Orissa Journal of Physics
ISSN 0974-8202

Vol. 26, No.1
February 2019
pp. 65-72

# Theoretical Model Study of Superconductivity of 122 type Iron-based Superconductors

S S JENA[1], S K AGARWALLA[1] and G C ROUT[2*]

[1] Dept of Applied physics and Ballistics, F.M.University, Balasore 756019, Odisha, India.
[2*]Physics Enclave, Plot No.664/4825, Lane-4A, Shree Vihar, Post: Patia, Bhubaneswar-751031, Odisha, India.
[1]Email: jena.sushreesangita93@gmail.com, [2*]E-mail: profgcrout@gmail.com

*Received: 28.11.2018* ; *Revised : 15.12.2018* ; *Accepted : 3.1.2019*

**Abstract.** We propose here a tight-binding model study of iron-based superconductors taking a one band model approach with the two different electron hopping integrals. Further the superconducting gap in this system is considered using three different pairing symmetries like $s_{\pm}$-wave, d-wave and s-wave. The total Hamiltonian is solved by Zuvarev's Green's function technique and the quasi-particle bands are calculated for the superconducting system. The electron DOS which is proportional to experimentally observed tunneling spectra is calculated from the imaginary part of the electron Green's function. The electron density of states (DOS) is computed numerically taking total Brillouin zone of the system. The electron DOS exhibits asymmetric gap structure with a V-shaped gap with a node for $s_{\pm}$-wave and d-wave, while it shows asymmetric U-shaped gap for s-wave. Finally the computed electron specific heat exhibits a sharp jump near the superconducting transition temperature.

**Keywords:** Iron-based superconductors, tunneling spectra, specific heat

**PACS Numbers:** 74.25.Jb**,** 68.37.Ef, 74.25.Bt

## 1. Introduction

The discovery of superconductivity in Fe-based oxypnictide LaFeAsO of the type-1111 with critical transition temperature $T_C$ = 26 K has inspired worldwide interests [1]. After that a series of superconducting materials with FeAs-layer were discovered: such as $AFe_2As_2$ (type 122 with A= K, Na, Rb) and $RFe_2As_2$ (type 122 with R = Ca, Ba, Sr) [2-4]. Upto now, the highest reported transition temperature $T_C$ = 50 K for iron-based superconductivity was achieved in SMFeAsO and the superconductivity in the iron based materials is

unconventional and non-BCS type [5-7]. The superconductivity at $T_C$ = 30 K in FeSe-layer compound $K_{0.8}$ $Fe_2As_2$ have reported by Guo et. al. [8]. The angle resolved photoemission spectroscopy (ARPES) experiments [9-15] and Local density approximation (LDA) calculations [16-18] have reported that only the electron Fermi surface (FS) pocket exists, but the hole Fermi surface disappears. This compound may be heavily electron doped superconducting material. Upto now the pairing is still unclear for the systems and $d_{x^2-y^2}$-wave, $s_{\pm} = s_{x^2y^2}$-wave and s-wave pairing symmetries have been proposed [19-27]. The band structure calculations [16, 18] of the compounds show that all the five 3d orbitals of iron atoms hybridize strongly to contribute to the electronic density of states. To simplify the problem, a two band model has proposed by Raghu. et. al. [28, 29]. We report here a one band tight binding model for the conduction band and superconducting interaction for different pairing symmetries for pnictide systems to study the temperature dependent superconducting (SC) gap and tunneling conductance spectra measured by scanning tunneling microscopy (STM).

The role of SDW [30], Jahn Teller (JT) distortion [31] and interplay of JT effect and superconductivity in Fe-based superconductors within one band model approach has reported by Jena. et. al. [32]. Recently Jena. et. al. have reported the tight-binding study of lattice distortion and the tunneling spectra within two band model approach [33, 34]. More Recently Jena. et. al. have reported the theoretical study of the interplay of the structural distortion and the superconductivity (SC) with s± pairing symmetry and the anisotropic tunneling conductance spectra [35, 36]. In the present communication, we present here the theoretical study of the superconductivity of the 122-type iron-based systems and interpretation of the experimentally observed tunneling spectra. Here we present the model Hamiltonian in section 2, calculation of SC gap and electron density of states (DOS) in section 3. Results and discussion in section 4 and the conclusion in section 5.

