Orissa Journal of Physics
ISSN 0974-8202

Vol. 23, No.1
February 2016
pp. 85-92

Theoretical study of pairing symmetry in iron-based superconductors

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Received : 2.*12.2015* ; *Accepted : 11.01.2016*

Abstract. For the newly discovered iron-based superconductors, we propose a one band model for conduction band with first and second-nearest-neighbor electron hoppings with s-wave, d-wave and $s_{\pm}$-wave pairing symmetries for the superconductivity. We have calculated the Green's functions from which the temperature dependent superconducting (SC) gap and tunneling conductance are calculated and computed numerically taking 100×100 grid points of electron momentum throughout the Brillouin zone. The evolution of the SC gap and the tunneling conductance spectra are investigated for different model parameters of the system.

Keywords: Superconducting material, pnictides

PACS: 74.20.Pq, 74.70.Xa

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1. Introduction

The discovery of superconductivity in Fe-based oxypnictide LaFeAsO (F doped) of the type-1111 with critical transition temperature T_C = 26 K has inspired worldwide interests [1]. Then a series of superconducting materials with FeAs-layer were discovered: such as AFe_2As_2 (type 122 with A= K, Na, Rb) and MFe_2As_2 (type 122 with M = Ca, Ba, Sr) [2-4]. Upto now, the highest reported 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]. Guo et. al. have reported the superconductivity at T_C = 30 K in FeSe-layer compound $K_{0.8}$ Fe_2As_2 [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. Up to 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, Raghu. et. al. [28, 29] have proposed a two band model. 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 SC gap and tunneling conductance spectra measured by scanning tunneling microscopy (STM).

2. Formalism and calculation of Green's functions

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 pockets 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 pnictide systems. The tight binding model Hamiltonian for the degenerate d_{xz} and d_{yz} orbitals of iron atom is written as

$$H = \sum_{k,\sigma} \varepsilon_k \, C^{+}_{k,\sigma} C_{k,\sigma} + \sum_{k} \Delta(k) \, (C^{+}_{k\uparrow} C^{+}_{-k\downarrow} + C_{-k\downarrow} C_{k\uparrow}) \qquad (1)$$

where ε_k is the single band dispersion within tight-binding approximation in the Fe-Se square lattice. The band energy for this single band model of the iron based superconductor is given by, $\varepsilon_k = -2t_1(\cos kx + \cos ky) - 4t_2 \cos kx.\cos ky$, 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 $\Delta(k)$ in the Fe-Se plane is written as,

$$\Delta(k) = \sum_{k'} V(k-k') \left\langle C^{+}_{k'\uparrow} C^{+}_{-k'\downarrow} \right\rangle \qquad (2)$$

where V(k-k$^{/}$) is the momentum dependent effective Coulomb potential responsible for the formation of the Cooper pairs.There are three kinds of pairing symmetries namely the d-wave pairing symmetry with SC gap

$\Delta k = \Delta 0(T)(\cos kx - \cos ky)$, the s±-wave pairing symmetry with $\Delta k = \Delta 0(T)(\cos kx \times \cos ky)$ and the isotropic s-wave pairing symmetry with $\Delta k = \Delta 0(T)$. We have calculated the electron Green's function for the Hamiltonian using Zuvarev's Green function technique [30]. The coupled equations are solved and written as,

$$A_1(k,\omega) = << C_{k\uparrow}; C_{k\uparrow}^{+} >>_{\omega} = \frac{1}{2\pi} \frac{\omega + \varepsilon_k}{\left(\omega^2 - \omega_k^2\right)} \tag{3}$$

$$A_2(k,\omega) = << C_{-k\downarrow}^{+}; C_{k\uparrow}^{+} >>_{\omega} = \frac{1}{2\pi} \frac{\Delta(k)}{\left(\omega^2 - \omega_k^2\right)} \tag{4}$$

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

$$\Delta(k) = \sum_{k'} V(k-k') \left[\Delta(k')/2\omega_{k'}\right] \tan h\left(\frac{1}{2}\beta\omega_{k'}\right) \tag{5}$$

The electron momentum spans over the Brillouin zone in the two-dimensional square lattice. The summation appears as $\sum_k \to \frac{S}{(2\Pi)^2}\int\int dk_x dk_y$ where 'S' is the area of the square lattice. The integration is carried out for 100×100 grid points of the kx and ky components of the electron momentum. 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, 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.

