Anisotropic pseudogap in the half-filling 2-d Hubbard model at finite T

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We have studied the pseudogap formation in the single-particle spectra of the half-filling two-dimensional Hubbard model. Using a Green’s function with the one-loop self-energy correction of the spin and charge fluctuations, we have numerically calculated the self-energy, the spectral function, and the density of states in the weak-coupling regime at finite temperature. Pseudogap formations have been observed in both the density of states and the spectral function at the Fermi level. The pseudogap in the spectral function is explained by the non-Fermi-liquid-like nature of the self-energy. The anomalous behavior in the self-energy is caused by both the strong antiferromagnetic spin fluctuation and the nesting condition on the non-interacting Fermi surface. In the present approximation, we find a logarithmic singularity in the integrand of the imaginary part of the self-energy. Concerning the energy dependence of the spectral function and the self-energy, two theorems are proved. They give a necessary condition in the self-energy to produce the pseudogap at the Fermi level. The pseudogap in the spectral function is highly momentum dependent on the Fermi surface. It opens initially in the $\pm \pi, 0, (0, \pm \pi)$ regions as the normal state pseudogap observed in the high-$T_c$ superconductors and if the interaction is increased, it spreads to other Fermi surface sectors. The anisotropy of the pseudogap is produced by the low-energy enhancement of the spin excitation around $Q = (\pi, \pi)$ and the flatness of the band dispersion around the saddle point.

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I. INTRODUCTION

The recent series of angle-resolved-photoemission experiments in high-$T_c$ superconductors have brought a large number of new insights concerning the low energy single-particle states of these materials. The experimental observations include a rather wide flat-band region around $(\pi, 0)$ in the effective band dispersion [1–3] and also the anisotropy of the normal state pseudogap [4–9] which is consistent with the $d$-wave symmetry superconducting gap. Many theoretical approaches and computer simulations have been performed to investigate the pseudogap. Naturally, our ultimate objective is to explain the existing experimental data. However, the main purpose of this work is not to give a direct explanation of the experiments, but rather, to study the pseudogap formation in the Hubbard model which is often used to describe the high-$T_c$ materials.

To avoid confusion, we should make clear what kinds of pseudogap we are dealing with in this paper. In reality, in the literature this term has been used to represent several different features. What it is common in all cases is the fact that the pseudogap indicates a suppression or disappearance of the spectral intensity at the Fermi level. We can list the following three different cases. The first one is a disappearance of the spectral intensity due to the downward shift of the band dispersion around $(\pi, 0)$ region [10]. For example, some of the quantum Monte Carlo (QMC) simulations show such behavior in the strong coupling regime and at very low dopings [11,12]. This phenomenon is quite interesting since it looks as if it violates the Luttinger theorem on the Fermi surface. The second case is an effective pseudogap in the spectral function between a strong quasiparticle peak and a weak satellite peak. It is possible to find this situation even in a normal Fermi liquid. The third one is a suppression of the single-particle peak at the Fermi level with a two peak structure in its place. The pseudogap of our interest is this latter case. It should be clearly distinguishable from the second case. One physical origin of this kind of pseudogap is of course the fact that it is a precursor of the spin density wave (SDW) transition which takes place in the 2-d Hubbard model for zero doping at $T = 0$. We are aware of some models which take into account precursor effects of the superconducting transition to explain the pseudogap behavior observed in the normal phase of high-$T_c$ materials [13,14]. We don’t consider the superconducting transition effects in this paper.

In our work, we provide an explanation of the origin of the pseudogap formation in the 2-d Hubbard model, at half-filling, in the weak coupling regime. To calculate the spectrum we use a single-particle Green’s function which has a paramagnon-like one-loop self-energy correction for both charge and spin channels. At first we show the results
of our numerical calculations of the density of states (DOS), the spectral function, and the self-energy. The analysis of the real and imaginary parts of the self-energy plays a crucial role in the understanding of the microscopic origin of the possible structures of the spectra. Following this, we discuss the detailed origin of the pseudogap formation within our formulation.

We found pseudogap formations at the Fermi level in both the spectral function and the DOS. The pseudogap in the spectral function is explained by the non-Fermi-liquid behavior of the self-energy, i.e., its imaginary part has a negative peak and its real part has a positive slope. We show that both the strong antiferromagnetic spin fluctuation and the nesting condition on the non-interacting Fermi surface are the origins of the anomalous behaviors in the self-energy. We also generally argue the relation between the spectral function and the self-energy at the Fermi level. We show, for example, that if the spectral function has a pseudogap, the real part of the self-energy has a positive slope at the Fermi level. An auxiliary relation is used to present the argument. This relation derived from the Kramers-Kronig transformation is proved in the appendix.

The numerically obtained pseudogap shows a strong momentum dependence. For a certain choice of the parameters, the pseudogap appears around \((\pi, 0)\) but not at \((\pi/2, \pi/2)\). We show that the anisotropic pseudogap comes from the low-energy enhancement of the spin excitation around \(\mathbf{Q} = (\pi, \pi)\) and the flatness of the band dispersion.

II. MODEL

In the momentum representation the Hubbard model, with a nearest-neighbor hopping, on a two-dimensional square lattice can be written as

\[
H = \sum_{\mathbf{k}, \sigma} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k} \sigma}^\dagger c_{\mathbf{k} \sigma} + \frac{U}{2} \sum_{\mathbf{k}, p_1, p_2, \sigma} c_{\mathbf{k} + \mathbf{p}_1 + \mathbf{p}_2 - \mathbf{k} \sigma}^\dagger c_{\mathbf{k} - \sigma} c_{\mathbf{p}_2 - \sigma} c_{\mathbf{p}_1 \sigma}
\]

with \(\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)\), \(\sigma\) representing the spin index and with \(U\) being the coupling constant of the on-site Coulomb repulsion between two electrons with opposite spins. We redefine the chemical potential \(\mu\) by adding the Hartree-Fock term and this is chosen as the origin of the energy for the half-filling case.