## 2. Hamilton Model

It is reasonable to believe that the electronic bands crossing the Fermi surface (FS) are essential for constructing a minimal tight binding model, while all other bands that do not cross the Fermi energy may be neglected. The unit cell of the system consists of two iron atoms. Only one kind of FS pocket around the Fermi level and its symmetric points are actually relevant in the Brillouin zone. We consider the one band model in the presence of the superconductivity for the Fe-based 122-types systems. The tight binding model Hamiltonian for the degenerate $d_{xz}$ and $d_{yz}$ orbitals of iron atom is written as

$$\mathbf{H} = \sum_{\mathbf{k},\boldsymbol{\sigma}} \boldsymbol{\varepsilon}_{\mathbf{k}}\ \mathbf{C}^{+}_{\mathbf{k},\boldsymbol{\sigma}}\,\mathbf{C}_{\mathbf{k},\boldsymbol{\sigma}} + \sum_{\mathbf{k}}\ \Delta(\mathbf{k})\,(\mathbf{C}^{+}_{\mathbf{k}\uparrow}\,\mathbf{C}^{+}_{-\mathbf{k}\downarrow} + \mathbf{C}_{-\mathbf{k}\downarrow}\mathbf{C}_{\mathbf{k}\uparrow}) \quad (1)$$

where $\varepsilon_k$is the single band dispersion within tight-binding approximation in the Fe-As square lattice. The band energy for this single band model of the iron based superconductor is given by,

$\varepsilon_k = -2t_1(\cos kx + \cos ky) - 42t_2 \cos kx\ \cos ky$where $t_1$ and $t_2$ are respectively the nearest- and the next-nearest-neighbor hopping integrals of electrons in the square lattice and kx and ky are the components of the electron momentum $\vec{k}$.

The momentum dependent superconducting (SC) gap $\Delta(\mathrm{k})$ in the Fe-As plane is written as,

$$\Delta(\mathrm{k}) = \sum_{\acute{\mathrm{k}}} \mathrm{V}\,(\mathrm{k}-\acute{\mathrm{k}})\ \langle \mathrm{C}^{+}_{\acute{\mathrm{k}}\uparrow}\,\mathrm{C}^{+}_{-\acute{\mathrm{k}}\downarrow}\rangle \quad (2)$$

where $\mathrm{V}\left(\mathrm{k}-\acute{\mathrm{k}}\right) = -\mathrm{V}_0\,\mathrm{f}\left(\acute{\mathrm{k}}\right)\mathrm{f(k)}$ is the momentum dependent effective Coulomb potential responsible for the formation of the Cooper pairs, where f(k) is defined below. There are three kinds of pairing symmetries namely SC gap $\Delta_k = \Delta_0(\mathrm{T})\mathrm{f(k)}$, where $\mathrm{f(k)} = \cos \mathrm{kx} - \cos \mathrm{ky}$ for the d-wave pairing symmetry, $\mathrm{f(k)} = (\cos \mathrm{kx} \times \cos \mathrm{ky})$ for the $s_{\pm}$-wave pairing symmetry and f(k) = 1 for the isotropic $s_0$-wave pairing symmetry.

## 3. Calculation of SC Gap and electron DOS

We have calculated the electron Green's functions for the Hamiltonian using Zuvarev's Green's function technique [37].

The coupled equations are solved and written as,

$$A_1(k,\omega) = \langle\langle \mathrm{C}_{\mathrm{k}\uparrow};\ \mathrm{C}^{+}_{\mathrm{k}\uparrow}\rangle\rangle_{\omega} = \frac{1}{2\pi}\frac{\omega+\varepsilon_k}{(\omega^2-\omega_k^2)} \quad (3)$$

$$A_2(k,\omega) = \langle\langle \mathrm{C}^{+}_{-\mathrm{k}\downarrow};\ \mathrm{C}^{+}_{\mathrm{k}\uparrow}\rangle\rangle_{\omega} = \frac{1}{2\pi}\frac{\Delta(\boldsymbol{k})}{(\omega^2-\omega_k^2)} \quad (4)$$

where the two quasi-particle bands are written as, $\omega_k = \pm\sqrt{\varepsilon_k^2 + \Delta^2(k)}$.From the correlation functions calculated from the Green's function in eqn. (4), the temperature dependent SC gap parameter is calculated as given below.

$$\Delta(\mathrm{k}) = \sum_{\acute{\mathrm{k}}} \mathrm{V}\,(\mathrm{k}-\acute{\mathrm{k}})\ \left[\frac{\Delta(\acute{\mathrm{k}})}{2\omega_{\acute{k}}}\right]\tanh\left(\frac{1}{2}\beta\omega_{\acute{k}}\right) \quad (5)$$

