Journal Homepage: - www.journalijar.com
INTERNATIONAL JOURNAL OF ADVANCED RESEARCH (IJAR)
Article DOI:10.21474/IJAR01/4618
DOI URL: http://dx.doi.org/10.21474/IJAR01/4618
ISSN NO. 2320-5407

RESEARCH ARTICLE

THEORETICAL MODEL FOR IRON-BASED MAGNETIC SUPERCONDUCTOR.

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Manuscript Info

Manuscript History

Received: 26 April 2017
Final Accepted: 28 May 2017
Published: June 2017

Key words:-
Antiferromagneticorder, Green's Function, Superconductor

Abstract

The newly discovered high transition temperature superconductor pnictides (iron-based superconductor) exhibit coexistence of magnetism and superconductivity. In this paper, we propose a phenomenological theory tostudy the interplay between the superconductivity and antiferromagnetism. By using two band BCS type Hamiltonian and following green's function technique and theequationof the motion method,we have derived the superconducting gap as well as staggered magnetic field for ahalf-filled band situation.

Introduction:-

The discovery of high transition temperature (Tc) superconductor is a landmark in the history of condensed matter physics. It boosts multidirectional investigation in both experimental as well as theoretical fields. The thirst for getting a higher and higher Tc has led to a handful of superconductors with highest Tc=135K at ambient pressure [1] in mercury based cupratesremain the record till today. The very interesting feature of these cuprate superconductors is, they share a common structure element CuO_2 plane, where copper atoms form a square lattice. In this system $R_{2-x}M_xCuO_4$, superconductivity (SC) is known to occur for a narrow concentration range $0.05 \leq x \leq 0.25$. The puzzling fact is, many cuprates superconductor with CuO_2 planes are not superconducting, though it is established that the CuO_2 plane play an important role in the SC of cuprate. The second class of high Tc materials are iron based superconductor which was discovered in 2008 by Hosono and co-workers [2] with Tc=26K in LaOFeAs, the part of O atoms replaced by F atoms. The highest Tc in bulk iron based superconductor was discovered at 55K by Ren et al [3] for $SmO_{1-x}F_xFeAs$. Since then many families of iron based superconductors have been discovered and study of their physical properties is one of the major activity in condensed matter physics for the past several years.

It would be very interesting to see whether or not such co-existence can be possible which can give clues about the fluctuation ofmagnetism (Ferro, antiferro and ferrimagnetism) and leadtoemanation superconductivity. A decade ago scientists managed to obtain evidence for a homogeneouscoexistence of antiferromagnetic (AFM) and SC in heavy fermion compounds, a special type of inter-metallic compound on a microscopic scale. At the early stage of the iron-pnictide study, some experiments suggested that these two orders i.e. AFM and SC are separated both temporarily and spatially when they occur in the same sample. They occurin different parts of the materials as a separated phase. Later on, in improved quality crystal, researchers found indications about AFM and SC residing in the same placewhich is predicted from the susceptibility measurement on the onset of SC. The relation between AFM and SC in Iron Pnictides remains controversial. The low energy electronic structure of iron-based superconductors is dominated by the Fe 3d states [4]. Theangle-resolved photoemission spectroscopy (ARPES)experiments and density functional theory indicates a multi-sheet Fermi surface composed of several small electrons and hole Fermi surface which is disconnected from each other. The d_{xy}, d_{xz} and d_{yz} orbitals contribute mainly to the one near the Fermi

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energy [5, 6].The concentration of carrier of the iron-based superconductor can be tuned by doping in the charge reservoir layer or at the Fe site. Electron and hole doping can be varied over a large range and this, in turn, varies the chemical potential and Fermi surface.

The band calculation based on transport and optical conductivity measurements predicted a collinear antiferromagnetic (or spin density wave, SDW) state in the parent compounds [7]. This was subsequently confirmed by neutron scattering experiments. Most of the iron pnictide superconductors have same magnetic state [8].

The existence of Fe moments in these materials shows that not all Fe 3d electrons are equally conducting, some of them are more localized than the others. From the first principle density functional calculations, it was found that the crystal splitting of the 3d orbitals is small but the hybridization between Fe and As/Se atoms and the onsite Coulomb interaction vary differently for different 3d orbitals. Fe 3d electrons possess both local and itinerant nature. These itinerant electrons and local moment are not independent, they are actually coupled together.

Despite extensive investigations of interaction between SC and magnetic moment, there is so far no unified theory for the co-existence of SC and magnetism. Due to lack of proper theory, the existing experimental findings led to two school of thoughts: one, both the orders [10] result from the same conduction electrons and the other,there are two separate set of electrons responsible for magnetic ordering and superconductivity respectively [11]. The discovery of Fe-based compounds creates large interest in the scientific community due to the fact that though Fe is well-known ferromagnet, all parent compounds of Fe-basedsuperconductor's exhibit AFM order. In this work, we are trying to explain the interplay of superconductivity and magnetism on iron-based superconductor by taking a model Hamiltonian same as that taken for quaternary borocarbide compounds [12].

