Theory of high-temperature superconductivity in strongly correlated fermions system

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Abstract. A unified theory to explain generally the properties of high-temperature superconducting cuprates and iron pnictides etc. is presented. The theory is based on the extended d-p model emphasizing that the electronic state of superconductors can be described by the composed fermions constructed with newly defined operators. The peculiarity in the theory is that the Hamiltonian is so modified by the unitary transformation using these fermion operators as to apply the mean field approximation. It is found that the results can provide a universal explanation about the various superconducting and normal properties of high-temperature superconductors.

1. Introduction
Despite much intensive study about high-temperature superconducting cuprates and iron pnictides etc, its mechanism still remains an unsolved problem [1-8]. Recently, the author proposed the composite fermions theories of these superconductors [9]. These theories are based on the extended d-p model emphasizing that the electronic state of superconductors can be described by the composed fermions constructed with newly defined operators. However, it is another problem to unite these theories into a unified theory to explain generally the properties of these superconductors. Here in order to find the unified theory, the high-temperature superconductivity is more generally investigated in strongly correlated fermions system.

2. Effective Hamiltonian
The Hamiltonian is assumed to be an extended d-p model for a single layer of square planar

\[ H = \sum_{\alpha \beta} \epsilon_{\alpha} d_{\alpha \sigma}^\dagger d_{\alpha \sigma} + \sum_{j} \sum_{l} \left( \epsilon_{\sigma} d_{l \sigma}^\dagger p_{j \sigma} + \sum_{\sigma} \sum_{m} \left( \epsilon_{\alpha} d_{m \sigma}^\dagger p_{j \sigma} + H.c. \right) + \sum_{\alpha \beta \gamma} U_{\alpha \beta} d_{\alpha \sigma}^\dagger d_{\beta \sigma}^\dagger d_{\gamma \sigma} d_{\gamma \sigma} + \sum_{\gamma \delta} V_{\gamma \delta} d_{\gamma \sigma}^\dagger d_{\delta \sigma}^\dagger p_{j \sigma} p_{j \sigma} \right) \] (1)

where the operator \( d_{\alpha \sigma}^\dagger \) creates electrons or holes of n-th M (Cu or Fe) 3d orbital at site i, \( p_{j \sigma}^\dagger \) creates l-th L (oxide or pnictide) p electrons or holes at site j, \( \epsilon_{\alpha} \) and \( \epsilon_{\sigma} \) is the nearest-neighbor hopping integral. \( U_{\alpha \beta} \) and \( U_{\alpha \beta} \) (\( n \neq m \)) are the Coulomb repulsion and Hund coupling at M site, respectively, and \( V_{l\beta \gamma} \) is the interaction between neighboring M and L sites. In (1), the vacuum is defined as M \( d_{\alpha \sigma}^\dagger \) and L \( p_{j \sigma}^\dagger \) states (\( x = 10, y = 6 \) in the cuprate, \( x = 0, y = 6 \) in the pnictide). Considering the d-p covalency effect, the operator combining the L states around M ion is defined as
\[ \vec{p}_{\sigma \nu} = \sum_{j \in \{i\}} \epsilon_{\sigma \nu} \hat{c}_{\sigma j}^\dagger \hat{c}_{\nu j}, \quad \epsilon_{\sigma \nu} = \sqrt{\sum_{j \in \{i\}} \epsilon_{\sigma \nu}^j}, \]

where \( j = i + \mathbf{x}_j \) and \( \mathbf{x}_j \) presents the directions of M-L bonding. Since the relation of
\[ \sum_j p^\dagger_{\nu j} p_{\sigma j} = N \sum_j \vec{p}_{\nu \sigma} \cdot \vec{p}_{\sigma \nu} \quad (N \text{ is the valence ratio of } d \text{ to } p) \] is satisfied in the M-L compounds, Hamiltonian (1) is so changed as

\[ H = N \sum_\nu p^\dagger_{\nu \sigma} \vec{p}_{\nu \sigma} + \sum_\nu (\epsilon_{\sigma \nu} d^\dagger_{\nu \sigma} \vec{p}_{\nu \sigma} + \text{H.c.)} + \sum_{\nu \sigma \sigma'} U_{\sigma \sigma'} d^\dagger_{\nu \sigma} d^\dagger_{\nu \sigma'} d_{\nu \sigma'} d_{\nu \sigma} + N \sum_\nu \epsilon_{\sigma \nu} d^\dagger_{\nu \sigma} d_{\nu \sigma} + \text{H.c.)} \]

(3)

Since the operator \( \vec{p}_{\nu \sigma} \) is not orthogonal between the neighboring M sites, it does not exactly satisfy anti-commutation relations. However it is approximated here that \( \vec{p}_{\nu \sigma} \) can be well-defined fermion operator.

