Theory of Pseudogap in Underdoped Cuprates

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Abstract. Recent theoretical studies on the origin of the pseudogap emerging in underdoped cuprate superconductors are overviewed, based on insights obtained by a cluster extension of the dynamical mean field theory (cDMFT) for the doped two-dimensional (2D) Mott insulator. The pseudogap obtained in the cDMFT shows an $s$-wave-like full-gap structure, distinct from the $d$-wave superconducting gap. The zero-temperature electronic structure supports that a non-Fermi liquid phase exists and underlies the pseudogap. The non-Fermi liquid phase is separated from the larger-doped Fermi liquid by topological transitions of the Fermi surface and an emergence of zeros of Green’s function. A coexisting evolution of the poles (Fermi surface) and zeros of the Green’s function is a unique feature of the pseudogap phase. The spectra well reproduce the arc/pocket formation, together with basic experimental properties of the pseudogap phase in the cuprates. Furthermore, a full-gap structure is supported by a comparison with the results of Raman experiments. The overall feature supports the proximity of the Mott insulator and the significance of the quantum criticality of the Mott transition. These numerical results are further favorably interpreted by extending the exciton concept, known in semiconductors, to doped Mott insulators. In this composite fermion (CF) theory, the pseudogap emerges as a gap arising from a hybridization of the quasiparticle (QP) with the CF. The pairing channel opening between a QP and a CF solves the puzzle of the dichotomy between the $d$-wave superconductivity and the precursory insulating gap in the same antinodal region. A mechanism of superconductivity emerges from this pairing.

1. Introduction

Pseudogap ubiquitously found in the underdoped cuprates above the superconducting critical temperature is a puzzling and controversial phenomenon not well understood for more than 20 years after the discovery. Theoretically as well as experimentally, there exist a number of interpretations and proposals attempting to account for the origin of the pseudogap, while it is still under active debates \cite{1, 2, 3, 4, 5, 6}. One scenario proposes that the pseudogap is a precursory gap of the $d$-wave superconductivity itself \cite{7}. According to this scenario, the phase fluctuation existing even under a well-developed preformed pair destroys the superconducting order. Its simple picture has been challenged by the experimental observation of different structures between the pseudogap and the superconducting gap \cite{8}. Another scenario proposes that the pseudogap emerges as a consequence of a real spontaneous symmetry breaking such as charge (stripe) or nematic orders \cite{9, 10}, $d$-density wave \cite{11}, and a phase with orbital current within a unit cell \cite{12}. Symmetry broken states have been reported in some of the cuprates such as Y- and Bi-based compounds \cite{13}, while it is not clear at this moment whether all of the
high-\textit{T}_c cuprates show the same symmetry breaking. Other scenarios, such as the resonating valence bond [14] and the nodal liquid [15, 16] theories, propose strong fluctuations as the origin of the pseudogap. In these scenarios, the pseudogap is absent in the nodal point, with a \textit{d}-wave symmetry as in the superconducting gap. This assumption is based on the experimental observation that the occupied part of the spectra indeed looks like \textit{d} wave. However, since it has been difficult so far to observe the unoccupied part of the spectra at a sufficiently high resolution, the experimental pseudogap structure is in fact largely unknown. In any of the scenarios, the mechanism of the pseudogap formation is widely believed to be intimately correlated with the mechanism of the high temperature superconductivity itself.

Recent theoretical and computational progress, particularly cDMFT combined with the comparison with various experimental results has renewed the understanding of the pseudogap [17, 18, 19, 20, 21, 22, 23, 24, 25] and has revealed it as a distinct phase characterized by an unconventional metal. In this article, based on these numerical results without any \textit{ad hoc} assumption, we examine various scenarios and conclude that the scenario by the preformed pair is not supported as a mechanism of the pseudogap. In addition, the numerical result shows that the pseudogap does not have the \textit{d}-wave symmetry but shows a full-gap structure when we take into account the unoccupied part of the spectra. This contradicts the scenarios of the preformed pair, the nodal liquid, \textit{d}-density wave and some of the resonating valence bond theories. The numerical results rather support that the pseudogap develops even without an explicit symmetry breaking such as the charge (nematic) order and the orbital current, whereas the pseudogap indeed grows solely as a consequence of the proximity (quantum criticality) to the Mott transition in the strong coupling region.

