Influence of multi-orbital hopping and anisotropy in intra and inter orbital Coulomb interactions on the electronic spectra in iron pnictide superconductors

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ABSTRACT

The present work deals with a theoretical study of the electronic spectral function in iron pnictide superconductors, like LaFeAs(O, F) material. We have attempted three orbital per site model Hamiltonian containing various orbitals hopping energies, onsite intra and inter orbital electronic correlations, and Hund's coupling energy in Fe $3d$ orbitals. The expression of single particle spectral function within mean-field Green's function approach for superconducting state of iron pnictides, is obtained. The single particle spectral function is numerically analyzed for extended s-wave pairing symmetry as a function of various model parameters applicable for these systems. It is pointed out that the nature of electronic states at different k-point of Brillouin zone is essentially influenced by various orbital hopping parameters, onsite Coulomb interaction and Hund's orbital coupling. At $X(0, \pi)$ point of Brillouin zone a well-defined three peak spectra is predicted while at $\Gamma(0, 0)$ and $M(\pi, \pi)$ point the electronic spectra show two peaks due to crossing of electronic state (at Γ-point). Our analysis also indicates that Hund's coupling pile up the spectral weight close to Fermi level and onsite Coulomb correlations suppress the electronic states close to Fermi level at $\Gamma(0, 0)$ point and show opposite influence on spectral weight at different location of Brillouin zone. Finally, the theoretically obtained behavior of single particle spectral function has been viewed in terms of recent photoemission ARPES measurements and existing theoretical results on electronic structure in iron pnictide superconductors.

1. Introduction

The iron based superconductors [1–14] possess two dimensional layered crystal structures and show a small anisotropy in electronic properties. Iron is known for its 3d-orbital originated ferromagnetism, while iron pnictide superconductors show a phase diagram (Tc versus doping or pressure) with the coexistence of antiferromagnetic and superconducting phase at moderate doping. Further, external pressure and doping of the parent compound (e.g. La, F, S, Se, etc.) play an important role to establize superconductivity in these systems [15,16]. To pinpoint the nature of superconducting state, and electronic properties, the recent highly refined Angle Resolved Photoemission Spectroscopic (ARPES) measurements have provided an important insight into the nature of electronic states close to Fermi level [17].

In iron pnictides, the ARPES data predicted the existence of a hole-like pocket centered around the (0, 0) point and electron like pocket at $(\pm\pi, 0)$ or $(0, \pm\pi)$ point of Brillouin zone. Based on the first principal calculations, Zhang et al. [18] predicted that the hole-type Fermi surface (FS) mostly contain the contributions from the d_{yz} and d_{zx} orbital states (of Fe atom), and electron-type FS around the M-point mostly arise from the d_{xy} and $d_{yz/zx}$ states. Hence, electronic band structure emphasized that mostly d_{xz}, d_{yz} and d_{xy} orbitals of Fe-atom contribute to the electronic states near the Fermi surface and dictate the evolution of superconductivity and electronic properties in these iron based systems [18]. Further, it is believed [19] that the band structure near the Fermi level in iron pnictides can be described qualitatively within these (d_{xy}, d_{yz} and d_{zx}) three orbitals per site models. Daghofer et al. [20] have emphasized the three orbital model by considering the hybridization of the As-p orbitals with the Fe (d_{xz}, d_{yz} and d_{xy}) orbitals. It is further argued that d_{xy} orbital significantly contribute to the electron pocket states close to Fermi surface. The ARPES analysis due to Lu et al. [17] revealed that there exist all three orbital states at the Fermi level, while [21] d_{xz} and d_{yz} orbitals states dominate

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the Fermi surface and d_{xy} orbital contribute to the electronic states far from the Fermi level. Therefore, the electronic properties in normal and superconducting state can be qualitatively described within two d_{xz}/d_{yz} orbitals scenario. Further, there are indications [22] that the Fermi level is crossed by d_{xy}, d_{xz}, and d_{yz} orbital states only with a small admixture of chalcogen/pnictogen $4p_z$ orbitals, thereby showing the less important role of p_z-orbital on electronic properties in these systems.

There have been several theoretical attempts made so far in order to analyze the multi-orbital overlapping and electron correlation on electronic spectra of these systems. The functional renormalized group [23] studies indicated the presence of the pocket of d_{xy} orbital character and the intra-orbital interactions with the d_{xy} part of electron FS supporting the nodeless superconductivity. Chen et al. [24] have carried out a comparative study on the electronic structure of iron pnictide/chalcogenide. They found that in iron-chalcogenides, there exist three quasi-particle bands close to the center of the Brillouin zone (Γ-point) with the distinct symmetry (even or odd), on the other hand in iron-pnictides one finds only two bands centered around hole-like pocket at Γ point and electron like pocket at M point of Brillouin zone, respectively. This unique band structure of Fe based materials may be a manifestation of multi-orbital character and play important role to underline the nature of the electronic properties in these systems. There have also been studies based on the orbitals character of multiband electronic structure in electron doped iron based superconductors ($BaFe_{1.85}Co_{0.015}As_2$) [25]. These studies emphasized the importance of the multi-orbital states close to the Fermi level along with the orbital dependent electron–electron correlations on the electronic properties in iron superconductors. Recently, on the basis of ARPES data, Ye et al. [26] have examined the role of orbital selective Fermilogy and superconductivity in $AFe_{1-x}Co_xAs$ (A = Li, Na) system. These authors predicted that the superconducting phase get suppressed just when hole pockets sink below the Fermi energy and evolve into an electron pocket above E_F. Further, it is important to note that d_{xz}/d_{yz} orbital based electronic states are much less sensitive to impurity scattering around the zone center in comparison to the d_{xy} orbital based states and give rise to a robust superconducting state in doped iron-based superconductors [26]. Recently, Nekarasov et al. [27] have investigated the electronic structure by approaching the local density approximation (LDA) and dynamical mean field theory (DMFT) in hole doped iron chalcogenide superconductors ($K_{1-x}Fe_{2-y}Se_2$). It is pointed out that all Fe-3d (t_{2g}) bands (means d_{xz}, d_{yz}, and d_{xy} orbitals) crossing the Fermi level, have equal renormalization and the electronic states at the Fermi level are of predominantly xy symmetry. On the other hand, ARPES results [28] on superconducting ($A_xFe_{2-y}Se_2$ (A = K, Rb)) systems have shown a temperature-induced crossover from a metallic state (in which all three orbital (d_{xz}, d_{yz}, and d_{xy}) are present near the Fermi level) to a state in which the d_{xy} orbitals have diminished spectral weight while the d_{xz}/d_{yz} bands show metallic behavior.

