Spin Density Wave Interaction in Two Band Model for the Iron-Based Superconductors

Rasmita Mohapatra, Govinda Chandra Rout

Abstract—The newly discovered Oxypnictide superconductors have triggered enormous research interests in the condensed physics.We propose a two band model in presence of spin-density-wave(SDW) interaction to investigate the behavior of itinerant electron on the temperature dependent SDW gap, density of states, effect of doping and specific heat. The SDW gap equation is calculated from electron Green's function and solved numerically. Using the temperature dependent SDW gap, the density of states,occupation number for the two bands and specific heat are calculated and results are discussed to explain experimental facts .

Index Terms— two band model,density of states,doping,iron based superconductors,occupation number,Oxypnictides,specific heat,spin density wave.

1 Introduction

THE discovery of iron-based superconductors $LaO_{1-x}F_x$ FeAs with critical temperature 26K has led to a great break through in the field of high temperature superconductivity [1]. Immediately, the T_c has been enhanced upto 50K by replacing La using rare-earth elements [2],[3],[4],[5]. A $SmO_{1-x}F_x$ FeAs(x=0.2) superconductor still remains highest at T_c= 54K in rare-earth family [6]. Up to now many families of iron-based superconductors namely REOFeAs(1111-type), $(Ba/Sr)_{1-x}K_xFe_2As_2$(122-type),LiFeAs(111-type) and FeTe/As (11-type) have been discovered. All these materials show common layer structure based on a planer layer of iron atoms joined by pnictogen or chalcogen anions. It is widely believed that their superconductivity is based on the common iron layers.

Before doping , the parent compounds of most iron-based superconductors show long range antiferromagnetic orders[7],[8],[9],[10],[11]. After doping , the antiferromagnetism(AFM) gradually is suppressed and superconductivity(SC) is developed. The correlation effects among the lattice structure, magnetism, spin fluctuation and superconductivity are important for studying pairing mechanism.The magnetism can be understood by the itinerant electron picture, because the parent compounds are bad metals.With this picture the long range magnetic order arises from the Fermi surface nesting. The thermodynamic and transport measurements show that LaFeAsO exhibits structural phase transition T_s =155K [12] and spin density wave(SDW) instability at $T_N \cong 135K$ with nesting vector Q(π,π) connecting the hole and electron pockets in Fermi surface [13].

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 property $\varepsilon(k+Q) = -\varepsilon(k)$. The SDW gap parameter, density of states, doping effects and specific heat are computed numerically. We present the formalism in section-2, calculation of gap equation,occupation numbers for two bands and the DOS from electron Green's function in section-3, results and discussion in section-4 and conclusion in section-5.

2 Formalism

The band structure calculations have shown a finite DOS near the Fermi level [14] suggesting the importance of itinerant electrons. The local density approximation(LDA) band structure calculations indicate that the Fe 3d-orbitals are strongly hybridized and play the key role in the DOS near the Fermi level especially d_{xz} and d_{yz} [15],[16].This character suggests that the iron based superconductors have a multi-orbital nature.The system is described by a model Hamiltonian[17] as given below

$$H_0 = \sum_{k\sigma} \varepsilon_{kx} d^{\dagger}_{kx\sigma} d_{kx\sigma} + \sum_{k\sigma} \varepsilon_{ky} d^{\dagger}_{ky\sigma} d_{ky\sigma} + \sum_{k\sigma} \varepsilon_{kxy} (d^{\dagger}_{kx\sigma} d_{ky\sigma} + d^{\dagger}_{ky\sigma} d_{kx\sigma}) \quad (1)$$

. The first term in the Hamiltonian represents the hopping of the electron in orbital, d_{xz} with $d^{\dagger}_{kx\sigma}$ ($d_{kx\sigma}$) as the creation (annihilation) operator corresponding to electron momentum k and spin σ and energy ε_{kx}. Similarly the second term in the Hamiltonian represents the hopping of the electron in orbital d_{yz} with $d^{\dagger}_{ky\sigma}$ ($d_{ky\sigma}$) as the creation (annihilation) operator with energy ε_{ky} . 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} .