The electron momentum spans over the Brillouin zone in the two-dimensional square lattice. The summation appears as $\sum_k \rightarrow$

$\frac{S}{(2\pi)^2}\int\int dk_x dk_y$where 'S' is the area of the square lattice. The integration is carried out for 100×100 grid points of the kx and ky component of the electron momentum. The electron DOS describes the tunneling spectra of the iron-based superconductor. The electronic DOS is defined as,

$$DOS = -2\pi \sum_{k,\sigma} [Im\, A\,(k, \omega + i\eta)] \quad (6)$$

where $\eta$ is the small spectral width assigned to the frequency $\omega$ and $A\,(k, \omega)$ is the electron Green's function given in equation (3). After evaluating the imaginary part of $A\,(k, \omega)$ from equation (3), the DOS reduces to,

$$DOS = 2 \times \frac{S}{(2\pi)^2} \times \int_0^{2\pi}\int_0^{2\pi} dk_x\, dk_y \left\{\frac{(\omega+\varepsilon_k)2\eta\omega}{(\omega^2-E_k^2-\eta^2)+4\eta^2\omega^2}\right\} \quad (7)$$

Here we have converted the summation over 'k' into integral relation in the momentum x and y-plane of the electron momentum. Here '2' appear for the two spin orientation of the orbital and 'S' is the area of the unit cell in the real space. The dimensionless parameters (scaled by nearest neighbour-hopping parameter $t_1$ = 0.2 eV) are written as: the second-nearest-neighbor hopping integral t2 = -2.25 in terms of t1, superconducting (SC) gap z = $\Delta_0$(T)/t1(with temperature dependent gap $\Delta_0$(T) ), temperature t = $k_BT/t1$ and the SC coupling g = $V_0$/t1 (with $V_0$ as the momentum independent effective Coulomb energy) and band energy C = ω/t1.

## 4. Results and Discussion

The superconducting gap equation written in equation (5) is solved self-consistently and numerically employing three different pairing symmetries by taking 100 × 100 grid points of the electron momentum in the xy-plane. The physical parameters are scaled with respect to the nearest neighbor electron hopping integral t1 taking into account of the SC transition temperature $t_c \approx 30$ K appropriate for the $AFe_2As_2$ type superconductors [2-4].

The superconducting gap parameter is calculated at temperature t = 0.1 from temperature-dependent SC gap. The electron DOS for the system is directly proportional to the tunneling conductance of the system. Therefore, we have calculated electron DOS from the imaginary part of the Green's function written in equation (3) and computed it numerically at a temperature t = 0.1 for different pairing symmetries. The different SC couplings are $gs_{x^2y^2}$ = 21.45 for $s_{\pm}$-wave pairing symmetry, $gd_{x^2-y^2}$ = 3.49 for d-wave pairing and $gs_0$ = 1.92 for $s_0$-wave pairing symmetry. Taking the SC gap parameter at temperature t = 0.1 the DOS is plotted as shown in figure 1. The figure 1 shows V-shaped SC gap for $s_{\pm}$-wave

and d-wave pairing symmetries with asymmetric DOS, while the $s_0$-wave pairing shows U-shaped gap near the Fermi surface.

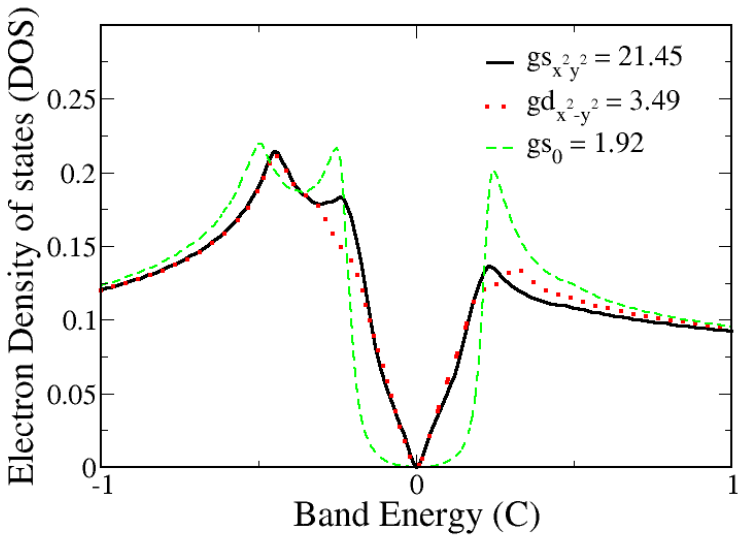


**Fig.1.** shows the plot of density of states (DOS) vs. band energy (C) for all different waves without chemical potential (μ), t1 = 1, t2 = -2.25.

