Fermi Surface Evolution, Pseudo Gap and Stagger Gauge Field Fluctuation in Underdoped Cuprates

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In the context of t-J model we show that in underdoped regime, beside the usual long wave length gauge field fluctuation, an additional low energy fluctuation, staggered gauge field fluctuation plays a crucial role in the evolution of Fermi surface (FS) as well as the line shape of spectral function for the cuprates. By including the staggered gauge field fluctuation we calculate the spectral function of the electrons by RPA (random phase approximation). The line shape of the spectral function near \((\pi, 0)\) is very broad in underdoped case and is quite sharp in overdoped case. For the spectral function near \((0.5\pi, 0.5\pi)\), the quasiparticle peaks are always very sharp in both underdoped and overdoped case. The temperature dependence of the spectral function is also discussed in our present calculation. These results fit well with the recent ARPES experiments. We also calculate the FS crossover from a small four segment like FS to a large continuous FS. The pseudo gap extracted from the ARPES data can be also interpreted by the calculation.

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The electronic structure of doped cuprates has been a challenge problem in condensed matter physics \([1]\). Recently, angle resolved photoemission spectra (ARPES) experiments have been done with both underdoped and overdoped samples \([2,3]\). In normal state the results show that for underdoped samples the FS only exists on a small segment near \((\pi/2, \pi/2)\) \([4,5]\). Away from this “Fermi Surface” segment the line shape of the spectra is very broad which makes the quasi particle peaks hard to detect. Also a gap which is called normal state gap (or pseudo gap) opens there, and will be closed above a critical temperature \(T^∗\) \([6,7]\). But for overdoped samples the FS forms a closed curve centered at \((\pi, \pi)\) and the quasi particle peaks are quite clear in all directions around the FS. The difference in ARPES line shape between the overdoped and underdoped samples attracts more research interests recently \([8,9,10,11]\).

The ARPES results could be explained by several approaches. In the nearly anti-ferromagnetic fermi liquid (NAFL) theory \([11]\), the anomalous features of the ARPES in underdoped case can be attributed to short range anti-ferromagnetic fluctuation on a special kind of FS \([11]\). The whole FS is divided into two regimes \([11]\) which are called hot particle regime and cold particle regime respectively. The hot particle regime which can be connected by wave vector \((\pi, \pi)\) feels the anti-ferromagnetic fluctuation strongly. It bears the pseudo gap and makes the line shape of the spectral function much broader. And the cold particle regime can not be connected by the wave vector \((\pi, \pi)\), so the quasiparticles there only weakly feel the anti-ferromagnetic fluctuation and the corresponding line shape is much sharper. Recently Chubukov et al. have calculated the FS crossover by varying the coupling constant from small to large \([12]\). The small FS appears in strong coupling case which can be understood as for the underdoped regime and the large FS is corresponding to weak coupling limit as for the overdoped regime. We will compare their results with ours later.

Another theory which may explain the pseudo gap behavior and FS evolution is the charge-spin separation scenario. In slave boson approach, the physical electron is the combination of the slave boson and pseudo Fermion. The U(1) mean field theory for the t-J model has been considered by many authors \([13,14]\) using the slave boson approach. The pseudo gap behavior can be attributed either to d-wave pairing state or staggered flux state. But if the U(1) gauge field fluctuation is considered, the d-wave pairing state loses its stability \([16]\). While for staggered flux phase, the missing of translation symmetry and time reverse symmetry has been considered as a sort of shortcoming \([15]\). In order to improve the above defects of the U(1) mean field theory, P.A.Lee and X.G.Wen proposed the SU(2) mean field approach for the t-J model \([17]\). In their approach, the SU(2) symmetry is preserved away from half filling by introducing two kinds of slave bosons. A segment like FS is obtained by their SU(2) mean field theory.

Inspired by the SU(2) mean field theory and our previous study \([18]\), we find that the staggered flux phase is energetically favorable in low doping regime. So the fluctuation of staggered flux may be important in underdoped regime, even if there is no symmetry breaking for the staggered flux due to the large quantum fluctuation in 2D. In order to explore this effect, we introduce a fluctuating U(1) staggered gauge field. The time reversal and translational symmetry get survived because there is no mean field value of staggered flux. The half pocket like FS is obtained in underdoped regime in which the staggered gauge fluctuation is strong. With the increment of doping concentration the staggered gauge fluctuation will be suppressed subsequently and meanwhile the FS evolves...
into a large one. We also calculate the spectral functions of physical electrons with the staggered gauge fluctuation being incorporated. The calculated line-shapes as well as the interpretation for the pseudo-gap are in good agreement with the ARPES data.

