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LETTER TO THE EDITOR

Incommensurate antiferromagnetic orders and peculiar electronic structures in the doped Hubbard model

Bang-Gui Liu

Centre of Theoretical Physics, CCAST (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China, and Institute of Physics, Chinese Academy of Sciences, PO Box 603, Beijing 100 080, People's Republic of China

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Abstract. In this letter we shall propose a new Hartree–Fock approach for the standard two-dimensional Hubbard model. Commensurate antiferromagnetic order exists only for half-filling. Upon doping, incommensurate spiral antiferromagnetic orders appear and electronic states build into the half-filling energy gap. Corresponding Fermi surfaces enclose areas proportional to the dopant concentrations so that the Hall concentrations scale with the dopant concentrations. These results are consistent with recent transport, neutron-scattering and photoemission experiments on the high-temperature cuprate superconductors.

Hubbard models attract widespread attention since they are believed to be useful in describing the high-T_c superconductivity of the cuprate materials. We are interested here only in the standard Hubbard (SH) model, i.e. the simplest one. It has the main properties of the other extended models, especially near the Fermi energy level. There have been many and various works on the SH model since Anderson first argued that the SH model could describe the high-T_c superconductivity in cuprate materials [1]. At half-filling, the SH model has an instability towards antiferromagnetic order [2]. To carry out a perturbation calculation one needs a suitable mean-field solution as a good starting point. The work by Schrieffer *et al* was based on a half-filling mean-field solution of an antiferromagnetic order [2]. Subsequently, many works have aimed to understand the Hubbard model [4, 5, 6]. For the doped Hubbard model, one usually took the half-filling energy bands as one's energy bands of doped systems in one's further works. This was the so-called rigid approximation. But upon doping there is an instability towards some incommensurate magnetic orders instead of the commensurate AFM order [5]. The rigid approximation is not a good approach to work with in the doping systems. Reference [6] suggested spiral magnetic orders for the doped SH model. Their free energy is not derived from the SH model, but from a statistical physics argument. In this letter we shall propose a systematic and consistent Hartree–Fock theory for the SH model.

Experimentally, it was found that there were incommensurate magnetic orders in the superconducting cuprates [6], electronic states were built into the energy gap of the corresponding undoped cuprates, and the Fermi surfaces of the superconducting cuprates have some peculiar properties [7, 9]. These phenomena can be understood easily in the framework of our Hartree–Fock theory.

We shall start with a general Hartree–Fock approximation and assume special forms for average spin and carrier concentration. Then we diagonalize the resulting Hamiltonian by

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a Bogoliubov transformation. Finally, we derive free energy and two constraint equations to determine the chemical potential μ, average spin s, and modulation vector (Q_1, Q_2). We shall obtain the phase diagram by demanding that the free energy takes a minimum. After obtaining μ, s and (Q_1, Q_2), we shall discuss the properties of electronic states. The half-filling ground state is an insulator of antiferromagnetic (AFM) orders. With doping, electronic states are built into the half-filling energy gap, the commensurate AFM order gives way to incommensurate spiral magnetic order, and the Fermi surface, locating mainly around the corner of the Brillouin zone, has a scale of dopant concentration instead of total electron (hole) concentration so that the Hall carrier concentration scales with the dopant concentration. These properties are consistent with recent experimental data on the cuprate superconductors [6, 7, 9].

We start with the following SH Hamiltonian:

$$H = -t\sum_{\langle ij\rangle}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + \mathrm{HC}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{1}$$

where, as usual, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are electronic operators, $n_i = \sum_\sigma c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator at site i, t is the hopping energy, and U is the on-site repulsive interaction energy. Our lattice is a two-dimensional square lattice. For our convenience we shall introduce in the Hamiltonian (1) a new term $\epsilon\sum_i n_i$, in which ϵ acts as our chemical potential. Besides this, we set such a unit that $2t = 1$. In this unit U and T will be scaled by $2t$. When making the Hartree–Fock approximation, usually one supposes that the spin operator $S^{\alpha}_i = c^{\dagger}_i\sigma^{\alpha}c_i$ has the following average values: $\langle S^{+}_i\rangle = \langle S^{-}_i\rangle = 0$ and $\langle S^{3}_i\rangle = s\mathrm{e}^{\mathrm{i}Q\cdot R_i}$. But this works only in the half-filling system where $Q = (\pi, \pi)$. In doped systems, the ground state of $Q = (\pi, \pi)$ is unstable. For the doped system with $Q \neq (\pi, \pi)$, it is impossible to diagonalize analytically the HF Hamiltonian. In our approach, we suppose $\langle n_i\rangle = \rho$, $\langle S^{3}_i\rangle = 0$, $\langle S^{+}_i\rangle = s\mathrm{e}^{\mathrm{i}Q\cdot R_i}$, and $\langle S^{-}_i\rangle = (\langle S^{+}_i\rangle)^{\dagger}$. This supposition means that $\langle S_i\rangle = \langle(S^{x}_i, S^{y}_i, S^{z}_i)\rangle = (s\cos Q\cdot R_i, s\sin Q\cdot R_i, 0)$. When $Q = (\pi, \pi)$, we obtain $\langle S_i\rangle = (s\cos\pi\cdot R_i, 0, 0)$ so that spin orders are antiferromagnetic in the x direction. When $Q = (0, 0)$, spin orders are ferromagnetic in the x direction. Otherwise the spins' orders are spiral in the xy plane. Our HF Hamiltonian takes the following form in k space:

