Influence of Anisotropy in Coulomb Interaction on Density of Electronic States in Iron Pnictide Superconductors

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Abstract— The present work deals with the tight binding modeling and numerical computation of quasi-particles energy dispersion and density of electronic states (DOS), taking into account electronic correlations and Hund's coupling along with 3d orbitals (d_{xz}, d_{yz}) features governing the electronic properties in iron pnictides superconductors. The tight binding Hamiltonian containing the inter-band coupling, intra-band and inter band Coulomb correlations has been employed for two orbital per site and two tight binding band scenario. Employing, the Green's function equation of motion approach within BCS mean field approximation in superconducting state of iron pnictides. We have obtained the expression of different quasi-particle energies and electronic density of states as a function of various model tight binding parameters. The energy dispersion at different k point (Γ (0, 0), X (π, 0) and M (π, π)) of Brillouin zone is numerically computed. It is noticed that the behavior of electronic states is different at each k-point of the Brillouin zone and highly influenced by next nearest neighbor hopping and Coulomb correlation. Through computer stimulation, it is further predicted that inter-band Coulomb correlation establize the superconducting states and quasi-particle energy spectrum possess four quasi-particle energy branches which represent the splitting of electronic states within two band iron pnictides. On increasing the inter band correlation, the quasi-particle energy peak in the spectra show prominent features lying above and below the Fermi surface and support in establizing the superconducting state in the presence of anisotropic Coulomb correlation in iron pnictides. Finally, the theoretically obtained behavior of quasi-particle energies and density of states has been viewed in terms of recent photoemission ARPES and STM data in iron pnictide superconductors.

Keywords: Iron based superconductors, Spectral properties, Tight binding two band model Hamiltonian and onsite electronic correlation.

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1 INTRODUCTION

The discovery of superconductivity in iron oxypnictides ReFeAsO (Re=rare earth) with Tc = 26K [1] has open up a new vistas in research activities related to experimental and theoretical aspects of electronic properties of iron based superconductors. Till now, there have been two series of iron based superconductors: iron pnictides [1-8] and iron chacogenides [9-12]. Iron is known for its 3d-orbital electron originated ferromagnetic material, while iron pnictides are metallic with the co-existence of anti-ferromagnetic and superconducting phase, which further depends on doping level. The crystal structure of iron based superconductors have a common planer layer of Fe atoms in a two dimensional square lattice along with tetrahedral pnictides/chalcogenides.

To clarify the nature of superconducting state, the knowledge of the electronic band structure of these materials is of vital importance. The experimental Angle Resolved Photoemission Spectroscopy and Scanning Tunnel Microscopy (STM) studies have revealed the information about the nature of electronic states near the Fermi level, band dispersion, multipocket structure of the Fermi surface and nature of the isotropic superconducting gaps [13-16] in these systems. In iron pnictides the ARPES data predicted the existence of hole-like pocket centered at around the Γ (0, 0) point and electron like pocket at X (±π,0) or (0,±π) point of Brillouin zone. The theoretical scenarios [17-19] have emphasized

that the superconducting state of these materials exhibits a sharp peak in the electronic density of states close to Fermi level along with a dominant role of Fe-3d and As-4p orbitals hybridization. Further, it is also emphasized that all five 3d orbitals (i.e. d_{xy}, d_{x2-y2}, d_{xz}, d_{yz} and d_{3z2-r2}) states of Fe contribute significantly to the electronic states close to the Fermi level and influence electronic properties, and hence superconductivity in iron based superconductors. Further, the existence of intra and inter orbital electronic correlations and Hund's coupling due to tendency of electrons occupation in different orbitals in high spin state in these system has also been emphasized.

Recently, we have theoretically analyzed the spectral function within two orbitals (d_{xz}, d_{yz}) per site tight binding model for iron pinictide superconductors and pointed out that the Hund's coupling term tries to accumulate spectral weight close to Fermi level and support to stabilize superconducting state [20]. It has been further emphasized that the intra-band Coulomb correlations suppressed the spectral weight around the Fermi level. The theoretical attempts [21] analyzed the band structure of LaFeAs(O, F) system by employing random phase approximation and revealed that d_{xz} / d_{yz} orbitals mainly contribute to the electronic states close to point (0, 0) and (π, 0) of Brillouin zone. The recent high resolution scanning tunneling spectroscopic (STS) measurements,

have also analyzed the quasi-particle local density of states (LDOS) with atomic resolution as the tunneling conductance is directly proportional to the local density of states of electronic states. Recently, Parish et al. [22] analyzed the LDOS as a function of doping and pointed out a fully gapped to gapless behavior with S_{x2-y2} pairing symmetry in these systems.

