Opening of pseudogaps due to superconducting critical fluctuations in quasi-two dimensions

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We examine the role of the anisotropy of superconducting thermal critical fluctuations in the opening of pseudogaps in quasi-two dimensions. When the anisotropy of coherence or correlation lengths of the fluctuations is large enough and critical temperatures $T_c$ are high enough, the energy dependence of the selfenergy derived from that of Landau’s normal Fermi liquid in critical regions; its imaginary part has no minimum at the chemical potential. Prominent pseudogaps open in such a non-Fermi liquid phase. Pseudogaps must be absent or subtle in quasi-two-dimensional superconductors with low $T_c$ and almost isotropic three-dimensional superconductors.

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Cuprate oxide superconductors, which are quasi-two dimensional ones, exhibit high superconducting (SC) critical temperatures $T_c$. On the other hand, no order is possible at non-zero temperatures in one and two dimensions; if $T_c$ were nonzero, thermal critical fluctuations would diverge at $T_c$. Even if observed $T_c$ are high in quasi-low dimensional superconductors, they must be $T_c$ substantially reduced by the fluctuations. One may argue that some anomalies must be accompanied by the reduction of $T_c$. It is plausible that the opening of the so called spin-gap or the pseudogaps is one of the accompanying anomalies. In actual, it has already been shown that the renormalization of quasiparticles caused by SC fluctuations gives rise to the opening of pseudogaps. The purpose of this paper is to clarify the role of the anisotropy of SC thermal critical fluctuations in the opening of pseudogaps in quasi-two dimensions.

In order to exhibit the essence of the issue in a simple manner, we consider first intermediate-coupling attractive models on a quasi-two dimensional lattice composed of square lattices:

$$\mathcal{H} = \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{1}{2} \sum_{ij\sigma\sigma'} U_{ij} a_{i\sigma}^\dagger a_{j\sigma}^\dagger a_{j\sigma'} a_{i\sigma}. \quad (1)$$

When transfer integrals $t_{ij}$ between nearest and next nearest neighbors on a plane, $-t$ and $-t'$, are considered, the dispersion relation of electrons is given by $E(k) = -2t \left| \cos(k_x a) + \cos(k_y a) \right| - 4t' \cos(k_x a) \cos(k_y a)$, with $a$ the lattice constant of square lattices; the bandwidth is $8|t|$. Denote attractive interactions $U_{ij}$ between onsite and nearest-neighbor pairs on a plane by $U_0$ and $U_1$. We consider two models: $U_0/|t| \simeq -4$ and $U_1 = 0$, and $U_0 = 0$ and $U_1/|t| \simeq -4$. Quasi-two dimensional features are phenomenologically considered as an anisotropy factor of SC fluctuations, which is introduced below.

When $U_0/|t| < 0$ and $U_1 = 0$, isotropic s-wave SC fluctuations are developed. When $U_0 = 0$ and $U_1/|t| < 0$, anisotropic s-wave, p-wave, or $d\gamma$-wave SC fluctuations can be developed. We consider only two cases, isotropic s wave ($\Gamma = s$) and $d\gamma$ wave ($\Gamma = d\gamma$). When fluctuations of a single wave, $s$ or $d\gamma$ wave, are considered, the selfenergy to linear order in fluctuations is given by

$$\Sigma_{\sigma}(i\epsilon_n, k) = -\frac{k_BT}{N} \sum_{\omega} \sum_{q} U_{ij}^2 \frac{1}{N} \langle -i\epsilon_n - i\omega, -k - q \rangle \chi_{\Gamma}(i\omega_l, q) \times G_{\sigma}(-i\epsilon_n - i\omega_l, -k - q), \quad (2)$$

where $N$ is the number of unit cells, $U_1 = U_0 = 0$ and $\eta_{\Gamma}(k) = 1$ for $\Gamma = s$, $U_1 = U_0 = 0$ and $\eta_{\Gamma}(k) = \cos(k_x a) - \cos(k_y a)$ for $\Gamma = d\gamma$, $G_{\sigma}(i\epsilon_n, k) = 1/|i\epsilon_n + \mu - E(k)| - \Sigma_{\sigma}(i\epsilon_n, k)$ is the renormalized Green function, with $\mu$ the chemical potential, and $\chi_{\Gamma}(i\omega_l, q)$ is the SC susceptibility for $\Gamma$ wave. The chemical potential shift caused by the Hartree and Fock terms is included in $\mu$. Other types of fluctuations such as charge ones also renormalize quasiparticles. They are ignored or a part of them is phenomenologically considered as lifetime width $\gamma$, which is introduced below.

