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Role of kinetic energy and spin density wave (SDW) interaction in iron-based superconductors: A model study

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Abstract: We report here the interplay of spin density wave (SDW) and kinetic energy hopping integrals in newly discovered oxypnictide iron-based superconductors. The system is described by a minimum two-band model consisting of nearest and next-nearest neighbour intra- and inter-orbital hoppings of electrons of iron ions. Besides, we propose here a Heisenberg type spin-spin interaction among the electrons of iron ions considered within a mean-field approximation. The electron Green's functions are calculated by Green's function technique of Zubarev and hence the gap equation for SDW order is calculated which is solved self-consistently. The interplay is investigated by the variation of temperature dependent SDW gap, the electron density of states (DOS) and temperature dependent electronic specific heat. The results are discussed according to the experimental observations.

Keywords : Two-band model, Spin density wave (SDW), Fe-Oxypinctide, Specific heat, Density of states (DOS).

1. Introduction

The discovery of a new class of high-T_c material $LaO_{1-x}F_xFeAs$ with critical temperature 26K[1] initiated enormous research interest in the field of high-T_c superconductivity. So far many families of iron based superconductors have been discovered [2,3, 4, 5, 6] with highest critical temperature 55 K in $SmO_{1-x}F_xFeAs$ [7] and 56K in $Gd_{1-x}Th_xFeAsO$ [8]. Though the parent compounds $LOFeAs$(L=La)[1], Sm[9], Ce[10], Nd and Gd) are not

superconductors, but according to the prediction of band structure calculations based on transport and optical conductivity measurement[11], there develops a spin density wave state below _ 150K due to Fermi surface nesting with structural transition from tetragonal to orthorhombic symmetry [11, 12, 13], which is also confirmed by neutron scattering experiment [12]. Also the transport [11] and neutron scattering measurements[12] in *LaOFeAs* have shown the spin density wave(SDW) magnetic order below T = 137K. Further in $SrFe_2As_2$ only one extremely sharp first order transition at TN = 205K is observed with both antiferromagnetic ordering and lattice distortion. In $BaFe_2As_2$, Rotter et. al. suggested the presence of a second-order phase transition at 140K with both SDW and lattice distortion[14]. From the susceptibility data of Pfisterer and Nagorsen [15, 16], the magnetic phase transition(AFM) occurs at 200K and 130K in SrFe2As2 and $BaFe_2As_2$ respectively. Also all the different families of iron-based superconductors share the common feature of an antiferromagnetic order[17]. The electronic structure of the iron-based superconductors is characterized by multi-band and multi-orbital nature[18]. All five 3d orbitals of Fe strongly hybridize with *As* 4p orbitals and have contribution to both itinerant conducting electrons and localized magnetic moments which bring complexity to understand and explain experimental phenomena. But to understand the mechanism of iron-based superconductors, five band[19, 20, 21] and four band[22] tight-binding models are proposed. For the unfolded one *Fe* ion/cell Brillouin zone, Mazin et. al.[23] reported that the band structure near the Fermi level involves the three *Fe* orbitals, d_{xz}, d_{yz} and d_{xy} (or $d_{x^2-y^2}$). Based upon these observations, Raghu et. al.[24] have considered a two-dimensional square lattice with two degenerate d_{xz} and d_{yz} orbitals per site and replaced the role of d_{xy} (or $d_{x^2-y^2}$) orbit by a nearest-neighbour hybridization between d_{xz} and d_{yz} orbitals.

In this present communication, we consider a minimal two band model(d_{xz}, d_{yz} bands) 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 condition near the Fermi surface with an electron wave vector $Q = (\pi, \pi)$, such that $\varepsilon_{(k+Q)x} = -\varepsilon_{kx}$ and $\varepsilon_{(k+Q)y} = -\varepsilon_{ky}$ .The paper is organized as follows. We introduce a tight-binding two-band model with SDW interaction in both the bands and also discuss the interplay of SDW order and kinetic energy in section-2. We calculate the electron Green's functions, expression for gap equation, tunneling conductance and electronic specific heat in

section-3. Then we present the results and discussion in section-4 and finally conclusion in section-5.