Therefore, in the light of above facts, it is interesting to theoretically analysis of quasi-particle energies spectrum and density of electronic states in iron pnictide superconductors as a function of Fe 3d orbitals (d_{xz}/d_{yz}) coupling, intra and inter band electronic interactions and Hund's coupling energy to pinpoint the nature of superconducting states close to Fermi level and hence underline their electronic properties. In the proceeding subsection, the theoretical formalism of quasi-particle energy dispersions and electronic density of states within tight binding two band model Hamiltonian with two d-orbitals per sites i.e. d_{xz} and d_{yz} in iron pnictide superconductors is presented.

2. THEORETICAL FORMALISM

The LaFeAsO (1111) iron based superconductor, where LaO and FeAs layers are stacked alternately in 2D square lattice. The Fe atoms are in a fourfold coordination taking shape of a $FeAs_4$-tetrahedron. The Fe atoms form square net with a Fe-Fe distance of approximately 2.8$\overset{\circ}{A}$ [18] as shown in figure [1]. We have considered two bands model characterized by d_{xz} and d_{yz} orbitals per Fe site. Both orbitals d_{xz} and d_{yz} dominate electronic states near the Fermi surface (E_F) in comparison to other orbitals. One can write the model Hamiltonian for pnictide superconductors within two band scenario in the following form [20]:

$$H = H_0 + H_{intra} + H_{inter} \quad (1)$$

Here $$H_0 = \sum_{r,k,\sigma} \varepsilon_{rk} C^+_{rk,\sigma} C_{rk,\sigma}$$

$$H_{intra} = \sum_{r,kk',\sigma} U_{kk'} C^+_{rk\sigma} C^+_{r-k-\sigma} C_{rk'\sigma} C_{r-k'-\sigma} + U' \sum_{r,kk',\sigma} n_{rk\sigma} n_{rk'-\sigma}$$

$$H_{inter} = \sum_{\substack{r\neq s,k,\sigma \\ 1,2}} \varepsilon_{rsk} \left(C^+_{rk\sigma} C_{sk\sigma} + C^+_{sk\sigma} C_{rk\sigma} \right) + U'' \sum_{\substack{r\neq s \\ kk',\sigma}} n_{rk\sigma} n_{sk'-\sigma}$$
$$+ J_H \sum_{r\neq s} \sum_{\substack{kk' \\ \sigma}} \left(C^+_{rk\sigma} C^+_{r-k-\sigma} C_{s-k'-\sigma} C_{sk'\sigma} + h.c \right)$$

Where, r and s denotes two band (1 and 2), and h.c means Hermitian conjuate. The $n_{rk\sigma} = C^+_{rk\sigma} C_{rk\sigma}$ and

$n_{rk-\sigma} = C^+_{rk-\sigma} C_{rk-\sigma}$, represents the occupation number of the electronic band states of rth band with momentum (k) and spin (ζ). $C_{rk\sigma} \left(C^+_{rk\sigma} \right)$ is the annihilation (creation) operator of electrons with spin ζ and momentum (k) in each bands. Here, $U_{kk'}$ is the effective BCS attractive interaction within each band. The ε_{rsk} is the term taking care of hybridization of electronic states of two bands. U' and U'' are intra-band and inter-band Coulomb repulsions between electrons, which describe the on-site electronic interaction, respectively. The term J_H represents Hund's coupling energy in Fe 3d orbitals [20].

