Theory of Electron Differentiation, Flat Dispersion and Pseudogap Phenomena

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Abstract

Aspects of electron critical differentiation are clarified in the proximity of the Mott insulator. The flattening of the quasiparticle dispersion appears around momenta $(\pi,0)$ and $(0,\pi)$ on square lattices and determines the criticality of the metal-insulator transition with the suppressed coherence in that momentum region of quasiparticles. Such coherence suppression at the same time causes an instability to the superconducting state if a proper incoherent process is retained. The d-wave pairing interaction is generated from such retained processes without disturbance from the coherent single-particle excitations. Pseudogap phenomena widely observed in the underdoped cuprates are then naturally understood from the mode-mode coupling of d-wave superconducting(dSC) fluctuations with antiferromagnetic ones. When we assume the existence of a strong d-wave pairing force repulsively competing with antiferromagnetic(AFM) fluctuations under the formation of flat and damped single-particle dispersion, we reproduce basic properties of the pseudogap seen in the magnetic resonance, neutron scattering, angle resolved photoemission and tunneling measurements in the cuprates.

KEYWORD: A. Oxides, A. Superconductors, D. Magnetic properties, Metal-insulator transition, High-Tc cuprates

1 Introduction

High-temperature cuprate superconductors show a variety of unusual properties in the normal state \cite{1}. Among others, we discuss two remarkable properties widely observed in the cuprates. One is the flat dispersion in single-particle excitations. Angle resolved photoemission spectra (ARPES) in Y and Bi based high-Tc cuprates show an unusual dispersion which is far from weak correlation picture \cite{2}. The dispersion around $(\pi,0)$ and $(0,\pi)$ is extremely flat beyond the expectations from usual van Hove singularities. The flat dispersion also shows rather strong damping. The other property we discuss is the pseudogap phenomenon observed in the underdoped region. It is observed both in spin and charge excitations in which gap structure emerges from a temperature $T_{PG}$ well above the superconducting transition point $T_c$. The gap structure is observed in various different probes such as NMR relaxation time, the Knight shift, neutron scattering, tunneling, ARPES, specific heat, optical conductivity, and DC resistivity. The ARPES \cite{3, 4} data
have revealed that the pseudogap starts growing first in the region around $(\pi, 0)$ and $(0, \pi)$ from $T = T_{PG}$ much higher than $T_c$. Therefore, the pseudogap appears from the momentum region of the flattened dispersion and it is likely that the mechanism of the pseudogap formation is deeply influenced from the underlying flatness. The superconducting state itself also shows a dominant gap structure in this flat spots, $(\pi, 0)$ and $(0, \pi)$, due to the $d_{x^2-y^2}$ symmetry. In fact, the pseudogap structure above $T_c$ continuously merges into the $d_{x^2-y^2}$ gap below $T_c$. To understand the pairing mechanism and the origin of the high transition temperatures, a detailed understanding of the physics taking place in the flat dispersion region is required.

2 Flat Dispersion

Theoretically, the emergence of the flat dispersion around $(\pi, 0)$ and $(0, \pi)$ has also been reported in numerical simulation results rather universally in models for strongly correlated electrons such as the Hubbard and $t$-$J$ models on square lattices \cite{5}. Furthermore, the emergence of the flat dispersion also leads to various unusual properties. For example, the electronic compressibility critically diverges as $\kappa \propto 1/\delta$ with decreasing doping concentration $\delta$ while the Drude weight is unusually suppressed as $D \propto \delta^2$ \cite{6, 7}. In more comprehensive understanding, the emergence of the flat dispersion is connected with the criticality of the transition from metals to the Mott insulator. All the numerical data are consistent with the hyperscaling relations with a large dynamical exponent $z = 4$ for the metal-insulator transition \cite{1, 8}. Such large exponent opposed to the usual value $z = 2$ for the transition to the band insulator is derived from the slower electron dynamics generated by the flat dispersion. This criticality is interpreted from a strong proximity of the Mott insulator where strong electron correlation generates suppressed dynamics and coherence. The coherence temperature (the effective Fermi temperature) is also scaled as $T_F \propto \delta^2$ and indicates unusual suppression.

