Journal of Sciences and Multidisciplinary Research
Volume 6, No. 2, 2014
ISSN: 2277-0135

MAGNETISM IN IRON BASED SUPERCONDUCTORS AT SUPERCONDUCTIVITY REGIME

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Abstract: This is proposed to answer for co-existences superconductivity (SC) in the orbital overlap and magnetism, i.e. antiferromgnetism (AF) in iron based superconductors. This theory shows a gradual transition in the Nambu generalization of the Bardeen Cooper Schrieffer model to the psudospin Hamiltonian representation leading up to SC and AF state.

Keywords: Magnetism, Iron, Based Superconductors, Superconductivity Regime

INTRODUCTION

Naturally the parent compound of these systems is not superconducting itself but it does exhibits both magnetic and structural phase transitions. This structural phase transition changes the crystal symmetry from tetragonal (space group P4/nmm) to orthorhombic (space group Cmma) leading up to an antiferromagnetical (AF) order with a spin structure [1], This is because the cuprates, the Fe magnetic moments along (1,1) direction are parallel while the two nearest neighboring Fe are antiparallel. Similarly the cuprates turns superconducting by introducing impurities that create electrons and holes in the parent compound. This transition is due to direct orbital interaction between Fe atoms at 285 pm, while there is no such direct d-orbital overlap observed in the cuprates [1-2]. The electronic states of iron in LaFeAsO and fluoride doped have been studied in detail by 57Fe Mossbauer spectroscopy [2-3]. The Mossbauer spectra proved spin ordering in LaFeAsO and its suppression upon doping. The isomer shifts of the arsenide oxides are close to the data observed for the phosphate. Below the antiferromagnetic ordering (T=138 K), LaFeAsO shows full magnetic hyperfine field splitting with a hyperfine field of 4.86 T [2-3]. The magnetic moment at the iron atoms was estimated to have values in the range of 0.25–0.35μB/Fe atoms [3]. In FeAs based superconductors both the structural and magnetic transition can be suppressed by impurities (dopant) such as fluorine or with the oxygen deficiency [4]. The addition of impurity elements affect superconductivity in the doped system and cause pair interaction in the presence of the applied field. This leads to magnetic spin fluctuation thereby distorting the ordering [1-4]. Given the system Hamiltonian representation [5-6] as

$$H=\sum_{k}\varepsilon_{-}+\varepsilon_{+}\left(d^{+}_{1k\uparrow}d_{1k\uparrow}+d^{+}_{1k\downarrow}d_{1k\downarrow}\right)+\sum_{k}\varepsilon_{-}-\varepsilon_{+}\left(d^{+}_{2k\uparrow}d_{2k\uparrow}+d^{+}_{2k\downarrow}d_{2k\downarrow}\right)-\sum_{kk'}V_{1kk'}\,d^{+}_{1k\uparrow}d^{+}_{1k\downarrow}d_{1k\downarrow}d_{1k\uparrow}$$
$$-\sum_{kk'}V_{2kk'}\,d^{+}_{2k\uparrow}d^{+}_{2k\downarrow}d_{2k\downarrow}d_{2k\uparrow}-\sum_{kk'}V_{12kk'}\left(d^{+}_{1k\uparrow}d^{+}_{1k\downarrow}d_{2k\downarrow}d_{2k\uparrow}+d^{+}_{2k\uparrow}d^{+}_{2k\downarrow}d_{1k\downarrow}d_{1k\uparrow}\right) \qquad 1.0$$

Where, ε_{ik} (i =1, 2), is the quasi- particle kinetic energy of the band electrons, $V_{1kk`}$,$V_{2kk`}$ ($V_{12kk`}$) are wave vector dependent intra-band (inter-band) electron interaction for the band. kk` is the crystal wave vector parameter estimated relatively to the screened Coulomb $d^{+}_{ik}\left(d_{ik}\right)$ potential. , represents the creation (annihilation) operators for the electron of spins orientation, s ($=\uparrow,\downarrow$).

By Gorkov factorization [7] and we obtain the form of Eq (1.0) in Eq(1.1)

$$H=\sum_k \varepsilon_{1k}\left(d^+_{1k\uparrow}d_{1k\downarrow}+d_{1k\downarrow}d^+_{1k\uparrow}\right)+\sum_k \varepsilon_{2k}\left(d^+_{2k\uparrow}d_{2k\downarrow}+d_{2k\downarrow}d^+_{2k\uparrow}\right)-\sum_{K'}\Delta_{1k}\left(d_{1k\downarrow}d_{1k\uparrow}+d^+_{1k\uparrow}d^+_{1k\downarrow}\right)-\sum_{K'}\Delta_{2k}\left(d_{2k\downarrow}d_{2k\uparrow}+d^+_{2k\uparrow}d^+_{2k\downarrow}\right) \quad 1.1$$

The gaps are defined, as well as, the pair correlations as follows;

$$H=\sum_k \psi^+_{1k}\left(\varepsilon_{1k}\tau_3-\Delta_{1k}\tau_1\right)\psi_{1k}+\sum_k \psi^+_{2k}\left(\varepsilon_{2k}\tau_3-\Delta_{2k}\tau_1\right)\psi_{2k}=\sum_k \psi^+_{1k}\bar{H}_1\psi_{1k}+\sum_k \psi^+_{2k}\bar{H}_2\psi_{2k} \quad 1.2$$