We next introduce the single-particle Green’s function at finite temperature in the paramagnetic regime. In general, we can write the full single-particle Green’s function as

\[
G(\mathbf{k}, \omega_n)^{-1} = G_0(\mathbf{k}, \omega_n)^{-1} - \Sigma(\mathbf{k}, \omega_n)
\]

where \(G_0(\mathbf{k}, \omega_n)^{-1} = i\omega_n - \varepsilon_{\mathbf{k}}\) and \(\Sigma(\mathbf{k}, \omega_n)\) is the proper self-energy. Here, in the weak-coupling regime, we consider the one-loop self-energy correction to the Green’s function. The formulation we use is based on the standard perturbation expansion over \(U/t\). These one-loop corrections are constructed with the free (mean-field) fermion line and the corresponding charge or spin fluctuation lines. The charge and spin fluctuations are described in terms of the susceptibilities calculated within the random phase approximation (RPA). We neglect higher-order contributions which appear in the diagrammatic series expansion. This kind of approximation has already been used in paramagnon theory [18]. Thus, the one-loop self-energy is simply

\[
\Sigma(\mathbf{k}, \omega_n) = U^2 T \sum_{\mathbf{q}, \nu_m} \left[ \frac{1}{2} \chi_c(\mathbf{q}, \nu_m) + \frac{3}{2} \chi_s(\mathbf{q}, \nu_m) - \chi_0(\mathbf{q}, \nu_m + \nu_m) \right] G_0(\mathbf{k} + \mathbf{q}, \omega_n + \nu_m)
\]

where we have defined the charge susceptibility as \(\chi_c(\mathbf{q}, \nu_m) = \chi(\mathbf{q}, \nu_m)/[1 + U\chi(\mathbf{q}, \nu_m)]\) and the spin susceptibility as \(\chi_s(\mathbf{q}, \nu_m) = \chi(\mathbf{q}, \nu_m)/[1 - U\chi(\mathbf{q}, \nu_m)]\). To avoid the double counting of the second-order self-energy diagram, we have subtracted \(\chi_0(\mathbf{q}, \nu_m)\) in the square brackets in \(\Sigma(\mathbf{k}, \omega_n)\). Here \(\chi_0\) is given by

\[
\chi_0(\mathbf{q}, \nu_m) = \sum_{\mathbf{k}} \frac{f(\varepsilon_{\mathbf{k} + \mathbf{q}}) - f(\varepsilon_{\mathbf{k}})}{\nu_m - (\varepsilon_{\mathbf{k} + \mathbf{q}} - \varepsilon_{\mathbf{k}})}
\]

with \(\nu_m = 2m\pi T\) and \(f(x)\) is the Fermi distribution function defined by \(f(x) = 1/[\exp(x/T) + 1]\).
III. NUMERICAL RESULTS

To calculate the spectra obtained from the above Green’s function, we made the analytic continuation of the energy variables of the self-energy and the Green’s function. In this way we obtained the retarded self-energy and the retarded Green’s function. As a result, the imaginary part of the self-energy becomes,

\[
\text{Im} \Sigma^R(k, \omega) = -U^2 \sum_q \left[ \frac{3}{2} \text{Im} \chi^R(q, \varepsilon_{k+q} - \omega) + \frac{1}{2} \text{Im} \chi_c^R(q, \varepsilon_{k+q} - \omega) - \text{Im} \chi^R(q, \varepsilon_{k+q} - \omega) \right] \\
\times [f(\varepsilon_{k+q}) + n(\varepsilon_{k+q} - \omega)]
\]

where \( n(x) \) is the Bose distribution function defined as \( n(x) = 1/(\exp(x/T) - 1) \). ‘R’ denotes the retarded function. The corresponding real part can be obtained from the imaginary part by means of the Kramers-Kronig transformation. Using those schemes, we have numerically calculated the susceptibilities, the self-energy, and the Green’s function. The momentum summation in \( \text{Im} \chi(q, \nu) \) was reduced to a contour integral in the Brillouin zone and roughly 4000 line-elements have been numerically summed up along the contour. The momentum summation in the imaginary part of the self-energy and the DOS have been done on a 120 × 120 mesh in the Brillouin zone. All parameters used in the calculation are within the Stoner instability condition in RPA.

A. Density of States

In Fig. 1 we show the \( U \) dependence of the DOS \( N(\omega) = \sum_k A(k, \omega) \) for \( T/t = 0.5 \) where the spectral function \( A(k, \omega) \) is defined by

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} G^R(k, \omega) \\
= -\frac{1}{\pi} \frac{\text{Im} \Sigma^R(k, \omega)}{[\omega - \varepsilon_k - \text{Re} \Sigma^R(k, \omega)]^2 + [\text{Im} \Sigma^R(k, \omega)]^2}.
\]

For \( U/t = 1.5 \), the overall structure still keeps the shape similar to the non-interacting case with a clear single peak on the Fermi level. For \( U/t = 2.5 \), a weak pseudogap can be seen, and finally, for \( U/t = 3.0 \), a rather wide pseudogap can be observed. The high-energy band tails are developed as \( U/t \) becomes large.

Figure 2 shows the temperature dependence of the pseudogap formation in the density of states for \( U/t = 2.0 \). The pseudogap develops as we lower the temperature. Using the Stoner condition, we numerically found that \( T/t = 0.21 \) is the SDW transition temperature for \( U/t = 2.0 \). The temperature effect appears only around the Fermi level and the overall high-energy structure is left almost unchanged.