In a simple picture, the correlation effects emerge as the isotropic mass renormalization, where the Coulomb repulsion from other electrons makes the effective mass heavier. This effect was first demonstrated by Brinkman and Rice \cite{9} in the Gutzwiller approximation and refined in the dynamical mean field theory \cite{10}. In the numerical results on a square lattice, the correlation effects appear in more subtle way where the electrons at different momenta show different renormalizations. When the Mott insulator is approached and the doping concentration becomes small, the mass renormalization generally becomes stronger. However, once the renormalization effect gets relatively stronger in a part of the Fermi surface, it is further enhanced at that part in a selfconsistent fashion because the slower electrons become more and more sensitive to the correlation effect. This generates critical differentiation of the carriers depending on the portion of the Fermi surface.

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On square lattices, the stronger renormalization happens around \((\pi, 0)\) and \((0, \pi)\). The trigger of this strong correlation effect concentrating near \((\pi, 0)\) and \((0, \pi)\) is intuitively understood from the carrier motion under the background of antiferromagnetic correlations. As we see a real space picture in Fig.1a, the carrier motion in the diagonal direction does not disturb the correlations due to the parallel spin alignment, while the motion in horizontal and vertical directions strongly disturbs the AFM backgrounds and the motion itself is also disturbed as a feedback. Such strong coupling of charge dynamics to spin correlations causes flattening and damping of electrons around \((\pi, 0)\) and \((0, \pi)\), but not around the diagonal direction \((\pm \pi/2, \pm \pi/2)\). The anisotropic renormalization effect eventually generates a singularly flat dispersion on particular region of the Fermi surface, which accepts more and more doped holes in that region due to the enhanced density of states. The transition to the Mott insulator is then governed by that flattened part, since the carriers reside predominantly in the flat region. The criticality of the metal-insulator transition on the square lattice is then determined from the doped carriers around the flat spots, \((\pi, 0)\) and \((0, \pi)\). The hyperscaling relation becomes satisfied because such singular points on the momentum space governs the transition.

We, however, should keep in mind that the relaxation time of quasiparticles and the damping constant of magnetic excitations do not have criticality at the transition point to the Mott insulator. A general remark is that the relaxation time is critical only in the case of the Anderson localization transition and not in the case of the transition to the Mott insulator. The DC transport properties and magnetic relaxation phenomena are contaminated by such noncritical relaxation times \(\tau\) and are influenced by the carriers in the other portion than the flat part because the flat part has stronger damping and less contributes to the DC properties. Large anisotropy of \(\tau\) masks the real criticality and makes it difficult to see the real critical exponents in the \(\tau\)-dependent properties. Relevant quantities to easily estimate the criticality is the \(\tau\) independent quantities such as the Drude weight and the compressibility.

Near the metal-insulator transition, critical electron differentiation and selective renormalization may lead to experimental observations as if internal degrees of freedom of the carriers such as spin and charge were separated because each degrees of freedom can predominantly be conveyed by carriers in different part of the Fermi surface. Another possible effect of the electron differentiation is the appearance of several different relaxation times which are all originally given by a single quasiparticle relaxation in the isotropic Fermi liquids, but now depend on momenta of the quasiparticles.

If the mass renormalization would happen in an isotropic way as in the picture of Brinkman and Rice, the renormalization can become stronger without disturbance when the insulator is approached. However, if the singularly renormalized flat dispersion emerges critically only in a part near the Fermi surface but the whole band width is
ratained, that flattened part has stronger instability due to the coupling to larger energy scale retained in other part of the momentum space. The instability can be mediated by local and incoherent carrier motion generated from two-particle processes derived in the strong coupling expansion [11]. The instability of the flat dispersion was studied by taking account such incoherent terms in the Hubbard and $t$-$J$ models [12, 13, 7]. The inclusion of the two-particle terms drives the instability of the flat part to the superconducting pairing and the formation of the gap structure. The paired bound particles formed from two quasiparticles at the flat spots have different dynamics from the original quasiparticle. In fact, when the paired singlet becomes the dominant carrier, the criticality changes from $z = 4$ to $z = 2$, resulting in the recovery of coherence and kinetic energy gain. It generates a strong pairing interaction from the kinetic origin. This pairing mechanism is a consequence of suppressed single-particle coherence and electron differentiation due to strong correlations.

