Origin of the pseudogap and its influence on superconducting state

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When holes move in the background of strong antiferromagnetic correlation, two spatial scales emerge which lead to a much reduced hopping integral with an additional phase factor. By taking these two effects into consideration, we propose an effective Hamiltonian to investigate pseudogap in cuprates. We argue that pseudogap is the consequence of dressed hole moving in the antiferromagnetic background and has nothing to do with the superconductivity. In the normal state, the pseudogap opens near the antinodal region and vanishes around the nodal region. In the superconducting state, the d-wave superconducting gap dominates the nodal region, while the pseudogap dominates the antinodal region. A two-gap scenario is concluded to describe the relation between the two gaps.

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I. INTRODUCTION

One of the most fascinating properties of the cuprates is the opening of a gap (pseudogap) above $T_c$ in the underdoped and optimally doped regime, where most abnormalities observed. The origin of the pseudogap and its relation to the superconducting (SC) gap are fundamental questions to realize the physics underlying the high-temperature superconductors. Although much progress has been made, the issue remains open. There are two distinct scenarios on the relation between the pseudogap and the SC gap:\textsuperscript{1} 1) The one-gap scenario: The pseudogap is viewed as the precursor of the SC gap, reflecting pair fluctuation above $T_c$, and would acquire phase coherence below $T_c$. The argument was based on angle-resolved photoemission spectroscopy (ARPES),\textsuperscript{2–4} electron tunnelling,\textsuperscript{5} and thermal transport measurements,\textsuperscript{6–8} etc. 2) The two-gap scenario: The pseudogap is not directly related to the SC gap, but emerge from some ordered states such as antiferromagnetic (AF),\textsuperscript{9–11} staggered flux,\textsuperscript{12} stripe,\textsuperscript{13} spin or charge density wave,\textsuperscript{14} and orbital circulating current,\textsuperscript{15} etc. and competes with SC gap. Models account for these ordered states capture some aspects of the pseudogap, but a theoretical framework which gives a full picture from the pseudogap to SC state is not yet established. Nevertheless, many experiments, including ARPES,\textsuperscript{16,17} electronic Raman scattering,\textsuperscript{18} and elastic neutron diffraction,\textsuperscript{19} etc. seem to favor the two-gap scenario. More recently, the improved ARPES data\textsuperscript{20–22} showed that the gap opens near the antinodal region, and vanishes near the nodal region in the pseudogap state, which leads to the arc structure of the Fermi surface. In the SC state, the pseudogap dominates the antinodal region, while the simple d-wave type gap dominates the nodal region.

In this Letter, an effective single particle Hamiltonian is proposed to study the pseudogap. The main idea came from the well known fact that moving holes in the antiferromagnetic background leads to two spatial scales: a long distance one and a short distance one. On the large spatial scale, the effective hopping integral is much reduced due to accumulated strong AF correlation, while on the small spatial scale, the moving holes obtain an additional phase factor due to the surrounding AF correlation. Thus, pseudogap came directly from the AF correlation and is irrelevant to the superconductivity. Based on the effective Hamiltonian, we find that the pseudogap opens near the antinodal regime and vanishes around the nodal region. Its doping and momentum dependence qualitatively agree with recent ARPES measurements. The arc structure of the Fermi surface is also obtained, with its length expanding from underdoping to overdoping. In the SC state, the simple d-wave SC gap dominates the node region, while the pseudogap dominates the antinodal region. The resultant gap also agrees well with experiments.

The neutron scattering\textsuperscript{11} and quantum oscillations measurements\textsuperscript{22} show that in the underdoped region, antiferromagnetic correlation remains on the CuO$_2$ plane. Its existence has also been found numerically.\textsuperscript{22} For each spin, its four nearest neighbors compose a plaquette. As a hole is introduced into the center of this plaquette, it will sense an effective magnetic field originated from its four neighboring opposite spins. Correspondingly, there is a doping dependent gauge flux $\Phi$ passing through the plaquette. In its journey of wanderings, the hole is affected by the staggered flux filed in which $\Phi$ and $-\Phi$ appear alternatively. Therefore, in the small spatial scale, when the hole hops, it encounters a phase shift $\delta/4$ (or $-\delta/4$) via Aharonov-Bohm effect, where $\delta = 2\pi\Phi/\Phi_0$ ($\Phi_0 = \hbar c/e$ is the flux quanta). On the other hand, in the large spatial scale, the effective hopping, represented
by the hopping matrix $I_n = \langle c_i^+ c_j + c_i^+ c_j \rangle_n (n = 1, 2, \text{ and } 3$ for the nearest, second nearest, and third nearest neighbor respectively), evaluated by all possible configurations, is substantially reduced by the strong AF correlation. Take the $t - J$ model as an example, we derive the following effective single particle Hamiltonian by considering the effects of two spatial scales as,