A similar calculation of the DOS was done in the work by Kampf and Schrieffer [19]. They have also obtained the pseudogap formation near the Fermi level \( \omega = 0 \) for a weakly doped Hubbard model at zero temperature. In their calculation they took into account only the spin fluctuation effects in an one-loop self-energy similar to ours. Since the spin fluctuation effect becomes much stronger than the charge contribution near the SDW transition, the similarity of our calculation and theirs is natural. Pseudogap openings in the DOS in the weak-coupling regime has been observed in a QMC simulation [20]. They obtained pseudogaps for \( U/t = 4.0 \) and \( T/t = 0.2 \) for several lattice sizes from \( 8 \times 8 \) to \( 12 \times 12 \). A similar behavior in the DOS obtained by the fluctuation exchange (FLEX) approximation [21]. They obtained a very narrow and deep pseudogap in the DOS for \( U/t = 1.57 \) and \( T/t = 0.05 \) at half-filling. All of those results including ours are at least qualitatively in good agreement with each other. The DOS for \( U/t = 3.0 \) in Fig. 1 has a rather large pseudogap. This may be due however to our simple approximation.

B. Spectral function and the self-energy

The existence of the pseudogap in the DOS enables us to guess the decrease of the intensity of the spectral function at \( \omega = 0 \). In Fig. 3 (a) we plot the temperature dependence of the spectral function \( A(k_F, \omega) \) at \( k_F = (\pi, 0) \) together with the real and imaginary parts of the self-energy. We have also calculated \( A(k, \omega) \) for other momenta and our results are a strong indication of the anisotropy of the pseudogap. We will discuss it in more detail in a later section.

As we have expected, Fig. 3 (a) shows the weight decrease in the spectral function as the pseudogap develops in the DOS shown in Fig. 2. The self-energy shows a specific behavior. The real part (Fig. 3 (b)) has a positive slope and the
imaginary part (Fig. 3 (c)) shows a negative peak. This tendency becomes stronger as we decrease the temperature. Moreover, the Green’s function has three poles which correspond to the solutions of \( \omega - \varepsilon_{kF} = \text{Re} \Sigma^R(k_F, \omega) \) for \( T/t = 0.22 \) as shown in Fig. 3 (b). Two of the poles are associated with two peaks of \( A(k_F, \omega) \) in Fig. 3 (a) and the other pole is linked to the pseudogap. Those features in the spectral function and the self-energy clearly indicate the destruction of the Fermi-liquid quasiparticle states. We will argue in more detail on the relation between the pseudogap and the anomalous behavior in the self-energy in the next section.

This same trend in the spectral function has already been shown in the so-called two-particle self-consistent (TPSC) approach by Vilk and Tremblay [22, 23]. In the FLEX approach [21], however, there is no pseudogap in the spectral function although their self-energy shows a similar non-Fermi-liquid behavior that both our result and TPSC approach have shown. The detailed analysis and comparisons between those approaches can be seen in Ref. [23].

For the weak coupling regime at half-filling, the finite temperature pseudogap formation in \( A(k, \omega) \) in a QMC simulation [24] was attributed to a finite size effect. Making a different analysis of the QMC simulation data, the pseudogap formation was confirmed by Creffield et al [20]. The latter authors have used a singular-value-decomposition method instead of the maximum-entropy method to obtain the spectral function from the calculated finite temperature Green’s function. They obtained a clear pseudogap opening even with a 12 \( \times \) 12 system size.

IV. PSEUDOGAP AND THE NON-FERMI-LIQUID BEHAVIOR IN THE SELF-ENERGY

In this section we discuss the origin of the non-Fermi-liquid behavior in the imaginary part of the self-energy. This section is organized in three subsections. Firstly we analyze the imaginary part of the self-energy within the present paramagnon theory. A log singularity is found in the integrand of the imaginary part of the self-energy around \( \mathbf{q} = (\pi, \pi) \equiv \mathbf{Q} \). Let’s consider the integrand of the spin component of the self-energy at \( \mathbf{k} = k_F \). The integrand is

\[
I_{k_F}(\mathbf{q}, \omega) = -\frac{3}{2} U^2 \text{Im} \chi^R(\mathbf{q}, \varepsilon_{k_F+q} - \omega) \left[ f(\varepsilon_{k_F+q}) + n(\varepsilon_{k_F+q} - \omega) \right].
\]

(4.1)

Considering the strong low-energy enhancement of \( \text{Im} \chi^s(Q, \nu) \), we suppose that the major contribution to the imaginary part of the self-energy comes from the integrand at \( \mathbf{q} = \mathbf{Q} \). By setting \( \mathbf{q} = \mathbf{Q} \), the spin fluctuation spectrum can be written as

\[
\text{Im} \chi^R(\mathbf{Q}, \varepsilon_{k_F+\mathbf{Q}} - \omega) = \frac{\text{Im} \chi^R(\mathbf{Q}, -\omega)}{[1 - \text{Re} \chi^R(\mathbf{Q}, -\omega)]^2 + [\text{Im} \chi^R(\mathbf{Q}, -\omega)]^2}
\]

(4.2)

with

\[
\text{Im} \chi^R(\mathbf{Q}, \nu) = \frac{\pi}{2} \rho_0 \left( \frac{\nu}{2} \right) \tanh \left( \frac{\nu}{4T} \right)
\]

(4.3)

and

\[
\text{Re} \chi^R(\mathbf{Q}, \nu) = \frac{P}{\pi} \int d\nu' \frac{\text{Im} \chi^R(\mathbf{Q}, \nu')}{\nu' - \nu}.
\]

(4.4)

