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Physics Procedia 81 (2016) 17 – 20

Physics Procedia

28th International Symposium on Superconductivity, ISS 2015, November 16-18, 2015, Tokyo, Japan

Unitary-transformed fermions theory of iron-based superconductors

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Abstract

Unitary-transformed theory of iron-based superconductors is presented. This theory is based on the *d-p* model emphasizing that the electronic state of superconductors can be described by the composed fermions constructed with newly defined operators. The Hamiltonian is so modified by the unitary transformation using these fermion operators as to apply the mean field approximation. The theory is extended to the case of superconducting pnictides in considering some characteristics such as multi orbitals, antiferromagnetic metal and so on. It is indicated that the effective interaction between these composite fermions can determine the several electronic properties in superconducting pnictides. It is found that the superconductive paring wavefunction is *s*-like state different from the *d* state of cuprates, but can be changeable depending on the various conditions of the electronic or crystal structures. The relations with structural modification and carrier doping are also discussed.

Peer-review under responsibility of the ISS 2015 Program Committee

Keywords: High Tc superconductivity; Iron-based superconductors; *d-p* model

1. Introduction

Since the discovery of superconducting iron pnictides, there has been much intensive study about many interesting properties in the normal and in the superconducting state [1]. However, what mechanism plays an essential role for determining these properties still remains an unsolved problem. Recently, the author has proposed the composite fermions theory of superconducting cuprates [2]. This theory is based on the *d-p* model emphasizing that the electronic state of superconductors can be described by the composed fermions constructed with newly defined operators. The Hamiltonian is so modified by the unitary transformation using these fermion operators as to

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Peer-review under responsibility of the ISS 2015 Program Committee
doi:10.1016/j.phpro.2016.04.008

apply the mean field approximation. In this paper the unitary-transformed theory is extended to the case of iron-based superconductors in considering some characteristics such as multi orbitals, antiferromagnetic metal and so on.

2. Basic equations

For the iron-based superconductors, there have been many theoretical studies such as spin or orbital fluctuation models and the models with localized spins [3,4]. Here the so-called *d-p* model will be modified in the formulation similar to the case of cuprates. The Hamiltonian is assumed to be an extended *d-p* model for a single layer of square planar

$$H=\sum_{in\sigma}\varepsilon_{dn}d^{+}_{in\sigma}d_{in\sigma}+\sum_{j\sigma}\varepsilon_{p}p^{+}_{j\sigma}p_{j\sigma}+\sum_{in\sigma}\sum_{j\in\{in\}}(\varepsilon_{inj}d^{+}_{in\sigma}p_{j\sigma}+\mathrm{H.c.})+U_{nmn'm'}\sum_{inm\sigma\sigma'}d^{+}_{in\sigma}d_{im\sigma}d^{+}_{in'\sigma'}d_{im'\sigma'}+\sum_{injo\sigma'}V_{inj}d^{+}_{in\sigma}d_{in\sigma}p^{+}_{j\sigma'}p_{j\sigma'}, \tag{1}$$

where the operator $d^{+}_{in\sigma}$ creates electrons of *n-th* Fe 3*d* orbital at site *i*, $p^{+}_{j\sigma}$ creates pnictide (Pn) 4*p* electrons at site *j*, and ε_{inj} is the nearest-neighbor hopping integral. $U_{nmn'm'}(n=n',\, m=m')$ and $U_{nmn'm'}(n\neq n',\, m\neq m')$ are the Coulomb repulsion and Hund coupling at Fe site, respectively, and V_{inj} is the interaction between neighboring Fe and Pn sites. In (1), the vacuum is defined as Fe d^0 and Pn p^6 states. Considering the Fe 3*d*-Pn 4*p* covalency effect, the operator combining the four pnictides states around a Fe ion is defined as

$$\tilde{p}^{+}_{in\sigma}=\sum_{j\in\{in\}}\varepsilon_{inj}\varepsilon_{n}^{-1}p^{+}_{j\sigma},\quad \varepsilon_{n}=\sqrt{\sum_{j\in\{in\}}\varepsilon^{2}_{inj}}, \tag{2}$$

where $j = i + \boldsymbol{x}_j$, and $\boldsymbol{x}_j$ presents the directions of Fe-Pn bonding. Since the relation of $\sum_j p^{+}_{j\sigma}p_{j\sigma}=\sum_i \tilde{p}^{+}_{in\sigma}\tilde{p}_{in\sigma}$ is satisfied in the Fe-Pn compounds, Hamiltonian (1) is so changed as

$$H=\sum_{in\sigma}\varepsilon_{dn}d^{+}_{in\sigma}d_{in\sigma}+\sum_{in\sigma}\varepsilon_{p}\tilde{p}^{+}_{in\sigma}\tilde{p}_{in\sigma}+\sum_{in\sigma}(\varepsilon_{n}d^{+}_{in\sigma}\tilde{p}_{in\sigma}+\mathrm{H.c.})+U_{nmn'm'}\sum_{inm\sigma\sigma'}d^{+}_{in\sigma}d_{im\sigma}d^{+}_{in'\sigma'}d_{im'\sigma'}+\sum_{in\sigma\sigma'}V_{in}d^{+}_{in\sigma}d_{in\sigma}\tilde{p}^{+}_{in'\sigma'}\tilde{p}_{in'\sigma'} \tag{3}$$