Because critical fluctuations are restricted to a narrow region around $\epsilon_n = 0$, Eq. (2) is approximately given by

$$\Sigma_{\sigma}(i\epsilon_n, k) = -U_1^2 \eta_{\Gamma}^2(k) \frac{k_BT}{N} \sum_{\omega} \sum_{q} G_{\sigma}(0)(-i\epsilon_n - i\omega_l, k) \times \frac{1}{N} \sum_{|q||\le q_c} \sum_{q_z} \chi_{\Gamma}(i\omega_l, q). \quad (3)$$

The summation over $q_{||} = (q_x, q_y)$ is restricted to $|q_{||}| \le q_c$, and $G_{\sigma}(0)(i\epsilon_n, k) = 1/|i\epsilon_n + \mu - E(k)| + i\gamma/|\epsilon_n|/|\epsilon_n|$ is used instead of $G_{\sigma}(i\epsilon_n, k)$ to avoid a selfconsistent procedure; the lifetime width $\gamma$ is introduced in $G_{\sigma}(0)(i\epsilon_n, k)$. We also use a phenomenological expression for the SC susceptibility to avoid another selfconsistent procedure:

$$\chi_{\Gamma}(i\omega_l, q) = \frac{\chi_{\Gamma}(0)\omega_l^2}{\kappa^2 + (q_{||} a)^2 + \delta^2(q_z c)^2 + \frac{|\omega_l|}{\Gamma_{\text{SC}}|t|}}, \quad (4)$$

with $\chi_{\Gamma}(0)$ the static homogeneous one, $\delta$ the anisotropy factor of SC fluctuations, and $c$ the lattice constant along the $z$ axis. The so called $\omega$-linear term is ignored in
Eq. (1)}. The density of states renormalized by SC fluctuations is given by
\[ \rho(\varepsilon) = \frac{1}{N} \sum_k \left( -\frac{1}{\pi} \right) \text{Im} \left[ G'_\sigma(\varepsilon + i0, k) \right], \]
with \( G'_\sigma(\varepsilon + i0, k) \) defined by\( 1/\left[ 1/G^{(0)}_\sigma(\varepsilon+i0, k) - \Sigma(\varepsilon+i0, k) \right] \).

Following the previous paper \[12\], we can show that \( \chi(0) \kappa^2 |t| / |g_0 R| \) for the coupling constant \( U_T, t' = -0.3t < 0 \) for transfer integrals, \( \mu/|t| = -0.5 \) for the chemical potential, \( a = c \) for the lattice constants, \( g_e = \pi \alpha a \) for the cut-off wave number, and \( \gamma/|t| = 0.5 \) for the lifetime width.

First, we consider SC critical points; \( T = T_c \) and \( \kappa = 0 \). Although \( T_c \) depends on other parameters, we treat it as an independent one; our free parameters are \( \delta \) and \( \Gamma_{SC} \) in addition to \( T_c \). Figure 1 shows \( -\text{Im} \left[ \Sigma(\varepsilon + i0, k) \right] / |g_0 R|^2(k)|t| \) as a function of \( \varepsilon \) for three cases of \( E(k) - \mu \); its \( k \) dependence comes through \( E(k) \).

When fluctuations are isotropic \( (\delta = 1) \), the selfenergy is small and its \( \varepsilon \) dependence is consistent with that of Landau’s normal Fermi liquid, as is shown in Fig. 1(d). When fluctuations are anisotropic \( (\delta \ll 1) \), the selfenergy can be large, as are shown in Figs. 1(a)-(c). Even when the anisotropy is large, the \( \varepsilon \) dependence is consistent with that of the Fermi liquid as long as \( T \) is low, as are shown in Figs. 1(a)-(c). When the anisotropy is large and \( T \) is high, \( \varepsilon = 0 \) is not any minimum point of \( -\text{Im} \left[ \Sigma(\varepsilon+i0, E(k)) \right] \), as are shown in Figs. 1(a)-(c).