H_1 and H_2 are the pseudospin Hamiltonians for the two bands [6] and ψ_{ks} *and* ψ^+_{ks}, are Nambu two-component spinors. From the pseudospin Hamiltonians of the two-bands in Eq.(1.2) and Nambu two component spinor[9] responsible for the spin ordering and disorder orientations.

$$\psi^+_{1k}=\begin{bmatrix} d^+_{1k\uparrow} & d_{1k\downarrow}\end{bmatrix},\ \psi_{1k}=\begin{bmatrix} d_{1k\uparrow}\\ d^+_{1k\downarrow}\end{bmatrix}\ for\ band\ one \quad 1.3$$

$$\psi^+_{2k}=\begin{bmatrix} d^+_{2k\uparrow} & d_{2k\downarrow}\end{bmatrix},\ \psi_{2k}=\begin{bmatrix} d_{2k\uparrow}\\ d^+_{2k\downarrow}\end{bmatrix}\ for\ band\ two \quad 1.4$$

Integrating over k-volume of the bands helps for the analytical evaluation of the band electron spin and Hamiltonian modification.

$$\sum_k \to \int dk\ ,\ H=\int \psi^+_{1k}\bar{H}_1\psi_{1k}dk\ +\int \psi^+_{2k}\bar{H}_2\psi_{2k}dk \quad 1.5$$

Following simplification in Eq(1.5), the exchange effect interaction of the electrons of atom '1', of spin (↑, ↓) in band-one of ψ_{1k} ,ψ^+_{1k} with the electrons of atom '2' of spin (↑, ↓) in band-two ψ_{2k} ,ψ^+_{2k} is seen as

$$J=\int \psi^+_{ik}\bar{H}_i\psi_{ik}dk,=\int \psi^+_{jk}\bar{H}_i\psi_{jk}dk\ ,\ i(j)=1,2 \quad 1.6$$

$$\frac{H\psi_{2k}}{\psi_{1k}}=\int \psi^+_{1k}\bar{H}_1\psi_{2k}dk\ =C \quad 1.7$$

$$H-\frac{H\psi_{2k}}{\psi_{1k}}=\int \psi^+_{1k}\bar{H}_1\psi_{2k}\psi_{1k}dk-\int \psi^+_{1k}\bar{H}_1\psi_{2k}dk=\int\left(\psi^+_{1k}\bar{H}_1\psi_{2k}\psi_{1k}-\psi^+_{1k}\bar{H}_1\psi_{2k}\right)dk\ =C-J \quad 1.8$$

$$H\left(1-\frac{\psi_{2k}}{\psi_{1k}}\right)=C-J\ \ ,\ \ H\left(1+\frac{\psi_{2k}}{\psi_{1k}}\right)=C+J \quad 1.9$$

Considering the linear combination of Nambu spinors, and the normalization factor N guarantees for the usual normalization condition for probability waves. These make it easy for simple simplification to apply:

$$\psi=N\left[\psi_{1k}+\psi_{1k}\right],\ \psi^2=N^2\left[\psi^2_{1k}+\left\{\psi^+_{1k}\right\}^2+2\psi_{1k}\psi^+_{1k}\right] \quad 1.10$$

$$\int \psi^2 dk = 1, \;\; N^2 \int \left| \psi_{1k}^2 + \left\{ \psi_{1k}^+ \right\}^2 + 2\psi_{1k}\psi_{1k}^+ \right| dk = 1 \qquad 1.11$$

$$\left(\frac{1}{2N^2} - 1 \right)^2 = S^2 - 1 \;, \left(\frac{1}{2N^2} \right)^2 = S^2 + 1 \qquad 1.12$$

Solving further simplification using Eq(1.12) and Eq(1.9) yields

$$\frac{H\left(1 - \frac{\psi_{2k}}{\psi_{1k}}\right)}{\left(\frac{1}{2N^2} - 2\right)^2} = \frac{C - J}{S^2 - 1} = E_P - 2E_\circ \;, \quad \frac{H\left(1 + \frac{\psi_{2k}}{\psi_{1k}}\right)}{\left(\frac{1}{2N^2} + 1\right)^2} = \frac{C + J}{S^2 + 1} = E_a - 2E_\circ \qquad 1.13$$

Eq. (1.13) is purely superconducting and antiferomagnetic. However, within the bands, Eq. (1.13) shows Coulomb's interaction energy between the electron spin density and nuclei charge. Exchange integral contains the product of wave function of both atomic orbital and characterize the quantum mechanical effect is partially in both SC state and AF state at the same time[9-12]. Two solutions arise from Eq.(1.13) due to qusi particle energy splite : where Ep, is the parallel spin ordering state energy, and E_a is the antiferromagnetic state or the energy of anti parallel spin orientation in iron based compound at singlet superconducting state and $E_\circ$ is the ground state energy.

SUMMARY

There is a mixed state that exists and the material becomes superconducting such that the magnetic order parameters can fluctuate leading to antiferromagnetic state.

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Reference to this paper should be made as follows: Igwe P. C., *et al* (2014), Magnetism in Iron Based Superconductors at Superconductivity Regime. *J. of Sciences and Multidisciplinary Research,* Vol. 6, No. 2, Pp. 1 – 8.

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