A link between the spin fluctuation and Fermi surface in high $T_c$ cuprates
— A consistent description within the single-band Hubbard model

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A link between the spin fluctuation and the “fermiology” is explored for the single-band Hubbard model within the fluctuation exchange (FLEX) approximation. We show that the experimentally observed peak position of the spin structure in the high $T_c$ cuprates can be understood from the model that reproduces the experimentally observed Fermi surface. In particular, both the variation of the incommensurability of the peak in the spin structure and the evolution of the Fermi surface with hole doping in La$_{2-x}$Sr$_x$CuO$_4$ may be understood with a second nearest neighbor hopping decreasing with hole doping.

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In the physics of high $T_c$ cuprates, it is of great importance to investigate how the states dominated by the electron-electron interaction are affected by the band structure and the band filling. This is especially so for the spin fluctuation, which has been recognized as one of the central normal state properties. So it is an important challenge to look into the link between the spin fluctuation and the “fermiology”.

The doping dependence of the spin fluctuation in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) has been well established from neutron scattering experiments, where incommensurate spin structures appear when holes are doped. $^{[4]}$ It has also been shown that such an incommensurate spin structure can be understood qualitatively within the single-band Hubbard or $t$-$J$ models. $^{[5,6]}$ However, the doping dependence of the incommensurability $\delta$ (the deviation of the peak in the spin structure from $q = (\pi, \pi)$) has not been, to our knowledge, understood quantitatively within single-band models. Namely, large $\delta$ appears with a small amount of hole doping (e.g., $\delta \simeq 0.2$ already at $x \sim 0.1$) in the underdoped regime, while $\delta$ saturates to 0.25 $\sim$ 0.30 in the overdoped regime. $^{[4]}$

More recently, the incommensurate spin structure is observed in the (underdoped) YBa$_2$Cu$_3$O$_{6.6}$ (YBCO$_{6.6}$) and (nearly optimally doped) Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi2212) samples as well, $^{[12]}$ which suggest that the phenomenon is not an accident for LSCO. Several authors have theoretically investigated the Hubbard $^{[8]}$ and $t$-$J$ models $^{[9]}$ in the context of these materials. By contrast, it is well known that the antiferromagnetic order is robust against electron doping in Nd$_{2-x}$Ce$_x$CuO$_{4-y}$ (NCCO). The difference is endorsed by a recent observation of a commensurate spin fluctuation in a superconducting NCCO sample ($x = 0.15$). $^{[11]}$

On the other hand, the shape of the Fermi surface has been revealed from the angle resolved photoemission (ARPES) studies for various high $T_c$ cuprates including YBCO $^{[14]}$, Bi2212 $^{[16,17]}$, LSCO $^{[18,19]}$, and NCCO $^{[20]}$. In particular, a recent ARPES experiment $^{[18,19]}$ has shown that the nesting of the Fermi surface in the underdoped LSCO is not so good as has been expected previously $^{[21-22]}$ from band calculations. $^{[23,24]}$

So the theoretical challenge is the following. We can simulate these shapes of the Fermi surface by taking appropriate values for the hopping parameters extended to distant neighbors in the tight-binding model, and the question is how the electron-electron interaction would dictate the spin structure. This is exactly the purpose of the present study. We employ here the single-band Hubbard model, one of the simplest models for repulsively interacting electrons. We shall show that the experimentally observed Fermi surface and the peak position of the spin structure can be understood consistently within the single-band Hubbard model by taking appropriate values for the hopping parameters. The spin susceptibility and the Fermi surface of the Hubbard model are calculated with the fluctuation exchange (FLEX) approximation, $^{[2]}$ which is appropriate for treating large spin fluctuations.