To study the quasi-particle energy spectrum with above (equation (1)) tight binding two bands Hamiltonian model for iron pnictide superconducting system, we have employed Green's function equation of motion approach [20] and finally obtained following desirable Green function $G_{11}(k,\omega) = \langle\langle C_{1k\sigma} | C^+_{1k\sigma} \rangle\rangle$:

$$G_{11}(k,\omega) = \frac{\begin{bmatrix} \left\{\omega^2 - (\varepsilon_2 + U'\langle n_2\rangle + U''\langle n_1\rangle)^2 - (\Delta_k + \Delta_H)^2 - \varepsilon_{12}^2\right\} \\ \left\{\omega + (\varepsilon_1 + U''\langle n_2\rangle + U'\langle n_1\rangle)\right\} + \\ \varepsilon_{12}^2\left\{\varepsilon_1 + \varepsilon_2 + (U' + U'')(\langle n_1\rangle + \langle n_2\rangle)\right\} \end{bmatrix}}{2\pi \begin{bmatrix} \left\{\omega^2 - (\varepsilon_2 + U'\langle n_2\rangle + U''\langle n_1\rangle)^2 - (\Delta_k + \Delta_H)^2 - \varepsilon_{12}^2\right\} \\ \left\{\omega^2 - (\varepsilon_1 + U'\langle n_1\rangle + U''\langle n_2\rangle)^2 - (\Delta_k + \Delta_H)^2 - \varepsilon_{12}^2\right\} - \\ \varepsilon_{12}^2\left\{\varepsilon_1 + \varepsilon_2 + (U' + U'')(\langle n_1\rangle + \langle n_2\rangle)\right\}^2 \end{bmatrix}} \quad (2).$$

By using simple algebra, one can rewrite the above Green's function in standard form:

$$G_{11}(k,\omega) = \frac{1}{2\pi}\left[\frac{A_{1k}}{(\omega - E^+_{1k})} + \frac{A_{2k}}{(\omega - E^-_{1k})} + \frac{A_{3k}}{(\omega - E^+_{2k})} + \frac{A_{4k}}{(\omega - E^-_{2k})} \right]. \quad (3)$$

Where, E_{1k} and E_{2k} represent quasi-particle energies with the two orbital per Fe site in iron pnictide superconductor are given as follows:

$$E^\pm_{1k} = \pm \left(\sqrt{ \frac{\begin{matrix} \left\{(\varepsilon_2 + U'\langle n_2\rangle + U''\langle n_1\rangle)^2 + (\varepsilon_1 + U'\langle n_1\rangle + U''\langle n_2\rangle)^2 + 2(\Delta_k + \Delta_H)^2 + 2\varepsilon_{12}^2\right\} + \\ \left\{\varepsilon_1 + \varepsilon_2 + (U' + U'')(\langle n_1\rangle + \langle n_2\rangle)\right\}\sqrt{\left\{\varepsilon_2 - \varepsilon_1 + (U'' - U')(\langle n_1\rangle - \langle n_2\rangle)\right\}^2 + 4\varepsilon_{12}^2} \end{matrix}}{2} } \right), \quad (4)$$

$$E^\pm_{2k} = \pm \left(\sqrt{ \frac{\begin{matrix} \left\{(\varepsilon_2 + U'\langle n_2\rangle + U''\langle n_1\rangle)^2 + (\varepsilon_1 + U'\langle n_1\rangle + U''\langle n_2\rangle)^2 + 2(\Delta_k + \Delta_H)^2 + 2\varepsilon_{12}^2\right\} - \\ \left\{\varepsilon_1 + \varepsilon_2 + (U' + U'')(\langle n_1\rangle + \langle n_2\rangle)\right\}\sqrt{\left\{\varepsilon_2 - \varepsilon_1 + (U'' - U')(\langle n_1\rangle - \langle n_2\rangle)\right\}^2 + 4\varepsilon_{12}^2} \end{matrix}}{2} } \right), \quad (5)$$

The above equations (4) and (5) show that there are total four branches of quasi-particle energies but they are equivalent to two by two and depend on various model parameters of the model Hamiltonian. Further, one can obtain spectral function $A(k, \omega)$ [20] and hence density of states from above Green's function using following relationship:

$$A_{11}(k,\omega) = -\frac{1}{\pi} \text{Im} G_{11}(k,\omega), \quad (6)$$

Where, Im stands for imaginary part of Green's function $G_{11}(k,\omega)$. We obtained final expression for spectral function by using equation (6) as follows:

$$A_{11}(k,\omega) = \frac{1}{\pi} \sum_{i=1}^{4} A_i \delta(\omega - E_i). \quad (7)$$

Here, spectral function ($A_{11}(k,\omega)$) contain δ- function which is just equivalent to broadening of the quasi-particle peak and one need to solve this δ- function. For this purpose, we have considered Lorentzian type of broadening and used the following approximation:

$$\delta\left(\omega\pm E_i\right) \approx \underset{\Gamma\to 0}{Lim}\frac{\Gamma}{\pi}\frac{1}{\Gamma^2 + \left(\omega\pm E_i\right)^2} \qquad . \qquad (8)$$

