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Spinor Transformation and Antiferromagnetism in Iron Based Superconductors

[1]Chijioke P. Igwe, [2]Nwakanma Mike, [3]Oguazu E. Chinenye
Department of Physics and Astronomy, University of Nigeria, Nsukka, Nigeria,
Department of Industrial Physics, Renaissance University Ugbawka,Enugu

Abstract: *This theory is proposed to account for the spinor transformation (ST), antiferromagnetism (AF) and superconductivity (SC) in the direct d-orbital overlap of iron based superconductors. The ST, shows the gradual transition in the pair representation by Nambu to the Fourier's Green function leading up to SC and AF state. The AF dominant in the band regime, is determining from the two component spinor describing its interaction effect on the band electrons, represented by the spin, Coulomb integral and exchange integral.*

I. Introduction

Naturally the quaternary equi-atomic REOFeAs compounds are rather simple structured containing alternating layers of Fe-As and Re-O layers, where FeAs layers are believed to be responsible for superconductivity. The undoped compound of these systems is not superconducting itself but it exhibits both a structural and magnetic phase transition. This structural phase transition changes the crystal symmetry from tetragonal (space group P4/nmm) to orthorhombic (space group Cmma) and leads to an antiferromagnetical (AF) order with a spin structure [1], This is because the Fe magnetic moments along(1,1) direction are aligned (parallel) while the two nearest neighboring Fe are antiferromagnetically (antiparallel) aligned, similar to the well known antiferromagnetic ordering of the cuprates. The cuprates turns superconducting by introducing impurities that create electrons and holes in the parent compound. Unlike the cuprates, the iron oxypnictides are metallic and the antiferromagnetic parent compound is a Mott insulator. 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 cuprates[1-2]. It is believed that this is caused by instability of the spin density wave (SDW). The electronic states of iron in LaFeAsO and fluoride doped have been extensively studied in detail by 57Fe Mossbauer spectroscopy [2-3]. The 57Fe 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 between 0.25–0.35μB/Fe atoms [3].In FeAs based superconductors both the structural and magnetic transition can be suppressed by 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]. To calculate this effect, ψ_{ks} *and* ψ_{ks}^{+} are functions containing both magnetic and superconducting elements of which according to exchange effect model of magnetism [5-6] are combination of d_{iks} *and* d_{iks}^{+} , expressible in matrix form. Since, it is well known that the electron spin and ions are the effective magnetic carriers [6], we proceed as follows; Superconductivity dual band Hamiltonian representation [7]:

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

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

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 potential. $d_{ik}^{+}\left(d_{ik}\right)$, represents the creation (annihilation) operators for the electron of spins orientation, s ($=\uparrow,\downarrow$).

The singlet pair is preserved by factorization [7] and we obtain the linear form of Eq (1.0) in Eq(1.1)

$$H=\sum_{k}\varepsilon_{1k}\left(d_{1k\uparrow}^{+}d_{1k\downarrow}+d_{1k\downarrow}d_{1k\uparrow}^{+}\right)+\sum_{k}\varepsilon_{2k}\left(d_{2k\uparrow}^{+}d_{2k\downarrow}+d_{2k\downarrow}d_{2k\uparrow}^{+}\right)-\sum_{K'}\Delta_{1k}\left(d_{1k\downarrow}d_{1k\uparrow}+d_{1k\uparrow}^{+}d_{1k\downarrow}^{+}\right)-\sum_{K'}\Delta_{2k}\left(d_{2k\downarrow}d_{2k\uparrow}+d_{2k\uparrow}^{+}d_{2k\downarrow}^{+}\right)1.1 \qquad (2.1)$$

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

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

H_1 and H_2 are the pseudospin Hamiltonians for the two bands and ψ_{ks} *and* ψ_{ks}^{+}, are Nambu two-component spinors.

II. Spinor transformation and Antiferromagnetism

The Nambu two component spinors are defined and upon mathematical transformation leads to four component spinors [8-10].

$$\psi_{1k}^{+}=\begin{bmatrix} d_{1k\uparrow}^{+} & d_{1k\downarrow}\end{bmatrix},\ \psi_{1k}=\begin{bmatrix} d_{1k\uparrow}\\ d_{1k\downarrow}^{+}\end{bmatrix}\ for\ \ band\ 1,\ \psi_{2k}^{+}=\begin{bmatrix} d_{2k\uparrow}^{+} & d_{2k\downarrow}\end{bmatrix},\ \psi_{2k}=\begin{bmatrix} d_{2k\uparrow}\\ d_{2k\downarrow}^{+}\end{bmatrix}\ for\ \ band\ 2 \qquad 1.3$$

$$\Pi_{ks}^{+}=\psi_{1k}^{+}\psi_{2k}^{+}=\begin{bmatrix} d_{1k\uparrow}^{+}d_{1k\downarrow}d_{2k\uparrow}^{+}d_{2k\downarrow}\end{bmatrix},\Pi_{ks}=\psi_{1k}\psi_{2k}=\begin{bmatrix} d_{1k\downarrow}\\ d_{1k\uparrow}^{+}\\ d_{2k\downarrow}\\ d_{2k\uparrow}^{+}\end{bmatrix}$$