Here \( \rho_0(x) = (1/(2\pi^2t))K \left( \sqrt{1 - [x/(4t)]^2} \right) \) is the density of states for the non-interacting band \( \varepsilon_k \) where \( K(k) \) is the complete elliptic integral of the first kind. In the same way, we also have

\[
f(\varepsilon_{k_F+\mathbf{Q}}) + n(\varepsilon_{k_F+\mathbf{Q}} - \omega) = -\frac{1}{2} \coth \left( \frac{\omega}{2T} \right).
\]

(4.5)
Note that we have used the nesting condition \( \varepsilon_{k_F+Q} = -\varepsilon_{k_F} = 0 \) on the Fermi surface. Then, we obtain

\[
I_{k_F}(Q, \omega) = \frac{-3}{2} \frac{U^2}{t^2} \left( -\frac{\pi}{4} \rho_0 \left( \frac{\omega}{2} \right) \tanh \left( -\frac{\omega}{4T} \right) \coth \left( \frac{\omega}{2T} \right) \right) \frac{\ln \left( \frac{32t}{|\omega|} \right)}{[1 - U \Re \chi^R_0(Q, -\omega)]^2 + [U \Im \chi^R_0(Q, -\omega)]^2}.
\]  

(4.6)

For \( \omega \sim 0 \), by the cancellation of the \( \omega/T \) dependence in \( \tanh \) and \( \coth \), we see that the numerator always has a log singularity since

\[-\frac{\pi}{4} \rho_0 \left( \frac{\omega}{2} \right) \tanh \left( -\frac{\omega}{4T} \right) \coth \left( \frac{\omega}{2T} \right) \sim \frac{1}{16\pi t} \ln \left( \frac{32t}{|\omega|} \right).\]

(4.7)

By approximating the denominator with its value at \( \omega = 0 \), the behavior of the integrand for \( q = Q \) is dominated by the log singularity,

\[
I_{k_F}(Q, \omega) \sim -\frac{3U^2}{32\pi t} \ln \left( \frac{32t}{|\omega|} \right) \frac{\ln \left( \frac{32t}{|\omega|} \right)}{[1 - U \Re \chi^R_0(Q, 0)]^2}.
\]

(4.8)

In lowering the temperature or by increasing \( U \), \( 1 - U \Re \chi^R_0(Q, 0) \) becomes smaller and the contribution from the region around \( Q = (\pi, \pi) \) dominates the other region’s contribution and it causes the larger peak of \( \Im \Sigma(k_F, \omega) \) at \( \omega = 0 \).

In Fig. 4 we plot the temperature dependence of \( I_{k_F}(Q, \omega) \) for \( U/t = 2.0 \) using Eq. (4.8). Fig. 5 (a) shows the low-energy enhancement of \( \Im \chi_s(Q, \nu) \). The log divergence at \( \omega = 0 \) exists for any finite values of \( T \). \( I_{k_F}(Q, \omega) \) shows a remarkable enhancement at the same time as \( \Im \chi_s(Q, \nu) \) has a sharp increase. Clearly, one can see that this enhancement of \( I_{k_F}(Q, \omega) \) around \( \omega = 0 \) causes the non-Fermi-liquid, i.e., the negative peak structure in the imaginary part of the self-energy.

### B. No log-singularity case

In the last subsection we have found a logarithmic behavior in the integrand of the imaginary part of the self-energy. This has a strong influence in producing the non-Fermi-liquid behavior in the self-energy. In general, however, the logarithmic van Hove singularity in the DOS will be smeared to some extent by any finite interaction between electrons. One might suppose that the non-Fermi-liquid-like behavior we have seen in the last section is an artifact of our approximation. In this subsection, we consider this question by introducing a model susceptibility which does not possess the log-singularity behavior. Again we take into account only the spin components and neglect other channels in the self-energy.

From \( \Im \chi^R_s(Q, \nu) \) given by Eq. (4.3), we see that the logarithmic behavior comes from the non-interacting density of states \( \rho_0(\omega) \). To consider the case that \( \rho_0(\omega) \) does not have any divergence at \( \omega = 0 \), we simply assume that \( \rho_0(\omega) \) is finite at \( \omega = 0 \). Then, from Eq. (4.3), we can approximate the imaginary part of \( \chi_0(Q, \nu) \) as \( \Im \chi^R_0(Q, \nu) = c\nu \) around \( \nu = 0 \) where \( c \) is a positive constant. Since we would like to see the low-energy behavior of the integrand of \( \Im \Sigma \), it is sufficient to approximate the spin susceptibility around \( \nu = 0 \). Furthermore, approximating \( \Re \chi_0(Q, \nu) \) by its value at \( \nu = 0 \), we obtain the imaginary part of the model susceptibility written as

\[
\Im \chi^R_s(Q, \nu) = \frac{c\nu}{[1 - U \Re \chi^R_0(Q, 0)]^2 + (c\nu)^2}.
\]

(4.9)

One can see that our model susceptibility is formally equivalent to the phenomenological model susceptibility in the nearly-antiferromagnetic-Fermi-liquid (NAFL) theory \[25\,26\]. This model was introduced by Millis, Monien, and Pines to explain the NMR experiments in the high-\( T_c \) materials \[25\]. By applying the NAFL theory to the effective models including the next-nearest-neighbor hopping, anisotropic pseudogap formation \[27\] and band dispersion \[28\] which explains the experimental data in the high-\( T_c \) materials have been obtained.