$$H = \sum_{k \sigma} \left( \gamma_k d_{k \sigma}^+ d_{k \sigma} + \text{h.c.} \right) + \sum_{k \sigma} \epsilon_k \left( d_{k \sigma}^+ d_{k \sigma} + c_{k \sigma}^+ c_{k \sigma} \right)$$

where $\gamma_k = -2(I_1 + J'\chi_0) \cos k_x + \epsilon_{k_x} - \epsilon_{k_y} \cos k_y$, and $\epsilon_k = -4J \cos k_x \cos k_y - 2\epsilon_0 (\cos 2k_x + \cos 2k_y) - \mu$. $\chi_0 = \sum_{q \sigma} \langle d_{q \sigma}^+ d_{q \sigma} + c_{q \sigma}^+ c_{q \sigma} \rangle$ is the uniform bond order, $J' = 3J/8$. The summation is restricted in the AF Brillouin zone. The effective Hamiltonian is diagonalized with the quasiparticle band shown in Fig. 1 is rather rigid against doping along the nodal line with much reduced bandwidth $0.6 - 0.7$ meV, well consistent with the ARPES measurements. The upper and lower band coincide at $(\pi/2, \pi/2)$. This means that no full gap opens, unlike the Mott insulator state. On the other hand, the lower band around $(\pi, 0)$ shows clear flatness below $E_F$. Correspondingly, a pseudogap (denoted by $\Delta_{PC}$) opens around the antinodal regime. The distance between the flatness part and Fermi level decreases with increasing doping. The results obtained here qualitatively coincide with the ARPES data. It should be noted that as far as the QP dispersion is concerned, even the effective single particle Hamiltonian (Eq. (1)) has already succeeded to describe the main features mentioned above shown in the insert of Fig. 1.

Fig. 2 shows the evolution of the pseudogap in the momentum space at different doping density. The magnitude of pseudogap is determined by evaluating the minimal distance of the lower band from Fermi energy in the given direction. $\Delta_{PC}(\theta)$ decreases with increasing $\theta$, and disappears at a critical value of $\theta$. This can be easily realized from Fig. 1 where the gap opens near the antinodal regime due to the flatness of QP dispersion induced by the staggered magnetic flux, while the gap closes due to the crossing of the QP dispersion over $E_F$. Such behavior had been confirmed by various experiments.

Both the pseudogap region and its magnitude decrease with doping as evidenced by ARPES data. The largest $\Delta_{PC}$ decreases from about 92 meV at deep underdoped region to about 40 meV at optimal doping with almost linear doping dependence. The numerical results consistent with ARPES measurement, but the range of angle

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**TABLE I:** The ED results of the spin-spin correlation function and hopping matrix in the 20-site cluster with different hole concentration.

| $n_h$ | $\langle S_i \cdot S_j \rangle$ | $I_1$ | $I_2$ | $I_3$ |
|-------|-------------------------------|-------|-------|-------|
| 0     | 0                             | 0     | 0     | 0     |
| 1     | -0.2745                       | 0.0703| -0.0297| 0.0125|
| 2     | -0.2179                       | 0.1483| -0.0350| 0.0355|
| 3     | -0.1670                       | 0.2116| -0.0469| 0.0510|
| 4     | -0.1399                       | 0.2635| -0.0594| 0.0732|
| 5     | -0.0855                       | 0.3126| -0.0709| 0.0960|