Here, broadening factor Γ is taken to be independent of momentum k and energy ω for simplicity. From above equation (6), one can calculate the density of states for two band iron pnictide superconducting systems at zero temperature by using the following relation:

$$N(\omega) = \int\limits_{-\pi}^{\pi}\ \int\limits_{-\pi}^{\pi} A_{11}(k,\omega)\,\mathrm{d}\left(k_x\right)\mathrm{d}\left(k_y\right). \quad (9)$$

From above Equation (9), one can analyze the influence of next neighbor energy, intra and inter-orbital Coulomb correlations on DOS in tight binding two band iron pnictides using numerical computation. In the preceding section, we have presented our numerical computation of theoretically obtained expression of density of electronic states $N(\omega)$ and nature of quasi-pariticle energies in iron pnictides.

3. RESULTS AND DISCUSSION

We have performed numerical computation and depicted the systematic diagram of band structure in two band iron pnictide system along with various values of next nearest neighbor hopping between (d_{xz} /d_{yz}) orbitals (t_3=-0.025eV and,-0.035) for different Γ (0, 0), X(π, 0) and M(π, π) points of Brillouin zone in figure 2(a). This figure clearly indicate that on increasing t_3, the quasi-particle energy bands get shifted far away from the Fermi surface at all above points of Brillouin Zones. Also corresponding to E_2 branch of quasi-particles, on increasing t_3, energy gap decreases at the Fermi surface at X(π,0) point of Brillouin Zones. One can also see a broad feature with higher binding energy dispersion close to M(π, π) point of Fermi surface. In figure (2b), we present the variation of density of states $N(\omega)$ versus energy(ω) for different values of next nearest neighbor hopping between orbitals of d_{xz} /d_{yz} (t_3=-0.025eV and -0.035) in extended s- wave pairing symmetry and we have kept all other parameters (t_1=-0.01eV, t_2= 0.04eV, t_4=-0.01eV, Δ_0=0.02eV, Δ_{ak}=$\Delta_0\cos(k_x)\cos(k_y)$, U=-0.4eV, U'=0.6eV, U''=0.2eV, J_H=-0.25eV, <n>=0.05, ε_{12}= 0.04eV, and Γ=0.015eV) fixed. Also, we have assumed uniform carrier density in each band (i.e. $\langle n_1\rangle = \langle n_2\rangle = \langle n\rangle$). It is clear from Fig. 2(b) that on increasing t_3, both the spectral peaks above and below the Fermi level show sharp increase in the spectral weight and the energy at the peak value of spectral weight remains unaltered. Further, it is also important to note that four quasi-particle energy branches represents splitting of two spectral bands below and above the Fermi surface, respectively. These results are in qualitative agreement with existing scanning tunneling results (STM) [23], where two pair of quasi-particle peaks in LDOS are predicted.

In fig 3(a), we have shown the variation of quasi-particles energy (E) along with momentum (k) for intra-band and inter-band correlations (U'=0.6eV, U'' =0eV and U'=0.6eV, U'' =0.2eV). On increasing the interband correlations, the energy bands get shifted far from the Fermi level at each point of BZ corresponding to quasi-particle energy branch E_1. Quasi-particle energy bands represent

higher dispersive energy at M (π, π) point of Brillouin zone corresponding to energy branch E_1. While corresponding to energy branches $E_{2k}{}^{+}$ and $E_{2k}{}^{-}$, energy bands becomes close to Fermi level at electron pocket X (π, 0) point of Brillouin zone.