2. Formalism for model Hamiltonian

In oxypnictide superconductors, all five iron 3d electrons have prominent electron density of states near Fermi surface. Therefore, five band model calculations are reported. However to simplify the calculation, a two-band model is considered here based on report by Raghu et. al.[24] taking hopping of d-electrons from site *i* and the nearest-neighbour site *j*, which is written as

$$H_I = -\sum_{<<i,j>>,\sigma}\left[t_{ij}^{\alpha,\beta} d_{\alpha i\sigma}^{\dagger} d_{\beta j\sigma}\right] \tag{1}$$

where, $t_{ij}^{\alpha,\beta}$ represents in general the hopping integral from site $\vec{r}_i$ to nearest site $\vec{r}_j$ from orbital α to β with $\alpha,\beta \equiv d_{xx}, d_{yz}$ orbitals. Here $d_{\alpha i\sigma}^{\dagger}(d_{\alpha i\sigma})$ represents the creation (annihilation) operator of the electron operator at site *i* and orbital α. The Fourier transformation of eq.(1) gives rise to the band dispersions, which are written as

$$\alpha_{kx} = -2t_1\cos k_x - 2t_2\cos k_y - 4t_3\cos k_x\cos k_y \tag{2}$$

$$\varepsilon_{ky} = -2t_2\cos k_x - 2t_1\cos k_y - 4t_3\cos k_x\cos k_y \tag{3}$$

$$\varepsilon_{kxy} = -4t_4\sin k_x\sin k_y \tag{4}$$

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 coulomb interaction among the electrons in the same orbital are considered within Hrtree-Fork approximation and the mean-field approximation gives rise to spin density wave(SDW) Hamiltonian H_{II} , which is written as

$$H_{II} = \Delta_S \sum_{\vec{k},\sigma}\left(d_{kx\sigma}^{\dagger} d_{k+Q,x,-\sigma} + d_{ky\sigma}^{\dagger} d_{k+Q,y,-\sigma}\right) \tag{5}$$

The SDW gap parameter is given by

$$\Delta_s = \sum_{\vec{k},\sigma} V_1(k)\left[< d^{\dagger}_{kx\sigma} d_{k+Q,x,-\sigma} > + d^{\dagger}_{ky\sigma} d_{k+Q,y,-\sigma} \right] \quad (6)$$

where V_1 is repulsive SDW interaction strength. The band dispersions satisfy the nesting condition near the Fermi surface with an electron wave vector $Q = (\pi, \pi)$, such that $\varepsilon_{(k+Q)x} = -\varepsilon_{kx}$ and $\varepsilon_{(k+Q)y} = -\varepsilon_{ky}$.

3. Calculation of SDW gap equation

In order to calculate the SDW gap equation, we introduce the Green's functions for electrons of the d_{xz} orbital as

$$G_1(k,\omega) = << d_{kx\sigma}; d^{\dagger}_{kx\sigma} >>_{\omega} \cdot G_2(k,\omega) = << d_{k+Q,x,-\sigma}; d^{\dagger}_{kx\sigma} >> \omega \quad (7)$$

The coupled Green's functions are calculated using double time single particle Green's function of Zubarev [25] and the solution of Eq(7) gives

$$G_1(k,\omega) = \frac{K_1(\omega)}{2\pi |D(\omega)|}\ ,\ G_2(k,\omega) = \frac{K_2(\omega)}{2\pi |D(\omega)|} \quad (8)$$

where $|D(\omega)|$ appearing in the denominator of all the Green's functions is written as

$$|D(\omega)| = \omega^4 - \omega^2\left(E^2_{kx} + E^2_{ky} + 2E^2_{kxy}\right) + E^2_{kx}E^2_{ky} + \varepsilon^4_{kxy} - 2E^2_{kxy}\,\varepsilon^2_{kxy} \quad (9)$$

where, $E^2_{kx} = \varepsilon^2_{kx} + \Delta^2_s, E^2_{ky} = \varepsilon^2_{ky} + \Delta^2_s, E^2_{kxy} = \varepsilon_{kx}\varepsilon_{ky} + \Delta^2_s$

and $K_i(\omega)$ with i =1, 2 appearing in numerator of the Green's functions are

$$K_1(\omega) = (\omega^2 - E^2_{ky})(\omega + \varepsilon_{kx}) - (\omega - \varepsilon_{ky})\varepsilon^2_{kxy}, K_2(\omega) = \Delta_s(\omega^2 - E^2_{ky} + \varepsilon^2_{kxy})$$