To the second order in perturbation theory on the condition of \( \epsilon_{\sigma \nu} < U_\nu (= U_{\nu \sigma}) \), let us find out the effective Hamiltonian of Eq. (3). For simplicity, Hund coupling and the interaction between different 3d orbitals are neglected. First the second term of Eq. (3) will be divided into three parts of \( H_1, H_2 \) and \( H_3 \) as follow as

\[ H_1 = \sum_{\alpha \beta} \epsilon_{\alpha \beta} (1 - n_{\alpha \sigma}) d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} (1 - n_{\beta \rho}) + \text{H.c.)} \]
\[ H_2 = \sum_{\alpha \beta \rho} \epsilon_{\alpha \beta \rho} d_{\nu \alpha} \vec{p}_{\nu \alpha} n_{\beta \rho} + \text{H.c.)} \]
\[ H_3 = \sum_{\alpha \beta \rho} \epsilon_{\alpha \beta \rho} n_{\alpha \sigma} d_{\nu \alpha} \vec{p}_{\nu \alpha} (1 - n_{\beta \rho}) + (1 - n_{\alpha \sigma}) d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} n_{\beta \rho} + \text{H.c.)} \]

(4)

where \( H_1 (H_2) \) is the hopping terms in the absence (presence) of fermions with the opposite spin at both \( d \) and \( p \) sites and \( H_3 \) indicates the terms in the presence of fermions with the opposite spin at either \( d \) or \( p \) sites. Thus, \( H_3 \) acts on the interaction \( U_\nu \) as a perturbation, but \( H_1 \) and \( H_2 \) do not so because the ground state is not assumed here to include the double occupancy states. Further, let us average the occupancy factors such as \( (1 - n_{\alpha \sigma}) \) by using \( (1 - n_{\alpha \sigma}) \). The Coulomb interaction \( U \) in the ground state can be effectively eliminated from the starting Hamiltonian because double occupancy states at \( \alpha \)-sites are inhibited by Coulomb repulsion. Thus, Hamiltonian (3) is modified by

\[ H = N \sum_{\alpha \beta} \epsilon_{\alpha \beta} p_{\nu \alpha} \vec{p}_{\nu \alpha} + \sum_\nu \left( \sum_{\alpha \beta} (1 - n_{\alpha \sigma}) (1 - n_{\beta \rho}) \epsilon_{\alpha \beta} d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} + \text{H.c.)} + \sum_{\alpha \beta \rho} \epsilon_{\alpha \beta \rho} n_{\alpha \sigma} d_{\nu \alpha} \vec{p}_{\nu \alpha} (1 - n_{\beta \rho}) + (1 - n_{\alpha \sigma}) d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} n_{\beta \rho} + \text{H.c.)} \right) \]

(5)

where \( J_1 = \epsilon_{\alpha \beta} (U - N \epsilon_{\alpha \rho} - N V_{\alpha \rho}) \), \( J_2 = \epsilon_{\alpha \beta} (N \epsilon_{\rho \rho} - N V_{\rho \rho}) \). Though the latter part of the forth term in (5) corresponds to the kinetic energy due to the hopping between sites, it is neglected here due to the second order kinetic energy. The former part corresponds to the effective anti-ferromagnetic interaction between \( d \)-\( p \) fermions. Thus, the effective Hamiltonian is finally obtained as

\[ H_{\text{eff}} = N \sum_{\alpha \beta} \epsilon_{\alpha \beta} p_{\nu \alpha} \vec{p}_{\nu \alpha} + \sum_\nu \left( \sum_{\alpha \beta} (1 - n_{\alpha \sigma}) (1 - n_{\beta \rho}) \epsilon_{\alpha \beta} d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} + \text{H.c.)} + \sum_{\alpha \beta \rho} \epsilon_{\alpha \beta \rho} n_{\alpha \sigma} d_{\nu \alpha} \vec{p}_{\nu \alpha} (1 - n_{\beta \rho}) + (1 - n_{\alpha \sigma}) d^\dagger_{\nu \alpha} \vec{p}_{\nu \alpha} n_{\beta \rho} + \text{H.c.)} \right) \]

(6)

where \( V = V_{\alpha \rho} + N \epsilon_{\rho \rho} \) ( \( V_{\alpha \rho} \) : interaction between the nearest neighboring sites in (1), \( V_{\alpha \rho} \) : anti-ferromagnetic interaction \( V_{\alpha \rho} = -\left( (1 - n_{\alpha \sigma}) n_{\beta \rho} + (1 - n_{\alpha \sigma}) n_{\beta \rho} \right) J_1 < 0 \quad \sigma \neq \sigma' \)).