2. General remark on the origin of gap formation

Let us begin with a general remark on the mechanism of the (pseudo)gap formation from a theoretical viewpoint. In the mean-field picture of any symmetry breaking, including magnetic and superconducting origins, gap formations are understood always as consequences of hybridizations of the QP, where a pole in the Green’s function of the hybridization partner causes the self-energy divergence of the QP Green’s function. The divergence of the self-energy means the presence of a zero in the QP Green’s function.

This mechanism is seen in the Hamiltonian given by the single-particle form as

\[ H = \sum_i \xi_{\alpha_i} \hat{c}_{\alpha_i}^\dagger \hat{c}_{\alpha_i} + \sum_i \epsilon_{\beta_i} \hat{c}_{\beta_i}^\dagger \hat{c}_{\beta_i} + \sum_i \Delta_i \hat{c}_{\alpha_i}^\dagger \hat{c}_{\beta_i} + \text{H.c.}, \]  

where the QP with the creation (annihilation) operator \( \hat{c}_{\alpha_i}^\dagger \) (\( \hat{c}_{\alpha_i} \)) hybridizes with the particle \( \hat{c}_{\beta_i}^\dagger \) (\( \hat{c}_{\beta_i} \)) with the quantum numbers \( \alpha_i \) and \( \beta_i \), respectively. Then a hybridization gap proportional to \( \Delta_i \) opens in the single-particle spectra after the diagonalization.

The antiferromagnetic gap in the mean field theory offers a typical example, where the gap is caused by the hybridization of electrons at a wave number \( k \) with the electrons at a different wavenumber \( k + Q_0 \), with \( Q_0 \) being the ordering vector. An \( \uparrow \)-spin electron with the momentum \( k \) hybridizes with a \( \downarrow \)-spin electron with the momentum \( k + Q_0 \), through the mean-field term \( \Delta_{\text{AFM}}[\hat{c}_{k\uparrow}^\dagger \hat{c}_{k+Q_0\downarrow} + \text{H.c.}] \). Then, the self-energy for the \( \uparrow \)-spin electron with the momentum \( k \) diverges at the pole of the \( \downarrow \)-spin electron with momentum \( k + Q_0 \).

When the bare dispersion of \( \hat{c}_{k\sigma}^\dagger \) in the absence of \( \Delta_{\text{AFM}} \) is given by \( \xi_k \) and it hybridizes with the electron \( \hat{c}_{k+Q_0\overline{\sigma}}^\dagger \), the Green’s function \( G \) and its self-energy \( \Sigma \) of the electron \( \hat{c}_{k\sigma}^\dagger \) are given as

\[ G(k, \omega) = \frac{1}{\omega - \xi_k - \Sigma(k, \omega)}, \quad \text{and} \quad \Sigma(k, \omega) = \frac{\Delta^2_{\text{AFM}}}{\omega - \xi_{k+Q_0}}, \]  

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where $\omega$ is the energy. With the symmetry breaking, a zero surface appears in the single-particle Green’s function. The zero surface is nothing but the self-energy pole, where $\Sigma = \pm \infty$ results in the breakdown of the perturbation expansion. The pole of the self-energy is nothing but the pole of the Green’s function of the hybridization partner, namely, the electron at $k + Q_0$ for the above antiferromagnetic order. The gap formation and the destruction of the Fermi surface are caused by the zero surface which splits the pole surface and leads to the insulating gap.

3. Numerical methods
Details of the cDMFT method is given in the literature [26, 21]. The cDMFT calculation has been performed on the 2D Hubbard model defined by

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} (\hat{c}_{i\sigma} \hat{c}_{j\sigma} + \text{H.c.}) + \sum_i U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

under doping of carriers with the concentration $\delta$ measured from half filling. The model was solved with two choices of impurity solvers. One is the exact diagonalization for a 4-site cluster to clarify the properties at zero temperature. The other is the continuous-time Monte Carlo method [27] up to 16-site clusters for finite temperatures. To compare with experimental momentum-resolved spectra, it is necessary to introduce a method to bridge between the cluster calculation and the translationally invariant system, by periodizing the cluster results. Recently, for this purpose, it was shown that the cumulant periodization scheme is the best way to reduce finite-size effects to infer the thermodynamic limit within limited cluster sizes [21, 23]. The largest cluster size employed for the studies on the pseudogap so far is 16 sites, where the self-energy as well as the spectral weight near the Fermi level already appears to show a good convergence to the thermodynamic limit in the studied parameter and temperature region [23].

