Pseudogap and Superconducting Fluctuation in High-$T_c$ Cuprates: Theory beyond 1-loop Approximation

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The pseudogap phenomena induced by the SC fluctuation are investigated in details. We perform a calculation beyond the 1-loop approximation. The SC fluctuation is microscopically derived on the basis of the repulsive Hubbard model. The vertex corrections are collected in the infinite order with use of the quasi-static approximation. The single-particle excitations, NMR $1/T_1 T$, spin susceptibility and superconducting transition temperature are discussed. The important role of the vertex correction is pointed out for the single particle spectral function. On the other hand, the validity of the 1-loop order theory is confirmed for other quantities. We shed light on the essential nature of SC fluctuation leading to the pseudogap from the comparison with spin and charge fluctuations.

KEYWORDS: Superconducting fluctuation; spin fluctuation; vertex correction; high-$T_c$ cuprates; pseudogap

1. Introduction

Since the discovery in 1986, many anomalous aspects of high-$T_c$ superconductors have been clarified by enormous studies. Among them, the pseudogap phenomena (Fig. 1) have indicated a break down of the Fermi liquid theory, which is a universal view on the low energy excitations in metals. The unusual nature has indicated an appearance of a new concept in the condensed matter physics.

From the experimental point of view, the pseudogap was found in the magnetic excitation by the nuclear magnetic resonance (NMR). At present anomalies have been observed in many experimental probes which include NMR, neutron scattering, electric transport, optical spectrum, tunneling spectroscopy and angle resolved photo emission spectroscopy (ARPES).

Among many theoretical proposals, we have adopted the “pairing scenario” in which the pseudogap is induced by the superconducting (SC) fluctuation. This scenario has been indicated by several experimental results cited above. In particular, ARPES, which presents a momentum resolved information, has provided a strong circumstantial evidence. The pseudogap in the single particle excitation first opens around the zone boundary $k \sim (\pi, 0)$ and gradually extends to the whole Fermi surface as approaching to the superconducting transition. The amplitude of the excitation gap does not change through $T_c$. The latter has been observed also in the tunneling spectroscopy and in the $c$-axis optical conductivity. These results have indicated a close relation between the superconductivity and pseudogap.

Since there are many approaches included in the pairing scenario, we have classified them into three kinds in order to avoid any confusion. One is the BCS-BEC cross-over formulated in the Nozières and Schmitt-Rink theory. However, this approach is not relevant for high-$T_c$ cuprates because this is basically justified in the low density system. We have adopted the second approach which is the perturbation theory with respect to the single particle spectral function. Then, the resonance scattering described by the electron self-energy plays an essential role. The 1-loop order theory which is called T-matrix approximation has been widely used and enabled us to perform a non-phenomenological treatment on the microscopic Hamiltonian. This approach is complementary with the third one, phase fluctuation theory.

It is our basic standpoint that non-Fermi liquid behaviors in cuprates should be derived from the Fermi liquid state. Because cuprates behave as a conventional metal in the over-doped region and there is no discontinuity between over-doped and under-doped regions, the origin of the anomalous behaviors should be inherent in the Fermi liquid state. Such understanding will be valuable for a universal understanding of the strongly correlated electron systems including transition metals, organic superconductors and heavy fermion systems. Then, the Fermi liquid theory will be a reasonable starting point. The microscopic study is suitable for this purpose since the characteristics of each system should be clarified from the microscopic point of view.

In the previous studies, a microscopic theory for the SC fluctuation is developed on the basis of the repulsive Hubbard model. Then, the T-matrix and self-consistent T-matrix approximations for the SC fluctuation have been used in combination with the FLEX approximation. It has been shown that single-particle, magnetic and transport properties are explained in a coherent way. The doping dependence including the particle-hole asymmetry is also reproduced without using any phenomenological assumption. The electron-doped cuprates are basically weak-coupling superconductors.

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and do not show pseudogap. The pseudogap state in the hole-doped region is described as a regime with spin and SC fluctuations, which have both cooperative and competitive aspects. We have shown that the pseudogap is essentially induced by the SC fluctuation.

The purpose of this study is an examination of the theory based on the 1-loop approximation. The previous studies have attributed the pseudogap to the serious correction arising from the 1-loop order term.\(^5\) This fact involves a naive question from the theoretical point of view. Do the higher order terms play a more serious role? There is no clear evidence for the validity of 1-loop order theory because so-called Migdal theorem is not generally applicable. In this paper we present a theory beyond the 1-loop approximation in order to answer this question. This study will clarify the roles of higher order corrections.

Theoretical studies beyond the 1-loop approximation have been developed mainly for the Lee-Rice-Anderson model\(^5\) which is an one-dimensional model with charge fluctuation. Then, the electronic system coupled to the classical Gaussian field has been investigated.\(^5\) The exact estimation is possible in the limit of infinite correlation length.\(^5\) An approximation for the finite correlation length has been suggested by Sadovskii\(^5\) and its validity has been investigated extensively.\(^5\) Theoretical method developed there has been applied to the two dimensional systems with charge fluctuation,\(^5\) spin fluctuation\(^5\) and SC fluctuation,\(^5\) respectively. We will explain in §3 that this method is formulated in the microscopic theory for the Hubbard-type Hamiltonian. It will be discussed that the estimation based on the infinite correlation length is applicable more robustly in the present case. We apply this method as well as the Sadovskii’s method to the repulsive Hubbard model in §4. The attractive Hubbard model is also briefly adopted as another typical example in §5.1.

We will show that higher order corrections are renormalized to be small, even if higher order terms develop in the scheme of naive perturbation calculation. It is concluded that the 1-loop order theory is qualitatively valid in many aspects (§4.2-4). On the other hand, the importance of the vertex correction will be illuminated for the single-particle spectral function, for which the 1-loop and self-consistent 1-loop approximations provide qualitatively incompatible results. It is shown that the non-self-consistent 1-loop approximation is qualitatively correct for this quantity (§4.1 and §5.1). This is an example in which the partial summation included in the self-consistent theory provides an unphysical result. We will show that this conclusion is non-trivial by comparing with the case of spin fluctuation and that of charge fluctuation (§5.2). Indeed, the roles of vertex corrections are determined by the symmetry of the order parameter. We furthermore illustrate that the differences between the order parameters are qualitatively understood from the naive perturbation theory (§5.3).

This paper is constructed in the following way. The 1-loop order theory is shortly summarized in §2. Higher order terms are classified in §3. We introduce the terms focused in this paper and formulate the infinite-order theory. A justification for the adopted approximation is given in Appendix A and B. The roles of vertex corrections are investigated in §4. The single particle excitations (§4.1), superconducting \(T_c\) (§4.2-3) and magnetic properties (§4.4) are discussed in details. The vertex corrections beyond the formulation in §3 are briefly discussed in the estimation of \(T_c\) (§4.3). The Sadovskii’s method is used in §4.4, where the naive perturbation is performed within the 4-loop order and compared with the Sadovskii’s method for a justification. The case of charge fluctuation and that of spin fluctuation are overviewed in §5, where the essential nature of SC fluctuation is clarified. The summary and discussion are given in the last section §6.

2. Theory in the 1-loop order

In this section, the 1-loop order theory is summarized before discussing the vertex corrections. After the basic mechanism of the pseudogap was described on the basis of the attractive model,\(^4\) the microscopic theory has been developed on the basis of the repulsive Hubbard model.\(^4\) An approach for the infinite-\(U\) \(d-p\) model has been also developed.\(^5\) Here we explain the formulation and typical results of the repulsive Hubbard model for a discussion in the following sections.

The Hubbard Hamiltonian is expressed as,

\[
H = \sum_{\mathbf{k}, \sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma} + U \sum_{i} n_{i, \uparrow} n_{i, \downarrow}.
\]

We consider the square lattice and choose the following tight-binding dispersion \(\varepsilon(\mathbf{k})\),

\[
\varepsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - \mu.
\]
Fig. 2. (a) The diagrammatic representation of the T-matrix. We denote the effective interaction between quasi-particles as $V_a$. (b) The self-energy in the T-matrix approximation.

represented by $V_a$. In the attractive models, the first order perturbation has been used for the estimation of $V_a$. In order to describe the superconductivity in the repulsive Hubbard model, we have to derive the effective interaction from the many body effects. Here we adopt the FLEX approximation which has been widely used as a microscopic description of the nearly anti-ferromagnetic Fermi liquid. The following calculation can be regarded as an improvement of the FLEX approximation so as to take account of the SC fluctuation. Then, the effective interaction is described by the spin and charge susceptibility in the following way,

$$V_a(k, k') = U + \frac{3}{2} U^2 \chi_s(k - k') - \frac{1}{2} U^2 \chi_c(k - k'),$$

(3)

where spin and charge susceptibility is estimated as,

$$\chi_s(q) = \frac{\chi_0(q)}{1 - U \chi_0(q)}, \quad \chi_c(q) = \frac{\chi_0(q)}{1 + U \chi_0(q)},$$

(4)

$$\chi_0(q) = -\sum_k G(k + q)G(k).$$

(5)

Here, the renormalized Green function is expressed as,

$$G(k) = \frac{1}{i\omega_n - \varepsilon(k) - \Sigma(k)}.$$  

(6)

The self-energy in the FLEX approximation is obtained as $\Sigma(k) = \Sigma_F(k)$, where

$$\Sigma_F(k) = \sum_q V_a(q)G(k - q),$$

(7)

$$V_a(q) = U^2 \left[ \frac{3}{2} \chi_s(q) + \frac{1}{2} \chi_c(q) - \chi_0(q) \right].$$

(8)

With use of these functions, the superconducting $T_c$ is estimated by the following eigenvalue equation (linearized Eliashberg equation),

$$\lambda_c \phi(k) = -\sum_{k'\neq k} V_a(k, k')|G(k')|^2 \phi(k'),$$

(9)

The transition temperature is determined by the criterion that the maximum eigenvalue is unity ($\lambda_c = 1$) at $T = T_c$. The FLEX approximation is regarded to be the mean field theory in the sense that the SC fluctuation is not taken into account. It should be stressed that the Eliashberg equation is derived from the strong coupling theory for the superconductivity which is needed for the quantitative estimation of $T_c$. This effort is important for the present purpose because the value of $T_c$ plays an essential role for the SC fluctuation. Note that the weak coupling theory significantly over-estimates the value of $T_c$.