Follow Lee and Nagaoa [20], the effective Lagrangian including the phase fluctuation for the uniform RVB state can be written as:

\[
\mathcal{L} = \sum_{i\sigma} f^+_i \left[ \frac{\partial}{\partial \tau} - \mu_F + i\lambda(r_i) \right] f_i + \sum_i b_i^+ \left[ \frac{\partial}{\partial \tau} - \mu_B + i\lambda(r_i) \right] b_i
\]

\[ - J' \chi_0 \sum_{i,r,\sigma} e^{i \theta_{r,i}} f_i^+ f_{i+r,\sigma} - t \chi_0 \sum_{i,r,\sigma} e^{i \theta_{r,i}} b_i^+ b_{i+r,\sigma} + \text{h.c.} \]

In the above equation, \( J' = \frac{2}{3} J \) [14], the label "r" represents the two directions in 2D plane and \( \chi_0 \) represents the two corresponding unit vectors. Then the three fields \( (\lambda_i, \theta_{1,i}, \theta_{2,i}) \) can be viewed as the three components of the U(1) lattice gauge field in 2D. The above Lagrangian is invariant under the local U(1) gauge transformation.

In Lee and Nagaoa’s approach [20], only the long wave length part of the U(1) gauge field is considered. So they treated the above lattice gauge field Hamiltonian in the long wave length limit and abandoned the short wave length part gauge field. Their treatment is understood to be valid only in the optimal doping case. In underdoped case there exists another low energy fluctuation which is the U(1) gauge field fluctuation near \((\pi, \pi)\). This kind of low energy fluctuation reflects the instability of staggered flux phase in very low doping area. With the increasing of doping, the U(1) gauge field fluctuation near \((\pi, \pi)\) loses its spectral weight rapidly as shown in Fig.5. Finally at optimal doping case this kind of fluctuation becomes unimportant and can be ignore reasonably as in Lee and Nagaoa’s paper [20]. In order to include this kind of fluctuation, we must consider the long wave length expansion of the gauge field near both \((0,0)\) and \((\pi, \pi)\). In real space, the low energy modes of the gauge field should include two low energy components, one is the uniform component and the other is the staggered component.

We have \( \theta_{r,i} = A_i(\vec{R}_i) + B_i(\vec{R}_i)(-1)^{ix+y+i} \) with \( r = 1, 2\), and \( \lambda_i = A_0(\vec{R}_i) + B_0(\vec{R}_i)(-1)^{ix+y+i} \).

Now a U(1) gauge transformation contains both uniform part and staggered part: \( \phi = \phi_a(\vec{R}_i) + \phi_b(\vec{R}_i)(-1)^{ix+y+i} \). The uniform part of the gauge field is transformed as the usual way: \( A_i(\vec{R}) \rightarrow A_i(\vec{R}) + \partial_{\vec{R}_i} \phi_a(\vec{R}) \) with \( r = 0, 1, 2 \). And the stagger part of the gauge field is transformed as: \( B_0(\vec{R}_{mn}) \rightarrow B_0(\vec{R}_{mn}) + \partial_{\vec{R}_i} \phi_b, B_r(\vec{R}) \rightarrow B_r(\vec{R}) - 2\phi_b(\vec{R}) \) in which \( r = 1, 2 \).

To treat the gauge fluctuation perturbatively, we should expand the eq.(1) in \( \theta_{r,i} \) to the second order. For reason of exploring the essential physics of the staggered gauge fluctuation, in this paper, we consider only the effect of staggered gauge field fluctuation. But we will discuss the effect of uniform gauge field fluctuation whenever necessary. We choose the gauge fixing condition for the staggered gauge field as \( B_1(\vec{r}) + B_2(\vec{r}) = 0 \). Then in k-space the Lagrangian with the staggered gauge field fluctuation incorporated can be written as

\[
H = \sum_{k,\sigma} (\epsilon_k - \mu_F) f^+_k f_k + \sum_k \frac{t}{J} (\epsilon_k - \mu_B) b^+_k b_k
\]

\[ + \sum_{k,\sigma} g(k, q) f^+_k f_{k+q} \phi_{k,\sigma} + \sum_{k,\sigma} \frac{t}{J} g(k, q) b^+_k b_{k+q} \phi_{k,\sigma}
\]

\[ + \sum_{q, q', k, \sigma} \frac{t}{J} \gamma(k, q, q') b^+_k b_{k+q+q'} \phi_{k,\sigma} \phi_{q,\sigma} \phi_{q',\sigma}
\]