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The contribution of additional phase factor in Eq. (1), the partial spin fluctuation has been taken into account for body effect. The effective hopping terms are all enhanced due to many $t$ terms, which is taken as energy unit, is also evaluated by the ED technique. The spectral function is obtained via $\hat{G}(k, i\omega) = \sum_{q, \omega} G(k, \omega) G(k, \omega)$, where $J = J_0 (\cos q_x + \cos q_y), \omega_n = \omega_m$ and $\omega_m$ are the fermionic and bosonic Matsubara frequency. Both the Green's function and self-energy are $2 \times 2$ matrices. The spectral function is obtained via $A(k, \omega) = -(1/\eta) \text{Im} G(k, \omega + i\delta)$. The quasiparticle band shown in Fig. 1 is rather rigid against doping along the nodal line with much reduced bandwidth $0.6 - 0.7(\sim 240-280\text{meV})$, well consistent with the ARPES measurement. The upper and lower band coincide at $(\pi/2, \pi/2)$. This means that no full gap opens, unlike the Mott insulator state. On the other hand, the lower band around $(\pi, 0)$ shows clear flatness below $E_F$. Correspondingly, a pseudogap (denoted by $\Delta_{PC}$) opens around the antinodal regime. The distance between the flatness part and Fermi level decreases with increasing doping. The results obtained here qualitatively coincide with the ARPES data. It should be noted that as far as the QP dispersion is concerned, even the effective single particle Hamiltonian (Eq. (1)) has already succeeded to describe the main features mentioned above shown in the insert of Fig. 1. Fig. 2 shows the evolution of the pseudogap in the momentum space at different doping density. The magnitude of pseudogap is determined by evaluating the minimal distance of the lower band from Fermi energy in the given direction. $\Delta_{PC}(\theta)$ decreases with increasing $\theta$, and disappears at a critical value of $\theta$. This can be easily realized from Fig. 1 where the gap opens near the antinodal regime due to the flatness of QP dispersion induced by the staggered magnetic flux, while the gap closes due to the crossing of the QP dispersion over $E_F$. Such behavior had been confirmed by various experiments. Both the pseudogap region and its magnitude decrease with doping as evidenced by ARPES data. The largest $\Delta_{PC}$ decreases from about 92 meV at deep underdoped region to about 40 meV at optimal doping with almost linear doping dependence. The numerical results consistent with ARPES measurement, but the range of angle
seem to have about 10% reduction. Results obtained by direct diagonalizing the Eq. (1) show similar doping and momentum dependence. However, the magnitude and the variation range of angle are more reduced. Comparing with the experiments, the present pseudogap vanishes somewhat slower with increasing $\theta$. In fact, the value of angle $\theta_0(\Delta_PG(\theta) = 0)$ is intimately related to the AF correlation in momentum space, large $\theta_0$ means smaller AF correlation. This implies that the present treatment is more appropriate to describe situations with strong AF correlation. In the present treatments, we do not adopt any pairing potential, which is distinct from the previous slave-boson calculation. Furthermore, the behavior of pseudogap differs from the early ARPES discovery, and is far from that of the simple d-wave gap. Therefore, the pseudogap is not related to the SC pairing. Our theoretical results imply that the pseudogap exists even in the overdoped range.

The evolution of the Fermi surface (FS) is depicted in Fig. 3. The intensity is strong near the nodal region, and becomes weak gradually toward antinode due to the opening of the pseudogap in this region. Thus, an arc FS structure forms around the nodal region. Its length expands with increasing hole concentration. The arc extends to a large hole FS above $x = 0.20$, where the pseudogap vanishes gradually. So, the arc structure is a direct consequence of the pseudogap. The evolution of the arc structure and its length also qualitatively agree with the recent ARPES experiment.

Now we discuss the existence and influence of pseudogap in the SC state. Based on experimental observations and above analysis, we start with the assumption that the total gap of the quasiparticle dispersion contains two components: the pseudogap, and the SC gap of the standard d-wave BCS form $\Delta_{P}(k, i\omega) = \Delta_{P}(0, 0) e^{-\gamma k}$. After some manipulations, the corresponding Green’s function is $\hat{G}(k, i\omega) = \hat{G}(k, i\omega) - \hat{G}(k, -i\omega))^{-1}$, where $\hat{G}(k, i\omega)$ contains pseudogap $\Delta_PG(0)$, is the diagonal Green’s function in the pseudogap state under RPA treatment.