What’s the ground state of this effective Hamiltonian? Here two ground states will be considered depending on the doping conditions. One of these is the states in the neighborhood of the insulator (so-called Mott insulator) and the other is the superconducting state based on the band picture. First let us consider the region in the neighborhood of the insulator. The effective Hamiltonian (6) is appropriate in this case because its representation in real space is very useful in the treatment of this region. In order
to enable to apply the mean field approximation, the operators \( d^*_\alpha n \), \( \tilde{\text{p}}^*_\alpha n \) are changed by unitary transformations of
\[
b^*_\alpha n = \alpha_n d^*_\alpha + \beta_n \tilde{\text{p}}^*_\alpha n, \quad c^*_\alpha n = \beta_n d^*_\alpha - \alpha_n \tilde{\text{p}}^*_\alpha n, \quad \alpha^*_\alpha + \beta^*_\alpha = 1
\]
(7)
where \( b^*_\alpha \), \( c^*_\alpha \) are defined as the mixing operators of M and L fermions. For the condition of \( \alpha_n \beta_n N \gamma \epsilon = (1 - n_{\alpha n})(1 - n_{\beta n})c_{\alpha n}(\beta^*_n - \alpha^*_n) \), the Hamiltonian (6) is transformed into
\[
H = N \sum_{k \in \text{m.c.}} \epsilon_k (\beta^* - \alpha^*) + (\beta^* b^* b - \alpha^* c^* c) + N \sum_{k \text{m.c.}} V(\alpha^* b^* b + \alpha^* b^* c + \beta^* c^* b + \beta^* c^* c + \cdots)
\]
(8)
Notice that the indexes \( n, l \) of \( \alpha_n, \beta_n, b_n, c_n \) etc are omitted to avoid the complex representation. Since there appear many interaction terms in the transformed Hamiltonian (8), this might make the problem somewhat difficult. However, the mixing of \( d \) and \( p \) fermions can be directly built in this Hamiltonian, which consists of two free fermions and the interaction terms between them. As a result this treatment has an advantage to enable to apply the mean field approximation because of the explicit representation of free fermions and their interaction terms. Next let us consider the case of the superconducting state based on the band picture. Since the representation in momentum space is appropriate in this region, the effective Hamiltonian (6) is transformed into
\[
H = \sum_{k \text{m.c.}} \epsilon_k p^*_k p_k + \sum_{k \text{m.c.}} (1 - n_{\alpha n})(1 - n_{\beta n})c_{\alpha n}(\alpha^*_n d^*_n + i p^*_n d_n) + N \sum_{k \text{m.c.}} V(\theta(k,k')d^*_n d_{k'}) p^*_k p_{k'} + \cdots
\]
(9)
Here \( \theta(k,k') = \sum_{j \text{m.c.}} \epsilon_j \exp[i(k-k') \cdot \mathbf{x}_j] \), \( \theta^*(k,k') = \sum_{j \text{m.c.}} \epsilon_j \exp[i(k-k') \cdot \mathbf{x}_j] \), \( x, y \) refer to the axis for the unit cell, and \( N \) is number of M sites in a single layer. The operators \( p^*_k d^*_n \), which are Fourier transformation of \( \tilde{\text{p}}^*_\alpha n, d^*_\alpha n \), are reconstructed with fermion operators defined by unitary transformation
\[
b^*_k = \alpha_k d^*_k + \beta_k \tilde{\text{p}}^*_k, \quad c^*_k = \beta_k d^*_k - \alpha_k \tilde{\text{p}}^*_k, \quad \alpha^*_k + \beta^*_k = 1
\]
(10)
where \( b^*_k \), \( c^*_k \) satisfy anti-commutation relations. Notice that the operators \( p^*_k \) satisfy anti-commutation relations exactly, but those are approximated operators of \( \tilde{\text{p}}^*_\alpha n \) in momentum space. For the condition of \( \alpha_{k l} \beta_{k l} L \epsilon = (1 - n_{\alpha n})(1 - n_{\beta n})c_{\alpha n}(\beta^*_l - \alpha^*_l) \), the Hamiltonian (9) is given by
\[
H = \sum_{k \text{m.c.}} \epsilon_k (\beta^* - \alpha^*) + (\beta^* b^* b - \alpha^* c^* c) + N \sum_{k \text{m.c.}} V(\theta(k,k') \alpha_k \beta_k c^*_k c_k b^*_k b_k + \beta^* \beta^* b^* b^* c^* c^* c_k c^* c_k + \cdots)
\]
(11)
where the indexes \( n, l \) of \( \alpha_n, \beta_n, b_n, c_n \) etc are omitted to avoid the complex representation. These effective Hamiltonian will be applied for the cuprate and pnictide superconductors in next chapter.