The T-matrix has been estimated by using the extended Eliashberg equation as,

$$T(k_1, k_2 : q) = \phi(k_1)t(q)\phi^*(k_2),$$

(10)

$$t(q) = \frac{g\lambda(q)}{1 - \lambda(q)},$$

(11)

$$\lambda(q) = -\sum_{k,p} \phi^*(k)V_a(k - p)G(p)G(q - p)\phi(p),$$

(12)

$$g = \sum_{k_1, k_2} \phi^*(k_1)V_a(k_1 - k_2)\phi(k_2),$$

(13)

where the wave function is normalized as

$$\sum_k |\phi(k)|^2 = 1.$$  

(14)

Since this estimation of the T-matrix is correct around $q = 0$, the role of SC fluctuation is appropriately represented. It should be noted that the parameter $\lambda(0)$ is equivalent to the maximum eigenvalue of the Eliashberg equation, namely $\lambda(0) = \lambda_c$. Thus, the divergence of the T-matrix is equivalent to the criterion in the Eliashberg equation.

The self-energy correction due to the SC fluctuation is obtained within the 1-loop order as (Fig. 2(b)),

$$\Sigma_S(k) = \sum_q T(k, k : q)G(q - k).$$

(15)

The total self-energy is obtained by adding it to the contribution from the spin fluctuation,

$$\Sigma(k) = \Sigma_F(k) + \Sigma_S(k).$$

(16)

The lowest order theory has been denoted as FLEX+T-matrix approximation (FTA) while the self-consistent calculation has been denoted as self-consistent FLEX+T-matrix approximation (SCFT). The basic role of the SC fluctuation is described by the FTA which is the 1-loop approximation with respect to the SC fluctuation. The SCFT is the self-consistent 1-loop order theory and furthermore includes the feedback effect on the magnetic fluctuation. The SCFT is needed to explain the transport phenomena in which the feedback effect plays an essential role.

Figure. 3 shows the spectral function and the self-energy obtained by FTA. We clearly see the anomalous behaviors. The imaginary part of the self-energy (Fig. 3(a)) shows the scattering peak of $|\text{Im} \Sigma^R (\mathbf{k}, \omega)|$ around $\omega = 0$. This feature is qualitatively different from the conventional Fermi liquid where the self-energy behaves as $|\text{Im} \Sigma^R (\mathbf{k}, \omega)| \propto \omega^2$. In this sense, the Fermi liquid theory breaks down in the pseudogap state owing to the SC fluctuation. The scattering peak around $\omega = 0$ leads to the pseudogap around $\mathbf{k} = (\pi, 0)$ as is shown in Fig. 3(b). This is the basic mechanism of the pseudogap phenomena induced by the SC fluctuation. The pseudo-
gap gradually occurs with decreasing the temperature and/or doping concentration.

Concerning the momentum dependence, the Fermi liquid behaviors appear around \( k = (\pi/2, \pi/2) \) which is denoted as “cold spot” in contrast to the “hot spot” around \( k = (\pi, 0) \). The \( \omega \)-linear behavior instead of \( \omega \)-square behavior is induced by the spin fluctuation. This momentum dependence induces the “Fermi arc” which has been observed in ARPES.\(^{25-28}\) Note that these anomalous behaviors are suppressed in the electron-doped cuprates where the SC fluctuation is very weak.\(^{36,52}\)

![Figure 3](image)

Fig. 3. (a) The imaginary part of the self-energy and (b) the spectral function on the Fermi surface. A, B and C show the results at \( k = (0.07\pi, \pi), k = (0.15\pi, 0.8\pi) \) and \( k = (0.43\pi, 0.45\pi) \), respectively. The parameters are chosen as \( U/t = 3.2, \delta = 0.1 \) and \( T = 1.2T_c \).

Because the SC fluctuation is characterized by the T-matrix around \( q = \Omega = 0 \), the following expansion (TDGL expansion) is instructive for a qualitative understanding.

\[
t(q, \Omega) = \frac{g}{\xi_0 + b|q|^2 - (a_1 + ia_2)\Omega}.
\]

We adopt a perturbation expansion with respect to the coupling between electrons and SC fluctuation, which is called loop expansion. In more general perturbation scheme for the Hubbard Hamiltonian,\(^{69}\) there appear other terms which are not included in the loop expansion. However, we simply ignore them and focus on the singular terms in the vicinity of the phase transition. The vertex corrections to the Green function are mainly discussed in this subsection. In addition to them, the vertex corrections to the pairing correlation function will be investigated in §4.3.

First of all, we show the Feynmann diagrams corresponding to the self-energy investigated in this paper (Fig. 4). Fig. 4(1) is equivalent to Fig. 2(b), and
Figs. 4(2), (3a) and (4a) are included in the self-consistent T-matrix approximation. The other terms are classified into the vertex correction. The diagrams including the electron loop are not included in Fig. 4. It should be noticed that the terms like Fig. 5(a) should be included in the 1-loop order term owing to the definition. Considering this fact, we understand that all of the ignored terms include the higher order mode couplings between SC fluctuations, which correspond to the nonlinear terms in the Ginzburg Landau expansion (4th, 6th, 8th,... order terms). For example, Fig. 5(b) and Fig. 5(c) include the fourth order vertex (Fig. 5(d)) and sixth order vertex (Fig. 5(e)), respectively. Therefore, the estimation of the terms in Fig. 4 is sufficient in the renormalized Gaussian region where the higher order mode coupling does not play any essential role, namely when the system is not too close to the critical point. We note that the mode coupling effect in the level of the self-consistent renormalization theory (SCR)\textsuperscript{67} is included by itself if we determine the fluctuation propagator self-consistently as in §4.2-4.

The diagrammatic expression in Fig. 4 is exact if we consider the Lee-Rice-Anderson model. Most of the previous studies beyond the 1-loop approximation\textsuperscript{56–63} have been devoted to this phenomenological model. The importance of these terms has been pointed out for the model with sufficiently long range attractive interaction where the calculation is reduced to the zero-dimensional problem.\textsuperscript{71} We will estimate these terms as an approximation for the microscopic model.

Fig. 5. Examples of diagrams which are not included in Fig. 4. (a) A diagram included in the 1-loop order term owing to the definition. (b), (c) and (f) are diagrams including higher order mode couplings. (d) and (e) are the forth order and sixth order vertex, respectively.

The higher order mode couplings are surely important when the system is close to the critical point. However, considerable part of them is represented by the renormalization of the fluctuation propagator. For example, the terms in Figs. 5(b) and (c) are the cases. These corrections are represented by the TDGL parameters (see eq. 17) and the shift of $T_c$. Therefore, the qualitative roles of SC fluctuation are not affected, although these corrections may be important for the estimation of $T_c$. In this sense we have mentioned that the corrections in Fig. 4 are important in the “renormalized” Gaussian region. Indeed, the renormalization of the fluctuation propagator has been investigated from 1980’s motivated by the theoretical issues on the BCS-BEC cross-over.\textsuperscript{71,72} Then, the higher order terms arising from the forth order vertex (Fig. 5(d)) have been investigated and concluded to be not important quantitatively. We will investigate the different kinds of mode coupling in order to discuss the doping dependence of $T_c$ in §4.3. They include the lower order terms with respect to the fluctuation propagator, rather than the terms investigated in Refs.\textsuperscript{71 and 72}.

There remain corrections including higher order mode couplings but not discussed above. We show the lowest order term in Fig. 5(f) which is the 4-loop order term. This term is more singular rather than the same order terms in Fig. 4. However, we will estimate this term, and conclude that this correction is small in the wide region of the pseudogap state (Appendix B).