The instability of the flat dispersion coexisting with relatively large incoherent process was further studied [11, 14, 15, 16]. It has turned out that promotion of the above scaling behavior and the flat dispersion offers a way to control potential instabilities. Even when a flat band dispersion is designed near the Fermi level by controlling lattice geometry and parameters, it enlarges the critical region under the suppression of single-particle coherence in the proximity of the Mott insulator mentioned above. In designed lattices and lattices with tuned lattice parameters, it was reported that the superconducting instability and the formation of the spin gap have been dramatically enhanced [14].

3 Theory of Pseudogap Phenomena

As is mentioned in §1, the pseudogap starts growing from the region of the flat dispersion. When the single-particle coherence is suppressed, the system is subject to two particle instabilities. As clarified in §2, the superconducting instability in fact grows. However, the antiferromagnetic and charge order correlations are in principle also expected to grow from other two-particle (particle-hole) processes and may compete each other. In particular, the antiferromagnetic long-range order is realized in the Mott insulator and its short-range correlation is well retained in the underdoped region. Therefore, to understand how the superconducting phase appears in the underdoped region, at least competition of dSC and AFM correlations have to be treated with underlying suppressed coherence in the region of $(\pi, 0)$ and $(0, \pi)$. The authors have developed a framework to treat the competition by employing the mode-mode coupling theory of dSC and AFM fluctuations where these two fluctuations are treated on an equal footing [17, 18].

It should be noted that the strong dSC pairing interaction is resulted from a highly correlated effect with electron differentiation while critical differentiations have not been
successfully reproduced from the diagrammatic approach so far. Then, within the framework of the mode-mode coupling theory, at the starting point, we have assumed the existence of correlation effects leading to the flattened dispersion and the d-wave pairing force. The AFM and dSC fluctuations are predominantly generated by the contributions from the quasiparticle excitations in the flattened regions $(\pi, 0)$ and $(0, \pi)$. These fluctuations are treated in a set of selfconsistent equations with mode couplings of dSC and AF. From the selfconsistent solution, the pseudogap formation is well reproduced in a region of the parameter space. The pseudogap emerges when the mode coupling between dSC and AFM is repulsive with a severe competition and dSC eventually dominates at low temperatures. Such competition suppresses $T_c$, while above $T_c$ it produces a region where pairing fluctuations are large. This region at $T_{PG} > T > T_c$ shows suppression of $1/T_1 T$ and the pseudogap formation around $(\pi, 0)$ and $(0, \pi)$ in $A(k, \omega)$. These reproduce the basic feature of the pseudogap phenomena experimentally observed in the underdoped cuprates. The pseudogap formation is identified as coming from the preformed pair fluctuations. In Fig.2, we show results obtained for the parameter values of the underdoped cuprates such as Bi2212 with $T_c \approx 83$K. The pseudogap formation in Im$G$ for $k$ close to $(\pi, 0)$ (actually $=(\pi, 3\pi/64)$) is plotted at several choices of temperatures in Fig.2(a). The momentum dependence shows that the pseudogap formation starts around $(\pi, 0)$ from higher temperatures and the formation temperature becomes lower with increasing distance from $(\pi, 0)$ as seen in Fig.2(b). When we see Im$G(k, \omega)$ around $(\pi, 0)$ it shows "fill-in" crossover with increasing temperature where the gap amplitude appears to be retained while the spectral weight inside the gap is gradually filled with the increase in temperature. All of the above reproduce the experimental observations.

We, however, note a richer structure of the gap formation observed in the transversal NMR relaxation time $T_{2G}$ and the neutron resonance peak. One puzzling experimental observation is that the pseudogap structure appears in $1/T_1 T$ [19, 20, 21, 22, 23], while in many cases $1/T_{2G}$, which measures Re$\chi(Q, \omega = 0)$ at $Q = (\pi, \pi)$, continuously increases with the decrease in temperature with no indication of the pseudogap. In addition, the so called resonance peak appears in the neutron scattering experiments [24]. A resonance peak sharply grows at a finite frequency below $T_c$ with some indications even at $T_c < T < T_{PG}$. This peak frequency $\omega^*$ decreases with lowering doping concentration implying a direct and continuous evolution into the AFM Bragg peak in the undoped compounds. The neutron and $T_{2G}$ data support the idea that the AFM fluctuations are suppressed around $\omega = 0$ but transferred to a nonzero frequency below $T_{PG}$.