Using our model susceptibility, the integrand of the imaginary part of the self-energy becomes

\[
I_{k_F}^s(Q, \omega) = -\frac{3}{2} \frac{U^2}{t^2} \frac{(c/2)\omega \coth(\omega/(2T))}{[1 - U \Re \chi^R_0(Q, 0)]^2 + (c\omega)^2}.
\]

(4.10)

In Fig. 4 (a), we show the \( U \) dependence of \( \Im \chi^R_s(Q, \nu) \) for \( T/t = 0.25 \). The necessary parameters in the model susceptibility are chosen as \( c/t = 0.5 \) and \( \Re \chi_0(Q, 0) = 0.4 \). We have roughly evaluated those parameters from the
C. Necessary condition for the pseudogap formation

As our numerical results have shown, the non-Fermi-liquid behavior of the self-energy and the pseudogap are related to each other. In all cases, as we have seen in our results, a pseudogap in \( A(k_F, \omega) \) accompanies the positive slope of the real part of the self-energy. In this subsection, we generally argue the relation between the self-energy and the spectral function at the Fermi level. We prove two theorems which hold between the self-energy and the spectral function. These theorems determine which conditions in the self-energy are necessary in order to have a pseudogap in the spectral function. Through the argument, we assume that: (i) the imaginary part of the (retarded) self-energy is always negative and finite, (ii) at \( \omega = 0 \), we have \((\varepsilon_{k_F} - \mu) + \text{Re}\Sigma^R(k_F, 0) = 0\). We leave the chemical potential \( \mu \) to keep the generality. Those assumptions are physically reasonable.

Next, we enunciate the two theorems, after that, we give the proofs of them.

Theorem I — If the imaginary part of the self-energy has a maximum at the Fermi level, the spectral function has a maximum at the Fermi level.

One easily sees that the conventional Fermi liquid satisfies the theorem I.

Theorem II — If the spectral function has a minimum at the Fermi level, the real part of the self-energy has a positive slope at the Fermi level.

Note that if the spectral function has a hollow at the Fermi level, we can say that the spectral function has a two peak structure around the hollow since the spectral sum over energy is finite. Hence, to discuss the existence of the pseudogap, it is sufficient to observe if the spectral function has a maximum at the Fermi level.

Proof of theorem I — If \( \omega \) is slightly different from 0, from the definition of the spectral function, we have

\[
A(k_F, \omega) = \frac{1}{\pi |\text{Im}\Sigma^R(k_F, \omega)| + \frac{1}{\left(\omega - (\varepsilon_{k_F} - \mu) - \text{Re}\Sigma^R(k_F, \omega)\right)^2 / |\text{Im}\Sigma^R(k_F, \omega)|}}. \tag{4.11}
\]

If \( \omega = 0 \), by the assumption (ii), we obtain

\[
A(k_F, 0) = \frac{1}{\pi |\text{Im}\Sigma^R(k_F, 0)|}. \tag{4.12}
\]

From the condition of this theorem, \( \text{Im}\Sigma^R(k_F, \omega) \) has a maximum at the Fermi level, and we have \(|\text{Im}\Sigma^R(k_F, \omega)| > |\text{Im}\Sigma^R(k_F, 0)|\). Moreover, the second term of the denominator of Eq. (4.11) is a positive finite, then we find \( A(k_F, 0) > A(k_F, \omega) \). The theorem I has been proved.

Before going to the proof of theorem II, we give the following lemma which is used in the proof.

Lemma — If \( \text{Im}\Sigma^R(k_F, \omega) \) has a maximum (minimum) at the Fermi level, then \( \text{Re}\Sigma^R(k_F, \omega) \) has a negative (positive) slope at the Fermi level. This lemma can be proved using a property of the Kramers-Kronig relation between \( \text{Im}\Sigma^R(k_F, \omega) \) and \( \text{Re}\Sigma^R(k_F, \omega) \). We give a proof of this property in the appendix, and the lemma follows immediately from it.

Proof of theorem II — From Dyson’s equation, we obtain that

\[
\text{Re}\Sigma^R(k, \omega) = \omega - (\varepsilon_k - \mu) - \frac{\text{Re}\Sigma^R(k, \omega)}{[\text{Re}\Sigma^R(k, \omega)]^2 + [\text{Im}\Sigma^R(k, \omega)]^2} \tag{4.13}
\]

and

\[
\text{Im}\Sigma^R(k, \omega) = \frac{\text{Im}\Sigma^R(k, \omega)}{[\text{Re}\Sigma^R(k, \omega)]^2 + [\text{Im}\Sigma^R(k, \omega)]^2}. \tag{4.14}
\]

At \( k = k_F \), the latter equation gives
\[ |\text{Im}\Sigma^R(k_F, \omega)| = \frac{1}{|\text{Im}G^R(k_F, \omega)| + |\text{Re}G^R(k_F, \omega)|^2 / |\text{Im}G^R(k_F, \omega)|}. \]  

(4.15)

At \( \omega = 0 \), from the assumption (ii) and Eq. (4.13), we find that \( \text{Re}G^R(k_F, 0) = 0 \). Then, from Eq. (4.13), we have

\[ |\text{Im}\Sigma^R(k_F, 0)| = \frac{1}{|\text{Im}G^R(k_F, 0)|}. \]  

(4.16)

Since the spectral function has a minimum at \( \omega = 0 \), we see \( |\text{Im}G^R(k_F, 0)| < |\text{Im}\Sigma^R(k_F, \omega)| \) for \( \omega \) near zero. Thus, we have

\[ \text{Im}\Sigma^R(k_F, 0) < \text{Im}\Sigma^R(k_F, \omega) < 0, \]  

(4.17)
i.e., \( \text{Im}\Sigma^R(k_F, \omega) \) has a minimum at \( \omega = 0 \). From the lemma, we see that \( \text{Re}\Sigma^R(k_F, \omega) \) has a positive slope at \( \omega = 0 \). The theorem II is finally proved.