### 3.2 Quasi-static approximation

According to these discussions, we consider the vertex corrections represented by Fig. 4. We adopt the quasi-static approximation in order to formulate an infinite-order theory. In this approximation, the thermal fluctuation is taken into account but the quantum aspect of the fluctuation is ignored. This procedure has been adopted in the studies of critical phenomena. In the formulation, the zero Matsubara frequency $\Omega_n = 0$ of the fluctuation propagator is taken into account. This procedure is generally justified at high temperature and/or in the vicinity of the critical point.

Indeed, the character of SC fluctuation emerges in the applicability of the quasi-static approximation. The condition for the quasi-static approximation is generally described as $\omega_{sc} \ll T$ where $T$ is the temperature and $\omega_{sc}$ is the characteristic frequency of the SC fluctuation. Interestingly, $\omega_{sc}$ is expressed as $\omega_{sc} \sim T_{c}$, where $\epsilon = (T - T_c)/T_c$ is the reduced temperature. Then, the quasi-static approximation is justified when $\epsilon \ll 1$. This fact should be contrasted to the case of AF spin fluctuation. Then, the characteristic frequency of the fluctuation is expressed as $\omega_{s} \sim E_F \varepsilon_s$, where $\varepsilon_s$ denotes the reduced temperature for the magnetic instability. It should be noticed that the factor appearing in $\omega_{sc}$ is smaller than that in $\omega_{s}$ by the order $T/E_F$. This fact implies the better accuracy of quasi-static approximation for the SC fluctuation rather than that for the spin fluctuation. This will be confirmed by the microscopic calculation based on the repulsive Hubbard model (see Appendix A). While the quasi-static approximation for spin fluctuation is basically justified at high temperature, that for SC fluctuation is effective in much lower temperature region.

Another interpretation of the quasi-static approximation is obtained from the application to the 1-loop order theory. In §2, we have shown the anomalous behavior of the self-energy induced by the SC fluctuation. It is easily confirmed that this anomaly arises from the quasi-static part of the T-matrix $t(q, \Omega_n = 0)$, which is singular in the vicinity of $T_c$. The remaining contribution from the dynamical part basically induces the Fermi liquid behavior. Thus, anomalous contribution leading to the pseudogap is appropriately included in the quasi-static approximation. Indeed, the applicability of quasi-static approxima-
tion is a requirement of the pseudogap phenomena because the pseudogap in the single particle spectral function appears when the former is more significant than the latter. Therefore, the quasi-static approximation is sufficient for the purpose of this paper, while the closing of pseudogap may be described inadequately.

Owing to the quasi-static approximation, only the momentum summation remains as a practical task. Although an exact estimation is still difficult, we can avoid this difficulty by considering the “dirty” region where the quasi-particle mean free path is much smaller than the GL correlation length, namely $l \ll \xi_{GL}$. In this region, the $q$-dependence of the Green function can be ignored, where $q$ is the momentum of fluctuation. It should be noticed that quasi-particle in the “hot spot” has a remarkably short mean free path owing to strong scattering due to the AF spin fluctuation.\textsuperscript{73–75} Therefore, the condition $l \ll \xi_{GL}$ is relevant in this region. Note that the superconductivity and magnetic properties are dominated by this region of the Fermi surface, while transport phenomena are not.\textsuperscript{53}

In the “dirty” region, the Green function in the $n$-loop order is equivalently estimated as,

$$G^{(n)}(k) = (-1)^n \Delta^{2n}(k) G^{(0)}(k)^n + G^{(0)}(-k)^n,$$  

(18)

where $\Delta^2(k) = \Delta^2|\phi(k)|^2$ and $\Delta^2 = T \sum_q |t(q, 0)|$, which is proportional to the thermal weight of the SC fluctuation. The equivalence of $n$-loop order diagrams will be briefly discussed in §4.4 where a justification is obtained from the numerical estimation. We have defined the Green function without including the SC fluctuation as $G^{(0)}(k)$. In the present case, the renormalization from the spin fluctuation is taken into account as $G^{(0)}(k) = G_F(k) = (i\omega_n - \varepsilon(k) - \Sigma_F(k))^{-1}$.

Counting the topological factor $n!$, the summation of the infinite series is obtained as an Euler’s error function,\textsuperscript{61} which is numerically tractable with use of the integral representation,

$$G(k) = G_F(k) \int_0^\infty \frac{e^{-t}}{1 + t \Delta^2(k) |G_F(k)|^2} dt.$$  

(19)

In this procedure the properties of the SC fluctuation are represented by the single parameter $\Delta$. We use this approximation in §4.1-3 where the single particle properties around $T = T_c$ and the value of $T_c$ are investigated. A more sophisticated estimation will be provided in §4.4 where the spatial fluctuation is taken into account. Note that the latter is reduced to eq. 19 in the limit $\xi_{GL} \rightarrow \infty$.

4. Microscopic Theory in the infinite-loop order

Hereafter, we investigate the role of vertex corrections on the basis of the repulsive Hubbard model. The basic formulation has been provided in §2 and §3.

Before going on to the main issue, we summarize the advantages of the microscopic theory. (1) the properties of the SC fluctuation is microscopically derived. This advantage has enabled us to discuss the doping dependence without using any phenomenological assumption. (2) The renormalization of the quasi-particles is taken into account. Owing to the electron correlation, the energy scale is renormalized to be smaller, and therefore the pseudogap occurs around $T \sim 0.01t \sim 100K$. Note that the pseudogap in the attractive Hubbard model appears in much higher temperature region (see §5.1). (3) The $d$-wave symmetry of the superconductivity is naturally derived. The characteristic momentum dependence of the superconducting gap is derived, which is different from the simple form $\Delta(k) \propto \cos{k_x} - \cos{k_y}$ especially in the electron-doped cuprates.\textsuperscript{36} (4) The strong enhancement of the AF spin fluctuation is taken into account. The magnetic properties, which will be discussed in §4.4 are dominated by the spin correlation around $q \sim (\pi, \pi)$. (5) The momentum dependence of quasi-particles is taken into account. The momentum dependent life time plays an essential role for the understanding of transport phenomena in the pseudogap state.\textsuperscript{53} The remarkably short mean free path at “hot spot” is induced by the spin fluctuation, which provides a consistency with the assumption $\xi_{GL} \gg l$.

In the following, we focus on the higher order corrections with respect to the SC fluctuation. The multiple scattering arising from the spin fluctuation has been investigated motivated by the indication of Schrieffer.\textsuperscript{76} The previous studies\textsuperscript{77, 78} have shown that this correction enhances the effective vertex, however does not affect qualitative roles of the spin fluctuation. We ignore the higher order coupling between the SC and spin fluctuations beyond the renormalization of Green function. The interests are focused on the roles of SC fluctuation.

4.1. Single-particle properties

In order to perform an infinite-loop calculation, we tentatively consider the neighborhood of $T_c$ and assume $\xi_{GL} \gg l$. Then, the Green function is expressed as eq. 19. Correspondingly, the self-energy in the 1-loop and self-consistent 1-loop approximation is expressed as,

$$\Sigma_F(k) = \Delta(k)^2 G_F(-k),$$  

(20)

$$\Sigma_F(k) = \Delta(k)^2 G_F(-k),$$  

(21)

respectively. We have ignored the frequency dependence of the coupling vertex $\phi(k)$, which gives no important effect in the vicinity of $T = T_c$. In this subsection, we ignore the feedback effects on the SC and spin fluctuations in order to fix fluctuation propagators in each approximation. A fully self-consistent calculation including the feedback effect is performed in §4.2-4. We have confirmed that qualitatively same results are obtained in the self-consistent calculation.

Here, we take into account the inter-layer coupling in order to avoid the singularity in the exactly two-dimensional system. The TDGL expansion for the Lawrence-Doniach model is adopted as,

$$t(q, 0) = \frac{g}{t_0 + bq^2 + 2br(1 - \cos q_x)},$$  

(22)

with introducing the phenomenological parameter $r$. Here the TDGL parameters $t_0$ and $b$ are microscopically determined. The phenomenological parameter is expressed by the anisotropy of the SC fluctuation as $r = \xi_\perp^2/\xi_\parallel^2$, where $\xi_\parallel$ is the coherence length along the $c$-axis in the unit of the inter-layer spacing. The exactly
two dimensional and isotropic three dimensional systems correspond to $r = 0$ and $r = 1$, respectively. The small value of $r \ll 1$ is a underlying assumption of eq. 22. We choose $r = 0.01 \sim 0.001$ as a typical value.

We show the results of the single particle spectral function in Fig. 6(a). The expressions 20, 21 and 19 are denoted as FLEX+T-matrix, FLEX+SCT and FLEX+QSG, respectively. It these estimations, the effect of SC fluctuation is represented by the single parameter $\Delta$. We find that the temperature dependence of $\Delta$ is not significant around $T = T_c$ owing to the inter-layer coupling. Therefore, the single particle properties are almost temperature independent, while they are rapidly altered below $T_c$. The experimental results have supported this result.