To understand these features, a detailed consideration on damping of the magnetic excitations is required. With the increase in the pairing correlation length $\xi_d$, the pseudogap in $A(k, \omega)$ is developed. Since the damping is mainly from the overdamped Stoner excitations, the gap formation in $A(k, \omega)$ contributes not only to suppress growth of
AFM correlation length $\xi$ but also to reduce the magnetic damping because, inside the domain of the $d$-wave order, the antiferromagnetic excitations are less scattered due to the absence of low-energy quasiparticle around $(\pi, 0)$. If the quasiparticle damping is originally large around $(\pi, 0)$, the damping $\gamma$ can be reduced dramatically upon the pseudogap formation. Under this circumstance, our calculated result reproduces the resonance peak and the increase in $1/T_2$ with lowering temperature at $T > T_c$ in agreement with the experimental observations in YBa$_2$Cu$_3$O$_{6.63}$, YBa$_2$Cu$_4$O$_8$ and some other underdoped compounds [17, 18].

A subtlety arises when the damping around $(\pi/2, \pi/2)$ starts contributing. This is particularly true under the pseudogap formation. If contributions from the $(\pi/2, \pi/2)$ region would be absent, the damping of the magnetic excitation would be strongly reduced when the pseudogap is formed around $(\pi, 0)$ as we mentioned above. However, under the pseudogap formation, the damping can be determined by the Stoner continuum generated from the $(\pi/2, \pi/2)$ region and can remain overdamped. This process is in fact important if the quasiparticle damping around the $(\pi/2, \pi/2)$ region is large as in the case of La 214 compounds [25]. The formation of the pseudogap itself is a rather universal consequence of the strong coupling superconductors. However, the actual behavior may depend on this damping. If the damping generated by the $(\pi/2, \pi/2)$ region is large, it sensitively destroys the resonance peak structure observed in the neutron scattering experimental results.

4 Summary and Discussion

Electron critical differentiation is a typical property of the proximity of the Mott insulator. The flattening of the quasiparticle dispersion appears around momenta $(\pi, 0)$ and $(0, \pi)$ on square lattices and determines the criticality of the metal-insulator transition with the suppressed coherence in that momentum region of quasiparticles. Such coherence suppression at the same time causes an instability to the superconducting state if a proper incoherent process is retained. The $d$-wave pairing interaction is generated from such retained microscopic process in the strong coupling expansion without disturbance from the coherent single-particle excitations. By assuming the $d$-wave attractive channel and the presence of strongly renormalized flat quasi-particle dispersion around the $(\pi, 0)$ region, we have considered the mode-mode coupling theory for the AFM and $d$SC fluctuations. The pseudogap in the high-$T_c$ cuprates is reproduced as the region with enhanced $d$SC correlations and is consistently explained from precursor effects for the superconductivity. The existence of the flat region plays a role to suppress the effective Fermi temperature $E_F$. This suppressed $E_F$ and relatively large pairing interaction both drive the system to the strong coupling region thereby leads to the pseudogap formation. The pseudogap formation is also enhanced by the AFM fluctuations repulsively coupled
with dSC fluctuations.

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Figure 1: Intuitive picture to understand anisotropic renormalization effects. An electron moving in diagonal directions under the AFM correlations are not severely renormalized as in (a) while they are for horizontal or vertical directions as in (b). In (b), frustrations are generated after the hole motion (denoted by circles) as shown by wavy bonds. These differences induce the differentiation between electrons around ($\pi$, 0) and ($\pi/2$, $\pi/2$).
Figure 2: Temperature dependence of (a) the imaginary part of the Green’s function for $k_F = (\pi, 3\pi/64)$ and (b) the leading-edge mid-point shift for several choices of momenta. In (a), the momentum point is on the Fermi surface and the closest to $(\pi, 0)$ in our calculation. Temperatures in the plotted data are 0.069, 0.06, 0.051, and 0.042 from the data with larger intensity at $\omega = 0$. In (b), the positive shifts indicate the pseudogap formation. The symbols represent the shifts at the momenta shown in the inset. The energies and temperatures are all scaled by the electron transfer amplitude ($t \sim 0.25$ eV) and the superconducting transition is signaled around $T \sim 0.02$. 