Equating $|D(\omega)|$ to zero, we find the quasi-particle dispersion bands, $\omega_{\alpha\vec{k}}$ with α= 1, 2 which are given by

$$\omega_{\alpha\vec{k}} = \pm\left[\varepsilon^{2+} + \Delta^2_s + \varepsilon^2_{kxy} - (-1)^{\alpha}\sqrt{((\varepsilon^{2-})^2 + 4E^2_{+}\varepsilon^2_{kxy})} \right]^{\frac{1}{2}} \quad (10)$$

where, we have $\varepsilon^{2\pm} = \frac{\varepsilon^2_{kx} \pm \varepsilon^2_{ky}}{2}$. Similarly we introduce the Greens functions for the electrons of d_{yz} orbital as

$$H_1(k,\omega) = << d_{ky\sigma}; d^{\dagger}_{ky\sigma} >>_{\omega}\ ,\ H_2(k,\omega) = << d_{k+Qy-\sigma}; d^{\dagger}_{ky\sigma} >>_{\omega} \quad (11)$$

These coupled equations are solved to find the final expression as

$$H_1(k,\omega) = \frac{K_5(\omega)}{2\pi|D(\omega)|}\,,\; H_2(k,\omega) = \frac{K_6(\omega)}{2\pi|D(\omega)|} \tag{12}$$

where $K_j(\omega)$ with j = 5,6 are written as

$$K_5(\omega) = (\omega^2 - E_{kx}^2)(\omega + \varepsilon_{ky}) - (\omega - \varepsilon_{kx})\varepsilon_{kxy}^2\,,\; K_6(\omega) = \Delta_s(\omega^2 - E_{kx}^2 + \varepsilon_{kxy}^2)$$

The expression for SDW gap defined in Eq(6) is calculated from the correlation function derived from the Greens function $G_2(k,\omega)$ and $H_2(k,\omega)$ and is written as

$$\Delta_s = \frac{1}{N}\sum_{\vec{k},\sigma} \left|\frac{(F_{21} - F_{22}) + (F_{61} - F_{62})}{2\left(\omega_{1\vec{k}}^2 - \omega_{2\vec{k}}^2\right)}\right| \tag{13}$$

where $F_{21} = \frac{K_2(\omega_{1\vec{k}})}{\omega_{1\vec{k}}} \tanh(\frac{1}{2}\beta\omega_{1\vec{k}})$, $F_{22} = \frac{K_2(\omega_{2\vec{k}})}{\omega_{2\vec{k}}} \tanh(\frac{1}{2}\beta\omega_{2\vec{k}})$,

$F_{61} = \frac{K_6(\omega_{1\vec{k}})}{\omega_{1\vec{k}}} \tanh(\frac{1}{2}\beta\omega_{1\vec{k}})$, $F_{62} = \frac{K_6(\omega_{2\vec{k}})}{\omega_{2\vec{k}}} \tanh(\frac{1}{2}\beta\omega_{2\vec{k}})$

The tunneling conductance spectra measured by the STM technique represents the DOS of electrons near Fermi surface. In the present work we calculate the DOS from the imaginary part of the electron Green's function given by the relation $\rho(\omega) = \sum_{\vec{k},\sigma}\rho_{\vec{k},\sigma}(\omega)$ where the spectral density function $\rho_{\vec{k}}(\omega) = ImG(\vec{\mathbf{k}},\omega)$, where G represents the sum of Green's function $G_1(\vec{\mathbf{k}},\omega)$ and $H_1(\vec{\mathbf{k}},\omega)$ with wave vector $\vec{\mathbf{k}}$ and spin σ. The free energy for the charge carriers in this system can be written as

$$F = -k_B T \sum_{\pm\alpha,\vec{k},\sigma} \ln\left[1 + \exp(-\beta\omega_{\pm\alpha\vec{k}}\right] \tag{14}$$

where $\omega_{\alpha,\vec{k}}(\alpha = 1,2)$ are the quasi-particle bands. The temperature dependent electronic specific heat and entropy at constant volume V and chemical potential μ are calculated from free energy(F) of the system by using the relation

$$S = -\frac{1}{N}(\frac{\partial F}{\partial T})_{V,\mu},\ C_V = k_B T(\frac{\partial S}{\partial T})_{V,N} \tag{15}$$