It is shown that the gap structure in the spectral function is suppressed in the FLEX+SCT, while it clearly appears in the non-self-consistent calculation (FLEX+T-matrix). This is the discrepancy explained in §2. We see that the non-self-consistent 1-loop approximation is qualitatively correct. The calculation including the infinite order vertex corrections (FLEX+QSG) shows the pseudogap in the spectral function, although the gap structure is reduced from the lowest order approximation. It is concluded that the self-consistent 1-loop order theory under-estimates the effects of SC fluctuation, while the non-self-consistent one over-estimates them. This qualitative conclusion will be clearly understood from the perturbative point of view (§5.3). It may be expected that the self-consistent 1-loop approximation is always incorrect as is discussed for the single particle spectrum. In the following, we show that this expectation is invalid and the SCFT is quite appropriate for the macroscopic quantities.

In the present case, the pseudogap in the infinite-loop calculation is broadened by the competition with the Fermi liquid behavior arising from the spin fluctuation. We note that the Fermi liquid behavior is basically obtained in the nearly AF Fermi liquid theory, although some deviations from the conventional Fermi liquid are derived. As a result, the difference between FLEX+SCT and FLEX+QSG is significantly reduced. This is an origin of the unimportance of vertex corrections for the macroscopic quantities.

The DOS is a typical one, which is shown in Fig. 6(b). It is shown that the pseudogap is similarly obtained in three calculations. We will show that the 1-loop approximation provides a rather different result if we assume $s$-wave superconductivity and neglect the spin fluctuation (§5.1). In the present case, the difference between approximations is significantly reduced by the $d$-wave symmetry, which allows low-energy excitations, and by the spin fluctuation. Thus, better convergence of the loop expansion is expected in this microscopic theory rather than the phenomenological models.

### 4.2 Phase diagram

In this subsection, we estimate the doping dependence of $T_c$. For this purpose we perform three kinds of calculation. In the previous paper we have performed the SCFT for the estimation of $T_c$ where eqs. 3-16 are self-consistently solved. Here we denote the calculation with eq. 21 instead of eq. 15 as the same abbreviation. In addition to that, we perform the self-consistent calculation with eq. 19 instead of eq. 15 which is denoted as self-consistent FLEX+Gaussian approximation (SCFG). The calculation with eq. 20 instead of eq. 15 is denoted as non-self-consistent FLEX+T-matrix approximation (NSCFT). These calculations correspond to the self-consistent 1-loop, infinite-loop and 1-loop approximation, respectively. In these calculations, the feedback effect on the spin fluctuation is self-consistently taken into account, which enhances the value of $T_c$.

In the previous paper, the critical point has been determined by the criterion $\lambda_c = 1 - \epsilon$ instead of $\lambda_c = 1$ as a phenomenological inclusion of the inter-layer coupling. In the present study, we explicitly take into account the inter-layer coupling with use of eq. 22. The value of $\epsilon$ roughly corresponds to the phenomenological cut-off as $\epsilon \sim 4br$. Since the value of $b$ is typically $b \sim 5$, the previously used value $\epsilon = 0.0252$ corresponds to $r \sim 0.001$, which is relevant for high-$T_c$ cuprates. Owing to the finite value of $r$, the logarithmic divergence in two-dimension is cut off and $\Delta$ at $T = T_c$ is obtained as

$$
\Delta^2 = \frac{|g|T}{4\pi b} \arccos \frac{q_c^2}{2r} \sim \frac{|g|T}{4\pi b} \log \frac{\pi^2}{r}.
$$

Here $q_c$ is the cut off momentum along the $ab$-plane, which is chosen to be $q_c = \pi$. This procedure enables us to avoid the finite size effect which is serious around $T = T_c$.

First, we show the effect of inter-layer coupling in Fig. 7(a) where the results of SCFG are shown. Even...
if the value of \( r \) differs by an order, the difference of \( T_c \) does not exceed the factor 2 in the whole doping range. This is owing to the logarithmic dependence of \( \Delta \) (see eq. 23). The qualitatively same doping dependence for \( r = 0.01 \) and \( r = 0.001 \) is an important property which allows a universal nature of the pseudogap independent of the inter-layer structure. Although the value of \( r \) is remarkably small in BSCCO, this difference affects only quantitatively.

It is shown that \( T_c \) has a maximum around \( \delta \sim 0.11 \), while the critical temperature in the mean field theory \( T^\text{MF}_c \) develops with decreasing \( \delta \) in the under-doped region (see Ref.36). This qualitatively different behavior between \( T_c \) and \( T^\text{MF}_c \) is consistent with our understanding of the phase diagram. That is, the onset temperature of the pseudogap follows \( T^\text{MF}_c \) below which the SC fluctuation becomes active more and more. On the contrary, the \( T_c \) is suppressed in the under-doped region owing to the fluctuation. We will show that the energy scale of the pseudogap is generally determined by \( T^\text{MF}_c \) and not by \( T_c \), independent of the inter-layer coupling (§5.1).

It is predominately believed that the inter-layer coupling is reduced with decreasing the doping. We have shown in Fig. 7(a) the result including the variation of \( r \). Then, we have chosen the linear interpolation \( r = 0.001 + 0.06(\delta - 0.08) \) so as to be \( r = 0.001 \) at \( \delta = 0.08 \) and \( r = 0.01 \) at \( \delta = 0.23 \). We see that the value of optimal doping is increased by the variation of inter-layer coupling.

We see from Fig. 7(b) that the higher order corrections do not change the qualitative behavior of \( T_c \). Three approximations give similar results. In particular, the close results are obtained between SCFT and SCFG. Therefore, it is concluded that vertex corrections beyond SCFT has no important role for the estimation of \( T_c \). This is not owing to the details of microscopic theory, since quite the same conclusion is obtained for the attractive Hubbard model (§5.1). Note that the feedback effect through the spin fluctuation furthermore reduces the differences. Since the pseudogap in the single particle excitations is under-estimated in the SCFT, the \( T_c \) is higher than SCFG. However, it will be shown that the \( T_c \) in the SCFT is still under-estimated compared with the calculation including the vertex correction on the pairing correlation function. Details are explained in the next subsection.

### 4.3 Vertex correction to the pairing correlation function

Thus far, we have investigated the vertex corrections on the Green function, which are shown in Fig. 4. Actually, more careful discussion is necessary in calculating the many body correlation function. The Maki-Thompson (MT) term and Aslamasov-Larkin (AL) term on the electric conductivity are typical ones which have been investigated since 1970's. These corrections on the magnetic properties have been investigated in Refs.82-84 where the unimportance of MT-term in the \( d \)-wave case has been pointed out. The microscopic treatment on the electric conductivity and Hall coefficient has been performed on the basis of the SCFT approximation.

Then, it has been shown that the dominant correction is the indirect feedback effect because of the characteristic momentum dependence of high-\( T_c \) cuprates. Then, the unimportance of the MT and AL terms has been concluded in contrast to the knowledges for the weak coupling superconductors. The correction to the Nernst effect has been also investigated on the basis of the SCFT approximation where the MT term plays an important role.
The increase of SC fluctuation is reduced by these corrections, while increases owing to the correction in Fig. 8. Therefore, the shown in Fig. 7(b).

In order to estimate the corrections in Fig. 8 as well as those in Fig. 4, we collect the all order terms by using the same approximation as in §4.1 and §4.2. Then, the q-dependence of Green functions is ignored. This simplification enables us to obtain a closed expression, which is the Eliashberg equation modified as,

$$\lambda_c \phi(k) = - \sum_{k'} V_a(k, k') P(k') \phi(k').$$ (24)

Correspondingly, the function $\lambda(q)$ is obtained in the following way,

$$\lambda(q) = - \sum_{k, p} \phi^*(k) V_a(k - p) Q(p, q) \phi(p).$$ (25)

Here, the functions $P(k)$ and $Q(p, q)$ are defined as,

$$P(k) = \int_0^\infty \frac{t e^{-t}}{|G_F(k)|^2 + t \Delta(k)^2} dt,$$ (26)

$$Q(p, q) = \frac{G_F(p) G_F(q - p)}{\Delta(p)^2 |G_F(p)|^2 - \Delta(p - q)^2 |G_F(q - p)|^2} \times \int_0^\infty \frac{\Delta(p)^2}{|G_F(p)|^2 + t \Delta(p)^2} \frac{\Delta(p - q)^2}{|G_F(q - p)|^2 + t \Delta(p - q)^2} e^{-t} dt, \tag{27}$$

respectively.

The role of $T_c$ has been shown in Fig. 7(b). We understand that the $T_c$ in the present calculation is larger than that obtained in the SCFT. Thus, the vertex corrections represented by Fig. 8 are larger than those included in the renormalization of Green function (Fig. 4).

Note that this conclusion is expected from the perturbative point of view. We see that the lowest order vertex correction included in Fig. 8 is in the 3-loop order. On the other hand, the 2-loop order term exists in the corrections represented by Fig. 8. It is understood from the simple estimation that this 2-loop order term enhances $T_c$. Therefore, the result in this subsection is consistent with the perturbative theory where the lowest order term is believed to determine the qualitative tendency.