Therefore, the impact of multi-orbital's coupling, intra and inter orbital Coulomb interactions on the electronic structure of iron based superconductors have not been clearly understood so far. The various theoretical attempts have been made based on the two orbital [29–32,33], three orbital [19,20,34,35] and also five 3d orbital per site models [36]. Recently, we have theoretically analyzed the spectral function of electronic states within two orbital per site tight binding model for iron pnictide superconductors and pointed out that the Hund's coupling term accumulate the spectral weight (i.e. electronic states) close to Fermi level and support to stabilize superconducting state [32] in these systems. On the basis of self-consistent FLEX (Fluctuation exchange) approximation approach in two orbital model Zhang et al. [33] studied

the superconducting state as a function of intra- and inter-orbital couplings within s± pairing superconductivity in iron pnictides. To achieve superconductivity in these systems, the role of the inter-orbital spin fluctuation pointed out to be more relevant. Further, studies [34] also show the band renormalization, Fermi surface and superconducting order parameters within three orbital model and employing FLEX approximations. It is pointed out that band renormalization is anisotropic due to Coulomb interaction and dominated by orbital physics close to $(0, \pi)$ point. Long et al. [35] found that in iron based system at the $(0, \pi)$ point, spin density wave (SDW) peak enhanced due to the intra-orbital Coulomb interaction, while it reduced with Hund's coupling energy. Therefore, the onsite intra and inter-orbital Coulomb interactions and Hund's coupling energy play an essential role in understanding the physics of multi-orbital in superconducting state of iron pnictide/chalcogenide systems.

The recent experimental and theoretical studies suggested that iron based superconductors exhibit extended s-wave pairing symmetry and nodeless superconductivity [37–42]. Jiang et al. [40] found that the superconducting order parameter with $S \pm (\Delta_0 \cos(k_x)\cos(k_y))$ symmetry is the most favorable for both the electron and hole-doped cases and the spin fluctuation thought to be the common origin of superconductivity in iron based superconductors [41]. Recently, Evtushinsky et al. [42] analyzed the correlation between orbital composition and superconducting gap magnitude and established a strong variation of the superconducting gap over the Fermi surface. It has been further emphasized that the nature of electronic states close to Fermi level and ARPES data in Fe based superconductors have not been properly understood so far and need attention from theoretical point of view.

Therefore, in the light of above ARPES data [17] and theoretical attempts [19,20,34,35], the influence of Fe 3d multi-orbital couplings, intra-orbital and inter-orbital electronic interactions and Hund's coupling term on the electronic spectra need to be analyzed properly in iron based superconductors. Hence, in the present work, we attempt the three orbital per site model Hamiltonian (a manifestation of three overlapping Fe 3d-orbitals per sites i.e. d_{xz}, d_{yz} and d_{xy}) for iron pnictide superconductors within BCS mean field scenario in order to maintain self-consistency. The theoretically obtained spectral function of electronic states has been numerically analyzed as a function of various model parameters by employing Green's function formalism and compared with the existing ARPES data [16] and other available theoretical investigations [19,20,35] related to electronic spectra in iron pnictide superconductors. We have taken into account the extended s-wave ($\Delta_{ak} = \Delta_0 \cos(k_x)\cos(k_y)$) pairing symmetry in superconducting state of iron pnictides as proposed by several workers [33,34,37–42]. In the next section, we have presented the theoretical formalism of spectral function of electronic states at various k-points of the Brillouin zone within the three orbital per site tight binding model applicable for iron based superconductors.

2. Model Hamiltonian and theoretical formalism

The FeAs layer in LaFeAsO form two dimensional square lattice, where Fe ions situated on the lattice sites corner and As-ion sites at the center of each square. The crystallographic unit cell contains two Fe-ions and two As-ions. In square lattice Fe is coordinated by As above and below the plane to form face sharing $FeAs_4$ tetrahedral. The splitting in the electronic states is attributed to coupling between the FeAs layers within unit cell. The Fe–Fe distance is 2.854 Å. The distance between Fe–As is 2.327 Å, while the As–As distance is 3.677 Å [43]. The degeneracy of d_{xz}, d_{yz} and d_{xy} orbitals play important role in describing three orbital per site model in iron pnictide [18,19].