The variation of the density of states $N(\omega)$ versus energy (ω) for interband correlations (U'=0.6, U'' =0eV and U'=0.6, U'' =0.2eV) in extended s- wave pairing scenario is shown in figure (3b). Further during the numerical computation, we have kept all other parameters fixed (t_1=-0.01eV, t_2= 0.04eV, t_3= -0.03eV, t_4=-0.01eV, Δ_0=0.02eV, Δ_{ak}=Δ_0 $\cos(k_x)\cos(k_y)$, U=-0.4eV, J_H=-0.25eV, ε_{12}= 0.04eV, and Γ=0.015eV). Also a uniform carrier density in each band (i.e.$\langle n_1\rangle = \langle n_2\rangle = \langle n\rangle$)) is assumed. It is clear from figure (3b) that on increasing the anisotropy in inter-band Coulomb correlations (U''), the quasi-particle energy peaks in the spectra show prominent feature both above and below the Fermi surface and indicate a clear superconducting gap at the Fermi level in the presence of anisotropy in Coulomb correlation in iron pnictides. These results are viewed in term of STM results in iron pnictides and show a gapped to gapless behavior in spectra at Fermi level as observed [22, 24-25]. One can also observed there is two separated quasiparticle peaks above and below the Fermi level. It will be interested to extend theses studies for using different carrier density i.e. for case $\langle n_1\rangle \neq \langle n_2\rangle$ and including other 3d-orbitals to improve the results cited here in iron pnictides.
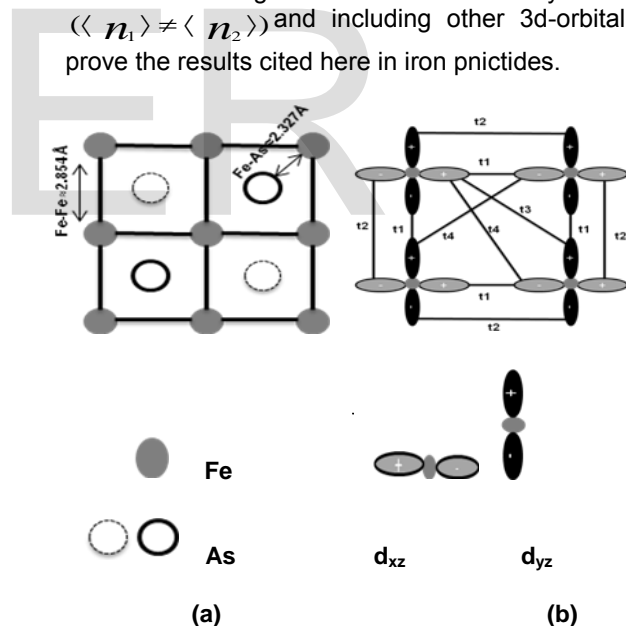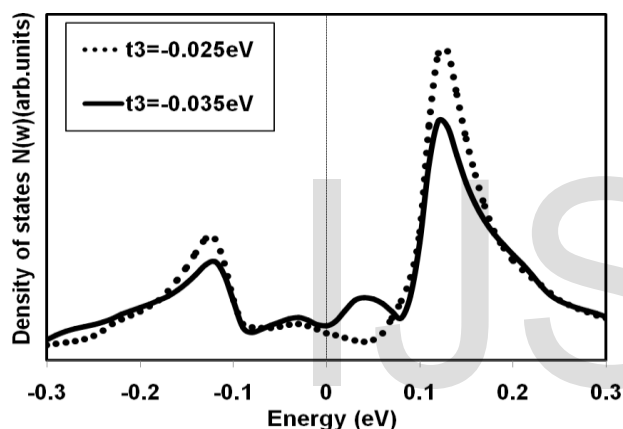

Fig.1 (a) The Fe ions form a square lattice and unit cell contains two Fe and two As ions are shown. **(b)** A schematic diagram of two orbital (d_{xz} and d_{yz}) model on Fe square lattice with hopping amplitude.

2(a)

2(b)