(2)

with \( \varphi = B_1 = -B_2, \epsilon_k = 2J(1) \chi_0(\cos k_x + \cos k_y), g(k, q) = \frac{t}{J} \chi_0 \left[ e^{-i\gamma} - e^{-i\gamma'} \right] \), \( Q = (\pi, \pi) \) and \( \gamma(k, q, q') = \frac{1}{\pi} \left[ -e^{-i\gamma} + e^{-i\gamma'} \right] \).

Using eq.(2), we calculate the electronic spectral function in RPA. First we obtain the effective propagator of staggered gauge field. The staggered gauge field propagator is given by: \(-D^{-1}(q, \omega_n) = \Pi_f(q, \omega_n) + \Pi_s(q, \omega_n) + \Xi_{f/s}(q, \omega_n)\), in which \( \Pi_f(q, \omega_n) \) and \( \Pi_s(q, \omega_n) \) are corresponding to the bubbles of spinons and holons \( (\text{Fig.1(a)} \text{ and Fig.1(b)}) \) respectively. And \( \Xi_{f/s}(q, \omega_n) \) are corresponding to Fig.1(c) and Fig.1(d). The dressed propagator of spinon and holon are calculated by considering the lowest order self energy corrections as shown in Fig.1(e) and Fig.1(f). Finally we obtain the physical electronic Green’s function by calculating the convolution of spinon and holon’s Green functions \( I_{13, 20} \).

The spectral weight of the staggered gauge field fluctuation at \( \vec{q} = (0,0) \) of different doping concentration are shown in Fig.2. With the increasing of doping the staggered gauge field fluctuation loses its spectral weight rapidly and becomes unimportant when \( \delta > 0.15 \).

We have calculated the electronic spectral functions for doping concentration \( \delta = 0.09 \) and 0.2 which represent the underdoped and overdoped case respectively. We choose the parameters as \( t/J = 3 \) and temperature as \( T = 0.19J \) in our calculation. For \( \delta = 0.09 \) which is shown in Fig.3(a), due to the strong staggered gauge field fluctuation the line shape of the spectral function is very
broad and the pseudo gap feature (suppressing the DOS near the Fermi level) is very clear near $(\pi, 0)$. But for the states near the diagonal line, the line shape is quite sharp and the quasi particle peaks are well defined here. This is in good agreement with the recent ARPES studies for underdoped samples [2,3]. In our present study and decrease when $\vec{k}$ is moved toward $(\pi/2,\pi/2)$. The spectral functions of $\vec{k} = (\pi, 0)$ and $\vec{k} = (0.9\pi, 0.15\pi)$ in two different temperature are shown in Fig.4. When

![Diagram](image1)

**FIG. 1.** The Feynman diagram considered in our RPA calculation. Solid line: spinon Green’s function. Dashed line: holon Green’s function. Wagged line: staggered gauge field Green’s function.

![Graph](image2)

**FIG. 2.** The spectral weight of stagger gauge field at $k = (0,0)$ as a function of doping concentration.

![Graph](image3)

**FIG. 3.** The spectral function of physical electrons for both underdoped(a) and overdoped case(b).

the large difference of the line shape in these two regimes are ascribed to the strong $k$ dependent coupling constant $g(k,q)$. So unlike the AF fluctuation approach, our results are not sensitive to the shape of zeroth order FS without considering the staggered gauge field fluctuation. Therefore the essential physics of our interpretation should be generic. The temperature dependence of the spectral function is also obtained by our RPA calculation. The pseudo-gap depression is only exist below a critical temperature $T_{cg}(k)$ which strongly depends on the wave vector $\vec{k}$. The $T_{cg}$ is very high at $\vec{k} = (\pi, 0)$, the temperature is raised the pseudo-gap depression is absent for $\vec{k} = (0.9\pi,0.15\pi)$ (dashed line in Fig.4(b)) but is still present for $\vec{k} = (\pi,0)$ (dashed line in Fig.4(b)). These results are also in good agreement with ARPES experiments [4,5].