The momentum vector and spin summations are converted in to integral form which leads to double integrals for k_x and k_y variables. The hopping integrals t_1, t_2, t_3, t_4 are scaled by hopping integral t_1. The SDW coupling $g_1 = \frac{V_1}{t_1}$ and the SDW gap $z_1 = \frac{\Delta_s}{t_1}$. The tight-binding calculation represents the band calculation for $t_1 = -1$, $t_2 = 1.3$, $t_3 = -0.85$, $t_4 = -0.85$. Here hopping integral t_1 is taken as $0.125eV \approx 1250K$.

4 Results and discussion

The effect of the nearest-neighbour kinetic hopping integral(t2) of electrons between π-orbitals on spin density wave(SDW) gap is shown in fig.1. This part of the kinetic energy competes with the insulating SDW gap. With increase of this kinetic energy from t_2 = 1.20 t_0 1.30, the magnitude of SDW gap is suppressed throughout the temperature range and the Neel temperature is also reduced correspondingly from t_N = 0.140(175*K*) to 0.108(135*K*) which satisfies for *LaFeAsO* with T_N = 135 [12]. This displays a strong competition between antiferromagnetic(AFM) order with the hopping energy (t_2) of the electron.

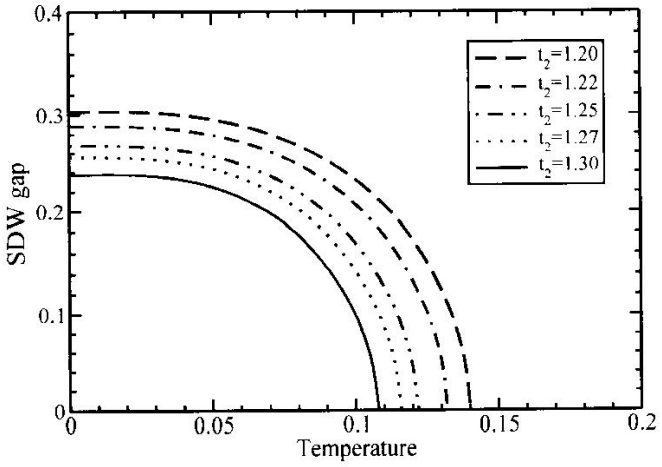

Fig. 1. The plot of SDW gap, z_1 (dimensionless form) vs. temperature, *t*(dimensionless form) for different values of kinetic energy parameter t_2 = 1.20, 1.22, 1.25, 1.27, 1.30 with SDW coupling g_1 = 2.0738 .

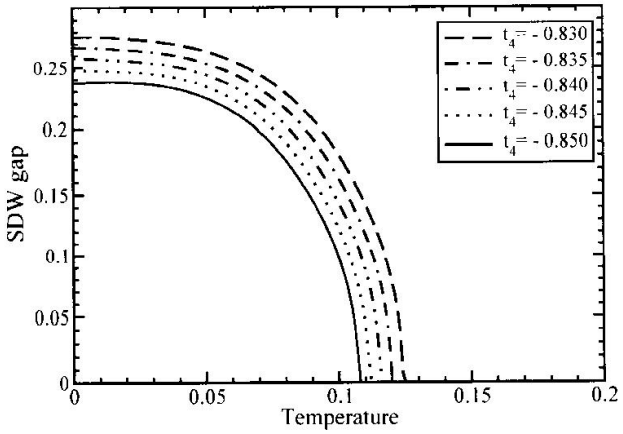

Fig. 2. The plot of SDW gap, z_1 (dimensionless form) vs. temperature, t(dimensionless form) for different values of hybridization parameter t_4 = -0.830, -0.835, -0.840, -0.845, -0.850 with SDW coupling g_1 = 2.0738 .