3. Cuprate superconductors
The characteristics of cuprate superconductors is that it is a single \( d \)-band \((n = 1)\), superconductive in hole doping, and insulator in non-doping state. Though \( p \)-band is multi-orbitals, a single band of \( l = 1 \) will be only considered here. First let us consider the case of the nearly non-doped region. Assuming that there is no \( p \)-holes in half-filling, the relations of \( (1 - n_{\alpha n}) \approx 0.5 + (1 - \kappa) \delta \approx 0.5 \), \( (1 - n_{\beta n}) \approx 1 - 0.5 \delta \approx 1 - 0.5 \delta \), \( \kappa \approx 1 \) are derived. Here \( \kappa \) is the doping ratio contributing to \( p \)-holes. For the condition of \( 2 \alpha \beta \epsilon_p = 0.5(1 - 0.5 \delta) \epsilon (\beta^* - \alpha^*) \), the Hamiltonian (6) is transformed into
\[ H = 2 \varepsilon_b (\beta^2 - \alpha^2)^{\dagger} (\sum c_i^\dagger \sigma c_i) + 2 \sum V (\alpha^2 \beta^2 b_i^\dagger b_i^\dagger b_i b_i + \alpha \beta^2 b_i^\dagger c_i c_i^\dagger + \beta^2 c_i^\dagger b_i b_i + \cdots) \]

(12)

Here \( N_\sigma \) (the valence ratio of \( d \) to \( p \)) = 2. For the copper oxides it is well known that its ground state shows antiferromagnets (so-called Mott insulator) in the non-doped region \([10,11]\). Using the composite operators defined here, the non-doped wave function corresponds to

\[ |\Psi \rangle = \prod (ab_{\uparrow}^\dagger + \beta c_{\uparrow}) \prod (ab_{\downarrow}^\dagger + \beta c_{\downarrow}) |0 \rangle \]

(13)

where \( A \) or \( B \) shows the sub-space of antiferromagnetic lattice and \( N \) is number of Cu sites in a single layer. Since there exists no \( p \)-hole in half-filling Mott insulator, it will not be necessary to consider the interaction \( V \) in this case. However, in the existence of \( p \)-holes, since \( V_{\sigma}(\sigma \neq \sigma') \) is interpreted to be attractive due to \( d-p \) exchange antiferromagnetic interaction, the case of \( V(=V_{\uparrow \uparrow} + N_{\downarrow \downarrow} V_{\downarrow \downarrow}) < 0 \) will play an important role for determining the ground state. Considering the experimental facts that the doping can almost supply the \( p \)-holes, doping holes are expected to occupy the quantum state corresponding to this situation. For the condition \( \beta^2 < \beta^2 \) which allows the reliable value of \( \varepsilon_b \) and \( \varepsilon_c \), the term \( b_i^\dagger c_i^\dagger c_i c_i^\dagger \) can be the most dominant interaction. This means that \( b-c \) or \( c-b \) pair will mainly contribute to determine the ground state. Thus, for the equivalency of sites, the normalized wave function is assumed to be

\[ |\Psi \rangle = \prod (s + tb_{\uparrow}^\dagger c_{\uparrow})(s + tc_{\downarrow}^\dagger b_{\downarrow}) \]