Now, following the formulation in the case of cuprates, let us find out the effective Hamiltonian of Eq. (3). It was assumed in the case of cuprates that the *d-p* interaction could prefer the antiferromagnetic coupling in order to avoid the Coulomb interaction at the *d* sites [2]. The similar *d-p* interaction will be adopted here. According to the second order perturbation theory for $\varepsilon_n < U_{nmn'm'}$, $\tilde{p}$ -states can combine with the *d*-states of Fe to form singlet-spin states. This also means that the Fe-Pn hybridization leads to an antiferromagnetic interaction between Fe and Pn electrons. For simplicity, neglecting Hund coupling and the interaction between different 3*d* orbitals, the effective $U_{nmn'm'}$ and V_{in} can be written as $U_{nmn'm'}\to U_n(\ll U_{nm})$, $V_{in}\to\tilde{V}_{in}=V_{in}+V_{n\sigma\sigma'}$ $(V_{n\sigma\sigma'}<0, V_{n\sigma\sigma}=0)$. Thus, in the band picture of iron-based superconductors, the effective Hamiltonian of (3) is transformed into momentum space

$$\begin{aligned}H=&\sum_{\mathbf{k}n\sigma}\varepsilon_{dn}d^{+}_{\mathbf{k}n\sigma}d_{\mathbf{k}n\sigma}+\sum_{\mathbf{k}\sigma}\varepsilon_{p}p^{+}_{\mathbf{k}\sigma}p_{\mathbf{k}\sigma}+\sum_{\mathbf{k}n\sigma}2^{-1/2}\varepsilon_{n}s_{n}(\mathbf{k})(-id^{+}_{\mathbf{k}n\sigma}p_{\mathbf{k}\sigma}+ip^{+}_{\mathbf{k}\sigma}d_{\mathbf{k}n\sigma})+N^{-1}\sum_{\mathbf{k}\mathbf{k}'n\mathbf{q}}U_{n}d^{+}_{\mathbf{k}n\uparrow}d_{\mathbf{k}'n\uparrow}d^{+}_{\mathbf{q}-\mathbf{k}n\downarrow}d_{\mathbf{q}-\mathbf{k}'n\downarrow}\\&+N^{-1}\sum_{\mathbf{k}\mathbf{k}''n\sigma\sigma'}\tilde{V}_{in}\theta_{n}(\mathbf{k},\mathbf{k}')d^{+}_{\mathbf{k}n\sigma}d_{\mathbf{k}'n\sigma}p^{+}_{\mathbf{k}''\sigma'}p_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'}\end{aligned} \tag{4}$$

Here $s_n(\mathbf{k})=\sum_{j\in\{in\}}\varepsilon_{inj}\varepsilon_n^{-1}\exp(i\mathbf{k}\cdot\mathbf{x}_j)$, $\theta_n(\mathbf{k},\mathbf{k}')=\sum_{j\in\{in\}}\varepsilon^{2}_{inj}\varepsilon_n^{-2}\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}_j]$, x, y refer to the axis for the unit cell, and N is number of Fe sites in a single layer. The operators $d^{+}_{\mathbf{k}n\sigma}$, $p^{+}_{\mathbf{k}\sigma}$ are reconstructed with fermion operators defined by unitary transformation

$$b^{+}_{\mathbf{k}n\sigma}=\alpha_{\mathbf{k}n}d^{+}_{\mathbf{k}n\sigma}+i\beta_{\mathbf{k}n}p^{+}_{\mathbf{k}\sigma},\quad c^{+}_{\mathbf{k}n\sigma}=\beta_{\mathbf{k}n}d^{+}_{\mathbf{k}n\sigma}-i\alpha_{\mathbf{k}n}p^{+}_{\mathbf{k}\sigma},\quad \alpha^{2}_{\mathbf{k}n}+\beta^{2}_{\mathbf{k}n}=1, \tag{5}$$

where $b^{+}_{\mathbf{k}n\sigma}$ and $c^{+}_{\mathbf{k}n\sigma}$ satisfy anti-commutation relations. For the condition of $\sqrt{2}\alpha_{\mathbf{k}n}\beta_{\mathbf{k}n}(\varepsilon_p-\varepsilon_{dn})=\varepsilon_n s_n(\mathbf{k})(\beta^{2}_{\mathbf{k}n}-\alpha^{2}_{\mathbf{k}n})$, the Hamiltonian (4) is given by