$$H_{\mathrm{HF}} = \sum_{k}\left[\epsilon_k n_{k\uparrow} + \epsilon_{k+Q}n_{k+Q\downarrow} - Us\left(c^{\dagger}_{k\uparrow}c_{k+Q\downarrow} + c^{\dagger}_{k+Q\downarrow}c_{k\uparrow}\right)\right] \tag{2}$$

where $\epsilon_k = \epsilon + U\rho/2 - tZr_k$ and $r_k = 2/Z(\cos k_x + \cos k_y)$. The HF Hamiltonian (2) can be diagonalized by the following Bogoliubov transformation:

$$c_{k\uparrow} = \mu_k a_k + \nu_k b_k \qquad c_{k+Q\downarrow} = -\nu_k a_k + \mu_k b_k \tag{3}$$

where $\mu^2_k + \nu^2_k = 1$. Our diagonalized Hamiltonian reads

$$H_{\mathrm{HF}} = \sum_{k}\left(e^{a}_k a^{\dagger}_k a_k + e^{b}_k b^{\dagger}_k b_k\right) \tag{4}$$

where $e^{a,b}_k = \epsilon_{k+} \pm \sqrt{U^2s^2 + \epsilon^2_{k-}}$. $\epsilon_{k\pm}$ is defined by $\epsilon_{k\pm} = (\epsilon_k \pm \epsilon_{k+Q})/2$. The consistency of the average values $\langle n_i\rangle = \rho$ and $\langle S^{+}_i\rangle = s\mathrm{e}^{\mathrm{i}Q\cdot R_i}$ requires that ρ and s satisfy the following constraint equations:

$$\rho = \frac{1}{N}\sum_{k}\left(\frac{1}{\mathrm{e}^{\beta e^{a}_k} + 1} + \frac{1}{\mathrm{e}^{\beta e^{a}_k} + 1}\right) \tag{5}$$

$$s = \frac{1}{N}\sum_{k}\frac{1}{2}\frac{Us}{\sqrt{U^2s^2 + \epsilon^2_{k-}}}\left(\frac{1}{\mathrm{e}^{\beta e^{b}_k} + 1} - \frac{1}{\mathrm{e}^{\beta e^{a}_k} + 1}\right) \tag{6}$$

where $\beta = 1/k_B T$. Free energy per site is given by

$$f = \frac{1}{N}\sum_k \left(\frac{e_k^b - \epsilon}{e^{\beta e_k^b} + 1} + \frac{e_k^a - \epsilon}{e^{\beta e_k^a} + 1} \right). \tag{7}$$

At zero temperature, $T = 0$ or $\beta = \infty$, equations (5–7) reduce to

$$\rho = \frac{1}{N}\sum_k \left[\theta(-e_k^b) + \theta(-e_k^a) \right] \tag{8}$$

$$s = \frac{1}{N}\sum_k \frac{1}{2} \frac{Us}{\sqrt{U^2 s^2 + \epsilon_{k-}^2}} [\theta(-e_k^b) - \theta(-e_k^a)] \tag{9}$$

$$f = \frac{1}{N}\sum_k \left[(e_k^b - \epsilon)\theta(-e_k^b) + (e_k^a - \epsilon)\theta(-e_k^a) \right]. \tag{10}$$

The above function $\theta(x)$ is defined by

$$\theta(x) = \begin{cases} 1 & x \geqslant 0 \\ 0 & x < 0 \end{cases}.$$

All properties will be determined by the parameters s, ϵ and Q. In our theoretical framework, s, ϵ and Q are determined by minimizing the free energy f under the constraints (5–6), or (8–9) in the limit of $T = 0$.