(14)

where the coefficient \( t \) indicates the probability of local-antiferro pair state. On the approximating us the relation of \( \langle \Psi | \sum p_i \rangle |\Psi \rangle \approx 2N s^\frac{1}{2} t = N \delta \) (\( \delta \): the doping ratio relative to half-filling), the ground-state energy is given by

\[ E_p = \langle \Psi | H |\Psi \rangle = N_\sigma \delta (\varepsilon_b + V), \quad V < 0 \]

(15)

The energy of the excited states will be evaluated by using the presumed excited state wave function as follow as

\[ |\Psi \rangle = \prod (s + tb_{\uparrow}^\dagger c_{\uparrow})(s + tc_{\downarrow}^\dagger b_{\downarrow})(\beta b_{\uparrow}^\dagger - \alpha c_{\downarrow}) |\Psi \rangle \]

(16)

This is orthogonal to the ground state function and corresponds to breaking up a \( b-c \) (\( c-b \)) pair in \( i \), the spin-up member going to \( b_{\uparrow}^\dagger, c_{\downarrow}^\dagger \). The excited energy is obtained as \( N_\sigma \delta (\varepsilon_b + V) - 2V \). This indicates that there is the energy gap between the ground and the excited states. Thus, the wave function (14) will be identified as the pseudogap state in the nearly non-doped region. The pseudogap energy is then estimated to be \( \Delta_\sigma = |V| \) and the pseudogap temperature \( T_p \) is approximated as the \( \lambda \Delta_\sigma (\lambda < 1) \).

Next let us consider the case in the neighborhood of optimally doped region. In this doping region the relation of \( \langle 1 - n_{\sigma} \rangle \approx 0.5 - (1 - \kappa) \delta \approx 0.5, \langle 1 - n_{\sigma} \rangle \approx 1 - 0.5 \kappa \delta \approx 1 - 0.5 \kappa (\kappa \approx 1) \) will be generally reasonable. On the condition of \( \alpha \beta \varepsilon_b = 0.5(1 - 0.5 \delta) \Delta(K) (\beta^2 - \alpha^2) \), the Hamiltonian (9) is represented by

\[ H = \sum_s \varepsilon_b (\beta^2 - \alpha^2)^{\dagger} (\sum c_i^\dagger \sigma c_i) + \sum_{k \kappa} V(\mathbf{k}, \mathbf{k}') (\alpha \alpha b_k^\dagger b_k^\dagger + \beta \beta c_k^\dagger c_k^\dagger + \cdots) \]

(17)
where $s(k) = \sin k + \sin k'$, $\theta(k,k') = \cos(k-k') + \cos(k - k')$, and the Cu-O distance is used as the length unit. Here $b^c_k$ and $c^c_k$ satisfy anti-commutation relations. Note that $V = V_p + V_0 = V_o < 0$ because in this doping region the Coulomb interaction $V_0$ can be neglected due to the screening effect of carriers. In (17) $b^c_k$ or $c^c_k$ fermion has the possibility of creating Cooper pairs, but $b^c_k$ will contribute to the Cooper formation because the Fermi surface exists in only $b^c_k$ band. Thus the BCS-like wave function is given by

$$|\Psi_s\rangle = \prod_k (u_k + v_k b^c_k, b^+_{-k}) |0\rangle, \quad u_k^2 + v_k^2 = 1 \quad (18)$$

The ground-state energy is

$$E = \langle \Psi_s | H | \Psi_s \rangle = 2\sum_k \epsilon_k v_k^2 + N^{-1} \sum_{p\alpha} \left[ V_{\alpha p} \alpha^c_p \beta^c_k u_k v_k u_p v_p \right] \quad (19)$$

where the relation $\epsilon_k = 0.5(\epsilon_k + [(1 - 0.5\delta)^2 \sigma^c \mathbf{s}(k) + \epsilon^c_k]^\alpha) - \epsilon_f$ is defined, measuring the energy relative to the Fermi level $\epsilon_f$. By minimizing $E$ with respect to $u_k$, $v_k$, the gap equation is obtained as

$$\Delta_k = -0.5\sum_p \Delta_p V_{\alpha p} (\Delta^c_p + \epsilon^c_p)^{-\alpha}, \quad V_{\alpha p} = N^{-1} V_{\alpha p} \alpha^c_p \beta^c_k u_k v_k u_p v_p \quad (20)$$