We easily see that the reverses of the two theorems do not always hold. For example, when \( \text{Re}\Sigma^R(k_F, \omega) \) has a positive slope, \( A(k_F, \omega) \) may have a single peak at the Fermi level. However, we can never have a simultaneous maximum in \( \text{Im}\Sigma^R(k_F, \omega) \) and a pseudogap in \( A(k_F, \omega) \) at the Fermi level. The argument we gave here does hold very generally and it does not depend on the models and the origin of the pseudogap.

The reverse of the lemma is not always true either. However, if we include an additional condition in the initial assumption such as the imaginary part of the self-energy has always a minimum or a maximum at the Fermi level, the reverse of the lemma is satisfied. To prove this let’s assume this new condition. From the lemma, \( \text{Re}\Sigma(k_F, \omega) \) always has a (positive or negative) slope at the Fermi level. Thus, the maximum (minimum) of \( \text{Im}\Sigma^R(k_F, \omega) \) is automatically linked to the negative (positive) slope of \( \text{Re}\Sigma^R(k_F, \omega) \). The reverse of the lemma follows from this.

By combining the reverse of the lemma and the theorem I, we immediately find that when \( \text{Re}\Sigma^R(k_F, \omega) \) has a negative slope at \( \omega = 0 \), the spectral function has a single peak at the Fermi level. In other words, as far as the Fermi-liquid-like negative slope remains in \( \text{Re}\Sigma^R(k_F, \omega) \) at \( \omega = 0 \), the pseudogap is never produced in the spectral function at the Fermi level.

**V. BAND DISPERSION AND ANISOTROPIC PSEUDOGAP**

In Fig. 6 (a) we show the band dispersion extracted from the numerical data of the spectral function \( A(k, \omega) \) for several momentum directions. The dot indicates the peak of the spectral function. The peaks roughly follow the original non-interacting band dispersion except around \( (\pi, 0) \). Clear (pseudo)gap structure can be seen around \( (\pi, 0) \). In contrast, around \( (\pi/2, \pi/2) \), there is no such pseudogap structure. This exemplifies the anisotropy of the pseudogap.

In Fig. 8, we show the band dispersion around \( (0, 0) \) and \( (\pi/2, \pi/2) \) also has a positive slope, but it is still weak. \( \text{Im}\Sigma^R(k_F, \omega) \) at \( k_F = (\pi/2, \pi/2) \) in Fig. 8 (b) has a large positive slope around \( \omega = 0 \). \( \text{Re}\Sigma^R(k_F, \omega) \) at \( k_F = (\pi/2, \pi/2) \) also has a positive slope, but it is still weak. \( \text{Im}\Sigma^R(k_F, \omega) \) at \( k_F = (\pi/2, \pi/2) \) in Fig. 8 (c) shows a sharp negative peak at \( \omega = 0 \). In contrast, \( \text{Im}\Sigma^R(k_F, \omega) \) at \( k_F = (\pi/2, \pi/2) \) has a weak minimum at \( \omega = 0 \). These remarkable momentum dependences of the real and imaginary parts around \( \omega = 0 \) determines the opening of the pseudogap.

For larger values of \( U/t \), we have obtained a pseudogap in \( A(k, \omega) \) also at \( k_F = (\pi/2, \pi/2) \). In Fig. 8 we show the spectral function for \( U/t = 3.0 \) and at \( T/t = 0.5 \). We chose the higher temperature to avoid the Stoner instability. The pseudogap at \( (\pi/2, \pi/2) \) is weaker than the one at \( (\pi, 0) \). Comparing with the spectral function for \( U/t = 2.0 \) shown in Fig. 8 (a), the intensity of \( A(k_F, \omega) \) in Fig. 8 is weak and its width are rather wide. This indicates band broadening effects due to the larger value of \( U/t \).

To understand the reason for the anisotropy of the pseudogap, it is sufficient to analyze the imaginary parts of the self-energy at \( \omega = 0 \) for \( k_F = (\pi, 0) \) and \( (\pi/2, \pi/2) \). There are two factors: the difference of the effective region of the \( q \) summation and the different behaviors of the bosonic excitation energy in the imaginary part of the self-energy. The first one is a kind of the selection rule of the momenta of the fermion-boson excitation and the latter is the restriction of energy on its excitation. We explain them as follows.
The distribution function term \( f(\varepsilon_{kF+q}) + n(\varepsilon_{kF+q} - \omega) \) produces an important restriction to the \( q \) summation in \( \text{Im}\Sigma(k_F, \omega) \). In Fig. 3, the approximated summation area in the \((q_x, q_y)\)-plane is shown by the shaded region in which \( q \) satisfies the condition \( |f(\varepsilon_{k_F+q}) + n(\varepsilon_{k_F+q})| > 0.5 \) for \( T/t = 0.22 \). We see that for both \( k_F = (\pi, 0) \) and \( (\pi/2, \pi/2) \) the region around \( q = Q \) contributes to the \( q \) summation. However, the shaded area around \( Q \) for \( k_F = (\pi, 0) \) is greater than that for \( (\pi/2, \pi/2) \). Thus, \( \text{Im}\Sigma(k_F, \omega) \) for \( k_F = (\pi, 0) \) has a larger contribution from the spin excitation around \( Q = (\pi, \pi) \).

