Pseudogap Induced by Superconducting Fluctuation in the $d$-$p$ Model

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In the high-$T_c$ superconductors, various anomalous properties have been observed at higher temperatures than the superconducting transition temperature $T_c$, especially in the underdoped region. Key issues on these anomalous properties must be on the existence of the pseudogap which has been suggested based on various experiments.

In-plane resistivities, Hall coefficients, and static uniform spin susceptibilities show peculiar temperature dependences below a certain characteristic temperature $T_0$ where the pseudogap is believed to become appreciable. Recently, photoemission experiments have revealed that the pseudogap is of the same size and has the same $k$-dependence as the superconducting gap. More recently, the temperature evolution of the pseudogap has been observed by the angle-resolved photoemission spectroscopy (ARPES).

There are several different views regarding the origin of the pseudogap. For example, it may be interpreted as a spin excitation gap in the singlet RVB states obtained by the $t$-$J$ model or it may be due to the Bose condensation of bound pairs or due to superconducting fluctuations.

In the present study, we demonstrate, using the $d$-$p$ model, that the pseudogap induced by the superconducting fluctuation (SC fluctuation) plays key roles in the determination of the phase diagram observed in high-$T_c$ superconducting materials. The pairing interaction mediated by the spin fluctuation and the single-particle spectrum by treating both the superconducting fluctuation and spin fluctuation in a consistent fashion. As temperature decreases, $1/T_1T$ increases at high temperatures, and it reaches a maximum followed by a sharp drop in the underdoped region, due to the evolution of the pseudogap in the single-particle spectrum. The evolution is also consistent with those of ARPES experiments.

KEYWORDS: pseudogap, NMR relaxation rate, superconductivity, superconducting fluctuation, spin fluctuation, superexchange interaction, $d$-$p$ model, $1/N$-expansion, slave-boson technique

Using the $d$-$p$ model, we demonstrate that the pseudogap, which is induced by the superconducting fluctuation, plays key roles in the determination of the phase diagram observed in high-$T_c$ superconducting materials. We take the pairing interaction mediated by the spin fluctuation and calculate the superconducting transition temperature $T_c$, the NMR relaxation rate $1/T_1$ and the single-particle spectrum by treating both the superconducting fluctuation and spin fluctuation in a consistent fashion. As temperature decreases, $1/T_1T$ increases at high temperatures, and it reaches a maximum followed by a sharp drop in the underdoped region, due to the effect of the AF fluctuation.

Then this $T_0$ corresponds to that determined by experiments on the Hall coefficient $R_H$.

First, we describe our model and formulation. We take the simplest version of the $d$-$p$ model as

$$H = \varepsilon_p \sum_{m=1}^{N} \sum_{k_m} c_{k_{m},m}^{\dagger} c_{k_{m},m} + \varepsilon_d \sum_{m=1}^{N} \sum_{i=1}^{d} d_{im}^{\dagger} d_{im}$$

$$+ N_{L}^{-1/2} \sum_{m=1}^{N} \sum_{k_{m},i} \{ t_i(k_m) c_{m,m}^{\dagger} d_{im} b_{i}^{\dagger} + h.c. \},$$

which is treated within the physical subspace where local constraints

$$\hat{Q}_i \equiv \sum_{m=1}^{N} d_{im}^{\dagger} d_{im} + b_{i}^{\dagger} b_{i} = 1 \quad (i = 1, 2, \cdots, N_L)$$

hold. In the above, $c_{k_{m},m}$, $d_{im}$ and $b_{i}$ are annihilation operators for a $p$-hole, a $d$-hole and a slave bo-
son, respectively, \(t_v(K) = t_v \exp(-iK \cdot R_v)\), where \(t_v = 2\sqrt{(1 - \cos k_x a + \cos k_y a)^2} \) and \(a\) is the lattice constant. The suffix \(m\) represents the spin-orbital degeneracy \((m = 1, 2, \cdots, N)\) introduced by dividing the phase space for \(K\) into \(N/2\) subspaces for \(K_m\), keeping the total degrees of freedom for spins and orbitals unchanged as \(\sum_{\sigma, k} = \sum_{m, k_m} \Sigma 1\). For numerical calculations in the present study, we set \(N = 2\). The local constraints in eq. (2) are strictly held when we calculate an expectation value of a physical quantity.