We consider the single-band Hubbard model,

$$
H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + H.c) + U \sum_i n_{i\uparrow} n_{i\downarrow},
$$

where we take $t_{ij} = t$ for nearest neighbors, $t_{ij} = t'$ for second nearest neighbors, and $t_{ij} = t''$ for third nearest neighbors. Using FLEX approximation, we calculate the RPA-type spin susceptibility $\chi(q, \omega)$ as well as the Fermi surface. In the actual calculation, we take $64 \times 64$ $k$-point meshes and the Matsubara frequencies $\omega_n$ from $-(2N_c - 1)\pi T$ to $(2N_c - 1)\pi T$, where $N_c = 1024$. The dynamical spin susceptibility for $\omega \neq 0$ is obtained by an analytical continuation of $\chi(q, i\omega_n)$ using Padé approximation. $^{[2]}$ For all the case studied, we take $U = 4t$ and $T = 0.05t$. We denote the band filling as $n$, the hole doping level as $p_h = 1 - n$, and the electron doping level as $p_e = n - 1$. 


First let us look at the case of YBCO, Bi2212, and NCCO. We find that the Fermi surface obtained by ARPES experiments for these materials can be reproduced by fitting \( t' = -0.40t \), \( t'' = +0.05t \). These values are close to the ones adopted in some of the previous studies. \([3, 15, 22, 27]\) In Fig.1, we superpose the experimentally obtained Fermi surface to that of the Hubbard model obtained with FLEX. The fit for YBCO is not so good as the others because the Fermi surface splits due to the interlayer coupling.

Fixing \((t', t'')\) at \((-0.40, 0.05)\), we have calculated the spin susceptibility \( \chi(q, \omega) \) for various band fillings. In Fig.2, we show typical results for the imaginary part \((\equiv \chi'')\) of \( \chi(q, \omega) \) with \( \omega = +0.05t \) for hole-doped (a) or electron-doped (b) cases. We can see that incommensurate peaks appear at \( q = (\pi, \pi (1 \pm \delta)) \), \((\pi (1 \pm \delta), \pi)\) for hole doping, while a commensurate peak appears at \( q = (\pi, \pi) \) for the electron doping.

The asymmetry between the hole and electron doping becomes even clearer if we plot the incommensurability \( \delta \) as a function of the band filling \([23]\) in Fig.3. One can immediately notice that a rather large incommensurability appears with a small amount of hole doping \((\delta \approx 0.25 \text{ at } p_h \sim 0.1)\), while the commensurate spin structure is robust against the electron doping up to \( p_e \sim 0.25 \). The robustness of the commensurate spin correlation in the electron doped regime is consistent with previous numerical studies for the Hubbard model \([3]\) and the \(t-J\) model. \([22, 24]\) We have further found that the obtained onset of the incommensurate spin structure around \( n \sim 1.3(p_e \sim 0.3)\) in the electron doped regime coincides with the situation at which the Fermi surface becomes too bloated to intersect the magnetic Brillouin zone boundary (the line \(|k_x| + |k_y| = \pi\)), as shown in the inset of Fig.3. \([23]\)

The result agrees quantitatively with experimental results for YBCO\(_{6.6}\), Bi2212, and NCCO, plotted as open symbols in Fig.3. Namely, YBCO\(_{6.6}\), in which the hole doping level in the CuO\(_2\) planes is around \( p_h \sim 0.1 \), \([31]\) is shown to have \( \delta \approx 0.22 \). \([11, 12]\) For Bi2212, a neutron scattering result has been obtained for a nearly optimally doped sample, in which an incommensurate spin structure has been detected. Although the actual spatial pattern of the spin structure has not been determined precisely, it has been concluded in Ref. \([12]\) that \( \delta \) would be around 0.32 if the spatial symmetry of the spin structure is the same as that in YBCO. The optimal hole concentration for Bi2212 is around \( p_h \sim 0.18 \) according to Ref. \([22]\), which is adopted in the plot. For NCCO, the commensurate antiferromagnetic order persists up to about \( x \approx 0.13 \). Quite recently, a commensurate spin fluctuation has been found in the superconducting samples Nd\(_{1.85}\)Ce\(_{0.15}\)CuO\(_{4-y}\). \([14]\) Here we plot this result by nominally taking \( n = 1.15 \), although the actual doping level may depend on \( y \).