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The chemical potential is adjusted to conserve the fermion occupation numbers for the variation of temperature. The hopping of the electrons from site to site gives rise to the energy dispersion as written below

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

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

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

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 -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 Hamilonian H_1 represents SDW interaction in d_{xz} and d_{yz} bands as given below

$$H_1 = \Delta_s \sum_{k,\sigma} (d^{\dagger}_{kx\sigma} d_{k+Q,x,-\sigma} + d^{\dagger}_{ky\sigma} d_{k+Q,y,-\sigma}) \qquad (2)$$

Here we introduce the spin-density-wave(SDW) interaction in both the orbitals d_{xz} and d_{yz} with nesting condition $\varepsilon(k+Q) = -\varepsilon(k)$ for both the orbitals. The SDW gap parameter is given by

$$\Delta_s = \sum_{k,\sigma} V_1(k)\left[\left\langle d^{\dagger}_{kx\sigma} d_{k+Qx-\sigma}\right\rangle + \left\langle d^{\dagger}_{ky\sigma} d_{k+Qy-\sigma}\right\rangle\right] \qquad (3)$$

where V_1 is repulsive SDW interaction strength.

3 CALCULATION OF GAP EQUATION

In order to calculate the gap equation, occupation numbers in different bands and the corresponding density of sates (DOS), we introduce the electron Green's functions for the d_{xz} orbital electrons as

$$A_1(k,\omega) = \langle\langle d_{kx\sigma}; d^{\dagger}_{kx\sigma}\rangle\rangle_{\omega} \qquad (4)$$

$$A_2(k,\omega) = \langle\langle d_{k+Qx-\sigma}; d^{\dagger}_{kx\sigma}\rangle\rangle_{\omega} \qquad (5)$$

$$A_3(k,\omega) = \langle\langle d_{ky\sigma}; d^{\dagger}_{kx\sigma}\rangle\rangle_{\omega} \qquad (6)$$

$$A_4(k,\omega) = \langle\langle d_{k+Qy-\sigma}; d^{\dagger}_{kx\sigma}\rangle\rangle_{\omega} \qquad (7)$$

The four coupled Green's functions are calculated using double time single particle Green's function of Zubarev [18].

The solution of Eq(4) , Eq(5), Eq(6) and Eq(7) gives

$$A_1(k,\omega) = \frac{1}{2\pi}\frac{k_1(\omega)}{|D(\omega)|} \qquad (8)$$

$$A_2(k,\omega) = \frac{1}{2\pi}\frac{k_2(\omega)}{|D(\omega)|} \qquad (9)$$

$$A_3(k,\omega) = \frac{1}{2\pi}\frac{k_3(\omega)}{|D(\omega)|} \qquad (10)$$

$$A_4(k,\omega) = \frac{1}{2\pi}\frac{k_4(\omega)}{|D(\omega)|} \qquad (11)$$

where |D(ω)| is written as

$$|D(\omega)| = \omega^4 + P\omega^2 + Q \qquad (12)$$

with

$$P = -\left(E^2_{kx} + E^2_{ky} + 2E^2_{kxy}\right)$$

,

$$Q = \left(E^2_{kx}E^2_{ky} + \varepsilon^4_{kxy} - 2E^2_{kxy}\varepsilon^2_{kxy}\right)$$

and

$$E^2_{kx} = \varepsilon^2_{kx} + \Delta^2_s$$

$$E^2_{ky} = \varepsilon^2_{ky} + \Delta^2_s$$

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

$$k_1(\omega) = \left(\omega^2 - E^2_{ky}\right)\left(\omega + \varepsilon_{kx}\right) - \left(\omega + \varepsilon_{ky}\right)\varepsilon^2_{kxy}$$

$$k_2(\omega) = \Delta_s\left(\omega^2 - E^2_{ky} + \varepsilon^2_{kxy}\right)$$

Equating |D(ω)| to zero, we find the quasi-particle dispersion bands which are given by

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

where

$$\varepsilon^{2\pm} = \frac{\left(\varepsilon^2_{kx} \pm \varepsilon^2_{ky}\right)}{2}$$

$$E_+ = \left(\varepsilon^2_+ + \Delta^2_s\right)^{1/2}$$

$$\varepsilon_{\pm} = \frac{\left(\varepsilon_{kx} \pm \varepsilon_{ky}\right)}{2}$$

Similarly we introduce the Green's functions for the electron in the d_{yz} orbital as given below

$$B_1(k,\omega) = \langle\langle d_{ky\sigma}; d^{\dagger}_{ky\sigma}\rangle\rangle_{\omega} \quad (13)$$

$$B_2(k,\omega) = \langle\langle d_{k+Qy-\sigma}; d^{\dagger}_{ky\sigma}\rangle\rangle_{\omega} \quad (14)$$

$$B_3(k,\omega) = \langle\langle d_{kx\sigma}; d^{\dagger}_{ky\sigma}\rangle\rangle_{\omega} \quad (15)$$

$$B_4(k,\omega) = \langle\langle d_{k+Qx-\sigma}; d^{\dagger}_{ky\sigma}\rangle\rangle_{\omega} \quad (16)$$