In Fig.3(b) we give the results in overdoped case. In this case, the staggered gauge field fluctuation is unimportant here and it does not change the spectral function of Lee and Nagaosa’s. So the quasi particle peak survives near $(\pi,0)$, but the width of the peak is much broader than the quasi particle peaks near $(\pi/2, \pi/2)$. The effect of the uniform gauge field fluctuation will give an additional width in both the two regime, but the effect of the uniform gauge field is nearly isotropic and it will not change our result qualitatively.

Since we can determine the electronic FS by searching for the quasi particle peaks moving across the Fermi level [4], a continuous crossover from small segment like FS to large FS is obtained by our calculation. Our results are shown in Fig.5. In low doping region, the strong staggered gauge field fluctuation smears the quasi particle peaks dramatically near $(\pi,0)$, so we can’t find any quasi particle peaks move across Fermi level in this regime. And in the other limit, along the direction from $(0,0)$ to $(\pi,\pi)$ the effect of staggered gauge field fluctuation is quite small, then the quasi particle peaks and the FS can be detected here. Between the above two limits there exist a critical point, the FS is present at one side and is absent in the other side. With the increment of doping concentration, this critical point moves toward $(\pi,0)$. The FS segment becomes larger and larger and finally the large FS restores at the optimal doping which is 15% in our present study. We can compare our approach with what is used in [12] by Chubukov and it et al. In general the two approaches are quite similar. The FS crossover in both approaches is caused by interacting with a bosonic fluctuation which is strongly enhanced near the momentum $(\pi,\pi)$. Therefore in our approach, the staggered gauge field fluctuation plays a similar role with the AF fluctuation in [12]. But also there exist subtle difference between them. In their approach, the cou-
pling constant is nearly isotropic and the pocket like FS is obtained only when the next nearest hopping term is included in the original Hamiltonian. But in our approach, the coupling constant $g(k, q)$ is strongly anisotropic. This cause a very large interaction with the staggered gauge field near $(\pi, 0)$ and a quite small interaction along the diagonal line. So in our study, the unclosed pocket like FS is caused by the strongly anisotropic coupling constant.

As shown in Fig.3(a) the pseudo gap feature is also very clear in the electronic spectral function near $(\pi, 0)$ in underdoped regime. We can also calculate the density of states(DOS) of the electrons by calculating the summation of the spectral function in k space as $\rho(\omega) = \sum_k A(k, \omega)$. The results are shown in Fig.6(a) for $\delta = 6\%$(solid line),$\delta = 9\%$ (dashed line) and $\delta = 15\%$(dotted line). The suppression of DOS near Fermi level is clear for $\delta = 6\%$ and is absent for $\delta = 15\%$. This may give an explanation for the pseudo gap behavior in underdoped regime. The temperature dependence of the DOS is also calculated and the results for $\delta = 10\%$ are shown in Fig.6(b). One can easily find that the pseudo gap is formed with the decrease of the temperature.

In U(1) mean field theory, the pseudo gap phase is ascribed to either d-wave pairing state or staggered flux state. The d-wave pairing state only gives four Fermi point and is known to be unstable against the gauge field fluctuation \cite{10}. The state which is stable should have ‘segment’ like but not ‘point’ like FS. In the present paper, we proposed a possible description for the pseudo gap phase in underdoped regime. We only include the strong fluctuation of staggered flux and do not need the symmetry broken staggered flux which breaks the translation symmetry and time reverse symmetry. We hope this will give a more reasonable explanation for the pseudo gap behavior in underdoped regime.

Very recently a phenomenological form of self energy which emphasizes the d-wave pairing fluctuation \cite{11} is proposed by M.R.Norman et al \cite{7} to fit the ARPES experiments. The different behavior in the regime near $(\pi, 0)$ and $(\pi/2, \pi/2)$ is ascribed to the symmetry of d-wave pairing. As hinted by the SU(2) approach of Lee and Wen, or SO(5) theory of Zhang, these two kinds of fluctuation may be accommodated together guided by certain underlying subtle physics.

It is rather encouraging that our simple approach fits various kinds of ARPES data with reasonable magnitude but without phenomenological parameters. We expect it catches certain essential physics of the pseudo-gap in the underdoped regime.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5}
\caption{The FS evolution with the increment of doping concentration.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig6}
\caption{(a) The density of state(DOS) of physical electrons with different doping concentration. (b) The density of state(DOS) of physical electrons with different temperature.
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