3(a)
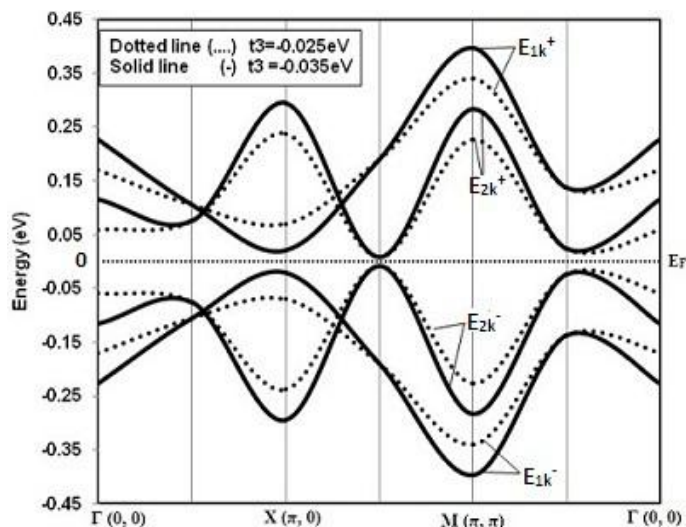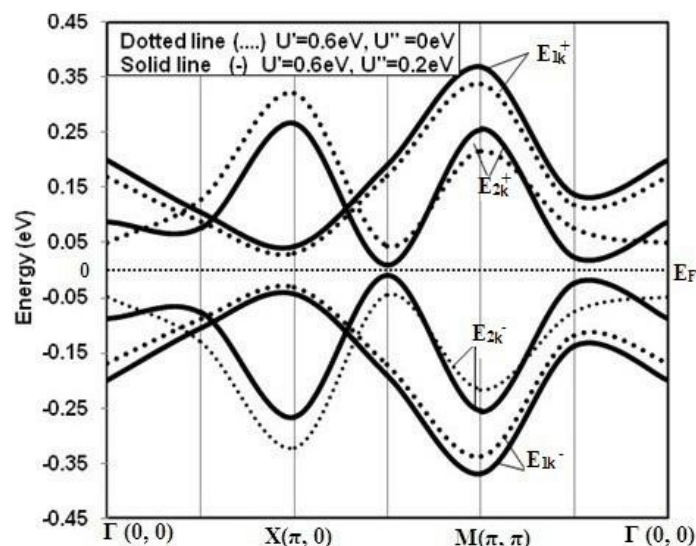
3(b)

Fig. 2 (a) The band structure of two band iron pnictide system for different value of next nearest neighbor hopping (t_3=-0.025eV, -0.035eV) at Γ (0, 0), X (π, 0), M(π, π) points of Brillouin zone. **(b)** Density of states N(ω) versus Energy(ω) for different value of next nearest neighbor hopping (t_3=-0.025eV and -0.035eV) in extended s- wave pairing symmetry and keeping (t_1=-0.01eV, t_2= 0.04eV, t_4=-0.01eV, Δ_0=0.02eV, Δ_{ak}=Δ_0 cos(k_x) cos(k_y), U=-0.4eV, U'=0.6eV, U''=0.2eV, J_H=-0.25eV, <n>=0.05, ε_{12}= 0.04eV, and Γ=0.015eV) as fixed, respectively.
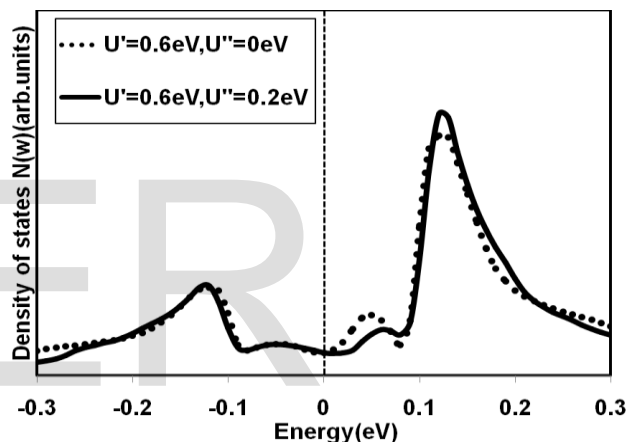
Fig. 3 (a) The band structure of two band iron pnictide system for different intraband and interband correlations (U'=0.6, U'' =0eV and U''=0.2eV) at Γ (0, 0), X(0,π) and (π,0) , M(π, π) point of Brillouin zone. **(b)** Density of states N(ω) versus Energy(ω) for (U'=0.6, U'' =0eV and U''=0.2eV) in extended s- wave pairing and keeping (t_1=-0.01eV, t_2=0.04eV, t_3=-0.03eV, t_4=-0.01eV, Δ_0=0.02eV, Δ_{ak}=Δ_0 cos(k_x) cos(k_y), U=-0.4eV, J_H=-0.25eV, ε_{12}= 0.04eV, <n>=0.05and Γ=0.015eV) as fixed, respectively.

References

[1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc 130, 3296 2008.

[2] H. Takahashi, K. Igawa, K. Arii, Y. Kamihara, M. Hirano, and H. Hosono, Nature 453, 376 2008.

[3] X. H. Chen, T. Wu, G. Wu, R. H. Liu, H. Chen, and D. F. Fang, Nature 453, 761 2008.

