the scaling energy $t_1 =0.125$ eV=1250 K, for the JT coupling $g_2=0.57$ and elastic constant $c_1=0.034$ and SDW coupling $g_1=1.9945$. The interplay of JT distortion and antiferromagnetism has been investigated by varying lattice constant, JT coupling, antiferromagnetic SDW coupling and chemical potential (not reported here) to explain experimentally observed electronic and lattice properties of oxypnictide systems. Hence different experimentally measured transition temperatures are T_{SDW} =

135K and T_S=154K for PrFeAsO [8], T_{SDW} = 140K and T_S=155K for CeFeAsO [9], T_{SDW} = 135K and T_S=155K or SmFeAsO [10].

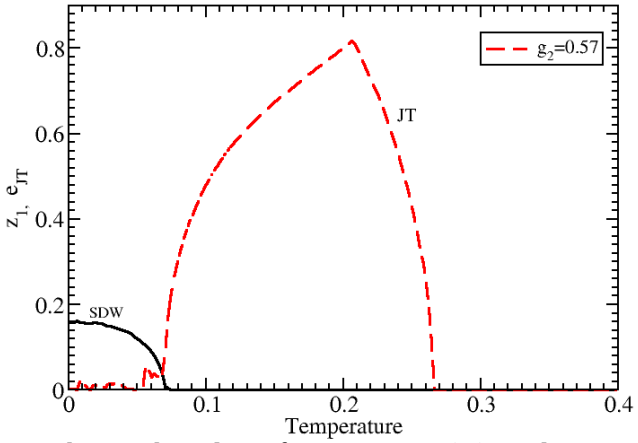

Fig.1(a) : Shows the plot of SDW gap (z_1) and JT energy gap (e_{JT}) vs. temperature (t) (dimensionless form), for SDW coupling g_1=1.9945, JT coupling g_2=0.57, elastic constant c_1=0.034 and chemical potential =zero.

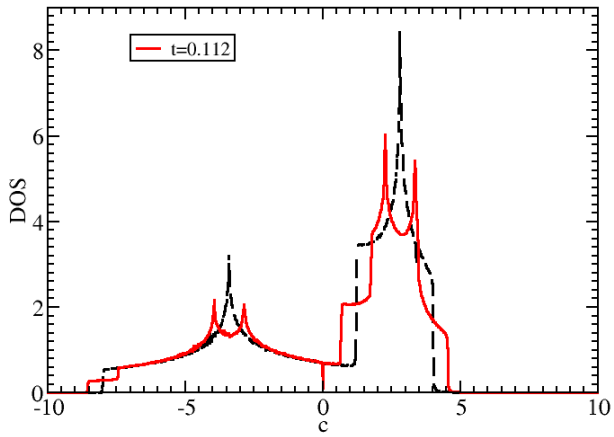

Fig.1(b) : Shows the plot of conduction electron DOS vs. conduction band energy(c) in absence of both SDW interaction and JT distortion(dotted line) and in presence of only JT interaction(continuous line) for SDW coupling g_1=1.9945, JT coupling g_2=0.57, elastic constant c_1=0.034, spectral width e_1=0.005 and temperature t= 0.112.

The electron DOS of the system in absence of both JT distortion and SDW interaction and in presence of only JT distortion is shown in Fig. 1(b). In absence of JT distortion and SDW interaction (as shown by dotted line), we observe two DOS for d_{xz} and d_{yz} bands i.e. one appearing below Fermi level (ϵ_F =0) with a sharp van-Hove singularity at energy $c_1 \simeq$ -3.416 and another one above Fermi level with sharp van-Hove singularity at energy $c_2 \simeq$+2.808. Similar electron DOS having two band calculations for oxypnictides have been shown by Raghu et. al.[14] and also from density functional theory (DFT) calculation for LaFeAsO and $BaFeAs_2$[15]. In presence of JT distortion at temperature t=140K, the van-Hove singularities splits into two symmetric peaks separated by the lattice distortion energy $2g_2e \simeq 1.086$ as shown by continuous lines. The JT splitted lower band two peaks appear in lower band at energies $c \simeq$ -3.906 and -2.823 in DOS. Similarly the upper band splits showing two peaks in DOS at energies $c \simeq$ +2.269 and +3.358 near the van-Hove singularity. There is no splitting of DOS at ϵ_F =0.

