Pseudogap due to Antiferromagnetic Fluctuations and the Phase Diagram of High-Temperature Oxide Superconductors

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A reduction of the density of states near the Fermi energy in the normal state (pseudogap) of high-temperature oxide superconductors is examined on the basis of the two-dimensional tight-binding model with effective interactions due to antiferromagnetic fluctuations. By using antiferromagnetic correlation lengths which are phenomenologically assumed, the doping dependence of the pseudogap is obtained. The superconducting transition temperature decreases and eventually vanishes due to the pseudogap as the hole concentration is reduced.

In high-temperature oxide superconductors (HTSCs), behaviors which can be attributed to a reduction of the density of states (DOS) near the Fermi energy (pseudogap) have been observed. For example, experimental results in photoemission spectroscopies, tunneling spectroscopies, NMR experiments, and neutron scattering. However, the origin of the pseudogap remains controversial: preformed Cooper pairs in the spinon condensation model, spin fluctuation in the nearly antiferromagnetic (AF) spin fermion model, and so forth. Therefore, we treat phenomenologically defined DOS near the Fermi energy in the normal state (pseudogap) of high-temperature superconductors.

Among these candidates, the decrease of $T_g$ (the temperature below which the pseudogap phenomena are observed) with hole doping seems to suggest a possibility that the pseudogap mainly originates from AF fluctuations at least at temperatures much higher than the superconducting transition temperature ($T_c$). The AF long-range-ordered phase occurs in the vicinity of the half-filling, where the real gap is open. It is likely to have a pseudogap structure in the DOS in its proximity due to strong AF fluctuations. In this mechanism, the decrease of $T_g$ can be explained naturally, since the AF fluctuations decrease with doping. On the other hand, if we assume that the pseudogap is due to pairing fluctuations, temperature $T_g$ can be regarded as the temperature at which pairing fluctuations begin to occur. Therefore, when $T_g$ increases, it is natural to consider that $T_c$ should increase as well. However, such behavior is inconsistent with the observed behavior of the opposite doping dependencies of $T_g$ and $T_c$ in the underdoped region.

In this paper we examine the pseudogap due to AF fluctuations. The reduction of the DOS near the Fermi surface should suppress $T_c$ in the underdoped region, and thus $T_c$ has a peak as a function of hole concentration. We intend to describe a minimum theory which reproduces the phase diagram of a HTSC. Hence, we omit some of the details which do not change the qualitative behavior of $T_c$. For example, we adopt the static approximation for the spin fluctuations. The static approximation does not produce the imaginary part of the self-energy and the broadening of the one particle weight. However, the real part of the self-energy could reproduce the reduction of the DOS near the Fermi surface, which is the most intuitive definition of the pseudogap. Therefore, the static approximation is sufficient for our purpose. In addition, Schmalian et al. argued that the characteristic frequency of the spin fluctuations $\omega_{\text{sf}}$ is much smaller than the temperatures of interest for HTSCs.

In our formulation, AF fluctuations are taken into account through a renormalization effect. The importance of the renormalization effect in the doping dependence of the $T_c$ of HTSC was discussed on the basis of the two-dimensional Hubbard model. It was shown that $T_c$ is considerably near the boundary of the AF long-range-ordered phase by the strong renormalization effect due to AF fluctuations. However, the pseudogap was not taken into account sufficiently.

This work was extended to include the pseudogap due to AF fluctuations in a quasi-one-dimensional (Q1D) Hubbard model as a model of Q1D organic superconductors. It was shown that the pseudogap suppresses $T_c$ markedly near the spin density wave boundary. As a result, phase diagrams of Q1D organic superconductors in the pressure and temperature plane were semiquantitatively reproduced.

In HTSCs, however, the same approach based on one of the microscopic models is difficult. The interlayer coupling is much smaller and the temperature range of interest is much higher in HTSCs than it is in the organic superconductors. Hence, the thermal fluctuations are very strong in HTSCs. This situation makes a quantitative argument difficult. In addition, there is no common consensus as to which microscopic model is appropriate for HTSCs: a single-band Hubbard, $d$-$p$, $t$-$J$ models, and so forth. Therefore, we treat phenomenologically determined AF fluctuations from the experiments instead of calculating them microscopically, and concentrate on their qualitative features.

In the calculation of $T_c$, for simplicity, we assume that
the coupling constant of the pairing interactions does not depend on the doping. Such interactions may be attributed to those mediated by phonons. It may appear that the d-wave pairing does not occur with phonon-mediated interactions. However, it is shown that pairing interactions mediated by screened phonons can give rise to a d-wave pairing superconductivity in the presence of AF fluctuations. Here, we do not specify the origin of the pairing interactions. To some extent there may be a contribution from the exchange of AF fluctuations.