3. Results and Discussion

We have taken the nearest-neighbor and the next- nearest-neighbor electron hopping parameters in conduction band dispersion, momentum dependent Coulomb potential V(k-k$^{/}$) and different pairing symmetries for the superconducting gap and computed the temperature dependent superconducting gap parameter $\Delta_0(T)$ given in equation (5) numerically and self-consistently. The plots are shown in figure 1(a). The SC transition temperature t_C nearly 30 K is observed for the superconductivity [8]. For a given SC transition temperature t_C = 0.15 ($T_C \approx 30$ K) corresponding to hopping parameter t_1 = 0.02 eV, the SC reduced parameter is plotted for SC coupling g = 1.92 for s-wave pairing, gd = 3.49 for d-wave pairing and for gs = 21.45 for $s_{\pm}$-wave pairing. It is observed that the magnitude of the SC gap (z) is the smallest for s-wave pairing. The z value is

slight higher for d-wave pairing and the gap is the highest for $s_{\pm}$-wave pairing. All the temperature dependent gaps exhibit perfect mean-field behaviour with $s_{\pm}$ symmetry showing the robust SC transition at t_C. The relation $2\Delta_0(T=0)/k_BT_C \approx 3.52$ for s-wave pairing, ≈ 4.5 for d-wave pairing and ≈ 13.3 for $s_{\pm}$-wave pairing, as compared to the universal BCS constant of 3.52 for isotropic metallic superconductors. It shows that this constant is much higher compared to BCS constant. This type of higher SC coupling and $s_{\pm}$ symmetry is reported by ARPES experiments and and Local density approximation (LDA) calculations [9, 10, 17, 31] experiments and band structure calculations.

Seo et.al. have emphasized that $s_{\pm}$ symmetry is most compatible with the electron band structure and superconductivity of iron-based superconductor [31]. Focussing on $s_{\pm}$ pairing symmetry, we study here the effect of SC coupling gs = 20.55, 21.0, 21.45 for $s_{\pm}$ symmetry on the SC gap parameter. It is observed that, with the increase of SC coupling, the temperature dependent gap parameter (z) increases with increase of gs with the enhancement of transition from $t_C = 0.1$ ($T_C \approx 20$ K) to $t_C = 0.15$ ($T_C \approx 30$ K) corresponding to different AFe_2Se_2 AND MFe_2Se_2 [2, 4]. Further the temperature dependent gap (z) exhibits perfect mean-field behaviour.

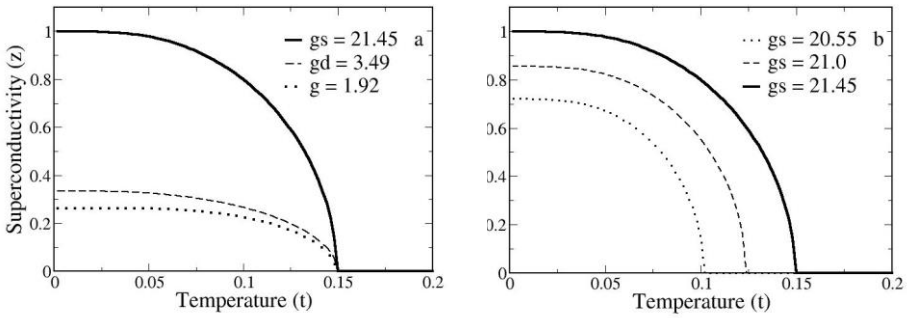

Fig. 1.(a) shows the plot of superconductivity(z) vs. temperature(t) for different waves of different values of g such as gs = 21.45, gd = 3.49, g = 1.92. **Fig. 1.(b)** shows the plot of superconductivity(z) vs. temperature(t) for $s_{\pm}$ wave of different values of g such as gs = 20.55, 21.0, 21.45.

The tunneling conductance spectra measured by scanning tunneling microscopy (STM) experiment is directly proportional to the electron density of states (DOS) which is calculated from the imaginary part of the electron Green's function A_1 (k, ω) given in equation (3). The computed DOS near the Fermi level i.e C = 0, is shown in figure 2(a). In the present one band model, we have considered nearest-neighbor-hoping parameter t1 and second- nearest-neighbor-

hoping parameter t2 in the conduction band dispersion. We study here the effect of hopping parameters on the DOS as shown in figure 2(a). for t1 = 1 & t2 = 0 (i.e, only contribution of the nearest neighbor hopping), the DOS exhibits a V-shaped asymmetric SC gap with a node at the Fermi point (C = 0) and the peak in DOS below the Fermi level is higher than the peak above the Fermi level. For the contribution of the only second-nearest-neighbor-hoping (i.e, t2 = -2.25 and t1 = 0), the DOS is symmetrically V-shaped with a narrow gap and a node at Fermi point. The contribution to DOS is mainly due to the nearest-neighbor-hoping. The total contribution to DOS is shown in continuous line as shown in figure 2(a). This shows asymmetric SC gap in DOS with a node. Parish et.al. [32] have reported a U-shaped SC gap in their model calculation for $s_{\pm}$ pairing symmetry for their two band model calculation.