4. Evolution of zero and pole surfaces with topological phase transitions
We first overview what the cDMFT has revealed. In the results on the 2D Hubbard model, the zero surface indeed appears at half filling at large onsite interaction $U$ even in the absence of the symmetry breaking [19, 21]. It separates the upper and lower Hubbard bands in the energy-momentum space and runs in the resultant Mott gap similarly to the symmetry broken cases (see Fig.1(a) of Ref. [19] or Fig.13(b) of Ref. [21]). The origin of the gap is not a simple mean field arising from the symmetry breaking but rather pure electron correlation itself.

In the lightly hole doped Mott insulator, the spectral weight transfers from the upper Hubbard to the top of the lower Hubbard band, at which the Fermi level is located. When $U/t$ is large, the backbone Mott gap structure with a zero surface is still retained at a high energy. At the same time, an intricate small-energy structure emerges hierarchically near the Fermi level after the spectral weight transfer from the original upper Hubbard band upon hole doping. This generates a low-energy pole surface (Fermi surface at the Fermi level) of QPs which is split and considerably deformed by a low-energy zero surface emerging from a partial collapse of the Mott gap and the spectral weight transfer. Whether the weight transfer from the upper Hubbard band on the verge of the Mott transition occurs by a continuous shift of the weight through the Mott-gap-energy region or the weight appears near the Fermi level without the shift is not clear at the moment. The zero surface, coexisting and residing between the split pole surfaces, makes a small energy gap, which is identified with the pseudogap. The cDMFT with the solvers of the exact diagonalization at temperature $T = 0$ and the continuous-time quantum Monte Carlo method at $T > 0$ for the available clusters up to 16 sites with the cumulant periodization in the Brillouin zone consistently show the coexistence [28, 19, 21]. The coexistence is indeed a generic feature of lightly doped Mott insulators relevant to the pseudogap region in the cuprates.

Figure 1 shows how zero and pole surfaces evolve with doping in the 2D Hubbard model. In heavily-doped region ($\delta > 0.14$), the electronic structure has only a large electron-like Fermi
Figure 1. Evolution of pole (Fermi surface) and zero of the single-particle Green’s function at the Fermi level $\omega = 0$. From the normal Fermi liquid (FL) with the electron-like Fermi surface to the Mott insulator (MI), several different quantum phase transitions caused by topological changes of the Fermi surface are designated by blue triangles. The red (light) and blue (dark) regions show negative and positive Re$G$, respectively. White boundaries indicate pole surfaces and dark boundaries indicate zero surfaces. The right triangle indicates a Lifshitz transition from an electron-like to a hole-like Fermi surface nearly simultaneously with the pair creation of the pole and zero surfaces. The middle triangle shows the location of a Lifshitz transition, where two open Fermi surfaces connect to a single closed Fermi pocket. The left triangle indicates the Mott transition where the Fermi surface pocket disappears with only the zero surface being left in the MI. The result was obtained by the cDMFT calculation at zero temperature with the 4-site cluster for the 2D Hubbard model only with the nearest neighbor transfer $t$ and the interaction $U = 8t$. The computational details are found in Ref. [21].