A few comments are in order at this point. Some previous studies have adopted a smaller \(-t' = 0.17t\) and a larger \( t'' = 0.20t\) for YBCO. \([3, 11]\) Although this parameter set approximately reproduces the experimentally obtained Fermi surface as well, \([4, 5]\) it only gives...
a broad commensurate spin structure in the underdoped regime \((p_h \leq 0.1)\), which crosses over to an incommensurate structure with peaks in the diagonal direction \((\pi(1 \pm \delta), \pi(1 \pm \delta))\) rather than for \((\pi, \pi(1 \pm \delta))\) in the overdoped regime \((p_h \geq 0.2)\).

In fact, we can reduce the value of \(-t'\) without much changing the shape of the Fermi surface by taking larger values of \(t''\), but with a slight reduction of \(-t'\) to \(t' = -0.30t\) (with \(t'' = 0.10t\)), the incommensurate spin structure at \(n = 0.90\), although still present, is already substantially degraded as compared with that for \(t' = -0.40t\). Thus, among the sets of parameters that reproduce the Fermi surface of YBCO, the ones with \(-t' \gg t''\) seem to be appropriate from the viewpoint of the spin structure. [23]

In Ref. [2], a relatively small \(-t'(= 0.25t\) with \(t'' = 0\)) has been concluded on the ground that a quantum Monte Carlo calculation shows an appearance of the peak in the spin structure in the diagonal direction for \(-t' \geq 0.3t\). We have also found that the diagonal peaks can appear for the present choice of \(-t' = 0.40t\) (with \(t'' = +0.05t\)), but that occurs only for band fillings \(n = 0.70\) (for which the calculation in Ref. [2] was performed) or less, so that there is no inconsistency. However, a smaller \(-t'\) is not acceptable in our view, since, not only the large curvature of the Fermi surface requires a large \(-t'\), but also the appearance of large \(\delta\) with a small amount of hole doping requires a large \(-t'\) as we shall see in Fig. 4 below. Since \(\delta\) is as large as \(\sim 0.22\) for YBCO\(x=0,6\) (with \(p_h\) being as small as 0.1), a large value of \(-t'\) such as the one adopted here is considered to be appropriate for this material.

Let us now turn to \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\), which provides an excellent test-bed for studying the link between the Fermi surface and spin structure, since (i) the material is unique in that the Fermi surface changes its topology (i.e., connectivity) between the underdoped \((x = 0.1)\) and overdoped \((x = 0.3)\) regimes, as has been observed by a recent ARPES experiment, [18,19] (ii) the overall doping dependence of the spin structure is well established from neutron scattering experiments. [2] First let us look into the Fermi surface. The ARPES result [18,19] suggests that the nesting of the Fermi surface for \(x = 0.1\) is not so good as has been expected previously from band calculations, so one needs to take relatively large values for \(-t'\) to reproduce that. We can then take \(t' = -0.35t\), \(t'' = +0.05t\), and \(n = 0.90\) to obtain a good fit to the experimentally obtained Fermi surface as shown in Fig. 4(a). On the other hand, the ARPES data at \(x = 0.3\) cannot be reproduced, as seen in Fig. 4(b), for fixed \((t', t'') = (-0.35t, +0.05t)\) with \(n = 0.70\). In fact, we have to assume \(-t'\) to be as small as 0.10t for a fixed \(t''(= 0.05t)\), or \(t' = -0.15t\) when \(t''\) is varied to zero, to reproduce the ARPES data. These values are actually close to the ones adopted for LSCO in many of the previous studies. [2,21,22] We show in Fig. 4(d) how the Fermi surface is well reproduced for \(t' = -0.10t\), \(t'' = 0.05t\) with \(n = 0.70\). A change in \(t'\) is really required, since if we fix \((t', t'')\) to these values to go back to \(n = 0.90\) in Fig. 4(c), the Fermi surface is seen to deviate from the ARPES data for \(x = 0.1\).

