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Tight-binding Model Study of Interplay of Spin Density Wave and Lattice Distortion in Iron-Oxypnictide Superconductors

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Abstract: We report here two-band tight binding model consisting the kinetic energy of the two bands with fourth nearest-neighbour electron hopping, antiferromagnetic spin density wave(SDW) interaction and lattice distortion. We calculate the Green's functions by using Zubarev's Green's function technique. The lattice strain and SDW gaps are calculated and computed self-consistently. The interplay of these two gap parameters are studied through the tunneling conductance and quasi-particle band dispersion of the pnictide superconductors.

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

The newly discovered iron-based superconductors 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] with critical temperature 55K in $SmO_{1-x}F_xFeAs$ [4] and 56K in $Gd_{1-x}Th_xFeAsO$[5]. 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[6]. Also the other parent oxypnictides like PrFeAsO with T_{SDW} = 135K and T_S=154K[7], CeFeAsO with T_{SDW} = 140K and T_S=155K [8] etc. are reported. After doping superconductivity appears with suppression of both the transition temperatures. The band structure calculations [9,10] have shown that the density of states(DOS) near Fermi level gets its maximum contribution from the Fe-3d orbitals. Kriiger et al. [11] 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-neighbour 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 and band dispersion of the system.

2. Formalism

We have considered here the simple tight-binding two band model proposed by Raghu et. al [12]. To account for Jahn-Teller distortion in the system, for degenerate d_{xz}andd_{yz} orbitals with orbital index α=1, 2, the present Hamiltonian appears as

$$H_1 = \sum_{\alpha,\boldsymbol{k},\sigma} (\varepsilon_{kx} - \mu) d^{\dagger}_{\alpha,kx,\sigma} d_{\alpha,kx,\sigma} + \sum_{\alpha,\boldsymbol{k},\sigma} (\varepsilon_{ky} - \mu) d^{\dagger}_{\alpha,ky,\sigma} d_{\alpha,ky,\sigma} + \sum_{\alpha,\boldsymbol{k},\sigma} \varepsilon_{kxy} (d^{\dagger}_{\alpha,kx,\sigma} d_{\alpha,ky,\sigma} + d^{\dagger}_{\alpha,ky,\sigma} d_{\alpha,kx,\sigma}) \quad (1)$$

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-neighbour hopping integrals. Here t_1 is the nearest-neighbour hopping integral between σ - orbitals and t_2 is the nearest-neighbour hopping integral between π-orbitals. Further, t_3 represents the second neighbour hopping integral between similar orbitals, while t_4 represents the second neighbour hopping integral between different orbitals. The static JT interaction and the SDW interactions are written as

$$H_2 = -Ge\sum_{\alpha,\boldsymbol{k},\sigma}(-1)^{\alpha}(d^{\dagger}_{\alpha,kx,\sigma}d_{\alpha,kx,\sigma}+d^{\dagger}_{\alpha,ky,\sigma}d_{\alpha,ky,\sigma})$$
$$+\sum_{\alpha,\boldsymbol{k},\sigma}\Delta_s(k)(d^{\dagger}_{\alpha,kx,\sigma}d_{\alpha,k+Q,x,-\sigma}+d^{\dagger}_{\alpha,ky,\sigma}d_{\alpha,k+Q,y,-\sigma})+\frac{1}{2}Ce^2 \qquad (2)$$

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

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

$$A_{1\alpha}(\boldsymbol{k},\omega)=\left\langle\left\langle d_{\alpha,kx,\sigma};d^{\dagger}_{\alpha,kx,\sigma}\right\rangle\right\rangle_{\omega}=\frac{1}{2\pi}\frac{k_{\alpha1}(\omega)}{|D_{\alpha}(\omega)|} \qquad (3)$$

where, $k_{\alpha1}(\omega)=\left(\omega^2_{\alpha k}-E^2_{\alpha ky}\right)\left(\omega_{\alpha k}+\varepsilon_{\alpha kx}\right)-(\omega_{\alpha k}-\varepsilon_{\alpha ky})\varepsilon^2_{kxy}$, $E^2_{\alpha ky}=\varepsilon^2_{\alpha ky}+\Delta^2_s$ 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 ($B_{1\alpha}(\mathbf{k},\omega)$) are found for d_{yz}b and. Equating $|D_\alpha(\omega)|=0$, we find the quasi-particle dispersion bands, which are given by

$$\pm\omega_{\alpha1\boldsymbol{k}}\,,\pm\omega_{\alpha2\boldsymbol{k}}=\pm\left[\varepsilon^{2+}_{\alpha}+\Delta^2_s+\varepsilon^2_{kxy}\pm\left(\left(\varepsilon^{2-}_{\alpha}\right)^2+4\left(E_{\alpha+}\right)^2\varepsilon^2_{kxy}\right)^{1/2}\right]^{1/2}$$