surface, characteristic to the Fermi liquid. With reducing doping, this Fermi surface changes its topology to hole-like. On top of that, between 12 and 14 % dopings, a zero surface emerges around $(\pi, \pi)$ in pair with a small pole surface. The emergence of the zero surface signals the breakdown of the perturbation theory. Below this quantum phase transition with the topological change in the Fermi surface structure, non-Fermi liquid phase appears adiabatically disconnected with the overdoped Fermi liquid. The pseudogap phase appears further after another topological transition that is characterized as a Lifshitz transition transforming the two open Fermi surfaces into a single pocket. Since the outer part of the pocket is close to the zero surface, it is strongly damped and may not be visible in the angle resolved photoemission spectroscopy (ARPES), leaving a truncated arc-like structure in the inner part of the pocket [28]. The Mott insulator is realized after the final topological transition where the Fermi pocket vanishes. The evolution from the overdoped Fermi liquid to the Mott insulator may not be unique depending on the model parameters, even without symmetry breakings, and Fig. 1 illustrates one of the cases. Nevertheless, the existence of the topological phase transition (with emergence of the zero surfaces) separating the pseudogap phase from the conventional Fermi liquid is inevitable. Aside from details such as the quantitative accuracy of the result, if the evolution is continuous, the conventional Fermi liquid in the overdoped region with only the pole surface can be evolved by doping to the zero-surface-dominating Mott insulator, only when an intermediate phase exists: In this intermediate phase, the poles (Fermi surface) and zeros of the Green’s function have to coexist to continuously bridge the pole-only Fermi liquid and zero-only Mott insulator.

This region of coexisting zero and pole surfaces with the emergence of the pseudogap cannot be adiabatically connected with the normal Fermi liquid in the largely-overdoped region, because, as we described above, the emergence of the zero surface implying the diverging self-energy of QP means the breakdown of the perturbation theory. Moreover, the emergence of the zero surface accompanies a simultaneous creation of a pole surface, which generates a quantum phase
transition caused by a topological change in the Fermi surface. This quantum phase transition has nothing to do with a spontaneous symmetry breaking by itself, while it is categorized to a topological transition [29, 30, 31]. When interaction effects are involved in topological transitions, unconventional universality classes with a “soft” quantum criticality, characterized by the critical exponents such as $\beta > 1/2$ and $\delta < 3$, emerges in general around this marginal quantum critical point. This is in marked contrast with the conventional quantum criticality driven by the spontaneous symmetry breaking and described by the Landau-Ginzburg-Wilson scheme [29, 31]. Interaction effects may drive the topological quantum phase transition to the first-order one beyond the marginal quantum critical point. This first-order transition may continue at nonzero temperature and terminate at a finite-temperature critical point with the Ising universality class. When the transition occurs by the filling control, it occurs as the phase separation into different electron concentrations. However, such a phase separation is prohibited in the presence of the long-ranged Coulomb interaction. Then a meso-scale inhomogeneity or charge order becomes an intrinsic possibility as has been suggested in many experiments for the cuprates. Such competing orders observed in several types of cuprates indicate that the cuprates are close to the marginal quantum critical point driven by the topological transitions. Recently, the proximity of the first-order transition driven by the topological transition has been studied by the dynamical cluster approximation [32]. An intriguing future issue is how this soft criticality accompanying inevitable large quantum fluctuations induces instabilities toward competing orders such as superconductivity.

5. Full gap structure of pseudogap

A striking fact in the cDMFT result is that the pseudogap structure does not satisfy the $d$-wave symmetry and it appears to open a full $s$-wave-like gap [19, 21]. The result has clarified that the pseudogap is $d$-wave like only below the Fermi level, while it opens a full gap in the unoccupied part even in the nodal point. In the nodal region, the arc or pocket like structure of the Fermi surface becomes gapped in the unoccupied energy part. The $s$-wave structure of the pseudogap including the nodal point is robust against finite-size effect: It is consistently seen in the cluster sizes from 4 to 16.

The $d$-wave-like structure below the Fermi level well accounts for the ARPES results. The structure of a full gap with the isotropic $s$-wave-like amplitude can be confirmed only when we consider the total structure including the part above the Fermi level. The unoccupied part above the Fermi level has not been well probed so far because of the experimental difficulties such as the poor resolution in the inverse photoemission spectroscopy. The present theory and proposal can be critically tested by measuring whether the full-gap structure indeed exists in the nodal region above the Fermi level. The pseudogap structure in fact critically poses restrictions to the theories as well as to the mechanism of the superconductivity. It is desired to develop a high-resolution momentum-resolved probe for the unoccupied part.