The figure 2 shows the effect of hopping integral dependant electron DOS for $s_{\pm}$-wave pairing. For second-nearest-neighbor electron hopping integral t2 = -2.25, in absence of nearest-neighbor electron hopping (t1 = 0), the DOS shows near the U-shaped gap to a very strong asymmetry in it. For nearest-neighbor electron hopping t1 = 1, in absence of second-nearest-neighbor electron hopping integral (t2 = 0), the DOS exhibits an asymmetric gap and the electron density below the Fermi surface becomes more as compared to above it. Finally the electron density is plotted in presence of t1 and t2 which shows two gap structures with reduced asymmetric structure. However, the DOS exhibits a small V-shaped gap near the Fermi surface with a node [38].

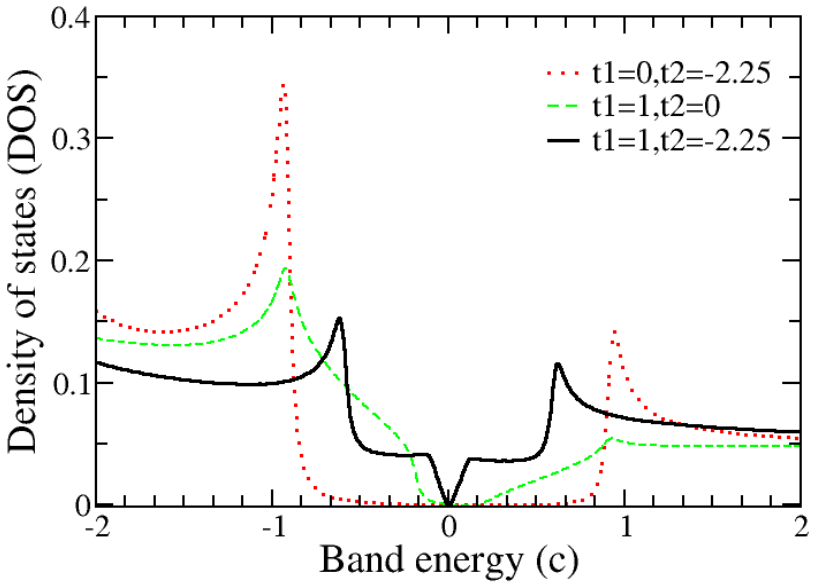


**Fig. 2.** shows the plot of density of states (DOS) vs. band energy (C) for $s_{\pm}$-wave of different values of t1 and t2 all are in one, gs = 21.45, μ =2.2.

We have framed the free energy of the system from which we have calculated numerically the temperature dependent entropy and electron specific heat for the system. We have computed the electron specific heat for different values of SC couplings for $s_{\pm}$-wave pairing symmetry, which is very often observed in iron-based superconductor. In figure 3 we show the temperature dependent electron specific heat for SC couplings gs = 20, 21 and 21.45. For gs = 20, we observe that the electron specific heat nearly increases linearly with temperature at low temperatures and finally exhibits a sharp jump at SC transition temperature at $t_C$ = 0.075. When gs is increased, we observe similar temperature dependence of electron specific heat. However, the specific heat jump is shifted to higher temperatures with higher specific heat jump at SC transition temperature. The specific heat becomes very very small beyond SC transition temperature.

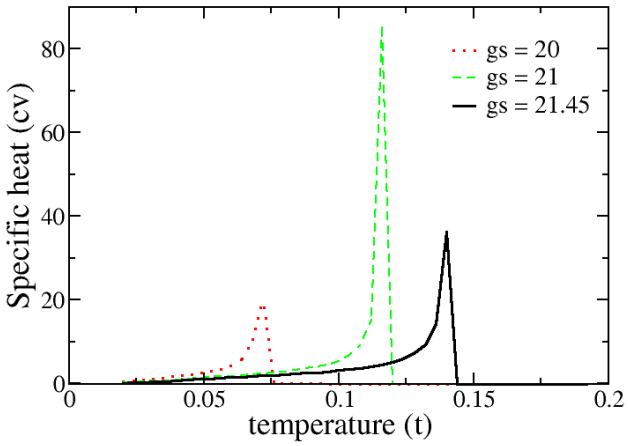


**Fig. 3.** shows the plot of specific heat ($C_v$) vs. temperature (t) for different values of superconducting coupling for $s_{\pm}$ wave, t1 = 1, t2 = -2.25.