The solution for Eq.(13) , Eq(14) , Eq(15) and Eq(16) gives

$$B_1(k,\omega) = \frac{1}{2\pi}\frac{k_5(\omega)}{|D(\omega)|} \quad (17)$$

$$B_2(k,\omega) = \frac{1}{2\pi}\frac{k_6(\omega)}{|D(\omega)|} \quad (18)$$

$$B_3(k,\omega) = \frac{1}{2\pi}\frac{k_7(\omega)}{|D(\omega)|} \quad (19)$$

$$B_4(k,\omega) = \frac{1}{2\pi}\frac{k_8(\omega)}{|D(\omega)|} \quad (20)$$

where

$$k_5(\omega) = \left(\omega^2 - E^2_{kx}\right)\left(\omega + \varepsilon_{ky}\right) - \left(\omega - \varepsilon_{kx}\right)\varepsilon^2_{kxy}$$

$$k_6(\omega) = \Delta_s\left(\omega^2 - E^2_{kx} + \varepsilon^2_{kxy}\right)$$

The expression for SDW gap defined in Eq(6) is calculated from the correlation function derived from the Green's function $A_2(k,\omega)$ and $B_2(k,\omega)$ and is written as

$$\Delta_S = \frac{1}{N}\sum_{k,\sigma}\left[\frac{(F_{21} - F_{22}) + (F_{41} - F_{42})}{2\left(\omega^2_{1k} - \omega^2_{2k}\right)}\right] \quad (21)$$

where

$$F_{21} = \frac{K_2(\omega_{1k})}{\omega_{1k}}\tanh\left(\frac{1}{2}\beta\omega_{1k}\right)$$

$$F_{22} = \frac{K_2(\omega_{2k})}{\omega_{2k}}\tanh\left(\frac{1}{2}\beta\omega_{2k}\right)$$

$$F_{41} = \frac{K_4(\omega_{1k})}{\omega_{1k}}\tanh\left(\frac{1}{2}\beta\omega_{1k}\right)$$

$$F_{42} = \frac{K_4(\omega_{2k})}{\omega_{2k}}\tanh\left(\frac{1}{2}\beta\omega_{2k}\right)$$

The electron occupation number is calculated from the correlation function derived from their corresponding Green's function . The occupation numbers n_x of the d_{xz} and n_y of the d_{yz} orbitals are defined as

$$n_x = \sum_{k,\sigma}\left\langle d^{\dagger}_{kx\sigma}; d_{kx\sigma}\right\rangle \quad (22)$$

$$n_y = \sum_{k,\sigma}\left\langle d^{\dagger}_{ky\sigma}; d_{ky\sigma}\right\rangle \quad (23)$$

The free energy for the charge carriers in this system can be written as

$$F = -k_B T\sum_{\pm ik\sigma}\ln\left[1 + \exp\left(-\beta\omega^{\pm}_{ik}\right)\right] \quad (24)$$

where ω_{ik} (i = 1, 2) are the quasi-particle bands . The expression for entropy and specific heat is
given by

$$S = -\frac{1}{N}\left(\frac{\partial F}{\partial T}\right)_{v,\mu} \text{ and } C = k_B T\left(\frac{\partial S}{\partial T}\right)_{v,N} \quad (25)$$

After simplification the final expression for specific heat is given by

$$\frac{S}{k_B} = \sum_{k,\sigma,i(i=1,2)}\left[\begin{array}{l}\ln 2(1+\cosh(\beta\omega_{ik})) \\ +\dfrac{\sinh(-\beta\omega_{ik})}{1+\cosh(\beta\omega_{ik})}(\beta\omega_{ik} - \Delta'_s)\end{array}\right] \quad (26)$$

where

$$\Delta'_s = \left(\frac{\partial\Delta_s}{\partial k_B T}\right) \text{ and } \beta = \frac{1}{k_B T}$$

The momentum and spin summations are converted in to integral form which leads to doule 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 tightbinding 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≃1250K. The SDW coupling and the SDW gap is defined as $g_1 = g_1\mu_B/t_1$ and $z_1 = \Delta_s/t_1$.