A set of self-consistent equations for single-particle Green’s functions of the leading order in the \(1/N\)-expansion was solved to yield the \(p\)-hole Green’s function given by

\[
G(k; \varepsilon_n) = \sum_{\gamma = \pm} \frac{A^\gamma_k}{\varepsilon_n - E_k^\gamma},
\]

with

\[
E_k^\gamma = \frac{1}{2} \left( \varepsilon_p + \omega_0 + \gamma \sqrt{(\varepsilon_p - \omega_0)^2 + 4b t_k^2} \right),
\]

(4)

\[
A_k^\gamma = \frac{E_k^\gamma - \omega_0}{E_k^\gamma - E_k},
\]

(5)

where \(\omega_0\) and \(b\) are the energy and the residue of the pole in the slave-boson Green’s function. The chemical potential \(\mu\) is determined by

\[
n = 1 + \delta = \frac{1}{N_L} \sum_{k, \sigma \gamma} f(E_k^\gamma),
\]

(6)

where \(n\) and \(\delta\) are the total hole number and the doped-hole number per unit cell, respectively, and \(f(E) = [\exp(E/k_B T) + 1]^{-1}\). Here, it is noted that the solution \(E_k^\gamma\) denotes the in-gap state emerging inside the charge transfer gap, \(\Delta \equiv \varepsilon_p - \varepsilon_d\), upon doping carriers to a Mott insulator. The band width of the in-gap states is proportional to \(\delta\) in the underdoped region. The effects of the interactions among the in-gap states are of higher-order terms in the \(1/N\)-expansion. Recently, it has been shown that quasi-particle interactions via the superexchange interaction play dominant roles in underdoped systems.

Now, we derive coupled equations to treat the effects of the SC fluctuation and the AF fluctuation in a consistent fashion (termed the extended self-consistent \(t\)-matrix approximation). The pairing interaction mediated by the AF fluctuation via the superexchange interaction \(J_a\) in RPA is given by

\[
V(q) \approx \frac{J_a(q)}{1 - J_a(q)\chi^{(0)}(q, 0)},
\]

(7)

with \(J_a(q) = -J_a(\cos(q_x a) + \cos(q_y b))\),

\[
\chi^{(0)}(q, \omega + i0^+) \approx \frac{\hbar^2}{N_L} \sum_k \frac{t_k^2}{(E_k^\gamma - \omega_0)^2 (E_k^\gamma - \omega_q)^2 \gamma},
\]

\[
\times \frac{1}{\pi} \int_{-\infty}^{\infty} df(x) \times \text{Im}G(k + q, x + i0^+) G(k, -\omega + x + i0^+)
\]

\[
1 - v_d \chi_0(0, 0) - v_d \chi_0(0, 0) = 0,
\]

(10)

where \(\chi_0\) is due to higher-order terms of the SC fluctuation, which is important in high-\(T_c\) superconducting materials because of the quasi 2-dimensionality of CuO growth.
In the normal state, close to the superconducting phase, $\chi_h(q,0)$ has a sharp $Q$-dependence, practically, $v_d\chi_h(q,0)$ is of $O(1)$ only at $q \cong 0$ and is zero otherwise in the limit of $T \to T_c$. Thus, $\chi$ does not contribute to the $q$-summation in the self-energy $\Sigma$ (eq.(11)) in this limit. In the present study, we simply assume that $v_d\chi_h(0,0) = 0.5$.

We also calculate the NMR relaxation rate, $1/T_1$, using the formula\[1\]
\[
\frac{1}{T_1T} = \frac{1}{N_L} \sum_q F_{ab}(q) \lim_{\omega \to 0} \text{Im} \chi_q^{\text{RPA}}(\omega)/\omega, \tag{15}
\]
with
\[
\chi_q^{\text{RPA}}(\omega) = \chi_q^{(0)}(q,\omega)/[1 - J_s(q)\chi_q^{(0)}(q,\omega)], \tag{16}
\]
\[
F_{ab}(q) = [A_{ab} + 2B(\cos q_x a + \cos q_y a)]^2/2
\]
\[
+ [A_c + 2B(\cos q_x a + \cos q_y a)]^2/2, \tag{17}
\]
\[
A_{ab} = -170, \quad A_c = 20 \quad \text{and} \quad B = 40. \tag{18}
\]

Here, $\chi_q^{(0)}(q,\omega)$ is given by eq. (8), where $G$ is replaced by $\tilde{G}$.

In actual numerical calculation, throughout the present study, we set $2t = 1.0$ (which is of $0(1eV$) in real systems), $\Delta = 2.5$ and $J_s = 0.1$. The total number of discrete points taken for the $q$-summation over the 2D first Brillouin zone is $32 \times 32$. The $\omega$-integral over the region from $-2\omega_0$ to $2\omega_0$ is replaced by the $\omega$-summation of 80 discrete points.