The bosonic energy \( \varepsilon^b(q) \equiv \varepsilon_{k_F+q} - \omega \) in the expression of \( \text{Im}\Sigma(k_F, \omega) \) for \( k_F = (\pi, 0) \) behaves in a totally different way from that for \( k_F = (\pi/2, \pi/2) \). To see the behavior for \( \omega \sim 0 \) and around \( q \sim Q \), we can write \( \varepsilon^b(Q + \delta q) \sim -\varepsilon_{k_F+\delta q} \), where \( \delta q \) is a small vector to represents deviation from \( Q \). Thus, we see that the behavior of \( \varepsilon^b(Q + \delta q) \) is determined by the band dispersion \( \varepsilon_k \) around \( k = k_F \). Hence, the bosonic energy contribution to \( \text{Im}\Sigma \) for \( k_F = (\pi, 0) \) is quite concentrated within a small region around 0 energy near the saddle point (flat-band) dispersion near \( (\pi, 0) \). In contrast, the bosonic energy for \( k_F = (\pi/2, \pi/2) \) can easily deviate from 0 as \( q \) moves in the summation region near \( Q \) since \( \varepsilon_{k_F} \) has a linear slope around \( k_F = (\pi/2, \pi/2) \). Thus, the low energy enhancement in the spin fluctuation around \( Q \) makes a stronger contribution to \( \text{Im}\Sigma(k_F, \omega) \) at \( k_F = (\pi, 0) \) than that at \( k_F = (\pi/2, \pi/2) \). As a result, the self-energy has a remarkable momentum dependence, and the anisotropy of the pseudogap is explained.

There are some QMC simulations of the spectral functions in the weak-coupling regime at half-filling \([20, 24, 31]\). With the exception of the results from Creffield et al. (Ref. [20]), a clear evidence of the anisotropic pseudogap in the spectral function is lacking in the QMC simulations. We think this is also due to the cluster size effect and the difference in method in extracting the information of the spectral function from the Green’s function as emphasized in Ref. [23]. We know of no other example of the anisotropic pseudogap in the \( t-U \) Hubbard model. However, in FLEX calculations, for the doped Hubbard model \([32, 33]\), a clear momentum dependence in the imaginary part of the self-energy at \( \omega = 0 \) near the Fermi momentum was obtained. They found that \( |\text{Im}\Sigma(k_F, 0)| \) has a large value along the Fermi surface which becomes larger and larger as \( k_F \) approaches the \( (\pi, 0) \) region. This tendency is consistent with our results at half-filling shown in Fig. 3 (c).

VI. CONCLUDING REMARKS

In this work we have studied the pseudogap formation in the two-dimensional Hubbard model at half-filling. We obtain a pseudogap formation in the density of states and in the spectral function. The pseudogap of the spectral function is produced when two conditions are satisfied: (i) a strong anti-ferromagnetic spin fluctuation, (ii) a nesting condition on the Fermi surface. The pseudogap on the Fermi energy is highly anisotropic and its associated symmetry is similar to the \( d \)-wave symmetry. The anisotropy is determined by the flatness of the band dispersion.

We emphasize that the pseudogap formation discussed is highly dependent on the specific character (perfect nesting) of the free band dispersion or the hopping term in the square lattice. Thus, the pseudogap is physically different from a gap formation such as the Mott insulator transition which takes place in a strong coupling regime. Our pseudogap can take place even in the weak coupling regime.

We have focused on the undoped single-band Hubbard model with nearest neighbor hopping. Unfortunately, the model we have used may be quite simple to make a quantitative comparison with the experimental data. Nevertheless, it is possible to apply the argument in the pseudogap originated, for example, in the Hubbard model with the next nearest neighbor hopping \((t-t'/U)\) model. In this model, the nesting condition associated with the momentum \( Q \) holds only around the \((\pi, 0)\) region (and, of course, also at the other symmetric three parts in the Brillouin zone). Hence, the pseudogap will open in this region. However, the region in the \( k_x = \pm k_y \) direction on the Fermi surface does not satisfy the nesting condition. Thus, we can predict that the electronic states around this diagonal region will remain in the Fermi liquid regime. Our argument is consistent with the physical picture of the so-called hot and cold quasiparticles by B. Stojković and Pines [26]. Investigation with more realistic models will be done in future works.

Very recently, the information of the self-energy has been extracted from the angle-resolved photoemission data [24]. In the work, it has been obtained that the observed normal state pseudogap accompanies a sharp negative peak in \( \text{Im}\Sigma^R \) and a positive slope in \( \text{Re}\Sigma^R \). The tendency of their data is qualitatively in good agreement with our results.

In the present work we have used a paramagnon-theory self-energy to calculate the electronic states. This treatment has a restriction due to the Stoner criterion in the RPA susceptibility. However, we believe that already in the level of this scheme, it contains important ingredients for the pseudogap formation and the partial destruction of the Fermi-liquid quasiparticles at the Fermi level. In particular, the anisotropic pseudogap formation in the spectral function in the calculated band dispersion indicates the coexistence of the Fermi-liquid-like quasiparticles and the SDW-like quasiparticles at the Fermi level.
APPENDIX: A RELATION IN THE KRAMERS-KRONIG TRANSFORMATION

In this appendix we give a simple proof of a relation obtained from the Kramers-Kronig transformation. We apply this relation to the real and imaginary parts of the self-energy in the main text of the present paper. The relation holds for any smooth functions. Suppose the following Kramers-Kronig relation for such two functions \( g(x) \) and \( h(x) \),

\[
g(x) = \frac{P}{\pi} \int_{-\infty}^{\infty} dx' \frac{h(x')}{x'-x}. \tag{A1}
\]

Then, the relation can be mentioned as follows. If \( h(x) \) has a maximum (minimum) at a certain point \( x = x_0 \), \( g(x) \) has a positive (negative) slope at \( x_0 \). We assume that \( h(x) \) has a peak at \( x = x_0 \) and it can be expanded around \( x_0 \) as \( h(x) \sim h(x_0) + (\gamma_h/2)(x-x_0)^2 \). This is reasonable as far as \( h(x) \) is a smooth function. Here, \( \gamma_h \) is the second derivative of \( h(x) \) at \( x = x_0 \). If \( \gamma_h > 0 \) \((<0)\), then the peak is a minimum (maximum).

