Research proposal:
The impurity effect in iron pnictide superconductors

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The superconductivity in LaOFeAs was first discovered in 2006 [1]; however, the transition temperature was low, T_c=3.5K, in the undoped parent compound. The achievement of raising the superconducting transition temperature was obtained in 2008, as reported by Kamihara *et al.*[2] that T_c=26K in $LaO_{1-x}F_xFeAs$ compound with doping of fluorine. Efforts by researchers have been made during the pase few years since the discovery of these novel superconducting materials aiming at understanding the normal state properties, the pairing mechanism, and the symmetry of the superconducting gap function[7–10].

Different from cuprate superconductors of which the parent compounds are Mott insulators, the parent compounds of Fe-based superconductors(FeSCs) are in most cases metals with an antiferromagnetic ordering[3]. First-principle electronic structure calculation[4] shows that the most prominent feature of the band structure of FeSCs is the multi-orbital nature at around the Fermi surface. Detailed projecting density of states calculation[5] indicates that in the vicinity of the Fermi level, Fe-3d orbitals dominates with a relatively small but considerable weight hybridization of As-p orbital, which gives rise to an efficient hopping of Fe-3d electrons over Fe sublattice via an intermediate As atom. Most iron pnictides share a similar Fermi surface including two hole bands centered at Γ and two electron bands emerging at M[4]. The flat character of the bands crossing the Fermi level along Γ-Z direction implies a weak energy dependence on k_z momentum of the hole qusiparticles, and consequently the superconductivity occurs in a qusi 2-dimensional electronic configuration.

The paring mechanism of high-T_c superconductors is a subtle question, and it has been a subject of great debates. Nonphononic mechanism of the pairing can be traced back to the discussion concerning superfluid ^{3}He[6], but did not become the mainstream before the discovery of cuprate superconductors. Many researchers believe that the "glue" that binds electrons into Cooper pairs, which induces the superconductivity, is generated by a type of bosons which plays a role of exchanging the antiferromagnetic spin fluctuation[7]. There are many possibilities concerning the paring symmetry in which the sign reversed $s_\pm$ wave pairing symmetry has been proposed to be the superconducting ground state[7, 8]. Still, the conventional s-wave and s_{++} paring are also be argued with some experimental evidence[9, 10].

The impurity in superconducting material affects the paring symmetry remarkably[11]. The isotropic s-wave superconductivity is insensitive to non-magnetic impurities according to Anderson's theorem, while the $s_{\pm}$ superconductivity is sensitive to non-magnetic impurities when inter-band electrons are scattered by the impurities, and insensitive when scattering happens between intra-band electrons. Zinc-doping is considered to induce the inter-band electrons scattering with a suppressing on $s_{\pm}$ superconductivity. It has been reported that an optimally doped $LaFeAsO_{0.9}F_{0.1}$ caused no influence on the superconductivity, whereas in the over-doped regime as $LaFeAsO_{0.85}F_{0.15}$, a severe suppressing was generated which results in a transition of paring symmetry from s_{++} to $s_{\pm}$[12, 13].

In this research project, we will study how the impurities affect on the superconductivity. A minimal two-orbital model[14] containing both on-site s_{++} pairing(g_0) and next nearest neighbor $s_{\pm}$ pairing(g_2) are introduced to study the effects caused by Zn impurities in the superconducting system. The Hamiltonian is of the following form:

$$H = H_0 + H_{pair} + H_{impurity} \tag{1}$$

where

$$H_0 = \sum_{<i\alpha, j\beta>,\sigma} t_{ij}^{\alpha\beta} a_{i\alpha\sigma}^{\dagger} a_{j\beta\sigma} \tag{2}$$

where the hopping parameters on a 2-dimensional square lattice are $t_{ii}^{\alpha\alpha} = -\mu$, $t_{ii+\hat{y}}^{11} = t_2$, $t_{ii+\hat{y}}^{22} = t_1$, $t_{ii=\hat{y}}^{22} = t_1$, $t_{ii+\hat{x}+\hat{y}}^{\alpha\alpha} = t_3$, $t_{ii+\hat{x}+\hat{y}}^{12} = t_{ii+\hat{x}+\hat{y}}^{21} = -t_4$, and $\mu = 1.6$, $t_1 = 1$, $t_2 = -1.3$, $t_3 = t_4 = 0.85$ in unit of t_1, respectively[14].

The pairing and impurity terms are:

$$H_{pair} = \sum_{i\alpha, j\beta} V_{\uparrow\downarrow\downarrow\uparrow}(i\alpha, j\beta; j\beta, i\alpha) a_{i\alpha\uparrow}^{\dagger} a_{j\beta\downarrow}^{\dagger} a_{j\beta\downarrow} a_{i\alpha\uparrow} \tag{3}$$

$$H_{impurity} = \sum_{i=1}^{N_{electron}} \sum_{l=1}^{N_{impurities}} V_0 \delta_{\hat{\vec{R}}_i \vec{R}_l} = V_0 \sum_{l\alpha\sigma}^{N_{impurities}} a_{l\alpha\sigma}^{\dagger} a_{l\alpha\sigma} \tag{4}$$

where

$$V_{\uparrow\downarrow\downarrow\uparrow}(i\alpha, j\beta; j\beta, i\alpha) = V_{ij} = g_0 \delta_{ij} + g_2 \sum_{\tau} \delta_{ji+\tau} \tag{5}$$

$$\Delta_{i\alpha\uparrow, j\beta\downarrow} = V_{ij} < a_{j\beta\downarrow} a_{i\alpha\uparrow} > \tag{6}$$

We assume that the intra-orbital pairing($\alpha = \beta$) contributes to the real space gap function much more than that of inter-orbital paring($\alpha \neq \beta$). The order parameter will be calculated using the real space Bogoliubov-de Gennes equation self-consistently.

$$\sum_{j\beta} \begin{pmatrix} t_{ij}^{\alpha\beta} & \Delta_{ij}^{\alpha\beta}\delta_{\alpha\beta} \\ \Delta_{ij}^{*\alpha\beta}\delta_{\alpha\beta} & -t_{ij}^{\alpha\beta} \end{pmatrix} \begin{pmatrix} u_{j\beta}^{n} \\ v_{j\beta}^{n} \end{pmatrix} = E_n \begin{pmatrix} u_{i\alpha}^{n} \\ v_{i\alpha}^{n} \end{pmatrix} \tag{7}$$

The superconducting gap function is given by

$$\Delta_{ij}^{\alpha\alpha} = \frac{V_{ij}}{4} \sum_{n} (u_{i\alpha\sigma}^{n} v_{j\alpha\bar{\sigma}}^{*n} + v_{i\alpha\bar{\sigma}}^{*n} u_{j\alpha\sigma}^{n}) \tanh(\frac{E_n}{2k_B T}) \tag{8}$$

Furthermore, we will study the interplay between g_0 and g_2 in the undoped system to investigate the influence of the impurity effect on the gap function. In general, we expect that this project will be able to qualitatively explain the results from various impurity-doping experiments reported recently.

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