[4] A.S. Sefat, R. Jin, M. A. McGuire, B. C. Sales, D.J. Singh, and D. Mandrus, Phys. Rev. Lett. 101, 117004 2008.

[5] M. Rotter, M. Tegel, and D. Johrendt, Phys. Rev. Lett. 101, 107006 2008.

[6] T. Hanna, Y. Muraba, S. Matsuishi, N. Igawa, K. Kodama, S.I. Shamoto , and H .Hosono, Phys. Rev. B 84, 024521 2011.

[7] X.C. Wang, Q.Q. Liu, Y.X. Lv, W.B. Gao, L.X. Yang, R.C Yu, F.Y. Li, and C.Q. Jin, Solid State Communications 148, 538 2008.

[8] X. Zhu, F. Han, G. Mu, B. Zeng, P. Cheng, B. Shen, and H.-H. Wen, Phys. Rev. B 79, 024516 2009.

[9] Y. Mizuguchi, F. Tomioka, S. Tsuda, and T. Yamaguchi, Appl. Phys. Lett. 93, 152505 2008.

[10] T. M. McQueen, Q. Huang, V. Ksenofontov, C, Felser, Q. Xu, H. Zandbergen, Y.-S. Hor, J. Allred, A. J. Williams, D. Qu, J. Checkelsky, N. P. Ong, and R. J. Cava, Phys. Rev. B 79, 014522 2009.

[11] K. Horigane, N. Takeshita, C.-H. Lee, H. Hiraka, and K. Yamada, J. Phys. Soc. Jpn.78, 063705 2008.

[12] X.-W, Yan, M, Gao, Z.-Y, Lu, and T. Xiang, Phys. Rev. B 84, 054502 2011.

[13] D.V. Evtushinsky, D.S. Inosov, V.B. Zabolotnyy, A. Koitzsch, M. Knupfer, B. Büchner, M.S. Viazovska, G.L. Sun, V. Hinkov, A.V. Boris, C.T. Lin, B. Keimer, A. Varyk-halov, A.A. Kordyuk, S.V. Borisenko, Phys. Rev. B 79, 054517 2009.

[14] D. H. Lu, M. Yi, S.-K. Mo, A. S. Erickson, J. Analytis, J.-H. Chu, D. J. Singh, Z. Hussain, T. H. Geballe, I. R. Fisher, Z. X. Shen, *Nature* 455, 81-84 2008.

[15] H. Ding, P. Richard, K. Nakayama, K. Sugawara, T. Ara-kane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Ta-kahashi, Z. Wang, X. Dai, Z. Fang, G. F. Chen, J. L. Luo, N. L. Wang Europhys. Lett. 83, 47001 2008.

[16] F. Chen, B. Zhou, Y. Zhang, J. Wei, H.-W. Ou, J.-F. Zhao, H. Cheng, Q.-Q. Ge, M. Arita, K. Shimada, H. Namatame, M. Taniguchi, Z.-Y. Lu, J. Hu, X.-Y. Cui, D. L. Feng, Phys. Rev. B 81, 014526 2010.

[17] D. J. Singh, L. Boeri, K. Koepernik, I. I. Mazin, M. D. Jo-hannes, Phys. Rev. B 78, 085104 2008.

[18] D. J. Singh, M.-H. Du, Phys. Rev. Lett. 100, 237003 2008.

[19] E. Akturk, S. Craci, Phys. Rev. B 79, 184523 2009.

[20] L. Rani, Ajay, J. Supercond. Nov. Magn. 26, 527-538 2013.

[21] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Konta-ni, H. Aoki, Phys. Rev. Lett. 101, 087004 2008.

[22] M.M. Parish, J. Hu, B. Andrei Bernevig, Phys Rev. B 78, 144514 2008.

[23] T. Hanaguri, K. Kitagawa, K. Matsubayashi, Y. Mazaki, Y. Uwatoko, H. Takagi, Phys Rev. B 85, 214505 2012.

[24] N-C. Yeh, M.L. Teaague, B. Shen, H-H. Wen, arXiv: 1107. 0697 2011.

[25] M. L. Teague, G. K. Drayna, G. P. Lockhart, P. Cheng, B. Shen, H.-H. Wen, N.-C. Yeh, Phys. Rev. Lett. 106, 087004 2011.