We calculate the electron self-energy up to the one-loop approximation as

\[ \Sigma_\sigma(k) = -T \sum_{n'} N^{-1} \sum_{k'} \sigma' V_{\sigma \sigma'}(k, k') G_{\sigma'}(k'), \tag{1} \]

with \( k = (k, i\omega_n) \), where \( V_{\sigma \sigma'} \) is the effective interaction due to the exchange of the fluctuations and \( G_{\sigma'}(k') \) is the renormalized electron Green’s function,

\[ G_{\sigma}(k) = \frac{1}{i\omega_n - \epsilon_k - \Sigma_{\sigma}(k) + \mu}. \tag{2} \]

We consider a two-dimensional tight-binding model with the electron dispersion

\[ \epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y, \tag{3} \]

where \( t \) and \( t' \) are the nearest- and next-nearest-neighbor hoppings, respectively.

We express the effective interactions due to exchange of magnetic fluctuations as

\[ V(k, k') = \frac{V_0}{(k - k' - q_m)^2 + q_0^2}, \tag{4} \]

within the static approximation. Here, \( V_0 \) and \( q_0 \) are the phenomenological parameters. Since the effective interactions due to the exchange of magnetic fluctuations are proportional to the spin susceptibility \( \chi(k - k') \), they must have a sharp peak at \( k = k' + q_m \), where \( q_m \)'s are the nesting vectors near \( (\pi, \pi) \) for the AF fluctuations which give the largest value of \( \chi(q) \).

There are four nesting vectors such as \( q_m = (\pi \pm \delta, \pi) \) or \( q_m = (\pi, \pi \pm \delta) \), when the incommensurate AF fluctuations occur \([\pi, \pi] \). In eq. (4), we take a nesting vector such as \( \pi \geq q_{mx} \geq q_{my} > 0 \) for \( k_x - k'_x \geq k_y - k'_y \geq 0 \). For other regions of \( k_x - k'_x \) and \( k_y - k'_y \), \( q_m \) is chosen so that \( V(k, k') \) satisfies the symmetry condition. The AF correlation length \( \xi \equiv 1/q_0 \) diverges at the critical hole concentration \( n^c_h \). We take

\[ \frac{1}{q_0} = \frac{C}{\pi(\mu_c - \mu)^{1/2}}, \tag{5} \]

which diverges at a critical chemical potential \( \mu_c \).

For small hole concentrations, the chemical potential \( \mu \) is roughly proportional to the hole concentration \( n_h \). Thus, the above form roughly implies \( \xi \propto 1/\sqrt{n_h} \), which is plausible in the sense that the AF correlation length is directly related to the average distance between holes \([\pi, \pi] \).

Thus, we finally obtain an equation to solve in a compact form

\[ \Sigma_\sigma(k) = \frac{1}{2} N^{-1} \sum_{k'} V(k, k') \tanh\left(\frac{\epsilon_{k'} + \Sigma_{\sigma}(k') - \mu}{2T}\right). \tag{6} \]

With the static approximation of eq. (5), we only need to solve the real part of the self-energy. Thus, it is found that the pseudogap appears as shown below, for example, in the DOS, which is given by

\[ \rho(\epsilon) = \int \frac{dk_x dk_y}{(2\pi)^2} \delta(\epsilon - \bar{\epsilon}_k), \tag{7} \]

where we have put \( \bar{\epsilon}_k = \epsilon_k + \Sigma_{\sigma}(k') \).

We solve the self-consistent equation for large discrete 512 × 512 momentum points in the first Brillouin zone. We confirmed that the results of 512 × 512 practically coincide with those of 256 × 256, within the width of the lines in our figures of DOS and \( T_c \). Thus, practically, the system size 512 × 512 can be regarded as being within the thermodynamic limit at the present temperature. We interpolate the obtained self-energy linearly in the momentum space so that the first Brillouin zone has 4096 × 4096 points for the calculation of DOS.

We consider the case of nearest-neighbor hoppings \( t \neq 0 \) and \( t' = 0 \). We choose \( V_0 = -0.4 \) and \( T = 0.01 \), and take \( C = 30 \) and \( \mu_c = -0.05 \) in eq. (6). We use the units in which \( t = 1 \). The value of \( \mu_c \) gives \( n^c_h \approx 0.02 = 2\% \), where \( n^c_h \) denotes the critical hole concentration of the AF long-range-order.

\[
\begin{align*}
\text{FIG. 1.} & \quad \text{Doping dependence of the AF correlation length } \\
& \quad \text{\( \xi \) (triangle), and the resulting densities of states } \rho_s(\epsilon_F) \text{ and } \\
& \quad \rho_d(\epsilon_F) \text{ (circles and squares, respectively). The solid lines are } \\
& \quad \text{guides for the eyes. } \rho_d(\epsilon_F) \text{ is the effective DOS for the d-wave pairing which is averaged with the weight } \\
& \quad (\cos k_x - \cos k_y)^2. \\
& \quad \text{Figure 2 shows the } n_h \text{ dependence of the AF correlation length } \xi, \text{ and the resulting DOS at the Fermi energy. In this figure, } \\
& \quad \rho_d \text{ is the effective DOS for the d-wave pairing in which the order parameter is } \Delta(k) \propto \\
& \quad (\cos k_x - \cos k_y),
\end{align*}
\]

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\[ \rho_\alpha(\mu) = \int \frac{d^2 k}{(2\pi)^2} \delta(\tilde{\varepsilon}_k - \mu) \left( \cos k_x - \cos k_y \right)^2. \] (8)

\( \rho_\alpha \) is that for the s-wave pairing, \((\Delta(\mathbf{k}) = \text{const.})\), which is equivalent to the usual DOS.