The scanning tunnel microscopy (STM) in principle probes the unoccupied part, although it does not have a momentum resolution. One problem in the underdoped region is the inhomogeneity which may mix the responses in the superconducting and non-superconducting regions with different amplitudes of the gap in the temperature range normally accessible by the STM. Nevertheless, when we focus on a strongly underdoped region by ignoring the influence of the superconducting region at small $\omega$, the STM appears to show a flatter bottom of the local density of states particularly in the large-gap (non-superconducting) region [33, 34, 35]. This result supports the existence of the full gap, if we eliminate the effects of the $d$-wave superconducting phase. It is an intriguing issue to investigate this region in more detail by examining the temperature dependence in the pseudogap phase and by using the Fourier-transform scanning tunneling spectroscopy (STS). This will serve for gaining more insight into the intrinsic momentum-resolved gap structure of the pseudogap phase particularly in the nodal
region above the Fermi level. Recent comparison of Raman intensity with the cDMFT result indeed supports that the full gap opens in the unoccupied part over the entire Brillouin zone including the nodal point [25]. By employing different light polarizations, Raman spectroscopy can separately probe particle-hole excitations in the nodal (B$_{2g}$) and antinodal (B$_{1g}$) regions in the Brillouin zone. It equally probes the energy region below and above the Fermi level. The Raman spectra show that the pseudogap grows more or less equally in the B$_{2g}$ and B$_{1g}$ polarizations in agreement with the prediction for the Raman spectra calculated from the cDMFT single-particle spectra that open the s-wave-like pseudogap. Furthermore, the Raman spectra show that the superconducting gap has an energy scale much smaller than the pseudogap and a peak outside the pairing gap appears in the pseudogap energy scale, suggesting entirely different origins of these two gaps.

6. Composite fermion theory
The pseudogap formation has been established in the numerical results on the doped Mott insulator. In this section, we discuss a generic mechanism of the pseudogap formation in lightly doped Mott insulators, by extending the exciton concept that has played a significant role in understanding excitations of semiconductors and insulators [36, 37].

Figure 2. Schematic illustration of two ways of adding electrons to lightly doped Mott insulators: (a) QP added in the sea of nearly half-filled electrons depicted as light-blue (gray) background (b) CF as a weakly bound state of the added electron and an existing hole. These two excitations both have 1/2-spins depicted by arrows. They also hop and become extended in real space, giving their dispersions. Gray circle in (b) represents a hole.

In the underdoped cuprates, the Mott gap is still a robust underlying structure, where a zero surface persists below the upper Hubbard band. At the same time, a low-energy-scale structure near the gap edge including the QP excitations also evolves with doping. In this circumstance, we have two possible ways of low-energy excitation of doped carriers. One is QP and the other is composite fermion (CF) excitations as are illustrated in Fig. 2. The QP is spatially extended as a single-particle state. This becomes a low-energy excitation because of the kinetic energy gain. On the other hand one may add an electron near a holon site, to form a weakly bound state of the added electron and the existing holon similarly to the case of excitons. In the Mott insulating state, such an exciton is a tightly bound state with the binding energy of the Mott gap. This exciton-type excitation is the only one allowed in the large $U$ limit. It is a localized excitation in the Mott insulator and observed at the Mott gap (more precisely, the charge transfer gap) edge of the optical conductivity [38]. At large but finite $U$, even in the lightly doped systems, this excitonic excitation may still be robust and distinguished from QPs when the added electron forms a state bound with the holon as one naturally expects. However,
the binding energy must be dramatically weakened, because the doublon-holon attractive force (that generates the binding into an exciton) is screened by other doped carriers. We note that the screening is expected to be efficient even with a tiny doping concentration especially in two dimensions because of a constant density of states at the gap edge for the normal quadratic dispersion. Then the bound state becomes extended over several sites. This bound state is called CF [36]. The binding energy of the CF is originally scaled by the Mott gap in the Mott insulator while it is scaled by \( t \) in the lightly doped insulator as is shown in Ref. [24].

The two types of excitations may physically represent “two sides of a coin”: The QP represents the coherent part whereas the CF picks up the incoherent part of the carrier. These two excitations are not perfectly the eigenstate of the Hamiltonian and they have finite life times and nonzero damping amplitudes. It means that the QP decays into the CF after a certain life time, while the CF mutually decays into the QP again. This process is nothing but the hybridization of the QP and CF as we will see below.

