Communication

Model study of coexistence of Jahn-Teller distortion, antiferromagnetism and superconductivity in iron pnictide superconductors

B. Pradhan [a,*], S.K. Goi [b,c], Srikanta Behera [a], P.K. Parida [a], R.N. Mishra [b]

[a] Department of Physics, B.J.B. College, Bhubaneswar, Odisha 751014, India
[b] Department of Physics, Ravenshaw University, Cuttack, Odisha 753003, India
[c] Department of Physics, N. C. College, Jajpur, Odisha 755007, India

ARTICLE INFO

ABSTRACT

We have proposed a theoretical model for the coexistence of superconductivity (SC), antiferromagnetism (AFM) and Jahn-Teller (JT) effect in the mean field approximation for iron based superconductors. The model is solved by using Zubarev's double-time Green's function technique to get their selfconsistent gap equations. Then these gap equations are solved numerically.

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1. Introduction

The history of interplay between magnetism and super-conductivity is a long discussed phenomenon. Within the BCS framework, magnetic impurities can act as pair breaking agents which suppress the superconductivity rapidly [1]. The super-conductivity always appears near the static antiferromagnetic (AF) order [2] for iron based unconventional superconductors [3–9]. Here, it suggests that magnetism may be a common feature for understanding the microscopic origin of unconventional super-conductors and high transition temperature superconductivity [10]. The AF order discovered in the iron based superconducting parent compounds in 2008 [11–13] provided a new opportunity to study the coexistence of magnetism and superconductivity.

The iron pnictides and iron chalcogenides are the two major classes of iron based superconductors [3,4]. The comparison between the hole-doped $La_{2-x}Sr_xCuO_4$ copper oxide and iron pnictide such as $BaFe_2As_2$ [14] shows that the substitution of the trivalent impurity induces superconductivity in cuprates whereas the substitution of ion at any element site of pnictide induces superconductivity. These include Ba by K/Na to form hole-doped $Ba_{1-x}K_xFe_2As_2$ [15,16], Fe by Co/Ni to form electron-doped $BaFe_{2-x}T_xAs_2$ (T=Co, Ni) [17,18] and As by P in the isovalent doped compound $BaFe_2As_{2-x}P_x$ [19]. The number of holes induced to FeAs layer is the same in $BaFe_2As_2$ due to K/Na doping but the Ni doping introduces the number of electrons be twice in the FeAs layer as from the electron counting of Co doping [3,4]. The evolution of the AF order with spin excitation can be provided by the doped $BaFe_2As_2$ which can be grown by self-flux method [5]. Some features of the magnetic order and spin excitation in the iron based superconductors are studied by the neutron scattering experiment [20–30]. Magnetism being responsible for super-conductivity is confirmed in both cuprate and heavy fermion systems [10]. In such systems, the magnetic fluctuations on each sub lattice [31–33] produce the orthorhombic distortion [33–36].

In the case of an unconventional high-T_c superconductor, there is an opening of a gap called pseudogap (PG) above the critical temperature T_c at a temperature $T^\star$ in the electronic excitation spectrum. The origin of this PG is still mysterious to the condensed matter physicists, which well describes the high-T_c super-conductivity. The interaction between localised orbital electronic states and the crystal lattice [37] drives for the JT effect phase transition. Through this JT effect, there is a splitting up of the electronic states and a symmetry lowering distortion in the lattice. Now, the change of energy of the electronic states can be measured easily. The orbital doublets and triplets can be split either by a magnetic field or by a strain. In the discovery of a family of transparent rare earth materials the understanding of JT effect becomes spectacular. The systems mentioned earlier may become either magnetically ordered or distorted if both the JT and

magnetic interactions are there in the system at low temperatures. Many of the pnictides suffer first order phase transitions involving magnetic ordering and structural distortions. This possibility exists because of the interplay between magnetic and JT interactions of the kind. With this prescription we proposed a model here to study the interplay of SC, AFM and JT effect on one another. The theoretical model is described in Section 2, the calculation of electron Green's functions which relate the order parameters of the SC, the AFM and the JT distortion are in Section 3. The discussions of the results obtained are described in Section 4 and concluded in Section 5.