From the obtained DOS, we calculate \( T_c \) by the conventional weak coupling formula

\[ T_c = 1.13 \omega_D e^{-1/\lambda_\alpha}, \] (9)

with \( \lambda_\alpha = g \rho_\alpha(\mu) \). We choose a value of the cutoff energy of bosons which mediate the pairing interactions as \( \omega_D = 1000 \) K. The value of \( g \) is chosen so that \( T_c \) takes reasonable values such as \( \sim 40 \) K or \( \sim 90 \) K at the peak.

Figures 2 and 3 show the doping dependence of the \( T_c \) for the s-wave pairing and d-wave pairing, respectively. From the sensitivity of the singular exponential form of eq. (9), we obtain marked suppressions of \( T_c \) near the AF boundary \((n_h \gtrsim n_h^c)\) and thus peak structures around \( n_h \sim 0.1 = 10\% \). In particular, for the d-wave pairing, the peak is narrow, and seems to coincide with the experimental phase diagram of HTSC.

In order to be more precise, we should take into account the temperature dependence of the DOS in the estimation of \( T_c \). However, for \( n_h \gtrsim n_h^c \), the AF correlation length \( \xi \) does not strongly depend on temperature at low temperatures \([31]\). When its temperature dependence is ignored, the DOS are almost independent of the temperature. For example, it can be confirmed that the results for \( T = 0.005 \) are almost the same as those for \( T = 0.01 \). On the other hand, even when the temperature dependence of \( \xi \) is taken into account, it does not change the qualitative result. It only emphasizes the peak of the \( T_c \), because the pseudogap becomes deeper for longer \( \xi \) and it reduces \( T_c \) more.

Figure 4 shows the DOS of the underdoped region \((n_h \approx 0.0237)\) and that of the overdoped region \((n_h \approx 0.227)\). It is seen that the pseudogap is deep and clear in the underdoped region, while it becomes very shallow in the overdoped region. We also find that the pseudogap becomes large in the direction of \((\pm \pi, 0)\) and \((0, \pm \pi)\), while it becomes small in the direction of \((\pm \pi, \pm \pi)\) \([32]\).

It is straightforward to extend the present calculation to the \( t' \neq 0 \) case. When we assume \( t' = -0.2 \) and a similar doping dependence of the AF correlation length which decreases with doping, we also have a peak structure of the \( T_c \) near \( n_h \approx 0.13 \) \([32]\). This peak structure is also consistent with the experimental phase diagrams except that the peak becomes very steep due to the van Hove singularity. However, it is easily verified by a phenomenological consideration that such steepness of the peak is not at all essential. If we assume that a large \( t' \) is appropriate for the HTSC, the Fermi surface crosses the van Hove singularities at a large hole concentration. Thus, the DOS at the Fermi energy and \( T_c \) have a sharp peak around the hole concentration. However, such singular behavior or marked enhancement of the DOS with hole doping has not been observed in any experiments, for example, the specific heat and susceptibility measurements. This suggests that the singularity is eliminated finally by some many-body effect. If we take this many-body effect into our phenomenological model beforehand, models with \( t' \approx 0 \) might be reasonable in order to describe a realistic situation, because it is consistent with the experimental facts that no singularity occurs in the overdoped region, and the AF correlation length increases near the half-filling.

FIG. 2. Doping dependence of \( T_c \) for the s-wave pairing. Circles, triangles and squares indicate the results for \( g = 2.3, 1.7 \) and \( 1 \), respectively. Solid lines are guides for the eyes.

FIG. 3. Doping dependence of \( T_c \) for the d-wave pairing. Circles, triangles and squares indicate the results for \( g = 0.9, 0.7 \) and \( 0.5 \), respectively. Solid lines are guides for the eyes.
We omit vertex corrections and dynamical effects. However, since these effects should reduce \( T_c \) in the underdoped region, it is likely that they only emphasize the peak structure of \( T_c \). Also, the strong coupling effects would not be essential regarding the qualitative behavior of the \( T_c \). The essential point is that \( T_c \) is very sensitive to the DOS, as explicitly written in the singular exponential form eq. (4) within the weak coupling theory. The quantitative improvement of the theory by including these effects remains for future study.

In conclusion, we propose a mechanism which explains the peak structure in the doping dependence of \( T_c \) of HTSCs. It is shown that the pseudogap due to AF fluctuations suppresses \( T_c \) in the underdoped region and eventually destroys the superconductivity at a finite doping. On the other hand, the pseudogap phenomena is less pronounced near the optimum doping at which \( T_c \) is maximum. Then, DOS is large since the Fermi energy is at the shoulder of the van Hove singularity. This leads to high \( T_c \). The decrease of \( T_c \) in the overdoped region is due to the decrease of the DOS \( \rho(\varepsilon) \), since the Fermi energy is distant from the van Hove singularity.

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