In such a non-Fermi liquid phase, quasiparticles on the whole Fermi surface are incoherent in case of \( s \) wave and those around \( (\pm \pi/\alpha, 0) \) and \( (0, \pm \pi/\alpha) \) are incoherent in case of \( d \gamma \) wave. Figure 1 implies that the reduction of \( T_c \) is large in quasi-two dimensional superconductors if observed \( T_c \) are high and it is small in almost isotropic three-dimensional ones even if observed \( T_c \) are high.

Figures 2 and 3 show \( \rho(\varepsilon) \) renormalized by \( s \)-wave and \( d \)-wave SC fluctuations, respectively. Prominent pseudogaps open in the non-Fermi liquid phase. Pseudogaps are more prominent for higher \( T_c \). However, \( T_c \) are mainly caused by larger \( g_r \), the tendency that pseudogaps are more prominent for higher \( T_c \) must be larger in actual superconductors than it is in Figs. 2 and 3.

Large anisotropy of critical fluctuations or a small \( \delta \) such as \( \delta < 0.1-0.3 \) is indispensable for the opening of prominent pseudogaps; pseudogaps are absent or subtle in the isotropic case \( (\delta = 1) \). Although spectra of \( \rho(\varepsilon) \) are slightly different between \( s \)-wave and \( d \)-wave cases, there is no essential difference between them as long as \( U_s \sim U_d \). The anisotropy of critical fluctuations within planes plays a minor role.

When cuprate oxides are treated, the theory should be extended to the strong-coupling repulsive regime, \( U_0 / |t| \gtrsim 8 \) and \( |U_1 / |t| \ll 1 \); we had better use the so called \( d \)-wave or the \( t-J \) model. A three-peak structure of the so called Gutzwiller’s quasiparticle band between the lower and upper Hubbard bands (LHB and UHB) is mainly because of strong local correlations. An intersite exchange interaction can be a Cooper-pair interaction. The main part of the exchange interaction in cuprate oxides is the superexchange interaction, which arises from the virtual exchange of pair excitations of electrons across LHB and UHB. An exchange interaction arising from that of Gutzwiller’s quasiparticles also work between Gutzwiller’s quasiparticles themselves. The strong local correlations, which give rise to the three-peak structure, and the exchange interactions can be treated by a Kondo-lattice theory. According to the single-site approximation (SSA) or the dynamical mean-field theory (DMFT), the three-peak structure is mapped to the so called Kondo peak between two subpeaks in the Anderson model or the Kondo problem. In the Kondo-lattice theory, an unperturbed state is constructed by including the local correlations in SSA or DMFT and intersite effects are perturbatively considered starting from the unperturbed state. Because SSA or DMFT is rigorous for infinite dimensions, this perturbation is nothing but \( 1/d \) expansion, with \( d \) spatial dimensionality. Then, a theory of superconductivity or SC fluctuations in the vicinity of the Mott transition or crossover can be developed almost in parallel to that of this paper \[12, 18, 19\]. Eventually, \( t \) of this paper is replaced by that of Gutzwiller’s quasiparticles, and the attractive interaction of this paper is replaced by the exchange interaction between nearest neighbors in such a way that \( U_d \rightarrow U_d^\gamma = \tilde{\gamma} \hat{I}_s (\tilde{\sigma}_o / \tilde{\sigma}_\gamma)^2 \), with \( \tilde{\sigma}_o \) and \( \tilde{\sigma}_\gamma \) the single-site vertex correction in spin channels and the mass renormalization factor in SSA or DMFT. Here, \( I_s \) is the exchange interaction constant between nearest neighbors, whose main part is \( J_s \) of the superexchange interaction. Phenomenological \( \gamma \) is mainly due to antiferromagnetic spin fluctuations instead of charge ones. Because \( T_c \) of \( d \gamma \) wave are much higher than \( T_c \) of other waves, we consider only \( d \gamma \) wave in the following part.