4 RESULT AND DISSCUTION

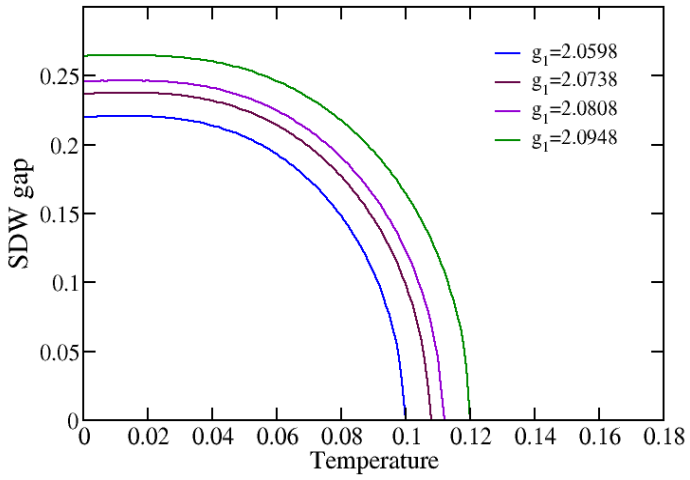

Fig. 1. The plot of SDW gap ,z_1 (dimensionless form) vs. temperature , t (dimensionless form) for different values of SDW coupling g_1 = 2.0598,2.0738,2.0808,2.0948 with zero chemical potential .

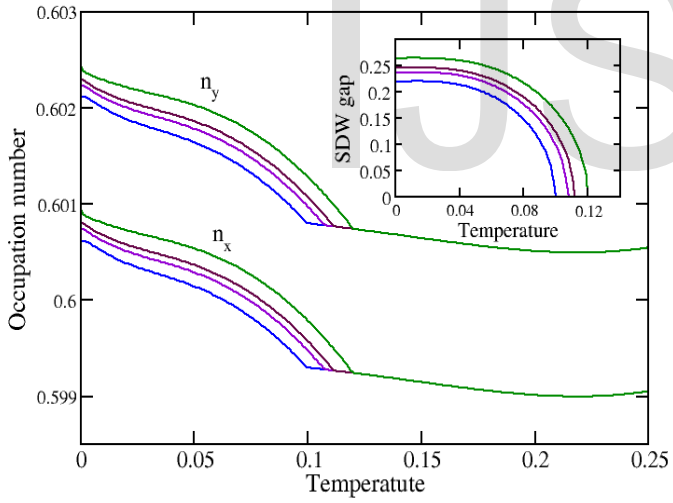

Fig. 2. The plot of occupation number n_x of the d_{xz} band and n_y of d_{yz} band vs. temperature , t (dimensionless form) for different values of SDW oupling from g_1 = 2.0598 to 2.0948.

Fig. 1. Shows the plot of SDW gap ,z_1 vs. temperature, t for different values of SDW coupling g_1 = 2.0598, 2.0738, 2.0808, 2.0948.The SDW coupling parameter is varied from g_1 = 2.0598 to 2.0948 in order to get the SDW transition temperatures from T_N = 125K to 150K for $t_1 \approx 0.125$ eV ≈ 1250K. This satisfies for T_N = 135K for LaFeAsO in thermodynamic and transport measurement [12] and T_N = 150K [19] from electron structure study.With increase of SDW coupling the magnitude of SDW gap is enhanced through out temperature as well as its Neel temperature .

Fig. 2. shows the plot of occupation number n_x of the d_{xz} band and n_y of d_{yz} band vs. temperature for different values of SDW coupling from g_1 = 2.0598 to 2.0948.The occupation number of the band d_{yz} becomes greater than the occupation number of the d_{xz} band .This indicates that d_{yz} band lies below d_{xz} band.With increase of SDW coupling g_1 the occupation number of the charge carriers in both the bands are enhanced through out the temperature up to T_N .With increase of SDW coupling g_1 , T_N is also enhanced to higher values. Since occupation numbers n_x and n_y are neither equal to one(for metals at T=0K) and (zero for insulators at T=0K) ,the system represents a bad metal or poor insulator.

Fig. 3 shows the effect of doping and hence chemical potential. It is observed that with the increase of chemical potential the SDW transition temperature(T_N) is suppressed.This is shown in the inset of Fig. 3 showing how T_N decrease with increase in doping as observed in experiments [20].