The effect of second neighbour hopping integral t_4 between two different orbitals of Fe-ion on SDW gap is shown in Fig.2. When this hopping kinetic energy of electrons is increased from t_4= -0.830 to -0.850, the SDW gap is suppressed throughout the temperature range and its Neel temperature is also reduced from t_N= 0.125 to 0.108. Under this condition the SDW gap retains its perfect mean-field behaviour and its robust transition from low temperature SDW phase to high temperature paramagnetic phase. This interaction displays a strong interplay between second neighbour kinetic hopping and the antiferromagnetic (AFM) magnetic order in which kinetic energy dominates over the AFM order.

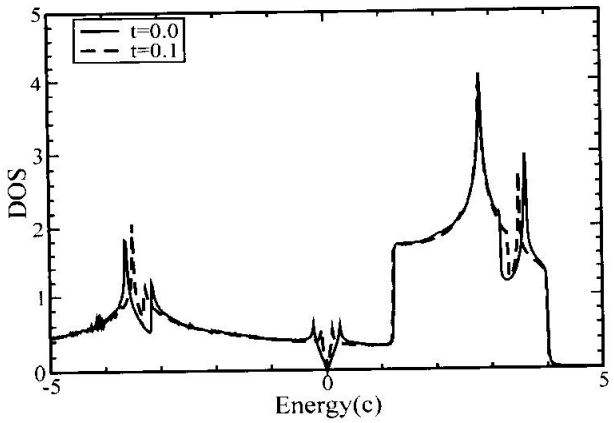

Fig. 3. The plot of the conduction electron DOS vs. energy for the fixed values of hopping integrals at t = 0.0, 0.1 .

The effect of temperature on electron density of states (DOS) is shown in Fig.3. At temperature t = 0.0, the DOS displays three gaps due to presence of spin density wave (SDW) gap present in the Oxypnictide system. The DOS shows a V-shaped d-wave type gap with a node at zero bias(band energy c=0.0). The two sharp peaks appearing due to Van-Hove singularities, each splits into two exhibiting SDW gap. Out of the two sharp peak, one appears in the valance band with band energy −3.632 to −3.154 and the other in conduction band with band energy +2.85 to +3.64. As shown in Fig.1 and variation of SDW gap with other parameters as reported by Mohapatra et al.[26], the SDW gap decreases with increase of temperature. Hence $\Delta_S(t=0.1) < \Delta_S(t=0.0)$. When we move from temperature t=0.0 to t=0.1, the all three SDW gaps appearing in DOS are reduced.

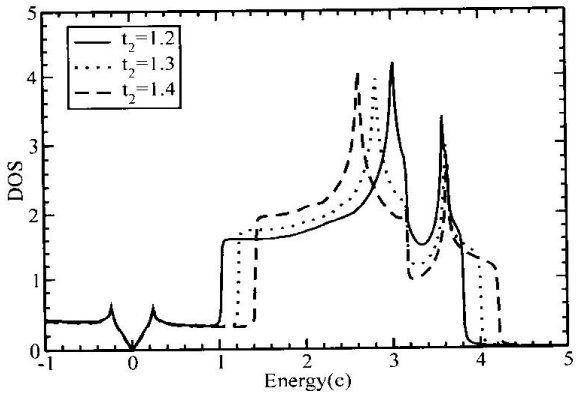

Fig. 4. The plot of the conduction electron DOS vs. energy for different values of kinetic energy parameter t_2 = 1.2, 1.3, 1.4 at t=0.0 .

The effect of nearest-neighbour hopping integral(t_2) of electron between the π-orbitals of Fe-ions on DOS is shown in Fig.4. It is observed that the part of the DOS i.e. in the valance band and that near the Fermi level (with band energy c = 0) is unaffected by the hopping integral t_2. The hopping integral interplays strongly with the SDW order as shown by the DOS appearing in the high energy (c > 0) conduction band. With increase of hopping integral t2 the SDW gap decreases and hence the gap edges in the DOS come closer. It is to note further that the second nearest-neighbour hopping integral(t_4) between different orbitals of Fe-ions have little effect on electron DOS.