The specific heat coefficient of the so called optimal doped cuprate-oxide superconductors is as large as 14 mJ/K²mol \[24\]. This implies that the Gutzwiller’s quasiparticle band width is about 0.3 eV or \( |t| \sim 0.04 \) eV. On the other hand, the superexchange interaction is as strong as \( |J_s| \sim 0.1-0.15 \) eV. Therefore, high-\( T_c \) superconductivity must occur in an intermediate coupling regime \( U_d^\gamma / |t| \sim 4 \). Because \( T_c / |t| = 0.2 \) corresponds to \( T_c \sim 100 \) K and \( \delta \lesssim 0.1 \) in cuprate oxides, Fig. 1(b) implies that the opening of pseudogaps at \( T_c \) must be caused by SC thermal critical fluctuations; even if other mechanisms work, the mechanism proposed here must play a major role, at least, at \( T_c \) and in critical regions.

If all the parameters such as \( \chi(0), \kappa, \delta, \) and \( \Gamma_{SC} \), were constant as a function of \( T \), pseudogaps would be
FIG. 1: $-\mathrm{Im}\left[\Sigma_{\nu}(\varepsilon+i0,\mathbf{k})/g_T^{\nu}\right](\mathbf{k})/|t|$ at critical temperatures ($\kappa = 0$) for $\Gamma_{SC} = 0.2$ as a function of $\varepsilon$: (a) $\delta = 0.01$, (b) $\delta = 0.1$, (c) $\delta = 0.3$, and (d) $\delta = 1$; (i) $E(\mathbf{k}) = \mu - 0.5|t|$, (ii) $E(\mathbf{k}) = \mu$, and (iii) $E(\mathbf{k}) = \mu + 0.5|t|$. In each figure, solid, dashed, broken, chain, and chain double-dashed lines show results for $k_B T_c / |t| = 0, 0.05, 0.1, 0.2, 0.4$, and 1, respectively. The selfenergy correction is larger for smaller $\delta$. When $\delta$ is small enough and $T$ is high enough, the $\varepsilon$ dependence is different from that of conventional normal Fermi liquids; there is no minimum at the zero energy or the chemical potential.

FIG. 2: $\rho(\varepsilon)$ at critical temperatures ($\kappa = 0$) for $s$-wave and $g_s = 4$: (a) $k_B T_c / |t| = 0.1$, (b) $k_B T_c / |t| = 0.2$, and (c) $k_B T_c / |t| = 0.4$; (i) $\Gamma_{SC} = 0.1$, (ii) $\Gamma_{SC} = 0.3$, and (iii) $\Gamma_{SC} = 1$. In each figure, solid, dashed, broken, chain, and chain double-dashed lines show $\rho(\varepsilon)$ for $\delta = 0.01, 0.03, 0.1, 0.3$, and 1, respectively. Pseudogaps are more prominent for higher $T_c$, smaller $\delta$, and smaller $\Gamma_{SC}$. Pseudogaps are absent in any spectrum for the isotropic case ($\delta = 1$).

FIG. 3: $\rho(\varepsilon)$ at critical temperatures ($\kappa = 0$) for $d$-wave and $g_d = 4$. See also the figure caption of Fig. 2. No essential difference can be seen between Fig. 2 for $s$ wave and this figure for $d\gamma$ wave.

FIG. 4: $\rho(\varepsilon)$ at $k_B T / |t| = 0.4$ for $d\gamma$ wave and $g_d = 4$: (a) $\delta = 0.01$, (b) $\delta = 0.03$, (c) $\delta = 0.1$, and (d) $\delta = 0.3$; (i) $\Gamma_{SC} = 0.1$, (ii) $\Gamma_{SC} = 0.3$, and (iii) $\Gamma_{SC} = 1$. In each figure, solid, dashed, broken, chain, and chain double-dashed lines show $\rho(\varepsilon)$ for $\kappa^2 = 0.5, 1, 2, 4$, and 8, respectively. When $\kappa^2$ or $\Gamma_{SC}$ are large enough, pseudogaps are absent or subtle. For example, pseudogaps are absent or subtle in any spectrum for $\kappa^2 \geq 2$; they are absent in any spectrum for $\Gamma_{SC} = 1$. 
developed with increasing $T$. Experimentally, however, pseudogaps close at high enough $T$. It is likely that the temperature dependences of $\chi_T(0)$, $\kappa$, $\delta$, and $\Gamma_{SC}$ are responsible for the closing of pseudogaps, for example, at $k_B T/|t| \simeq 0.4$ or $T \simeq 200$ K. Then, we examine what parameters are needed in order to reproduce a situation that pseudogaps that open at $k_B T/|t| = 0.2$ close at $k_B T/|t| = 0.4$. It is obvious that $\kappa^2$ increase with increasing $T$; $\chi_T(0)/\kappa^2$ is almost constant. It is likely that $\Gamma_{SC}$ increase with increasing $T$. Figure 4 show that when $\kappa^2$ and/or $\Gamma_{SC}$ are large enough at $k_B T/|t| = 0.4$ no prominent pseudogap can be seen. For example, no prominent pseudogap can be seen for $\kappa^2 \gtrsim 2$ even when $\Gamma_{SC} = 0.1$. It is interesting to complete the selfconsistent procedure, which is avoided in this paper, in order to confirm whether or not such temperature dependences of $a/\kappa$ and $\Gamma_{SC}|t|$, the correlation length and the energy scale of fluctuations, can be actually reproduced.