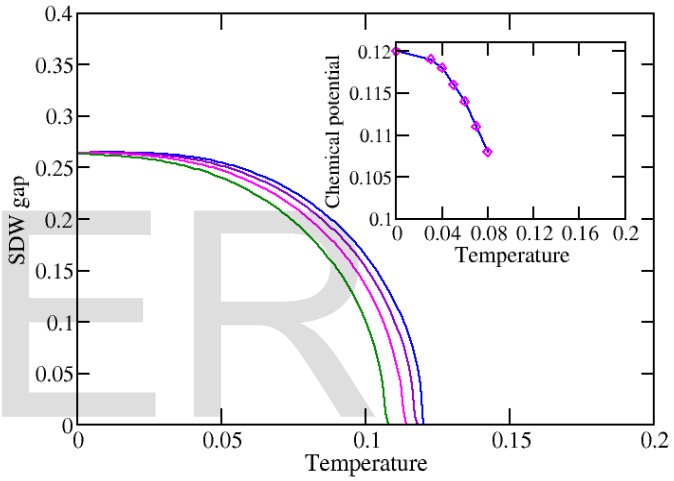

Fig. 3 The plot of SDW gap, z_1 (dimensionless form) vs. temperature , t (dimensionless form) with different values of chemical potential.

Fig. 4 shows the plot of the conduction electron DOS vs. band energy in absence of SDW gap as shown by blue line . In this case electronic density of states is higher showing narrow peaks at energy $c_1 \approx -3.36$ and $c_2 \approx +2.8$. The plot of DOS vs. band energy in presence of SDW gap is shown by pink line. The DOS is suppressed considerably through out the energy range indicating the insulating character of SDW interaction . The sharp peaks at c_1 and c_2 split asymmetrically into two separate peaks by a gap of energy $2z_1$. Further the DOS shows a d-wave type V-shaped gap near the Fermi level E_F = 0.

Fig. 5 shows the plot of specific heat vs. temperture for different values of SDW coupling g_1= 2.0598,2.0738,2.0948 . A sharp specific heat jump appears near Neel temperature and this jump gradually decreases towards lower temperature.This type of specific heat jump is reported for LaOFeAs at Neel temperature T_N = 155K[13] . With increase of SDW coupling the Neel Temperatureis extended to higher temperatures

and results in higher values of specific heat jump.This indicates that the Sommerfeld co-efficient γ and hence the effective mass is enhanced in the SDW phase of the system.

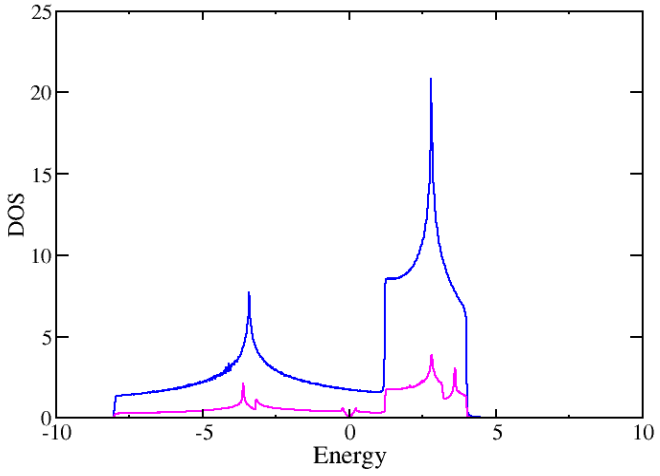

Fig. 4 The plot of the conduction electron DOS vs. energy for the fixed values of hopping integral at T = 0K.

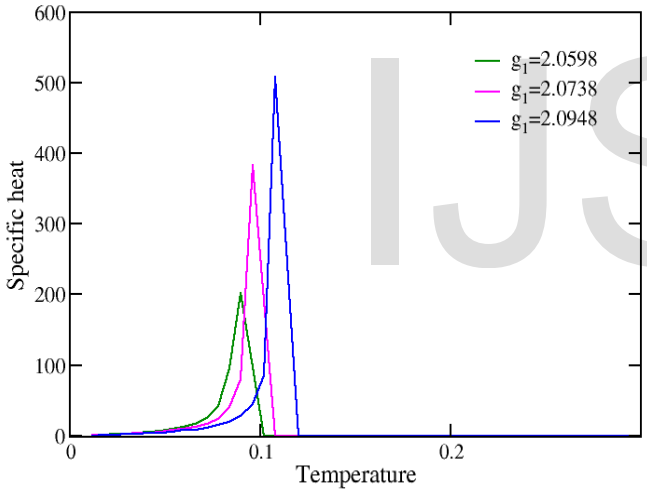

Fig. 5 The plot of specific heat vs. temperture for differentvalues of SDW coupling g_1= 2.0598,2.0738,2.0948 .

5 Conclusion

The present two band model including SDW interaction can explain qualitatively some experimental observations of iron-based superconductors.

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