2. Theoretical model

It is assumed that the *FeAs* tetrahedron contains an Fe^{2+} ion in $3d^6$ configuration where Fe $3d$ orbitals are $3d_{xz}$, $3d_{yz}$, $3d_{xy}$, $3d_{x^2-y^2}$ and $3d_{z^2}$. The density of states at the Fermi energy should be contributed by these five orbitals but for low energy physics, all these five orbitals are not equally important. These five fold Fe $3d$ orbitals split for the representations of the crystal symmetry. Now the $3d_{xz}$ and $3d_{yz}$ bands have largest itinerary among the five bands for hybridisation with the $4p$ orbitals of As. The other three orbitals, $3d_{xy}$, $3d_{x^2-y^2}$ and $3d_{z^2}$ have less effect for their hybridisation with the As $4p$ orbitals. The assumption of the crystal field splitting and the orbital hopping effect considers the $3d_{xz}$ and $3d_{yz}$ orbitals of Fe for low energy physics discussions [38]. The iron based superconductors belong to multiband/multigap class of superconductors [39]. The multigap superconductivity arises when the gap amplitudes on different sheets of the Fermi surface (FS) are radically disparate, e.g. due to different dimensionality of the bands for the usual phonon mediated pairing. In the case of iron based superconductors, the multigap arises due to the appearance of multiple FS pockets dictated by the crystalline symmetry. Two different s-wave gaps are observed in the case of $Ba_{0.6}K_{0.4}Fe_2As_2$ ($T_c = 37$ K) in different sheets of FS: a large gap of $\Delta_2 = 12$ meV in the small FS and a small gap $\Delta_1 = 6$ meV in the large FS [40]. The SC gap in iron based superconductors is believed to be an s-wave symmetry with its sign changing property between electron and hole pockets [41–44]. For the simplicity of the calculations the particle-hole symmetry may be considered in which the hole and electron Fermi surfaces are identical leading to perfect nesting. The limit of perfect nesting is straight forward to conclude that the multiband superconducting gaps merge into one gap (i.e., $\Delta = |\Delta_1| = |\Delta_2|$, where Δ_1 and Δ_2 may be the electron and hole band gaps) [45]. But the experimental results of Zhang et al. [46] suggest that the inter band hopping might not be so substantial. Thus, the so called $s_\pm$ wave characterised by the sign change of the SC orders between electron and hole pockets is not the proper description of the SC state, however, the s-wave type symmetry is a more proper description for the iron based superconductors. With this prescription, we have considered a model Hamiltonian for the coexistence of SC, AFM and JT interactions in the s-wave symmetry and solved selfconsistently.

The AFM order is characterised by the spin alignment on *Fe* lattice sites of iron based superconductors, which leads to the Néel ground state from the antiferromagnetic exchange. Due to the above reason, the *Fe* lattice is divided into two sub lattices with electron operators $a_{k\sigma}$ and $b_{k\sigma}$ for electron momentum k and spin σ. The hopping of the conduction electrons between the neighbouring sites of the two degenerate orbits of Fe^{2+} is described by H_c, where

$$H_c = \sum_{k,\sigma} \epsilon_0(k)\left[(a_{1k,\sigma}^\dagger b_{1k,\sigma} + b_{1k,\sigma}^\dagger a_{1k,\sigma}) + (a_{2k,\sigma}^\dagger b_{2k,\sigma} + b_{2k,\sigma}^\dagger a_{2k,\sigma}) \right.$$
$$\left. + (a_{1k,\sigma}^\dagger b_{2k,\sigma} + b_{1k,\sigma}^\dagger a_{2k,\sigma}) + (a_{2k,\sigma}^\dagger b_{1k,\sigma} + b_{2k,\sigma}^\dagger a_{1k,\sigma}) \right]. \tag{1}$$

Here, $a_{1k,\sigma}^\dagger$, $b_{1k,\sigma}^\dagger(a_{1k,\sigma}, b_{1k,\sigma})$ and $a_{2k,\sigma}^\dagger$, $b_{2k,\sigma}^\dagger(a_{2k,\sigma}, b_{2k,\sigma})$ are creation (annihilation) operators of the conduction electrons of iron ions at two JT distorted orbitals 1 and 2 respectively with momentum k and spin σ. The hopping takes place between neighbouring sites of iron with dispersion $\epsilon_0(k) = -2t_0(\cos k_x + \cos k_y)$.