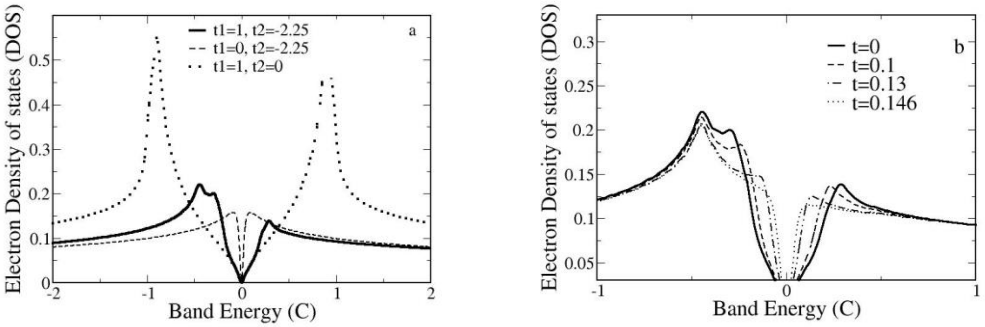

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Fig. 2.(a) shows the plot of density of states (DOS) vs. band energy (C) for different values of t1 and t2 such as t1 = 1 & t2 = -2.25, t1 = 0 & t2 = -2.25, t1 = 1 & t2 = 0. **Fig. 2.(b)** shows the plot of density of states (DOS) vs. band energy (C) for $s_{\pm}$ wave for different values of temperature t = 0, 0.1, 0.13,0.146.

The figure 2(b) shows the effect of temperature on the DOS i.e, on the conductance spectra of Fe-based superconductors taking the magnitudes of the SC gap for different pairings as shown in figure 1(a). We find that the SC gap (z) gradually increases from SC transition temperature t = t_C = 0.15 to t = 0. Therefore, it is expected that the DOS should display the enhancement of the SC gap with decrease of temperature. For temperature t = 0.146 near t_C, the DOS shows a narrow SC gap with a node at Fermi point. The SC gap gradually widens with the decrease of temperature with the gap edges of the SC gap shifting away from the Fermi point. However, the DOS nearly remains constant away from the Fermi point having constant electron DOS in the paramagnetic phase

Figure 3(a) shows the DOS for s-wave pairing g = 1.92, for d-wave pairing g = 3.49 and $s_{\pm}$-wave pairing g = 21.45. The DOS exhibits a U-shaped SC gap as observed in BCS type superconductors having s-wave type pairing symmetry. However, the gap edge below the Fermi point shows two peaks arising due to the contributions of first and second- nearest-neighbor-hoping parameter. The DOS exhibits a perfect V-shaped asymmetric SC gap for d-wave pairing symmetry. Similarly the DOS exhibit a V-shaped SC gap with a node at the Fermi point for $s_{\pm}$ pairing symmetry. However the DOS differs slightly for $s_{\pm}$ pairing from the other two pairings near the SC gap edges. This type of SC gaps having predicted by Parish et.al. [32] from their two band model calculations. On the contrary, they have reported symmetric SC gap in DOS for the two band model.

Figure 3(b) shows the effect of SC coupling gs = 20.55, 21.0, 21.45 for $s_{\pm}$ pairing symmetry which is most plausible pairing mechanism associated with iron-based superconductors. It is observed that the SC gap near Fermi point widens with increase of SC coupling gs.

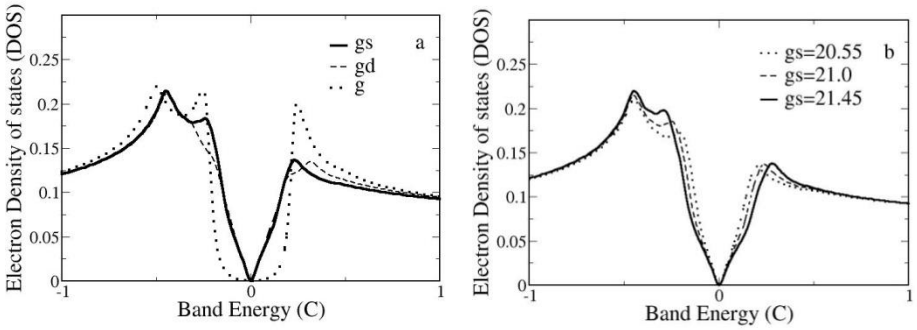

Fig. 3.(a) shows the plot of density of states (DOS) vs. band energy (C) for different values of g such as gs = 21.45, gd = 3.49, g = 1.92. **Fig. 3.(b)** shows the plot of density of states (DOS) vs. band energy (C) for $s_{\pm}$ wave for different values of g such as gs = 20.55, 21.0, 21.45.

4. Conclusions

We have considered here a single band model with two types of electron hopping parameters with different superconducting pairing symmetries. The effect of different types of pairing symmetries, coupling constants and temperature is investigated in the model calculation of SC gap and tunneling conductance.

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