We have confirmed that the TDGL parameter $b$ increases owing to the correction in Fig. 8. Therefore, the SC fluctuation is reduced by these corrections, while the increase of $T_c$ enhances the thermal fluctuation. We have confirmed that this effect is not serious, quantitatively. Therefore, we ignore the corrections in Fig. 8 in the following discussion about the magnetic properties. We close this subsection by noting that the qualitative feature of the doping dependence is still not altered, as shown in Fig. 7(b).

### 4.4 Magnetic properties

At the last of this section, we show the temperature dependence of NMR $1/T_1$ and uniform susceptibility $\chi_s(0)$. They are typical quantities showing the pseudogap.\textsuperscript{5,11} In order to discuss the magnetic properties, we perform another calculation proposed by Sadovskii.\textsuperscript{56} While we have only to consider the situation $\xi_{GL} > l$ for the estimation of $T_c$, the spatial fluctuation may be an essential nature above $T_c$. Sadovskii’s method has provided a simple and reasonable estimation for the spatial fluctuation. A justification will be obtained by the comparison with the numerical estimation within the 4-loop order. A Monte Carlo simulation is a method of use, as has been performed for the phenomenological model with spin fluctuation and that with charge fluctuation.\textsuperscript{86} However, we carry out an approximate but analytic treatment in order to obtain a clearer understanding and to compare several approximations in an equal footing.

In general, a spatial fluctuation gives rise to the broadening of self-energy in each order. In the method proposed by Sadovskii, this effect is taken into account by linearizing the inverse of Green function as $G_F(k - q) = 1/(i \omega_n - \varepsilon(k) + \imath \nu(k) q - \Sigma_F(k))$ and replacing the $q$-summation with adding an imaginary quantity. The imaginary quantity is chosen to be the inverse of typical length scale, namely $\xi_{GL}^{-1}$. Then, the self-energy in the n-loop order is expressed as,

$$\Sigma^{(n)}(k) = |\Delta(k)|^2 \Pi_{r=1}^{n+1} (i \omega_n - (-1)^r \varepsilon(k)) \quad (-1)^r \Sigma_F((-1)^r k) \pm i p(i) \tilde{\nu}(k) \xi_{GL}^{-1}. \tag{28}$$

The integer $p(i)$ is the number of SC fluctuation propagators enclosing the Green function appearing in the $i$-th order. The sign $(-)$ should be chosen in the upper (lower) half plane. The quasi-particle velocity is obtained as $\tilde{\nu}(k) = |\tilde{\nu}(k)|$ where $\tilde{\nu}(k) = \nu(k) + \partial \Re \Sigma_F(k, \imath \nu T) / \partial k$.

This method was first proposed for one-dimensional charge fluctuation systems as an exact solution.\textsuperscript{56} Although this procedure has been proved to be not exact beyond 1-loop order,\textsuperscript{57} a good accuracy as an approximation has been numerically confirmed in case of the complex order parameter.\textsuperscript{58,59} Here this method is applied to the two-dimensional SC fluctuation.

The infinite summation of eq. 28 is expressed as a recursive fraction,

$$\Sigma_S(k) = \frac{\Delta(k)^2}{-G_F^{-1}(-k) + \imath n(1) \tilde{\nu}(k) \xi_{GL}^{-1} + \Delta(k)^2 \Sigma_F^{-1}(k) + \imath n(2) \tilde{\nu}(k) \xi_{GL}^{-1} + \ldots}.$$ (29)

where $n(i) = [(i + 1)/2]$ and $[\ldots]$ is the Gauss symbol. It is easily confirmed that this expression is attributed to eq. 19 in the limit $\xi_{GL} \rightarrow \infty$. On the other hand, this expression is attributed to the zeroth order theory in the opposite limit $\xi_{GL} \rightarrow 0$. Thus, the expression 29 can be regarded as an interpolation between the limiting cases. It should be noted that the applicability of this method to the two dimensional case will need more discussion. In the previous application for AF spin fluctuation\textsuperscript{62} and
CDW fluctuation,\textsuperscript{61} the displacement of the fluctuation propagator \( \frac{1}{\xi_{GL}^2 + q^2} \) is implicitly performed. This displacement is accurate in the interested region \( q \sim 1/\xi_{GL} \). Owing to this procedure, the momentum summation is attributed to the one-dimensional problem. Therefore, the accuracy of Sadovskii’s method is similarly expected in the two-dimensional case. It should be stressed that the one-dimension is not particular for the phenomenological Gaussian fluctuation model, while the quantum fluctuation is essential in the one-dimensional microscopic models. Note that two or higher dimensional models where the Sadovskii’s method is exact have been proposed.\textsuperscript{61,70}

Fig. 9. Results of the loop expansion. (a), (b), (c) and (d) show the imaginary part of the self-energy in the 1-, 2-, 3- and 4-loop order, respectively. The dashed lines denoted as S’sM show the results of Sadovskii’s method. The indices (3a), (3b) and (4a-4d) correspond to the diagrams in Fig. 4. The parameters are chosen as \( U/t = 3.2 \) and \( T = 0.0084 \) where \( T = 1.035T_c^{MF} \).

In order to provide another ground, we perform the loop expansion up to the 4-loop order. Then, the quasi-static approximation is adopted and the dominator of Green function is linearized. The imaginary part of the self-energy in each order is estimated by the numerical integration. The result of the Sadovskii’s method (eq. 28) is shown together in Fig. 9. We see the qualitatively same behaviors between the Sadovskii’s method and naive loop-expansion in each order.

Another interesting finding is that the crossing diagram and non-crossing one are almost equivalent in the results of loop expansion. For example, the difference between Fig. 4(3a) and Fig. 4(3b) is almost invisible in Fig. 9(c). We see the same feature in the 4-loop order terms. This feature is obtained even if we do not linearize the dominator of Green function.\textsuperscript{87} It should be stressed that this feature is an essential assumption of the Sadovskii’s method. The results shown in Fig. 9 have confirmed that this assumption is satisfied with remarkable accuracy. From these results we believe that Sadovskii’s method is appropriate at least for qualitative discussions, although quantitative accuracy has not been proved.

The numerical factor \( n(i) = [(i + 1)/2] \) in eq. 29 is precisely obtained by counting the diagrams. This factor is replaced with \( n(i) = 1 \) in the self-consistent 1-loop approximation (SCFT) and with \( n(i) = \delta_{i,1} \) in the 1-loop approximation (NSCFT). The role of vertex corrections are clarified by the comparison between these calculations.

We show the results of NMR \( 1/T_1T \) and uniform spin susceptibility in Fig. 10. Here the estimation of \( \sum_{q<q_c} |t(q,0)| \) is numerically performed with the cut-off \( q_c = \pi/2 \). Because the inter-layer coupling is not important except for the vicinity \( T_c \), we perform the calculation in the two-dimension. The NMR \( 1/T_1T \) is estimated by using the fluctuation-dissipation theorem, which is expressed as

\[
1/T_1T = \sum_q F_\perp(q) \mid \frac{1}{\omega} \text{Im} \chi^R(q,\omega) \mid_{\omega \rightarrow 0},
\]

where

\[
F_\perp(q) = \frac{1}{2} \{ A_1 + 2B(\cos q_x + \cos q_y) \}^2 + \{ A_2 + 2B(\cos q_x + \cos q_y) \}^2.
\]
The hyperfine coupling constants $A_1, A_2$ and $B$ are chosen as $A_1 = 0.84B$ and $A_2 = -4B$. We have added the results obtained by the SCFT without using the quasi-static approximation. Then, the momentum and frequency summations are performed by using the fast Fourier transformation (FFT) and taking account of the same cut-off $q_c = \pi/2$.

It is clearly shown that the pseudogap phenomena appear in all of the calculations in a similar way. NMR $1/T_1T$ shows a maximum above $T_c$. On the other hand, the uniform susceptibility decreases with decreasing temperature from much higher temperature. This qualitatively different behavior is one of the characteristics of under-doped high-$T_c$ cuprates. This is owing to the interplay of the AF spin fluctuation and SC fluctuation.

We see that the vertex correction beyond SCFT is almost negligible. The unimportance of the vertex correction in the present case is very significant compared with the previous subsections. The result for $1/T_1T$ is particularly surprising because this quantity is very sensitive to the approximation, owing to the strong enhancement of the spin fluctuation. This fact indicates an extremely precise cancellation of the vertex corrections for magnetic properties.

It is noted that the same conclusion is obtained by neglecting the $q$-dependence of the Green function as is performed in §4.1-3. Then, the effect of spatial fluctuation is obviously neglected. This nature of approximation should be contrasted with the Sadoskii’s method where the spatial fluctuation is over-estimated. It is expected that the unimportance of vertex corrections for the magnetic properties is a robust conclusion, since it is confirmed by two complementary approximations.