## 5. Conclusions

We have proposed a tight-binding model study of superconductivity gap taking three different types of pairing symmetries for 122-types systems in electron DOS using Zuvarev's Green's function technique. We observe V-shaped SC gap for $s_{\pm}$-wave pairing symmetry and d-wave pairing symmetry and U-shaped gap for s-wave pairing symmetry. In all these cases, we observe asymmetric electron DOS. The two gap structure in the DOS arises due to two different hopping integrals. Finally electron specific heat exhibits a very sharp jump at SC transition temperature.

## References

[1] Y Kamhira et. al., *J. Am. Chem. Soc.***130,** 3296 (2008)

[2] K Sasmal et. al., *Phys. Rev. Lett*. **101.** 107007 (2008)

[3] F Han, H H Wen et. al., *Phys. Rev. B* **80**, 024506 (2009)

[4] M Rotter et. al., *Phys. Rev. Lett*. **101,** 107006 (2008)

[5] A D Christianson et. al., *Nature (London)* **456,** 930 (2008)

[6] I I Mazin et.al., *Phys. Rev. Lett*. **101.** 057003 (2008)

[7] T Hanaguri et. al., *Science* **328.** 474 (2010)

[8] J Guo, S. Jin et. al., *Phys. Rev. B* **82,** 180520 (R) (2010)

[9] Y Zhang et. al., *Nature Mater.***10,** 273 (2011)

[10] D Mou and X. J. Zhou, *Phys. Rev. Lett*. **106,** 107001 (2011)

[11] Lin Zhao et. al., *Phys. Rev. B* **83,** 140508 (R) (2011).
[12] X Wang et. al., *Europhys. Lett.***93,** 57001 (2011)
[13] T Qian et. al., *Phys. Rev. Lett*. **106,** 187001 (2011)
[14] M Xu et. al., arxiv: 1205.0787
[15] X-P. Wang et. al., arxiv: 1205.0996
[16] I R Shein et. al., *Phys. Lett*. A **375,** 1028 (2011)
[17] Xun-Wang Yan et. al., *Phys. Rev. B* **84,** 054502 (2011)
[18] Chao Cao et. al., *Phys. Lett.* **28,** 057402 (2011)
[19] Fa Wang et. al., *Europhys. Lett.*93, 57003 (2011)
[20] T A Maier et. al., *Phys. Rev. B* 83, 100515 (R) (2011)
[21] T Das et. al., *Phys. Rev. B* **84,** 014521 (2011)
[22] H Kotegawa et. al., *J. Phys.Soc. Jpn* **80**, **043708** (2011)
[23] Chen Fang et. al., *Phys. Rev. X* **1,** 011009 (2011)
[24] I I Mazin et.al., *Phys. Rev. B* **84,** 024529 (2011)
[25] T Saito et. al., *Phys. Rev. B* **83,** 140512 (R) (2011)
[26] Y Zhou et. al., *Europhys. Lett.***95**, 17003 (2011)
[27] R Yu et. al., *arxiv:* **1103.3259**
[28] Q Han, Z D Wang et. al., *Europhys. Lett.* **82,** 57003 (2011)
[29] S Raghu et. al., *Phys. Rev. B* **77,** 140512 (R) (2011)
[30] S S Jena and G C Rout, *Adv. Sc. Letts*, **22(** 2), 327-330(4) (2016)
[31] S S Jena, S K Panda and G C Rout, *AIP Conf. Proceedings* **1728** 020082 (2016).
[32] S S Jena, S K Agarwalla and G C Rout, *AIP Conf. Proceedings* (In Press) (2015)
[33] S S Jena, S K Agarwalla and G C Rout, *Orissa Journal Physics* **23(**2) 169 (2016)
[34] S S Jena, S K Agarwalla and G C Rout, *Orissa Journal Physics* Vol. **24(**1), 39 (2017)
[35] S S Jena, S K Agarwalla and G C Rout., *AIP Conf. Proc.* **1832**, 130025 (2017)
[36] S S Jena, S. K. Agarwalla and G C Rout., *Int. J. Nano and Biomaterials*, (2017)(Communicated)
[37] D N Zubarev, *Sov. Phys*. Usp.**3**, 320 (1960)
[38] Parish et. al., *Phys. Rev. B* **78**, 144514 (2008)