We then compare our results with the experiments to see if $\Delta_{P}(0)/\Delta_{SC} << 1$ (one-gap scenario) or it is substantial (two-gap scenario). We take the $x = 0.15$ case, which is near the optimal doping, as an example. In the nodal region, the gap increases almost linearly with decreasing angle $\theta$ as shown in Fig. 3. This is the typical d-wave behavior, showing that d-wave SC pairing dominates this region. In fact, the gap comes from the SC condensation entirely because the pseudogap vanishes along the arc. In the antinodal region, large deviation from the standard d-wave is rather obvious. The shape and the value

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**FIG. 1:** Lower band QP dispersion for different hole concentration under RPA treatments. Insert is the results obtained by direct diagonalizing the Eq. (1).

**FIG. 2:** Pseudogap as functions of angle $\theta$ for different doping. Solid lines, and open squares correspond to results with and without RPA treatment, respectively. Insert shows the experimental data on Bi2212 obtained from Ref. 15, squares, circles, and triangles are for UD75K, UD92K, and OD86K, roughly corresponding to underdoped ($x=0.1$), optimal doped ($x=0.15$), and overdoped ($x=0.2$) case. The dotted line are roughly corresponding to underdoped ($x=0.1$), optimal doped ($x=0.15$), and overdoped ($x=0.2$) case. The dotted line are guided for eyes.

**FIG. 3:** Density plots for integration of spectral intensity times Fermi function over an energy interval $[-0.025, 0.025]t$ around the Fermi energy for different doping density.
of the gap in the SC state with small value of $\Delta_{SC}$ are quite similar to that of the pseudogap state. Even one increases $\Delta_{SC}$ up to 0.06 such that $2\Delta_{SC} > \Delta_{PG}(0)$, the shape keeps unchanged and the value of the gap enhances little. Therefore, the pseudogap dominates the antinodal region. Between the two regions, the pseudogap and the SC gap coexist and compete with each other, so the deviation from the simple d-wave enhances gradually when approaching to the antinodal region. These features consist well with recent experiments on the optimal doped Bi2212$^{18}$, Bi2201$^{19}$, and LSCO$^{20}$, as shown in the inset of Fig. 4.

The degree of the deviation depends on the ratio of $\Delta_{SC}/\Delta_{PG}(0)$. Smaller ratio means larger deviation. Such effect has been manifested in optimal doped Bi2201$^{15}$ and Bi2212$^{22}$. The pseudogap in the two cuprates is almost the same at optimal doping, but the SC critical temperature in the former is three times of the latter. Correspondingly, the deviation from the simple d-wave is much enhanced in Bi2201. The enhancement of the deviation with decreasing doping can also be explained following this way. Such deviation had also been obtained in the previous one-gap scenario by applying the spin fluctuation theory$^{22}$. However, the correction was too small to account for the large deviation in underdoped Bi2201 and Bi2212. Based on our analysis, the two-gap scenario seems more appropriate to account for the observed gap behavior. The experiments support the one-gap scenario, mostly came from the earlier measurements$^{24}$. The data near the nodes were not easy to distinguish at that time. Additionally, some measurements, such as the thermal transport properties$^{25}$ may concern mainly on the nodal region, where the simple d-wave SC gap dominates. At last, we would like to point out that the enhancement of the SC gap with doping in the underdoped cuprates is an outcome of the decreasing pseudogap, which leads to the suppression of the density of state near the Fermi energy.

In conclusion, we have proposed an effective single particle Hamiltonian extracted from the exact diagonalization studies of the $t-J$ model to investigate pseudogap in the high-Tc cuprates. The main idea is to take the effects of two spatial scales, one leads to much reduced hopping and one adds to a phase factor, both reflect physics of doped holes moving in AF background, into account. Our results revealed that the pseudogap is the single particle property, and is not directly related to the SC state. It opens near the antinodal region and vanishes around nodal region. The doping and momentum dependence of the pseudogap are qualitatively consistent with recent ARPES measurements. The arc shape of the Fermi surface is a natural product of the pseudogap. In the SC state, the simple d-wave SC gap dominates the nodal region, while the pseudogap dominates the antinodal region. The two-gap scenario is therefore concluded.

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