At the last of this section, we comment on the closing of the pseudogap. As has been shown in §4.1, the pseudogap appears in the spectral function around $T = T_c$. As the temperature increases, the gap structure is gradually broadened. In the present parameters, the pseudogap at the hot spot disappears around $T = 0.005$ which corresponds to the maximum of NMR $1/T_1T$. We have confirmed that the closing of the pseudogap is yielded by the spatial fluctuation but not by the decrease of $\Delta$. Indeed, the temperature dependence of $\Delta$ is weak since the increase of temperature enhances the thermal fluctuation. Therefore, the closing of the pseudogap occurs as a blurring but not as a shrinking. This is quite consistent with the experimental observation in ARPES. Note that the quasi-static approximation is not valid far above $T_c$. Then, the dynamical fluctuation is also important as well as the spatial fluctuation.

5. Phenomenological Theory: More General Aspects

In this section, the comparison to spin fluctuation and charge fluctuation is performed on the basis of the phenomenological theory. We will see that the qualitative role of vertex corrections discussed in §4 is non-trivial and determined by the symmetry of order parameter. An analysis of the infinite order calculation within the phenomenological theory has been reported for the charge fluctuation, AF spin fluctuation and SC fluctuation, respectively. Here, we provide a comprehensive view and shed light on the essential character of SC fluctuation.

5.1 In case of SC fluctuation

First, we summarize the phenomenological theory for the SC fluctuation. The results on the single particle properties are clearly understood. In this section, we ignore the $k$-dependence of $\Delta(k)$ and phenomenologically assume the value of $\Delta$ for simplicity. This situation corresponds to the attractive Hubbard model which is briefly discussed at the last of this subsection. Since another scattering process is not taken into account here, the retarded Green function in the 1-loop, self-consistent 1-loop and infinite-loop calculations are described, respectively,

\[
G_R^R(k, \omega) = \frac{\omega + \epsilon(k)}{(\omega + \epsilon(k))(\omega - \epsilon(k)) - \Delta^2} \quad (32)
\]

\[
G_{\text{CS}}^R(k, \omega) = \frac{1}{\omega - \epsilon(k)} \left[ \frac{2}{1 + \sqrt{1 - \frac{4\Delta^2}{\omega^2 - \epsilon^2(k)^2}}} \right] \quad (33)
\]

\[
G_{\infty}^R(k, \omega) = \int_0^\infty \frac{\omega + \epsilon(k)}{(\omega + \epsilon(k))(\omega - \epsilon(k)) - t\Delta^2} e^{-t\Delta^2} dt \quad (34)
\]

\[
= \int_0^\infty \frac{\omega + \epsilon(k)}{(\omega + \epsilon(k))(\omega - \epsilon(k)) - \pi^2} e^{-\pi^2/\Delta^2} 2\pi x dx \quad (35)
\]

Strictly speaking, the condition $l \ll \xi_{\text{GL}}$ is not relevant in the present case since $l = \infty$. However, these expressions are sufficient for the qualitative discussion.

The Green functions in eqs. 32 and 34 imply the relation to the normal Green function in the superconducting state. We see that eq. 32 is equivalent to the normal Green function in the BCS theory. The square of the order parameter in the latter is replaced by the thermal weight of the fluctuation. The expression in the infinite-loop calculation corresponds to the normal Green function averaged by the Gaussian distribution of the order parameter. Quasi-particles propagate under the fluctuating order parameter which is approximated to be classical and Gaussian in the present case. If the mean free path is shorter than the correlation length, the spatial fluctuation of the order parameter is not effective for quasi-particles. Therefore, a physically relevant result is obtained as eq. 34. Thus, the quasi-static approximation provides a clear interpretation. On the other hand, it is difficult to find a clear interpretation of self-consistent 1-loop approximation (see eq. 33). This fact implies a potentiality that higher order terms are inappropriately taken into account in this approximation.

This possibility has been realized in §4.1 where the single particle spectral function has been discussed. We illustrate the spectral function obtained from eqs. 32-34 (Fig. 11(a)). The failure of the self-consistent 1-loop order theory is clearly understood. The single peak structure appears in the self-consistent 1-loop approximation (SCT), while the double peak structure is clearly observed in the 1-loop (T-matrix) and infinite-loop (QSG) approximations. The gap structure in the QSG is broad compared with the 1-loop approximation owing to the
not been shown in the microscopic theory (Fig. 6(b)). Then, the 1-loop order theory has been much improved owing to the $d$-wave symmetry and to the scattering from spin fluctuation.

At the last of this subsection, we provide results for the attractive Hubbard model in Fig. 13. Then, the Green function is expressed as eqs. 32-34 and the value of $\Delta$ and the propagator of fluctuation are self-consistently determined. Here the inter-layer coupling is taken into account with use of eq. 22. Fig. 13(a) shows that the vertex correction beyond the SCT is not serious for the estimation of $T_c$. This conclusion is in common to the microscopic theory in §4.2.

The relation between the excitation gap $\Delta$ at $T = T_c$ and the transition temperature in the mean field theory $T_c^{MF}$ is shown in Fig. 13(b). We clearly see the universal behavior independent of the indicator of three-dimensionality $r = (\xi_d / \xi_0)^2$. $T_c^{MF}$ and $\Delta$ has a universal relation, although the value of $T_c$ depends on the inter-layer coupling. This is an important finding for the whole understanding of cuprate superconductors. The result in Fig. 13(b) shows that the energy scale of the pseudogap is not determined by $T_c$, but by $T_c^{MF}$, which is robust for the variation of the inter-layer structure.

It should be noted that this relation is derived in the renormalized Gaussian fluctuation region focused in this paper. Therefore, the experimental observation is not an evidence for the fixed amplitude expected in the phase fluctuation region.\cite{46,51}

5.2 Comparison to spin and charge fluctuations

Next, the possibility of the pseudogap phenomena induced by spin fluctuation or charge fluctuation is discussed in order to extract the essential properties of SC fluctuation. The possibility on the AF spin fluctuation has been investigated extensively in the studies of high-$T_c$ cuprates.\cite{32,34,62} Although we will stress the invalidity of the quasi-static approximation for the spin fluctuation (Appendix A), this approximation is used for a comparison. The role of charge fluctuation has been interested in the context of the stripe order.\cite{92} In our opinion, the charge fluctuation is not important for a unified understanding of high-$T_c$ superconductors. However, the

Gaussian distribution of the pair field. Thus, the result obtained in §4.1 is qualitatively understood from this phenomenological theory.

This observation implies that the vertex corrections significantly cancel the higher order corrections included in the SCT. Note that the SCT applied to the attractive Hubbard model is one of the conserving approximations formulated by Baym and Kadanoff. The present calculation is an example that the preservation of some conservation laws unsatisfied in the SCT are satisfied phenomenologically.\cite{90,91} Then, the property of fluctuations and the coupling vertex to them are basically discussed. However, the present diagrammatic method indicates that the improvement of SCT should be performed by including the multiple scattering like Fig. 4.

The characteristics of each approximation will be clarified by showing the self-energy in Fig. 11(b). It is shown that the anomalous scattering peak around $\omega = 0$ almost disappears in the SCT. This is the reason of the broad single peak in the spectral function. The scattering peak remains in the infinite order calculation, while it is reduced from the 1-loop order theory.

Here, we show the DOS in Fig. 12. We see that the SCT is appropriate with regard to the DOS. This is because the spectral function slightly apart from the Fermi surface is not so different between the SCT and QSG. On the other hand, the result of the T-matrix approximation is rather different from that of QSG. This discrepancy has

Fig. 11. (a) The spectral function on the Fermi surface ($\epsilon(k) = 0$) obtained by eqs. 32-34. (b) The imaginary part of the self-energy. We have chosen the parameter as $\Delta = 0.2$.

Fig. 12. Results of the DOS. The dispersion relation eq. 2 is used with $t'/t = 0$ and $n = 1$.

\begin{align*}
\rho(\omega) &= 1 - |A(k, \omega)|^2 \\
\Im \Sigma(k, \omega) &= 2 T \rho(\omega) A^2(k, \omega) \sinh(\beta \omega) / \cosh(\beta \omega) + \frac{\Im \Sigma_0(k, \omega)}{\alpha(t')} \sinh(\beta \omega) / \cosh(\beta \omega).
\end{align*}
obtain the factor longitudinal mode but also the transverse one exist. We not easy in case of the spin fluctuation since not only the estimation of the numerical factor is

\[ G_x^R(k, \omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega - \varepsilon(k + Q)}{(\omega - \varepsilon(k))(\omega - \varepsilon(k + Q)) - \frac{\Delta^2}{2} / 2} \times e^{-t^2/2} dt, \]

respectively. The estimation of the numerical factor is not easy in case of the spin fluctuation since not only the longitudinal mode but also the transverse one exist. We obtain the factor \( \frac{2}{2n + 1}!! \) from the recurrence formula. Here we have defined the thermal weight of the charge and spin fluctuation as \( \Delta^2_g = g_s^2 T \sum \chi_c(Q + q, 0) \) and \( \Delta^2_s = g_s^2 T \sum \chi_s(Q + q, 0) \) where \( g_c \) and \( g_s \) are the effective coupling constants. In the RPA or FLEX for the Hubbard model, these coupling constants are equivalent to \( U \). Summing up the infinite series, the Green function is obtained as,

\[ G_x^R(k, \omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega - \varepsilon(k + Q)}{(\omega - \varepsilon(k))(\omega - \varepsilon(k + Q)) - \frac{\Delta^2}{2} / 2} \times e^{-t^2/2} dt, \]

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the maximum at $x = 0$, while the functions $x \exp(-x^2)$ and $x^3 \exp(-x^2)$ have the maximum at $|x| > 0$. This is the reason why the SC fluctuation and spin fluctuation are classified into the same class. Fig. 14(b) shows that the scattering peak leading to the pseudogap in the spectral function almost disappears in case of the charge fluctuation.