Following Kadanoff and Martin and define the Fourier's Green function by Zubarev [10-12],

$$G_s(k,iw_n)=\langle\langle\Pi_{ks}\Pi_{ks}^{+}\rangle\rangle=\begin{bmatrix} <d_{1k\uparrow}^{+}d_{1k\uparrow}> & <d_{1k\uparrow}^{+}d_{1k\downarrow}^{+}> & <d_{1k\uparrow}^{+}d_{2k\downarrow}^{+}> & <d_{1k\uparrow}^{+}d_{2k\uparrow}^{+}>\\ <d_{1k\downarrow}d_{1k\uparrow}> & <d_{1k\downarrow}d_{1k\downarrow}^{+}> & <d_{1k\downarrow}d_{2k\downarrow}> & <d_{1k\downarrow}d_{2k\uparrow}^{+}>\\ <d_{2k\uparrow}^{+}d_{1k\uparrow}> & <d_{2k\uparrow}^{+}d_{1k\downarrow}^{+}> & <d_{2k\uparrow}^{+}d_{2k\downarrow}> & <d_{2k\uparrow}^{+}d_{2k\uparrow}^{+}>\\ <d_{2k\downarrow}d_{1k\uparrow}> & <d_{2k\downarrow}d_{1k\downarrow}^{+}> & <d_{2k\downarrow}d_{2k\downarrow}^{+}> & <d_{2k\downarrow}d_{2k\uparrow}^{+}>\end{bmatrix} \qquad 1.5$$

The transformations of the two component spinor to a four component spinor showing the exchange effect interaction of the electrons of band '1', of spin (↑, ↓) in ψ_{1k} ,ψ_{1k}^{+} with the electrons of band '2' of spin (↑, ↓) in ψ_{2k} ,ψ_{2k}^{+}. Thus, yielding AF function ($d_{1k\uparrow}^{+}d_{2k\downarrow}$, $d_{1k\downarrow}d_{2k\downarrow}$) for the first and second bands respectively and determine possible AF gaps in this regime[10], except in a case where magnetic order may exist in both bands[1,3,6].Expressed by the equations(1.3-1.5) are elements containing both superconducting and ordered and disordered magnetic spin orientations[10].This also apply to the regime of two component spinors, hence, we show the effect of this exchange electron spin interactions as by Heisenberg[13]. Taken within the regime of two component spinors, the scalar product of ψ_{1k}^{+} and ψ_{1k} and integrate over volume of band-1

$$S_{1k}=\int\psi_{1k}^{+}\psi_{1k}dv_1=\int\begin{bmatrix} d_{1k\uparrow}^{+}d_{1k\uparrow} & d_{1k\uparrow}^{+}d_{1k\downarrow}^{+}\\ d_{1k\downarrow}d_{1k\uparrow} & d_{1k\downarrow}d_{1k\downarrow}^{+}\end{bmatrix}dv_1\ ,\ S_{ik}=\int\psi_{ik}^{+}\psi_{ik}dv_i\ ,\ i=1,2 \qquad 1.6$$

$$\left(S_{ik}\pm1\right)^2=\left(\int\psi_{ik}^{+}\psi_{ik}dv_i\pm1\right)^2;\left(S_{1k}+1\right)^2=\left(\int\psi_{1k}^{+}\psi_{1k}dv_1+1\right)^2,\left(S_{2k}-1\right)^2=\left(\int\psi_{2k}^{+}\psi_{2k}dv_2-1\right)^2 \qquad 1.7$$

Taking scalar product of ψ_{1k}^{+} and ψ_{2k} across v and integrating over the volumes of band-1 and band-2

$$h_{ijk}=\int\psi_{ik}^{+}V\psi_{jk}dv_idv_j\ \ \text{where, V is the potential, i(j)}=1,2,i\neq j \qquad 1.8$$

$$C=\int\psi_{1k}^{+}V\psi_{1k}dv_1\ ,\ J=\int\psi_{1k}^{+}V\psi_{2k}dv_1dv_2\ ,\ h_{11k}-h_{12k}=C-J\ ,\ h_{11k}+h_{12k}=C+J \qquad 1.9$$

S_{ik}, defines the overlap integral of the ith spin orientation, where C and J are the Coulomb and exchange integral respectively. Following simplification, we obtain

$$\frac{h_{ijk}}{\left(S_{ik}\pm1\right)^2}=\frac{h_{ijk}}{\left(\int\psi_{2k}^{+}\psi_{2k}dv_2-1\right)^2}\ ,\ \frac{C+J}{S_{1k}^2+1}=\varepsilon_a-2E_\circ\quad or\quad \frac{C-J}{S_{2k}^2-1}=\varepsilon_p-2E_\circ \qquad 1.10$$

Two solutions arise from Eq(1.10) due to splitting: Ep, which is the parallel spin ordering state energy and E_a which is the energy of anti parallel spin orientation in iron based compound (antiferromagnetic state) at singlet superconducting state. There is a mix state that exist once the material becomes superconducting such that the magnetic order parameter can fluctuate into two states at high and low temperatures. But at the superconducting state the material is predominately antiferromagnetic. Where, E_o is the ground state energy of the bands.

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