Numerical results for the $T$-dependence in $1/T_1T$ are shown in Fig. 1 for the hole-doping rate $\delta = 0.06 \sim 0.19$. At high temperatures, $1/T_1T$ increases as $T$ or $\delta$ decreases, due to the development of the AF fluctuation. We define $T_0$ as the characteristic temperature where the effects of the AF fluctuation begin to be appreciable. Explicit values of $T_0$ are determined by the condition $\left| T / (1/T_1T) \right|_{T=T_0}/\left| (1/T_1T) \right|_{T \to \infty, \delta = 0.1} = 2 \times 10^2$. At $\delta < 0.11$, $1/T_1T$ has a maximum at a certain temperature denoted by $T_{sg}$. Curves of $1/T_1T$ on the lower temperature sides terminate at $T_c$ for $\delta \gtrsim 0.1$, but we have not yet obtained $T_c$ for $\delta \lesssim 0.09$ due to the poor convergency of the numerical calculation at $T \cong T_c$. In the inset, the $T$-dependence of $1/T_1T$ obtained at $\delta = 0.1$ as above (solid line) is compared with that calculated by neglecting the effects of the SC fluctuation (dashed line). We note that the SC fluctuation also becomes appreciable at $T \sim T_0$ and continues to develop along with the AF fluctuation as $T$ decreases, while the SC fluctuation induces the pseudogap in the single-particle spectra (see Figs. 3 and 4), which suppresses the AF fluctuation. Eventually, the developed pseudogap eliminates the AF fluctuation, which leads to a sharp drop in $1/T_1T$ at $T \lesssim T_{sg}$. Recently, Kontani showed that the Hall coefficient $R_H$ is also enhanced by the AF fluctuation.\[2\]

Thus, the initial enhancement of $R_H$ at high temperatures can be assumed to have the same origin as that of $1/T_1T$. In this sense, we may argue that $T_0$ obtained in the present study corresponds to $T_0$ determined by $R_H$ experiments.\[3\]

We plot the three characteristic temperatures $T_0$, $T_{sg}$ and $T_c$ as functions of $\delta$ in Fig. 2. Note that $T_{sg}$ appears at $\delta \cong 0.11$ and increases as $\delta$ decreases, whereas $T_0$ appears at $\delta \cong 0.26$ and is much higher than $T_{sg}$. We also note that $T_c$ has a maximum at $\delta \cong 0.11$. The dotted curve of $T_c$ at $\delta \lesssim 0.09$ is determined by eq. (14) with the help of the extrapolation of numerical results for the $T$-dependence of $(1 - v_d\chi(0,0) - v_d\chi_h(0,0))$, because we had difficulty in obtaining fully convergent solutions for the self-consistent equations (7)-(13) at $T \cong T_c$ for $\delta \lesssim 0.09$. At $\delta$ decreases, the quasi-particle band narrows and the nesting effect increases, which enhances the AF fluctuation and then pushes $T_{sg}$ higher. The AF fluctuation enhances the pairing interaction and then the SC fluctuation, which develops the pseudogap and then suppresses $T_c$ in the underdoped region. $T_{sg}$ is determined by the competition between the AF fluctuation and the SC fluctuation. The phase diagram shown in Fig. 2 accounts for essential features of the anomalous metallic phase observed in high-$T_c$ superconducting materials.\[4\]

The single-particle density of states, $\rho(\omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\hbar} \sum_k G(k, \omega + i0^+)$, at $T = 0.02$, $0.025$, $0.03$ and $0.02$ with $\delta = 0.1$ where $T_0 = 0.057$ are shown in Fig. 3. At $T = 0.2$, $\rho(\omega)$ is nearly equal to that of the bare in-gap states without the effects of the SC fluctuation. At $T \lesssim T_0$, $\rho(\omega)$ decreases near the Fermi energy ($\omega = 0$) and increases at $|\omega| \gtrsim 0.05$ as $T$ decreases. The size of the pseudogap is roughly 0.1, which corresponds to the strength of the pairing interaction of order of $J_s$.

Lastly, we show contour plots of the $k$-dependence on the first Brillouin zone of the single-particle spectrum at the Fermi energy $\rho(k,0) = -\frac{1}{\pi} \text{Im} G(k,0)$ with $\delta = 0.1$ at $T = 0.2$ in Fig. 4 (left) and at $T = 0.02$ in Fig. 4 (right). The single-particle spectrum $\rho(k,0)$ has a large value in bright regions, where the energy of a quasi particle with $k$ is close or equal to the Fermi energy. Thus, the bright regions represent the shape of the Fermi surface. In the
dark regions, $\rho(k, 0)$ is nearly zero, where the energy of a quasi particle with $k$ is far from the Fermi energy. The Fermi surface exists in all directions at $T = 0.2$. As the temperature decreases, the single-particle spectra near the $[\pi, 0]$ and $[0, \pi]$ directions decrease due to the SC fluctuation with $d_{x^2-y^2}$ symmetry, and then the Fermi surface remains only near the $[\pi, \pi]$ direction at $T = 0.02$. These features are consistent with the results of ARPES experiments.\(^\dagger\)

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Pseudogap Induced by Superconducting Fluctuation in the $d$-$p$ Model

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