These two faces of excitations are successfully expressed by the slave boson theory originally formulated by Kotliar and Ruckenstein [39], by extending and improving it. The original Kotliar-Ruckenstein formalism is equivalent to the Gutzwiller approximation, where the band narrowing is represented by the decreasing amplitude of the slave boson condensate in the mean-field framework. Castellani et al. [40] extended it by including the Gaussian fluctuation of the boson condensate, which enables to describe the upper and lower Hubbard bands. Further improvement has been achieved by considering the fluctuation beyond the Gaussian level by incorporating the excitonic bound state formation of the QP with a holon [36, 37].

More concretely, in the slave boson formalism, an electron \( \epsilon \) is described as a particle composed of a boson (slave boson representing holon \( \epsilon \), doublon \( \delta \) and singly occupied up- and down-spin bosons \( p_\uparrow \) and \( p_\downarrow \)) and a fermion representing the QP \( f_\sigma \) with spin \( \sigma \) in the form \( \hat{c}_{i\sigma} = (\hat{p}_{ia}^{\dagger} \hat{e}_i + \hat{d}_{ia}^{\dagger} \hat{e}_i) \hat{f}_{i\sigma} \). Then the transfer term \( t_{ij} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} \) in the original Hubbard model is rewritten in the summation of terms such as \( t_{ij} \hat{p}_{ia}^{\dagger} \hat{p}_{ja} (\hat{\Upsilon}_{ia}^{\dagger} - \hat{C}_{ia}) (\hat{\Upsilon}_{ia} - \hat{C}_{ia}) \), where \( \hat{C}_{ia} = \hat{e}_i \hat{f}_{i\sigma} \). A Stratonovich-Hubbard field \( \Upsilon \) introduced here plays the role of the CF. The present formalism naturally takes into account the CF substantiated by this Stratonovich-Hubbard field [36, 37]. Now it becomes clear that the above rewritten transfer contains the hybridization of a QP \( f \) with a CF \( \Upsilon \) after averaging out fluctuating charge bosons and spin bosons as \( \langle \hat{p}_{ia}^{\dagger} \hat{p}_{ja} \rangle \) in the decoupling approximation. The hybridization is scaled by \( t_{ij} \) and represents the physical process that the CF is dissolved into and recombined from a QP and a holon (or doublon) in binding-unbinding fluctuations. The effective Hamiltonian reads

\[
H = \sum_k \xi(k) \hat{f}_{k\uparrow}^{\dagger} \hat{f}_{k\uparrow} + \sum_k \alpha(k) \hat{\Upsilon}_{k\uparrow}^{\dagger} \hat{\Upsilon}_{k\uparrow} + \sum_k \Delta(k) \hat{f}_{k\uparrow}^{\dagger} \hat{\Upsilon}_{k\uparrow} + H.c.,
\]

where \( \alpha(k) \) is the CF dispersion, while the QP dispersion \( \xi(k) \) is also a renormalized one in the absence of the CF. Here, the CF has been defined so far as the bound state of a holon and an added electron, while another CF can equally be formed from the bound state of a doublon and an added hole. The formulation for the latter type is obtained straightforwardly from the former type, and for simplicity of the description, we do not explicitly introduce the latter type of the CF here.

Now the hybridization of QP and CF generates a hybridization gap, which is identified with the pseudogap in the cuprates. This hybridization gap is entirely different from the Mott gap precursor and from the superconducting gap as well. In fact, the pseudogap requires the underlying remnant of the Mott gap to exist but is generated as a lower-energy hierarchy developed with the CF.

The CF theory reproduces a number of puzzling experimental results as well as remarkable numerical results obtained by the cDMFT [21] and quantum Monte Carlo simulations [41].
instance, in addition to the consistent doping dependence of the pseudogap with the full-gap
structure, the whole structure of the spectral weight $A(k, \omega)$ with upper and lower Hubbard
bands and the QP dispersion, the hole pocket/arc structure of the Fermi surface at $\omega = 0$,
asymmetry of the density of states with respect to the $\omega > 0$ and $\omega < 0$ parts, and growth of the
density of states with increasing doping concentration, indicated in the specific heat, are very
consistent with the experimental and cDMFT indications[36].