It should be stressed that qualitatively the same result is obtained for three kinds of fluctuations, when we adopt the 1-loop or self-consistent 1-loop approximation. The differences obtained above are essentially owing to the role of vertex corrections. It is understood from the above discussion that the qualitative role of vertex corrections essentially depends on the symmetry of order parameter. In this sense, the results on the SC fluctuation are non-trivial. The $U(1)$-symmetry of the order parameter plays an essential role. In case of the charge fluctuation, the appropriate result is obtained from the self-consistent 1-loop approximation rather than the non-self-consistent one.

It is shown in Fig. 14(c) that the charge fluctuation induces the gap structure of DOS, which has been focused in the previous studies. Thus, the pseudogap in the quantities including the momentum summation is robust for the properties of order parameter as well as those of approximations. The suppression of DOS around $\omega = 0$ is more remarkable when the symmetry of the order parameter is higher.

Before closing this section, we comment on the realistic problem for high-$T_c$ cuprates. Then, the pseudogap induced by the AF spin fluctuation is not clearly observed in the FLEX approximation. We consider that this is not owing to the nature of the FLEX approximation, which is the self-consistent 1-loop approximation, but owing to the dynamical fluctuation which is important as will be shown in Appendix A.

5.3 Perspective from the perturbation theory

The qualitatively different role of the vertex corrections discussed in §5.2 is clarified from the perturbative point of view. Fig. 15 shows the diagrammatic representation of the loop expansion in case of the spin or charge fluctuation. We have shown the diagrams within the 3-loop order. Note that Figs. 15(1), (2a), (3a) and (3b) are included in the self-consistent 1-loop approximation, which is the FLEX approximation in the microscopic theory. The other terms are classified into the vertex correction.

In order to make a discussion clear, we introduce a common expression for each term. In case of the charge and spin fluctuation, we denote

$$
\Sigma^{(2a)}(k) = \sum_{q_1, q_2} V(q_1)V(q_2) \\
\times G(k + q_1)G(k + q_1 + q_2)G(k + q_1),
$$

and so on. The vertex $V(q)$ is defined as $V(q) = \frac{1}{2} g_2^c \chi_c(q)$ and $V(q) = \frac{1}{2} g_2^s \chi_s(q)$ for charge and spin fluctuation, respectively. We have chosen the notation in which the coefficient of the terms included in the self-consistent 1-loop approximation is unity. It is easily confirmed that odd order terms generally introduce the anomalous contribution leading to the pseudogap, while even order terms reduce it.

We see that the lowest order vertex correction is in the second order (Fig. 15(2b)). In case of the charge fluctuation, all of the terms contribute to the self-energy with a coefficient 1. Then, the self-energy in the second order is $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) + \Sigma^{(2b)}(k)$ and that in the third order is $\Sigma^{(3)}(k) = \Sigma^{(3a)}(k) + \Sigma^{(3b)}(k)$. In this case, the lowest order vertex correction reduces the anomalous contribution. Therefore, the effect of the charge fluctuation is still overestimated in the self-consistent 1-loop approximation.

On the other hand, the coefficients are complicated in case of the spin fluctuation. We obtain the second order term as $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) - \frac{1}{3} \Sigma^{(2b)}(k)$. The negative coefficient $-1/3$ arises from the coupling between

55, 56, 58–61

Thus, the pseudogap is robust for the properties of order parameter as well as

In this sense, the results on the SC fluctuation are non-trivial. The $U(1)$-symmetry of the order parameter plays an essential role. In case of the charge fluctuation, the appropriate result is obtained from the self-consistent 1-loop approximation rather than the non-self-consistent one.

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Before closing this section, we comment on the realistic problem for high-$T_c$ cuprates. Then, the pseudogap induced by the AF spin fluctuation is not clearly observed in the FLEX approximation. We consider that this is not owing to the nature of the FLEX approximation, which is the self-consistent 1-loop approximation, but owing to the dynamical fluctuation which is important as will be shown in Appendix A.

5.3 Perspective from the perturbation theory

The qualitatively different role of the vertex corrections discussed in §5.2 is clarified from the perturbative point of view. Fig. 15 shows the diagrammatic representation of the loop expansion in case of the spin or charge fluctuation. We have shown the diagrams within the 3-loop order. Note that Figs. 15(1), (2a), (3a) and (3b) are included in the self-consistent 1-loop approximation, which is the FLEX approximation in the microscopic theory. The other terms are classified into the vertex correction.

In order to make a discussion clear, we introduce a common expression for each term. In case of the charge and spin fluctuation, we denote

$$
\Sigma^{(2a)}(k) = \sum_{q_1, q_2} V(q_1)V(q_2) \\
\times G(k + q_1)G(k + q_1 + q_2)G(k + q_1),
$$

and so on. The vertex $V(q)$ is defined as $V(q) = \frac{1}{2} g_2^c \chi_c(q)$ and $V(q) = \frac{1}{2} g_2^s \chi_s(q)$ for charge and spin fluctuation, respectively. We have chosen the notation in which the coefficient of the terms included in the self-consistent 1-loop approximation is unity. It is easily confirmed that odd order terms generally introduce the anomalous contribution leading to the pseudogap, while even order terms reduce it.

We see that the lowest order vertex correction is in the second order (Fig. 15(2b)). In case of the charge fluctuation, all of the terms contribute to the self-energy with a coefficient 1. Then, the self-energy in the second order is $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) + \Sigma^{(2b)}(k)$ and that in the third order is $\Sigma^{(3)}(k) = \Sigma^{(3a)}(k) + \Sigma^{(3b)}(k)$. In this case, the lowest order vertex correction reduces the anomalous contribution. Therefore, the effect of the charge fluctuation is still overestimated in the self-consistent 1-loop approximation.

On the other hand, the coefficients are complicated in case of the spin fluctuation. We obtain the second order term as $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) - \frac{1}{3} \Sigma^{(2b)}(k)$. The negative coefficient $-1/3$ arises from the coupling between

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Thus, the pseudogap is robust for the properties of order parameter as well as

In this sense, the results on the SC fluctuation are non-trivial. The $U(1)$-symmetry of the order parameter plays an essential role. In case of the charge fluctuation, the appropriate result is obtained from the self-consistent 1-loop approximation rather than the non-self-consistent one.

It is shown in Fig. 14(c) that the charge fluctuation induces the gap structure of DOS, which has been focused in the previous studies. Thus, the pseudogap in the quantities including the momentum summation is robust for the properties of order parameter as well as those of approximations. The suppression of DOS around $\omega = 0$ is more remarkable when the symmetry of the order parameter is higher.

Before closing this section, we comment on the realistic problem for high-$T_c$ cuprates. Then, the pseudogap induced by the AF spin fluctuation is not clearly observed in the FLEX approximation. We consider that this is not owing to the nature of the FLEX approximation, which is the self-consistent 1-loop approximation, but owing to the dynamical fluctuation which is important as will be shown in Appendix A.

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\times G(k + q_1)G(k + q_1 + q_2)G(k + q_1),
$$

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On the other hand, the coefficients are complicated in case of the spin fluctuation. We obtain the second order term as $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k) - \frac{1}{3} \Sigma^{(2b)}(k)$. The negative coefficient $-1/3$ arises from the coupling between
the longitudinal and transverse modes. Thus, the sign of the lowest order vertex correction is opposite to the case of charge fluctuation. Therefore, the qualitatively different role of the vertex correction is expected. The self-consistent 1-loop approximation underestimates the effects of spin fluctuation. Note that the 1-loop approximation overestimates them since the vertex correction term $-\frac{1}{2}\Sigma^{(2b)}(k)$ has smaller coefficient 1/3 than $\Sigma^{(2a)}(k)$. The Monte Carlo study has reported the qualitatively consistent 1-loop approximation underestimates the effective for the anisotropic superconductivity rather than the charge fluctuation, owing to the vertex corrections as well as the numerical factor 3.