Replacing the sum in gap equation by an integral, the solution which is even in $k$ is given by $\Delta_k = \Delta_{0k} \delta_k (\cos k - \cos k')$. The solution decreasing the Coulomb interaction is $\Delta_k = \Delta_{0k} \delta_k \cos k - \cos k'$ which agrees with the experimental fact about the anisotropic gap of high-temperature cuprate superconductors [12]. Thus $\Delta_0$ is determined by the relation

$$1 = -0.5\pi^{-2} V \left[ \alpha^c_p \beta^c_k (\cos k - \cos k') \cos k \left[ \Delta^c_p \alpha^c_p \beta^c_k (\cos k - \cos k') \right] + \epsilon^c_k \right]^{-1/2} \exp(-\Delta^c_p \alpha^c_p \beta^c_k (\cos k - \cos k')) \exp(1/1N, V) \quad (21)$$

Using several approximation on the band structure, the superconductive maximum gap energy and the ground-state energy are given by

$$\Delta_k = 2\epsilon_p \delta[(1 + (1 - 0.5\delta)^2 \epsilon^c_k / \epsilon_f)^{1/2} \exp(1/1N, V), \quad \epsilon_f = N \delta \epsilon_p - N \epsilon_p \delta^2 [(1 + (1 - 0.5\delta)^2 \epsilon^c_k / \epsilon_f)^{1/2} \exp(2/1N, V) \quad (22)$$

where $N_f$ is the density of states at Fermi level. Note that the energy relative to Cu $3d$ level is measured and the contribution of the $c_{\alpha\beta}$ fermions to the total system energy is considered.

In order to evaluate the intermediate state between two doped regions, it is necessary to estimate the doping dependency of the free energy of the pseudogap and the superconductive states. First let us consider the $d$-$p$ interaction $V$ which is the variable of the free energy. The value of $V_{\alpha\beta}$ is proportional to $\epsilon^c_k$ due to $d$-$p$ anti-ferromagnetic exchange interaction. However, increasing of doping rate $\delta$, $\epsilon$ will be effectively $\epsilon((1 - 0.5\delta)$, because the hopping probability from Cu sites to O sites can be proportional to $(1 - 0.5\delta)$ due to exclusion principle. As a result, $V$ can be approximated as $V = V_0 \epsilon^c_k \epsilon^c_k (1 - 0.5\delta)^2$. Thus, the free energy and gap energy of the pseudogap and superconductive states can be obtained as a function of $\delta$. In those states, the interaction term of the free energy initially decreases with increasing doping, and passes a minimum point. Since these minimum points are generally different, it is plausible that there exists the mixed state in the intermediate region. Of course, there may be unknown states in the intermediate doped region. However, if the energy of those ground-states is smaller than the mixed states, they should be evidently detected in various experiments. There is so far no evidence about the existence of those intermediate states. Though those unknown states can contribute to the excited states, they could be at least neglected as the ground-state. This also agrees with the recent research in which the
pseudogap state competes with the superconductivity [13]. Thus, an overall wavefunction is assumed to be

$$ |\Psi(\delta)\rangle = f^{\alpha\beta}[\Psi_\alpha(\delta_\alpha)] + (1 - f)^{\alpha\beta}[\Psi_\beta(\delta_\beta)] $$

(23)

where $\delta_p$, $\delta_s$ are the doping quantity of PG and superconductive states and the total doping quantity is defined to be $\delta = f\delta_p + (1 - f)\delta_s$. The total free energy is then given by $G = fE_p(\delta_p) + E_s(\delta_s) + (1 - f)E_s(\delta_s)$, $0 < f < 1$ and the intermediate region is determined by minimizing $G$ with respect to $\delta$, $\delta_p$, $\delta_s$. Let us evaluate the doping quantity $\delta_{pm}$, $\delta_{sm}$ by minimizing $E_p(\delta_p)$ and $E_s(\delta_s)$ and the minimum point of the total free energy in the condition of $\delta_p$, $m < \delta_{sm}$. As the case of $\delta < \delta_{pm}$ means $\delta_p = \delta$, $\delta_s = 0$, the system will show a pure PG state. At $\delta = \delta_{pm}$ superconductivity appears in the PG state and the mixed state will be maintained until the PG state disappear at the doping quantity $\delta_{sm}$ satisfying $\delta = \delta_s$. In more increasing of $\delta$ there exists a pure superconductor. Thus, the overall wave function will be represented as three regions of $f = 1$ ($\delta < \delta_{pm}$), $f = (\delta_{pm} - \delta)(\delta_{pm} - \delta_{sm})^{-1}$ ($\delta_{pm} < \delta < \delta_{sm}$), and $f = 0$ ($\delta > \delta_{sm}$), respectively. For both regions of $\delta < \delta_{pm}$ and $\delta_{pm} < \delta < \delta_{sm}$, $\Delta_p$ and $T_p$ will decrease with increase of $\delta$ and vanish at $\delta = \delta_{sm}$. Since the superconductive region appearing at $\delta = \delta_{pm}$ can be identified to be composed of very small superconductive region, the sufficient coherency to detect the net superconductivity will be less formed. Therefore, the superconductive state for $\delta_{pm} < \delta < \delta_{sm}$ could be given by the effective gap $\Delta_{eff} = (\delta - \delta_{pm})\Delta_s(\delta_s/\delta_{sm})^{1/2}$. This also indicates that the superfluid density $\delta_{f}$ changes as $\delta - \delta_{pm}$ in the region of $\delta_{pm} < \delta < \delta_{sm}$. The superconductor will be the optimal doped state at the neighborhood of $\delta = \delta_{sm}$, and in the over-doped region $\Delta_s$ and $T_p$ will decrease with $\delta$ according to doping dependency. Thus, an overall phase diagram is theoretically obtained by considering three types of electronic states.