where,

$$E^2_{\alpha+}=(\varepsilon^{+}_{\alpha})^2+\Delta^2_s\,,\quad \varepsilon^{\pm}_{\alpha}=0.5\left(\varepsilon_{\alpha kx}\pm\varepsilon_{\alpha ky}\right),\quad \varepsilon^{2\pm}_{\alpha}=0.5\left(\varepsilon^2_{\alpha kx}\pm\varepsilon^2_{\alpha ky}\right)$$

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

The expressions for lattice strain(e) and SDW gap are defined as

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

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

The 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-bindingparameters aret_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

The 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}≃0.106(T_{SDW}≃132.5K) for the SDW coupling g_1 =2.2945.The JT gap is suppressed in the interplay region at low temperature with

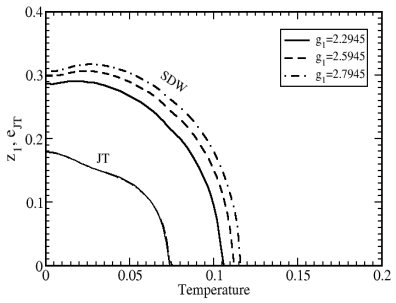

Fig.-1(a)

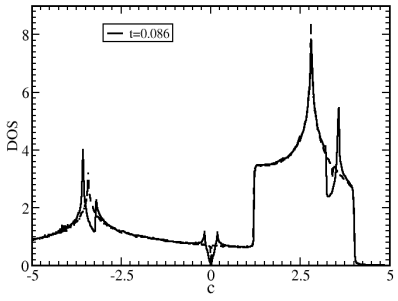

Fig.-1(b)

Fig.1(a) – Shows the plot of SDW gap (z_1) and JT energy gap (e_{JT}) vs. temperature(t)dimensionless form), for different values of SDW coupling g_1=2.2945, 2.5945, 2.7945 with JT coupling g_2=0.62, 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 SDW interaction(continuous line) for SDW coupling g_1=2.2945, JT coupling g_2=0.62, elastic constant c_1=0.034, spectral width e_1=0.005 and temperature t= 0.086.

JT transition temperature $t_s \simeq 0.074 (T_s \simeq 92.5K)$ for the scaling energy $t_1 = 0.125$ eV=1250 K, for the JT coupling $g_2=0.62$ and elastic constant $c_1=0.034$. With increase of SDW coupling (g_1), the SDW gap is enhanced throughout the temperature range while JT gap remains unchanged with the spin ordering. The different experimentally measured transition temperatures are T_{SDW} = 135K and T_S=154K for PrFeAsO [7], T_{SDW} = 140K and T_S=155K for CeFeAsO [8], T_{SDW} = 135K and T_S=155K or SmFeAsO [13].

Fig.-1(b) shows the plot of electron density of state (DOS) corresponding to two bands of the system. 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 $DOS = -2\pi \sum_{\alpha} \sum_{\mathbf{k},\sigma} \mathrm{Im}\left[A_{1\alpha}(\mathbf{k}, \omega) + B_{1\alpha}(\mathbf{k}, \omega) \right]$

Here we observe one van-Hove singularity below Fermi level(c=0) another singularity above c=0 shown in dotted line. At temperature t=0.086 i.e. in the pure SDW phase these two singularities splits into two separated by the SDW gap. Further, the two bands are separated by another V-shaped gap at c=0 with a node due to hybridization between two bands.

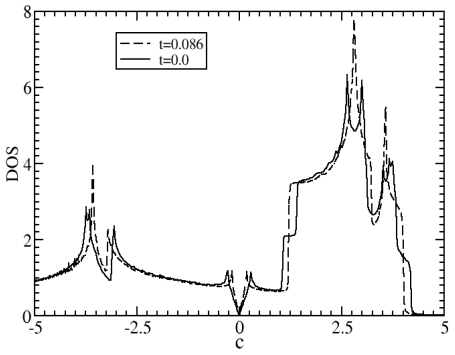

Fig.-2(a)

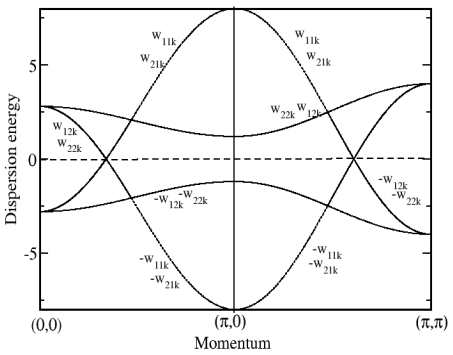

Fig.-2(b)