At last, we clarify the case of SC fluctuation. Then, the diagrams in Figs. 15(2b) and (3c-i) are absent. The number of the vertex correction terms is remarkably small in this case. Indeed, this is a characteristic property of the complex order parameter. We introduce the expressions for the remaining terms as,

$$\Sigma^{(2a)}(k) = \sum_{q_1, q_2} V(q_1)V(q_2) \times G(-k + q_1)G(k - q_1 + q_2)G(-k + q_1),$$

$$\Sigma^{(3a)}(k) = \sum_{q_1, q_2, q_3} V(q_1)V(q_2)V(q_3) \times G(-k + q_1)G(k - q_1 + q_2)G(-k - q_1 + q_2 + q_3) \times G(k - q_1 + q_2)G(-k + q_1),$$

$$\Sigma^{(3j)}(k) = \sum_{q_1, q_2, q_3} V(q_1)V(q_2)V(q_3) \times G(-k + q_1)G(k - q_1 + q_2)G(-k - q_1 + q_2 + q_3) \times G(k - q_2 - q_3)G(-k + q_3),$$

where $V(q) = t(q, 0)$. The second and third order terms are obtained as $\Sigma^{(2)}(k) = \Sigma^{(2a)}(k)$ and $\Sigma^{(3)}(k) = \Sigma^{(3a)}(k) + \Sigma^{(3b)}(k) + \Sigma^{(3j)}(k)$, respectively. Because the coefficient of each term is unity, the lowest order vertex correction $\Sigma^{(3j)}(k)$ has qualitatively the same role as $\Sigma^{(3a)}(k)$ which enhances the pseudogap phenomena. Thus, the role of vertex corrections clarified in §4 is expected from the perturbative point of view. Because the vertex correction in this case is higher order than that of spin and charge fluctuations, it is expected to be less important. This is an underlying origin of the unimportance of the vertex correction on the macroscopic quantities.

Summarizing, the results obtained in §§5.1 and §5.2 are qualitatively consistent with the expectation from the perturbation theory. The qualitatively different role of vertex corrections is explained from the lowest order vertex correction, even if the contribution from the higher order term is larger. Thus, the perturbation theory provides another understandings for the results, although we have to perform an infinite order calculation in order to obtain the results in a closed form.

6. Summary and Discussion

In this paper, we have investigated the role of higher order corrections beyond the T-matrix approximation for SC fluctuation. The results obtained from the detailed analysis are summarized in the following way. The first one is the importance of the vertex correction for the single particle spectral function. Then, the self-consistent T-matrix approximation is qualitatively incorrect, while the non-self-consistent one is appropriate. The second one is the unimportance of the vertex correction for the macroscopic quantities. We have explicitly estimated the DOS, superconducting transition temperature, NMR $1/T_1T$ and magnetic susceptibility on the basis of the repulsive Hubbard model. It has been shown that the self-consistent 1-loop order theory is rather precise for these quantities. We have found that the cancellation of the vertex correction for the magnetic properties is especially precise. These results basically provide a justification of the 1-loop order theory, although a care is necessary for the interpretation of ARPES measurements. The present study provides a clear point of view to the previous studies within the 1-loop order calculation.$^{36, 42-45, 52, 53}$

We have pointed out that the d-wave symmetry of the superconductivity and the renormalization from the spin fluctuation significantly reduce the effect of vertex corrections. This fact is natural since the higher order terms are generally suppressed by these properties. Therefore, a better convergence of the loop expansion is expected in the realistic situation rather than in the situation adopted in the phenomenological models.

It should be stressed again that the justification of the 1-loop order theory is obtained even when the naive perturbation calculation fails. Then, the higher order corrections are renormalized by summing up infinite series. Note that the cancellation occurs between the even order terms and odd order ones which have qualitatively opposite behaviors at low energy. The same order terms enhance rather than cancel each other. Therefore, the calculation within the finite order is remarkably inaccurate. The results in 3-loop order, 4-loop order...... seriously oscillate. The 1-loop order theory is significantly precise rather than the other finite order calculation. However, we have pointed out in §5.3 that the qualitative roles of vertex corrections are generally determined by the lowest order term. The unimportance of the vertex corrections arising from the SC fluctuation rather than that from the charge and spin fluctuations is also expected from the perturbative point of view. Thus, the perturbation theory is still valid in this qualitative sense.

| 2nd order | charge | SC | spin |
|-----------|--------|----|------|
| 3rd order | 8      | 1  | -22/9|

Table 1. The coefficient of vertex correction terms. The cases of the charge, SC and spin fluctuation are shown, respectively. We show the coefficient of the second order term $\Sigma^{(2b)}$ and the summation of the coefficients of third order terms $\Sigma^{(3c)}, \Sigma^{(3)}$. 

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Note that the 1-loop order theory has been used widely in the fluctuation theory including the FLEX approximation. The simplicity of the 1-loop order theory has enabled us to investigate rich issues in a coherent way. At the moment, there is no conclusive evidence for the validity because so-called Migdal theorem is not generally applicable. It may be considered that this problem is serious in the strongly correlated electron systems because the strong coupling nature of the fluctuation is a characteristic property of them. However, the present study implies a wide applicability of the 1-loop order theory, although it inevitably fails in the deeply critical region. For example, we believe that the 1-loop order theory for the spin fluctuation is more effective than expected from the lowest order estimation for the vertex correction. In many cases, the contribution which is not included in the fluctuation theory is more important rather than the vertex correction, as a quantitative correction. We expect that the observation in the present study will be a typical example in the rich field of the fluctuation theory in the correlated electron systems.

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Appendix A: On the validity of quasi-static approximation

This Appendix is provided as a ground for the quasi-static approximation which is used in this paper. For a quantitative estimation needed for this purpose, we show the results obtained in the microscopic theory developed in §4.4. Then, the quasi-static approximation has been used in combination with Sadovskii’s method. We show the result of SCFG at $T = 0.0035$. Fig. A-1 shows the $\Omega_n$-dependence of the pairing correlation function at $q = 0$. The spin correlation function at $q = (\pi, \pi)$ is shown for a comparison. In order to perform a comparison in an equal footing, we show the functions $|t(q)/g| = |\lambda(q)/(1 - \lambda(q))|$ and $U\chi_s(q) = U\chi_0(q)/(1 - U\chi_0(q))$ and choose the parameters so that the values at $\Omega_n = 0$ are almost equivalent.

It is clearly shown that the pairing correlation function rapidly decreases for a finite Matsubara frequency. Therefore, it is expected that the dynamical part of the T-matrix does not play any important role. This conclusion has been confirmed also in the explicit calculation within the 1-loop order theory (§4.4). Then, the SCFT approximations with and without quasi-static approximation provide similar results for magnetic properties. We have confirmed this fact also for the single particle spectral function, although the result has not been shown.

On the other hand, the spin correlation function takes not so small value at finite Matsubara frequency. In other words, the characteristic frequency of the spin fluctuation remains to be larger than the temperature. Thus, it is concluded that the quasi-static approximation for the spin fluctuation is not valid for the relevant region in the pseudogap state. We wish to stress again that such a remarkable difference between the SC fluctuation and spin fluctuation is not owing to the enhancement factors $1/(1 - \lambda(q))$ and $1/(1 - U\chi_0(q))$, but owing to the essential property of each fluctuation. As has been explained in §3.2, the characteristic frequency of the fluctuation is expressed as $\omega_{sc} \sim T\epsilon$ and $\omega_{ps} \sim E_F\epsilon_n$ for SC fluctuation and for spin fluctuation, respectively. We see a smaller coefficient in case of the SC fluctuation. Indeed, this is one of the characteristics of the phase transition with logarithmic divergence at $T \to 0$. For example, the superconductivity and SDW with perfect nesting are the cases.

It should be noted that the validity of the quasi-static approximation is related to the formation of the pseudogap in a straightforward manner. While the anomalous contribution leading to the pseudogap arises from the quasi-static part, the dynamical part basically smears it. The validity of the quasi-static approximation is actually an underlying origin of the clear pseudogap induced by the SC fluctuation.

Note that the invalidity of the quasi-static approximation for the spin fluctuation is concluded in the pseudogap state, but it is not a general consequence. This approximation for the spin fluctuation theory will be appropriate in higher temperature region and/or sufficiently close to the magnetic instability. In the present case, the pseudogap in the magnetic excitation itself is an origin of the invalidity, since it means the reduced damping of spin fluctuation.

Appendix B: Self-energy represented by Fig. 5(f)

In this paper, we have ignored the contribution from the non-Gaussian terms which include higher order mode couplings. Although considerable part of them is represented by the renormalization of fluctuation propagator (see Figs. 5(b) and (c)), the role of remaining terms is not clear. The lowest order term included in the remain-
The unimportance of the non-Gaussian term is remarkable in the result obtained in this paper. They do not seriously affect the qualitative conclusions. Although the role of higher order non-Gaussian terms is still unclear, we believe that the 4-loop order vertex corrections taken into account in this paper.

The result is shown in Fig. B-1. It is understood that the non-Gaussian term is much smaller than the same order vertex corrections taken into account in this paper. Because there are much more terms in the 4-loop order in Fig. 4 and they are almost equivalent (see §4.4), the unimportance of the non-Gaussian term is remarkable in the 4-loop order. This is partly owing to the fact that the 4-th order vertex \( \Gamma = \Sigma_4(G(k))^{\dagger} \) is significantly reduced by the self-energy arising from the spin fluctuation as well as the SC fluctuation. Although the role of higher order non-Gaussian terms is still unclear, we believe that they do not seriously affect the qualitative conclusions obtained in this paper.

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