4. Pnictide superconductors

The characteristics of pnictide superconductors is that it is multi orbitals, metal in non-doping, and superconductive in electron doping [14]. Since pnictides is metal in non-doping, the momentum representation is appropriate in the neighborhood of this doping region. Then, it seems that it isn’t needed to consider PG state on the condition of electron doping. However, if hole doping can enhance the strongly correlation between fermions, PG state may appear in the suitable condition of hole doping.

The BCS-like wave function, which is the ground state of (11), is given by

$$ |\Psi_s\rangle = \prod \langle u_s + v_s b_s^{+} b_{s^{+}} |0\rangle, \quad u_s^2 + v_s^2 = 1 \quad (24) $$

Thus, the following gap equation is given by

$$ \Delta_s = -0.5\sum_\alpha \sum_\nu \Delta_{\nu\alpha} \nu_{\alpha\nu} (\Delta_{\nu\alpha} + \nu_{\alpha\nu})^{-1/2}, \quad \nu_{\alpha\nu} = N \nu_\alpha \alpha_\nu \beta_\nu \beta_\nu \theta (k,k') \quad (25) $$

Since Fe-3$d$ electrons are multi orbitals, it is needed to select the dominant orbitals of Fe contributing to superconductivity [15]. The orbitals of $d_{xz}$, $d_{yz}$ that have the strong hopping transition to the nearest Pn sites and intersect the Fermi surface are considered here. First let us consider the symmetry of superconductive paring wavefunctions [16]. The gap equation (25) is then considered in the case of only orbitals $d_{xz}$, $d_{yz}$. For simplicity single $p$-orbital will be only considered. Considering that the square lattice of Fe$^{2+}$ is tetrahedrally coordinated with Pn anions $s_x(k), s_y(k), s_z(k), t_x(k,k')$, and $t_y(k,k')$ are calculated as $s_x(k) = \cos k_x, s_y(k) = \cos k_y, s_z(k) = \cos(k_z - k'), t_x(k,k') = \cos(k_x - k'), t_y(k,k') = \cos(k_y - k')$ where the half of Fe-Fe distance is used as the length unit. In the case of $d_{xz}$ ($n = 1$), replacing the sum in (25) by an integral, the solution which is even in $k$ is given by $\Delta_{k} = \Delta_{y} \alpha_k \beta_{k'} \cos k$. Then, $\Delta_0$ is then determined by the relation
$$1 = -0.5\pi^2 V_1 \sum \alpha_k^2 \beta_k^2 \cos^2 k \cdot (\Delta_k^2 \alpha_k^2 \beta_k^2 \cos^2 k + \varepsilon_{k1}^2)^{-1/2} \, dk$$