The lattice distortion via JT effect [47–50] may be from the degeneracy of $3d_{xz}$ and $3d_{yz}$. The structural transition from tetragonal to orthorhombic distortion is exhibited by the iron pnictide superconductors. This is described by a two level configurational distortion at each distorted tetrahedron where the Fe ion exists. The population difference between the two bands is observed in the degenerate conduction band due to the presence of the tetragonal distortion. The lattice strain splits the single degenerate band into two band energies $\epsilon_{1,2}(k) = \epsilon_0(k) \pm Ge$ with the increase of the population difference. Here, the strength of the electron-lattice interaction is denoted by G and the strength of the static lattice strain by e. Now the JT Hamiltonian is described as

$$H_{e-L} = Ge \sum_{k,\sigma} \left[(a_{1k,\sigma}^\dagger b_{1k,\sigma} + b_{1k,\sigma}^\dagger a_{1k,\sigma}) - (a_{2k,\sigma}^\dagger b_{2k,\sigma} + b_{2k,\sigma}^\dagger a_{2k,\sigma}) + \frac{1}{2}C_0 e^2 \right], \tag{2}$$

where the lattice strain e is defined as

$$e = -\left(\frac{G}{C_0}\right) \sum_{k,\sigma} \left[\left\langle a_{1k,\sigma}^\dagger b_{1k,\sigma} \right\rangle + \left\langle b_{1k,\sigma}^\dagger a_{1k,\sigma} \right\rangle - \left\langle a_{2k,\sigma}^\dagger b_{2k,\sigma} \right\rangle + \left\langle b_{2k,\sigma}^\dagger a_{2k,\sigma} \right\rangle \right]. \tag{3}$$

Here, $\frac{1}{2}C_0 e^2$ represents the elastic energy of the system with C_0 being the elastic constant. Under the condition that the gain in electronic energy is more than the elastic energy $\frac{1}{2}C_0 e^2$ then the strain is stabilised.

The Heisenberg exchange interaction between the magnetic moments at the neighbouring sites produces the sub lattice magnetisation. The AFM Hamiltonian within the mean field approximation for the staggered sub lattice magnetisation can be written as

$$H_s = \frac{h}{2} \sum_{k,\sigma} s\left[(a_{1k,\sigma}^\dagger a_{1k,\sigma} - b_{1k,\sigma}^\dagger b_{1k,\sigma}) + (a_{2k,\sigma}^\dagger a_{2k,\sigma} - b_{2k,\sigma}^\dagger b_{2k,\sigma}) \right], \tag{4}$$

where $a_{i\sigma}$ and $b_{j\sigma}$ describes the electron operators at sites i and j of two neighbouring sub lattices respectively. Here, $s = \pm 1$ for up and down spins respectively. The strength of sub lattice magnetisation ($=$AFM order parameter) is described by h which is defined as

$$h = -\frac{1}{2}g_L\mu_B \sum_{k,\sigma} s\left[\left\langle a_{1k,\sigma}^\dagger a_{1k,\sigma} \right\rangle - \left\langle b_{1k,\sigma}^\dagger b_{1k,\sigma} \right\rangle + \left\langle a_{2k,\sigma}^\dagger a_{2k,\sigma} \right\rangle - \left\langle b_{2k,\sigma}^\dagger b_{2k,\sigma} \right\rangle \right]. \tag{5}$$

Here, g_L and μ_B are the Lande-g factor and Bohr magnetron respectively. The superconductivity is introduced to the system through the BCS pairing interaction. The Cooper pairing is assumed to be existing only within the same orbitals and the same strength of the interactions. So the mean field pairing Hamiltonian is written as

$$H_I = -\Delta \sum_{\alpha,k} \left[(a_{\alpha k\uparrow}^\dagger a_{\alpha,-k\downarrow}^\dagger + b_{\alpha k\uparrow}^\dagger b_{\alpha,-k\downarrow}^\dagger) + h.\,c. \right], \tag{6}$$