The so called coherence peaks are missing in Figs. 2 and 4. We also note that $\rho(0)|s_1| = O(1)$ even when pseudogaps are developed. This is quite different from $\rho(0)|s_1| \ll 1$ at $T \ll T_c$ in SC phases. The origin of the so called zero-temperature pseudogap 26, which is characterized by $\rho(0)|s_1| \ll 1$, must be different from that proposed in this paper.

The density of states in SC phases of cuprate-oxide superconductors is different from that of conventional ones: dips outside SC gaps in cuprate oxides and no dips in conventional ones 8, 3, 11. Low-energy SC fluctuations $|\omega| \lesssim \varepsilon_G(T)$, with $\varepsilon_G(T)$ being SC gaps, must be suppressed below $T_c$, but high-energy fluctuations such as $|\omega| \simeq \varepsilon_G(T)$ or $|\omega| \gtrsim \varepsilon_G(T)$ must be developed. Pseudogaps may open at high-energy regions because of high-energy SC fluctuations even in SC phases. A possible scenario is that dips appear because of the superposition of SC gaps and pseudogaps.

Because low-energy SC fluctuations $|\omega| \lesssim \varepsilon_G(0)$ cannot developed at $T = 0$ K, the reduction of $\varepsilon_G(0)$ at $T = 0$ K must be very small. In the mean-field approximation for $d\gamma$ wave 13, where the reduction of $T_c$ is not considered, $\varepsilon_G(0)/k_B T_c \simeq 4.35$. Observed large ratios 8, 3, 11 of $\varepsilon_G(0)/k_B T_c \gtrsim 8$ are pieces of evidence that $T_c$ are actually reduced by SC critical fluctuations.

Transition-metal dichalcogenide and organic superconductors are another possible low dimensional high-$T_c$ ones 26, 27. If $T_c$ are high and $\varepsilon_G(0)/k_B T_c$ are large, pseudogaps must also be prominent in critical regions.

It is straightforward to extend the theory of this paper to pseudogaps due to spin and charge fluctuations. When $T_c$ of spin or charge density wave are high and the anisotropy of fluctuations is large, pseudogaps must also be prominent in critical regions.

Mercury-based cuprate oxides show very high $T_c$ under pressures 28, 29. Pressures must reduce the anisotropy so that the reduction of $T_c$ becomes smaller with increasing pressures. It is interesting to search for almost isotropic cuprate-oxide superconductors with no prominent pseudogap. Because the reduction of $T_c$ by critical fluctuations is small, their $T_c$ can be higher than $T_c$ of quasi-two dimensional ones. A simple argument implies that if $\varepsilon_G(0)/k_B T_c = 4-5$ are realized $T_c$ can exceed 200 K.

In conclusion, pseudogaps can open in critical regions of quasi-two dimensional superconductors with high critical temperatures $T_c$ because of thermal critical fluctuations, which can be well developed only in low dimensions. They can open for not only anisotropic superconductors but also isotropic or BCS ones in quasi-two dimensions. Because it is difficult for the fluctuations to be developed in quasi-two dimensional superconductors with low $T_c$ and almost isotropic three dimensional ones, even with high $T_c$, it is unlikely that prominent pseudogaps open in such superconductors.