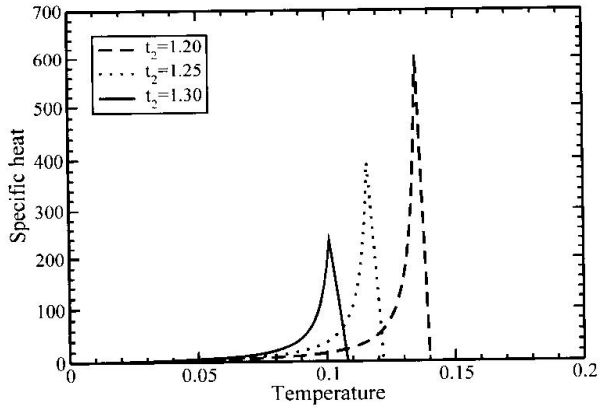

Fig. 5. The plot of specific heat vs. temperture for different values of kinetic energy parameter t_2 = 1.20, 1.25, 1.30 with SDW coupling g_1=2.0738.

In order to study the thermal properties of oxypnictide superconductors, we have calculated the electronic specific heat of the system in presence of SDW magnetic order based upon our two-band model by differentiating free energy with temperature at constant volume to calculate temperature dependent entropy and hence specific heat(C_V) of the system. The effect of nearest-neighbour hopping integral(t_2) of electron between π-orbitals on temperature dependent specific heat is shown in Fig.5. For a given SDW coupling g_1=2.0738 and a given hopping integral t_2=1.2, the C_V shows a sharp jump at Neel temperature t_N=0.14(t=175 K). The change in specific heat at t_N is nearly 603, which corresponds to a very large value of Sommerfeld specific heat co-efficient. With decrease of temperature the C_V sharply decreases and approaches zero at t = 0K. With further increase of hopping integral t_2=1.2 to 1.3, the Neel temperature reduces and the magnitude of specific heat jump also reduces considerably. However, the robust character of SDW order near t_N remains as indicated by the sharpness of jump in C_V. This type of specific heat jump is reported for *LaOFeAs* at Neel temperature T_N = 155 K [11]. The increase of kinetic energy(t_2) suppresses the SDW order indicating the strong interplay between kinetic energy and SDW order in the system.

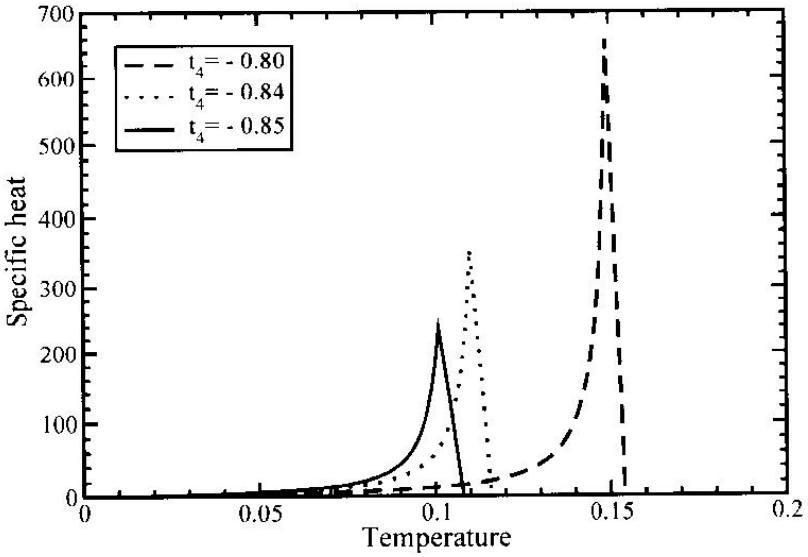

Fig. 6. The plot of specific heat vs. temperature for different values of hybridization parameter t_2 = -0.80, -0.84, -0.85 with SDW coupling g_1=2.0738 .

The effect of second nearest-neighbour hopping integral (t_4) between two different orbitals of Fe-ions is shown in Fig.6. The hopping integral t_4 has the similar effect on C_V as that of t_2 indicating once again the dominate bahavior of kinetic energy over the SDW order in oxypnictide systems. With increase of hopping integral t_4, Neel temperature as well as specific heat jump are reduced considerably.

5. Conclusion

We have considered here a two band model with spin density wave(SDW) interaction to describe the oxypnictide system in normal phase. The temperature dependent SDW gap is solved numerically. It is observed that there is strong interplay between the SDW order parameter and different hopping integrals of electrons. This strong interplay is evidenced by the variation of SDW coupling and hopping parameters on SDW gap, density of states(DOS) and electronic specific heat.

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