Let’s observe the difference between \( g(x_0 + \varepsilon) \) and \( g(x_0) \) with \( \varepsilon \) being a small shift from \( x_0 \). We obtain that

\[
g(x_0 + \varepsilon) - g(x_0) = \frac{P}{\pi} \int_{-\infty}^{\infty} dx' \frac{\varepsilon h(x')}{(x'-x_0)^2 - \varepsilon(x' - x_0)}. \tag{A2}
\]

We easily see that the function \( \varepsilon/[(x'-x_0)^2 - \varepsilon(x' - x_0)] \) decreases rapidly as \( x' \) deviates from \( x_0 \) and \( x_0 + \varepsilon \). We can approximate the integration using the expansion of \( h(x) \) around \( x_0 \) as

\[
g(x_0 + \varepsilon) - g(x_0) \approx \frac{P}{\pi} \int_{x_1}^{x_2} dx' \varepsilon \left[ h(x_0) + (\gamma_h/2)(x' - x_0)^2 \right] \frac{1}{(x'-x_0)^2 - \varepsilon(x' - x_0)}. \tag{A3}
\]

where \( x_1 < x_0 < x_2 \), and besides, \(|x_2 - x_0|, |x_1 - x_0| \gg |\varepsilon| \). We have chosen \( x_1 \) and \( x_2 \) in a way which the expansion of \( h(x) \) is valid. By evaluating the integral up to the leading order of \( \varepsilon \), we obtain

\[
g(x_0 + \varepsilon) - g(x_0) \sim \frac{(x_2 - x_1)\gamma_h}{2\pi}. \tag{A4}
\]

Thus, for \( \gamma_h > 0 \) \((\gamma_h < 0)\) at \( x = x_0 \), the slope of \( g(x_0) \) is positive (negative).

By applying the same argument to the opposite transformation defined as

\[
h(x) = -\frac{P}{\pi} \int_{-\infty}^{\infty} dx' \frac{g(x')}{x'-x}. \tag{A5}
\]

we find that if \( g(x) \) has a maximum (minimum) at \( x = x_0 \), the slope of \( h(x) \) at \( x = x_0 \) is negative (positive).

In the above derivation, we assumed that the functions of our interests can be approximated with a quadratic form around a peak point we have interests. One can show the same relation in the case that the function behaves as \( h(x) \propto |x-x_0| \) around \( x = x_0 \). This is what happens if \( h(x) \) is the imaginary part of the self-energy of a marginal Fermi liquid \([35]\). Even if the peak is a \( \delta \)-function, the relation we argued is still applicable although the slope becomes infinite. One example of this can be seen in the mean-field Green’s function for the spin-density-wave states.

[1] K. Gofron, J. C. Campuzano, A. A. Abrikosov, M. Lindroos, A. Bansil, H. Ding, D. Koelling, and B. Dabrowski, Phys. Rev. Lett. 73, 3302 (1994).
FIG. 1. $U$ dependence of the density of states $N(\omega)$ at $T/t = 0.5$.

FIG. 2. Temperature dependence of the density of states $N(\omega)$ for $U/t = 2.0$. Inset shows the overall structures of $N(\omega)$.

FIG. 3. Temperature evolution of (a) the spectral function and (b) the real and (c) imaginary parts of the self-energy for $U/t = 0.2$ and at $k_F = (\pi, 0)$.

FIG. 4. Temperature dependence of (a) $\text{Im} \chi_s(Q, \nu)$ and (b) the integrand $I_{k_F}(Q, \omega)$ of the imaginary part of the self-energy for $U/t = 2.0$.

FIG. 5. $U$ dependence of the excitation spectra of (a) the model susceptibility (see the text) $\text{Im} \chi^*_s(Q, \nu)$ and (b), (c) the integrand $I_{k_F}(Q, \omega)$ of the imaginary part of the self-energy for the model susceptibility.
FIG. 6. (a) Band dispersion for several momentum directions and (b) $A(k,\omega)$ around $(\pi,0)$ region calculated for $U/t = 2.0$ and at $T/t = 0.22$.

FIG. 7. (a) Spectral function at $k_F = (\pi,0)$ (solid line) and $(\pi/2,\pi/2)$ (dotted line), and the corresponding (b) real and (c) imaginary parts of the self-energy. The parameters are $U/t = 2.0$ and $T/t = 0.22$.

FIG. 8. Spectral function at $k_F = (\pi,0)$ (solid line) and $(\pi/2,\pi/2)$ (dotted line) for $U/t = 3.0$ and at $T/t = 0.5$. Note the differences in scale compared with Fig. 7 (a).

FIG. 9. Main contribution area (shown with shade) to the $q$ summation in $\text{Im}\Sigma(k_F,0)$ for $T/t = 0.22$ and at (a) $k_F = (\pi/2,\pi/2)$ and (b) $k_F = (\pi,0)$. Momenta $q$’s in the region satisfy $|f(\varepsilon_{k_F+q}) + n(\varepsilon_{k_F+q})| > 0.5$. 

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Fig. 1: T. Saikawa and A. Ferraz
Fig. 2: T. Saikawa and A. Ferraz
Fig. 3: T. Saikawa and A. Ferraz
Fig. 4: T. Saikawa and A. Ferraz
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Fig. 6: T. Saikawa and A. Ferraz
Fig. 7: T. Saikawa and A. Ferraz
Fig. 8: T. Saikawa and A. Ferraz
Fig. 9: T. Saikawa and A. Ferraz