7. Dichotomy and superconductivity
In this section, we discuss plausible consequences inferred from the results based on the cDMFT
and the CF theory in the previous sections. Since QP and CF represent the coherent and
incoherent part of the single-particle excitation, respectively, they may both play roles in pairing.
The QP pairing leads to the conventional Cooper pair, while the CF may also form a bound state
with another CF or with a QP. This is regarded as an incoherent pair, which contributes to the
superconducting gap without the phase coherence. In this sense, the CF offers a novel mechanism
of superconductivity. The pairing of the CF and QP is already considered explicitly in a
perturbative treatment[37]. We here note that the CF dynamically has a large dipole moment
consisting of the hole and the electron (doublon) because of the spatially extended structure of
their bound state, and the pairing may occur through this dynamical dipole fluctuation as in the
case of the attraction through the van der Waals interaction, but with a much larger energy
scale. Polarizable CF fluctuations are a natural source of the glue for the pairing that has a
conceptual similarity to the exciton mediated pairing. Internal degrees of freedom of a CF have
not been explored in detail in the literature, although the CF self-energy has to some extent
been considered[37].

The CF degrees of freedom give a solution to the puzzle of the dichotomy known in the
cuprates. Here the dichotomy means that experimentally the insulating pseudogap coexists
with the superconducting $d$-wave gap in the superconducting phase both mainly in the antinodal
region[42]. Since the pseudogap in the antinodal region enhances the insulating behavior rather
than the pairing precursor, it must severely compete with the superconducting $d$-wave gap in
this antinodal region. Then the question is why such a $d$-wave gap having the largest gap in the
antinodal region grows under the insulating pseudogap in the same region without destroying
each other.

Our numerical and theoretical findings solve this puzzle: In the antinodal region, the QP
dispersion is gapped and the coherent pairing is killed. However, this gapped region is nothing
but the region where the CF poles run. This means that the polarizable CF fluctuations most
efficiently couple with QPs and offer glues for QP pairings particularly in the nodal region.
The pairing with the CF involved may also most efficiently occur in the antinodal region. In
the antinodal region, the Cooper pairs of the QPs and the incoherent pairs of the CFs appear
strongly mixed and it is not meaningful to distinguish them. In this way, the CF pair and QP
pair are mutually transferable as the coherent and incoherent parts of the same pair, and the
CF pair reinforces the QP Cooper pair. Despite the reinforcement, we expect that the QP gap
appears following a conventional $d$-wave symmetry and is still smaller than the CF incoherent
gap.

Spatially inhomogeneous gap has been observed in the STS [34, 43]. Two distinct energy
scales of the gap have also been pointed out in ARPES[8, 42]. Since the pairing mechanism
discussed here has a dual character of coherent and incoherent contributions, respectively from
QPs and CFs, it is tempting to assign the large gap region observed in STS as that arising from
the CF pair presumably trapped near the dopant position thus contributing to an incoherent
and large gap. The large gap in the antinodal region not necessarily correlated with the
superconductivity with the $d$-wave form may also be accounted for by the contribution from the
incoherent CF pairing. The incommensurate charge modulation found in STS[44] may also
represent localized pairs involving CFs or their real-space condensation into the charge order.
8. Concluding Remark

We have discussed recent progress made for the understanding of the pseudogap observed in the cuprate superconductors. The pseudogap phase is identified as the phase with the coexistence of the poles and zeros of the QP Green’s function. This phase is separated from the conventional Fermi liquid by the topological transitions and distinguished by the existence of the zero surface at the Fermi level. The quantum criticality of the topological transitions is described by an unconventional universality class beyond the scheme of Landau, Ginzburg and Wilson. The full s-wave-like gap structure of the pseudogap revealed in the cDMFT and supported by the Raman experiments imposes a severe constraint on the origin of the pseudogap and high-$T_c$ superconductivity as well. The pseudogap as a generic phenomenon of the lightly doped Mott insulator has a consistent interpretation as the hybridization gap of the QP and the excitonic CF. The pairing of the CF solves the dichotomy of the pairing in the antinodal region coexisting with the insulating pseudogap in the same region. Experimental detection of the CF by an appropriate probe is a real challenge, because it is charge neutral. Studies on the unoccupied part of the spectra also provide an experimental challenge. These hidden parts are crucial to understand the pseudogap and the mechanism of the superconductivity in the cuprates. Further detailed studies on the hidden CF physics is a challenging issue for future.

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