Theoretical Model:-

The Hamiltonian composed of conduction electron band, F-electron band, the hybridization of conduction electron and F-electron band, BCS like pairing band and intra-atomic Coulomb interaction of F-electron. Here we have considered BCS like pairing Hamiltonian as

$$H_c = \sum_{k\sigma} \epsilon_0(k)\left(a^{\dagger}_{k\sigma} b_{k\sigma} + h.c\right) + (h/2)\sum_{k\sigma} \sigma\left(a^{\dagger}_{k\sigma}(a_{k\sigma}) - b^{\dagger}_{k\sigma}(b_{k\sigma})\right) + V\sum_{k\sigma}\left(a^{\dagger}_{k\sigma} f_{1,k\sigma} + b^{\dagger}_{k\sigma} f_{2,k\sigma} + h.c\right) - \Delta\sum_k\left[\left(a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} + h.c\right) + \left(b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} + h.c\right)\right] \text{----------(1)}$$

The first term in the Hamiltonian describes the conduction which represents the hopping of the quasi-particles between the neighbouring sites of the two sub-lattices.$a^{\dagger}_{k\sigma}(a_{k\sigma})$ and $b^{\dagger}_{k\sigma}(b_{k\sigma})$are the creation (annihilation) operators of electrons at site 1 and 2 of Ni respectively with momentum k andσ. Hopping takes place between nearest neighbour site of Ni with dispersion,

$$\epsilon_0(k) = -2t_0\left(cosk_x + cosk_y\right) \text{---------- (2)}$$

where t_0 is the nearest neighbor hopping integral. Strongly AFM correlation of conduction Ni d-electrons is simulated by a staggered magnetic field of strength h and this contributes to the Hamiltonian as given by the second term in equation (1). Effective hybridization between the f-electrons of the rare earth atom and the conduction electrons of Ni atom contributes to the Hamiltonian as given by the third term in the Hamiltonian. $f^{\dagger}_{ik\sigma}(f_{ik\sigma})$ is the creation (annihilation) operator of the f-electrons and V is the strength of hybridization. Only on-site hybridization is included here. The last term in the Hamiltonian represents the attractive part of intra-band interaction term which leads to superconductivity.

Here BCS type of phonon-mediatedCooper pairing of conduction electrons of different sites is taken into account. The inter sub-lattice pairing may be significant here but has not been taken into consideration for simplicity of numerical calculation. The superconducting order parameterΔ is given as

$$\Delta = -\sum_K \tilde{V}_k \left(< a^{\dagger}_{k\uparrow}\, a^{\dagger}_{-k\downarrow} > + < b^{\dagger}_{k\uparrow}\, b^{\dagger}_{-k\downarrow} >\right) \text{---------- (3)}$$

$\widetilde{V_k}$is the strength of the attractive interaction between two electrons mediated by the phonons. By using double time electron green function of Zubarev type and theequation of motion method we have solved the Hamiltonian as given in equation 1.

We have obtained the equation for superconducting gap and staggered magnetic field as

$$\Delta(T) = V_0 N(0) \int_{\omega_D}^{\omega_D} d\epsilon_0(k) \times [F_1(k,T), + F_2(k,T)] \text{---------- (4)}$$

and

$$h = -\frac{1}{2} g\mu_B N(0) \int_{+\frac{W}{2}}^{-\frac{W}{2}} d\epsilon_0(k) \times [F_1(k,T) - F_2(k,T)] \text{---------- (5)}$$

where

$$F_1(k,T) = \frac{(\Delta - h/2)}{2\sqrt{E_{1k}^4 - 4V^4}} [\omega_1(k) \tanh\left(\frac{1}{2}\beta\omega_1\right) - \omega_2(k) \tanh\left(\frac{1}{2}\beta\omega_2\right)] \text{---------- (6)}$$

$$F_2(k,T) = \frac{(\Delta + h/2)}{2\sqrt{E_{2k}^4 - 4V^4}} [\omega_3(k) \tanh\left(\frac{1}{2}\beta\omega_3\right) - \omega_4(k) \tanh(\frac{1}{2}\beta\omega_4)] \text{---------- (7)}$$

As

$$E_{1,2}^2(k) = \epsilon_0^2(k) + (h/2 \pm \Delta)^2 \quad \text{---------- (8)}$$

$$\pm\omega_{1,2} = \left[\frac{E_{1k}^2 \pm \sqrt{E_{1k}^4 - 4V^4}}{2}\right]^{1/2} \quad \text{---------- (9)}$$

$$\pm\omega_{3,4} = \left[\frac{E_{2k}^2 \pm \sqrt{E_{2k}^4 - 4V^4}}{2}\right]^{1/2} \quad \text{---------- (10)}$$

Conclusion:-

In our model Hamiltonian, we have taken all the interaction term along with the hybridization term. Neutron diffraction experiment on $BaFe_{2-x}Co_xAs_2$ [14] shows that the commensurate antiferromagnetic order appears below the structural transition temperature and superconductivity coexists with an antiferromagnetic order for $0.06<x<0.102$.For the pnictides, there are strong indications that they are itinerant systems with magnetism arising from a nesting induced spin density wave. Thus our model which we have already used to describe the co-existence of antiferromagnetism and superconductivity for rare earth superconductors [12,15] can also be able to describe the coexisting properties ofiron-based superconductors.

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