Fig. 2(a) – Shows the plot of conduction electron DOS vs. conduction band energy(c) in presence of SDW interaction (dotted line) and in presence of bothSDW interaction and JT distortion (continuous line) for SDW coupling $g_1=2.2945$, JT coupling $g_2=0.62$, elastic constant $c_1=0.034$, spectral width $e_1=0.005$ and temperature t= 0.0. **Fig. 2(b)** – Shows the band structure of two-band model in absence of spin density wave(SDW) interaction and JT distortion with SDW gap $z_1=0.0$ and JT energy $e_{JT}=0.0$, plotted along the path $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi)$.

Fig.-2(a) shows the effect of temperature on the tunneling conductance. In the pure SDW phase at t=0.086, the two van-Hove singularities splitinto two dueto SDW gap with a V-shaped gap at c=0(shown in dotted line). The DOS is plotted in the region of interplay between lattice distortion and SDW interaction at temperature t=0.0. It is observed that the van-Hove singularities again split due to JT-gap and SDW gap is further enhanced due to lattice distortion in the system. The splitted peaks at the van-Hove singularities exhibit asymmetric behavior. This type of multiple spectra is observed experimentally in scanning tunneling microscopy(STM) measurements of the oxypnictide superconductors.Fig.-2(b) shows the plot of band dispersion in absence of both SDW interaction and JT distortion. Here, we observe two bands i.e. w_{11k} and w_{21k} for d_{xz} orbitals. Similarly, we observe two bands i.e. w_{12k} and w_{22k} for d_{yz} orbitals. Further, we have also plotted the negative of these bands in the dispersion curve shown in fig.-2(b). The band do not show a gap at electron momentum ($\pi/3$, 0) and (π, $2\pi/3$) at Fermi energy(c=0).

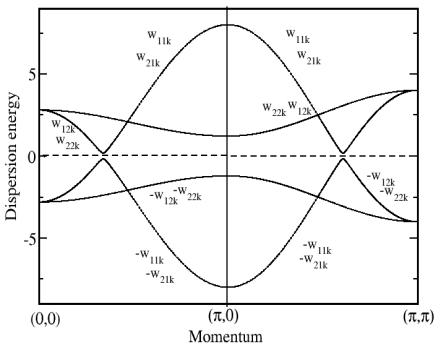

Fig.-3(a)

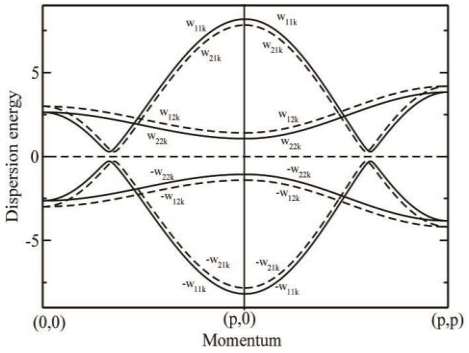

Fig.-3(b)

Fig. 3(a) – Shows the band structure of two-band model in presence of spin density wave(SDW) interaction with SDW gap z_1=0.179 and JT energy e_{JT}=0.0, plotted along the path (0,0) → (π,0) → (π,π) .**Fig. 3(b)** – Shows the band structure of two-band model in presence of both spin density wave(SDW) interaction and JT distortion with SDW gap z_1=0.286 and JT energy e_{JT}=0.178, plotted along the path (0,0) →(π,0) → (π,π) .

Fig.-3(a) shows the plot of band dispersion in presence of SDW interaction. It is observed that the band dispersion shows the upper conduction band and lower valance band is separated by insulating SDW gap $2z_1 \simeq 0.358$ at Fermi level(c=0), at electron momentum ($\pi/3$, 0) and (π, $2\pi/3$). The magnitude of this gap is important for electronic property oxypnictide system.Fig.-3(b) shows the electron band dispersion of the system in presence of JT distortion and SDW gap. Due to presence of JT distortion each band splits into two as shown by

continuous and dotted lines in fig.-3(b). The SDW gap at c=0 at momentum ($\pi/3$, 0)shifts to higher momentum and the SDW gap at c=0, at (π, $2\pi/3$)shifts to lower momentum due to JT distortion.

5. Conclusion

We have proposed here a two-band model for oxypnictide superconductors taking JT distortion and SDW interaction. The gap equations for JT energy and SDW energy, the tunneling conductance and band dispersion are calculated. The interplay of these order parameters on density of states and band dispersions are studied.

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