Eq. (26) is also represented as $1 = -\pi^2 V_1 \sum \alpha_k^2 \beta_k^2 \cos^2 k \cdot (\Delta_k^2 \alpha_k^2 \beta_k^2 \cos^2 k + \varepsilon_{k1}^2)^{-1/2} N_\sigma \varepsilon \, d\varepsilon$. Here $l$ is the length of Fermi line in Brillouin zone, $E_0$ is the energy width contributing to the Cooper formation, and $N_\sigma$ is the density of states at Fermi surface. The gap energy $\Delta_n$ is then obtained by solving the gap equation regarding $\Delta_0$. In the case of $d_{yz}$ ($n = 2$), using the transformations of $k_x \to k_x$, $V_x \to V_z$, $\alpha_{k1} \to \alpha_{k2}$, $\beta_{k1} \to \beta_{k2}$, the similar gap equation is obtained. Since the band of $d_{xz}$, $d_{yz}$ are almost the same configuration, the value of $\varepsilon_1$ will be equal to that of $\varepsilon_2$. These conditions mean the equivalency of $\varepsilon_x$, $\varepsilon_y$, $\varepsilon_{kx}$, $\varepsilon_{ky}$, $\varepsilon_{kz}$ etc and indicate that the total gap energy is presented as $\Delta_k = \Delta_{k1} + \Delta_{k2} \propto \cos k_x + \cos k_y$. Notice that the total gap energy is given by $\Delta_k = \sum \Delta_k$, because the gap equations can be separated in the ground state energy. It is thus concluded that the superconductive paring of Fe-Pn is $s$-like state different from the $d$-state of cuprates. Also, it is suggested that $d_{xx}$, $d_{yy}$ orbitals contribute to superconductivity in a cooperating way. However, if the equivalency of these orbitals is broken, it may lead to the different pair symmetry due to the modification such as the change of the crystal structure. Second let us consider the structural dependency of the critical temperature $T_c$. It is well known as an empirical rule that the optimal $T_c$ is obtained when the bond angle of Pn-Fe-Pn approaches $109.5^\circ$ of a regular tetrahedron [17,18]. Surprisingly, the superconductivity of Fe-Pn is very sensitive to the change from the regular tetragonal structure of Pn anions. This suggests that Fe-Pn bonding state is strongly correlated with superconductive properties. Since the crystal structure is determined by the state with the maximum atomic bonding energy, the regular tetrahedron indicates that the Fe-Pn bonding energy is in the maximum state. On the other hand, according to this theory, the superconductivity is determined by the state of the Fe-Pn composite system and the antiferromagnetic interaction forming Cooper pairs is proportional to $\varepsilon_{k1}^2$, that is the square of Fe-Pn hopping integral. The Fe-Pn bonding energy will be approximately proportional to the value of Fe-Pn hopping integral. Thus, the modification of the regular tetrahedron will weaken the superconductivity of Fe-Pn. Third let us discuss the doping dependency of the superconductive properties. Though some Fe-Pn materials exhibit low-temperature ($T_c \sim 4$K) superconductivity without doping, the high $T_c$ iron-based superconductors appear by a partial replacement of F or H on the oxygen site [19,20]. In general these iron-based superconductors indicate the phase diagram that the $T_c$ appears when the antiferromagnetism disappear or weaken, and disappear with increasing of doping level. This phase diagram can be explained in a similar way to the case of cuprates. In non-doping state, Fe ions are the superexchange antiferromagnetic state through the sites of pnictides that are non-magnetic materials (closed shell). However, it is recognized that there is the change from the closed shell state related to the mechanism of superexchange antiferromagnetism. This means that the doped electrons will be supplied in Fe-3d sites and the partial empty sites of pnictide. Therefore, in the similar situation with the case of cuprates, the doping will create the antiferromagnetic interaction contributing the superconductive state and reversely will weaken the superexchange antiferromagnetic interaction between Fe ions.

5. Conclusions
In order to find the unified theory to explain generally the properties of high-temperature superconductors such as cuprates and iron pnictides, a theory of high-temperature superconductivity in strongly correlated fermions system is derived from an extended $d$-$p$ model reconstructed with unitary-transformed fermions. It is indicated that the effective interaction between these newly defined fermions can determine the pseudogap and the superconductive states in cuprates and pnictides superconductors. It is also found that the theory can explain the various properties such as pseudogap energy, superconductive gap energy, critical temperature, superconductive anisotropy, and doping dependency and structural dependency of the electronic states in those superconductors. The important conclusion is that the pseudogap state and the Cooper pair formation in high-temperature superconductors could be only caused by the interplay between the $d$-$p$ hybridization and the $d$-$p$ exchange antiferromagnetic interactions.
interaction. This also suggests that the new selection of composite fermions may open an alternative root to improve the critical temperature of superconductors.

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