One might suspect that the reason why we have to take different values for the hopping parameters in the underdoped and overdoped regimes might be because the FLEX approximation did not take into account properly the electron correlation effect, which should become more significant in the underdoped regime. This, however, cannot be the case, since it is known that the electron correlation effect tends to enhance the nesting in Fermi surfaces as the system approaches half-filling, while the experimental data suggest that the nesting becomes worse for smaller \(x\). Thus we can assume that the decrease of \(-t'/t\) with hole doping is not an artefact.

Keeping the above analysis for the Fermi surface in mind, we have calculated \(\chi(q, \omega)\) for three values of \(t'\), namely, \(t'/t = -0.35, -0.25,\) and \(-0.10\), fixing \(t'' = 0.05t\). A typical result for \(t' = -0.25t\), \(t'' = +0.05t\), and \(n = 0.80\) is given in the inset of Fig. 4. Again, incommensurate peaks are found at \(k = (\pi, \pi(1 \pm \delta))\), \((\pi(1 \pm \delta), \pi)\). The band filling dependence of the incommensurability is plotted in Fig. 4. Here, a result similar to that for \((t', t'')(=-0.10t, 0.05t)\) can also be obtained for \((t', t'')(=-0.15t, 0.0)\), i.e., the other choice of parameter set that reproduces the ARPES data for \(x = 0.3\). The doping dependence of \(\delta\) for small values of \(-t'\) is similar to those obtained in previous theoretical studies for LSCO.[2,22] As already stated previously, \(\delta\) is essentially zero in the underdoped regime \((n \geq 0.90)\) for
small values of $-t'$, which is inconsistent with experimental observations. It can be seen that the appearance of large $\delta$ with a small amount of hole doping, which is observed experimentally ($\delta \sim 0.2$ for $x \sim 0.1$), can only be obtained for large enough $-t'$. On the other hand, the incommensurability increases monotonically with hole doping if we stick to a fixed ($t'$, $t''$). Thus we conclude that we have to have $-t'/t$ (and possibly $t''/t$) decreasing with hole doping in order to obtain the experimentally observed saturation of $\delta$. The doping dependence of both the Fermi surface and the spin structure can then be understood within a single scenario.

To conclude, the main message of the present paper is that the experimental observations such as the saturation of the incommensurability in LSCO and the sharp contrast of the spin structure between electron doped and hole doped systems can be understood within a single-band model, and that we do not have to go back, as one might suspect, to the original three-band model that explicitly takes into account Cu 3d and O 2p orbitals.

A remaining problem is why, if our picture is correct, $-t'/t$ (and possibly $t''/t$) decreases with hole doping in LSCO. As for the discrepancy between the ARPES result and the band calculation in the underdoped regime, we may make a following conjecture at the present stage. If we closely look at the band calculation for LSCO, [23,24] there is, in contrast to that of YBCO, a large dispersion between $\Gamma$ ($k = (0,0)$) and $G_1$ ($k = (\pi,0)$) in the band lying near the Fermi level. In a tight-binding model, this corresponds to a small $-t'$. A large energy difference between $\Gamma$ and $G_1$ is known to be due to the mixing between the Cu $d_{x^2-y^2}$ - O $p_{x,y}$ orbital and the Cu $d_{3z^2-r^2}$ - O $p_z$ orbital. [23] If, for some reason, this hybridization is weaker than expected in the underdoped regime, so that the main character of the band near the Fermi level is Cu $d_{x^2-y^2}$ - O $p_{x,y}$, then the energy difference between $\Gamma$-$G_1$ would be smaller, amounting to a larger $-t'$. If this is correct, the reason why the hybridization is weak in the underdoped regime, or why it is recovered in the overdoped regime becomes a future problem. Experimental observation in Ref. [33] showing that the Cu $d_{3z^2-r^2}$ - O $p_z$ character grows with hole doping may have some relevance to this point.

The relation between the present result and the so-called ‘1/8-problem’ or ‘charge stripes’ [50] is another interesting future problem.

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This turns out to be the case for other values of $(t', t'')$ we studied, e.g., $t' = -0.2t$, $t'' = 0.0$.

Conversely, if spin structures qualitatively different from that of YBCO are to be present in other materials with similar Fermi surfaces, a smaller $-t'$ with a larger $t''$ could be the cause.

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