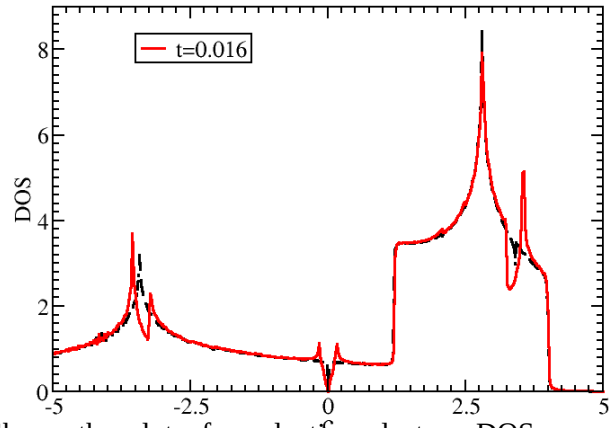

Fig. 2(a) – Shows the plot of conduction electron DOS vs. conduction band energy (c) in absence of both SDW interaction and JT distortion (dotted line) and in presence of only SDW interaction(continuous line) for SDW coupling g_1=1.9945 , JT coupling g_2=0.57, elastic constant c_1=0.034, spectral width e_1=0.005 and temperature t= 0.016.

Fig.-2(a) shows the electron DOS at lower temperature t = 20K in presence of only SDW interaction. For clear understanding, in the same graph we have plotted the DOS in absence of both JT distortion and SDW gap (as shown by dotted line) and we observe two sharp van-Hove singularities in lower and upper band. In presence of only SDW gap z_1= 0.157, at temperature t = 20K, both the

van-Hove singularities splits into two separated by the SDW gap $2z_1 \simeq 0.316$. It is to note further that the splitting of DOS at van-Hove singularities exhibit asymmetry in structure and peak height. Again there appears a d-wave type V-shaped gap in DOS near the Fermi level $\epsilon_F = 0$.

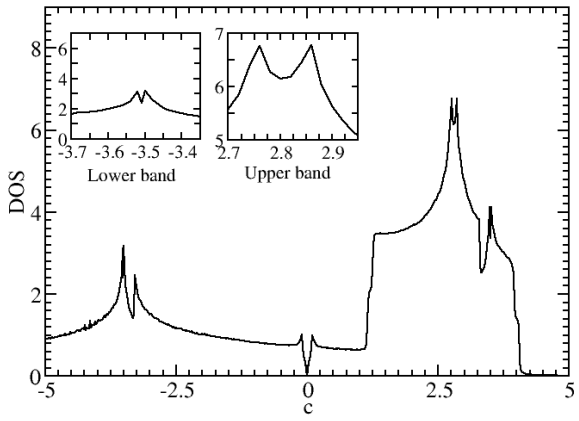

Fig. 2(b) – Shows the plot of conduction electron DOS vs. conduction band energy(c) in presence of both SDW interaction and JT interaction for SDW coupling g_1=1.9945, JT coupling g_2=0.57, elastic constant c_1=0.034, spectral width e_1=0.005 and temperature t= 0.056.

The Fig.-2(b) shows the DOS at temperature t =70K in the interplay region of JT distortion and antiferromagnetic SDW interaction, with lattice energy e_{JT} = 0.051 and SDW gap energy z_1= 0.104. As a result, the lower and upper densities corresponding to the two bands exhibits a V-shaped gap near Fermi level appearing due to the hybridization between the two bands. The JT splitted two peaks in the lower band and upper band further split into two separated due to the SDW gap energy. In the interplay region the JT energy gap is suppressed and the gap energy value is very small. So the splitting due to JT distortion is weak. However, the splitting of the DOS in the upper band is more prominent as compared to the lower band (as shown in inset of Fig.-2(b)). It is to note further that the splitted peaks in the DOS exhibit asymmetric behavior due to presence of SDW interaction (see Fig.-2(b)).

5. Conclusion

We have considered a tight-binding two-band model in presence of JT distortion and SDW interaction and calculated temperature dependent lattice energy and SDW gap, and computed them self-consistently. The lattice energy is

suppressed at low temperatures, where SDW interactions persist. The electron DOS exhibits multiple splitting as observed experimentally in conductance spectra of oxypnictides.

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