At half-filling, $Q = (\pi, \pi)$ and $\epsilon = -U/2$. s is determined by

$$s = \frac{1}{N}\sum_k \frac{1}{2} \frac{Us}{e_k} \tanh(\beta e_k/2) \tag{11}$$

where $e_k = \sqrt{U^2 s^2 + \epsilon_{k-}^2}$. In the limit of $T = 0$, we obtain $\tanh(\beta e_k/2) = 1$, and s is a function of the on-site coupling U divided by $2t$. Figure 1 demonstrates the dependence of s on the ratio $U/2t$. For large $U/2t$, we derive such an asymptotic behaviour of s as $s = 1/2 - 4t^2/U^2$. The corresponding free energy is given by $f = -4t^2/U$ in leading order of $2t/U$. For small $U/2t$ we derive another s asymptotic behaviour

$$s = \frac{2t}{U} \exp(2.76 - \pi\sqrt{4t/U}).$$

This small-U behaviour is accurate if $U < 0.5t$. Our half-filling s and f values are the same as the results of Schrieffer *et al* [3].

In doped systems, we expect that Q is not equivalent to (π, π). But if $1 - \rho$ is small enough, it is still expected that the deviation of $(\pi, \pi) - Q$ will be very small. Generally, we define $Q = (Q_1, Q_2)$. Equations (5–7) are invariant under transformations $Q_1 \to -Q_1$ and/or $Q_2 \to -Q_2$ so that we can confine Q_1 and Q_2 to the region of $[0, \pi]$ in our following calculations. For our convenience, we define $\delta = 1 - \rho$ and $q = (q_1, q_2) = (\pi, \pi) - Q$. When δ is small enough, we expect that q_1 and q_2 are small. As a result, we can analytically solve the constraints and minimize the free energy. We take s_0 of the half-filling as our average spin s of small δ. The zero-temperature free energy is given by

$$f = f_0 + \frac{B}{4}\left[(q_1 - \delta/B)^2 + (q_2 - \delta/B)^2 \right] \tag{12}$$

where f_0 is independent of q_1 and q_2, and $B = Us_0\left[\gamma(-1) - \gamma(1)^2/\gamma(3)\right]/4$. $\gamma(K)$ is defined by $\gamma(K) = (1/N)\sum_k \left(1 + \epsilon_k^2/U^2 s_0^2\right)^{-K/2}$. Because (12) holds only when δ is small enough, $q_1 = q_2 = \delta/B$ holds only near $\delta = 0$. B is always positive for all U. $B = 2/\pi^2$ for very small U and $B = 2.5/U^3$ for very large U. If U is very large, $q_1 = q_2 = \delta/B$

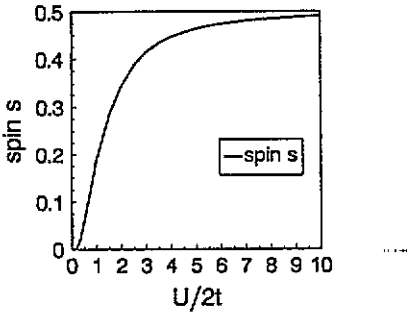

Figure 1. Dependence of average spin s on the on-site correlation strength $U/2t$. The correlation is considered to be weak if $U < 0.5t$.

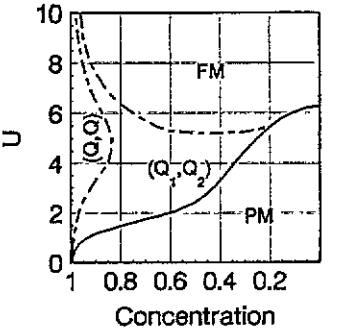

Figure 2. U–ρ phase diagram. The phase boundaries are not clearly defined except the paramagnetic edge. $Q = (Q_1, Q_2)$ changes continuously in all areas except the paramagnetic edge.

will be very large as long as $\delta \neq 0$. This means that a phase transition to FM takes place at $\delta \sim 0$ for infinitely large U, being consistent with Nagaoka's theorem [10]. In the lightly doped systems, q_1 and q_2 are small so that the magnetic orders are a kind of deformed AFM order. For this kind of order the AFM structure is kept locally but the commensurate property is broken. It is expected experimentally that neutron-scattering peaks will become more broad and the single-peak structure will be replaced by a two-peak structure [6].

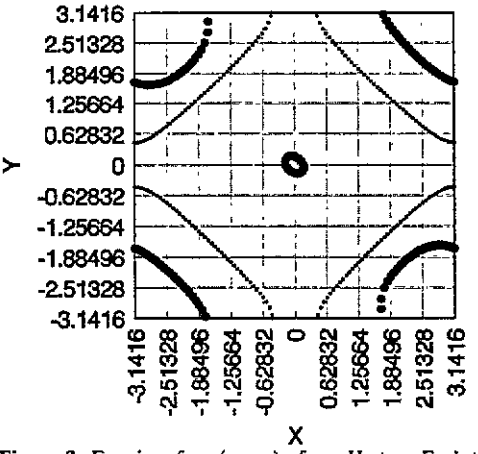

Figure 3. Fermi surface (curve) of our Hartree–Fock theory. Its symmetry is so low that only the parity symmetry remains. The area it contains is equivalent to the dopant concentration multiplied by $4\pi^2$.

Generally it needs digital calculations to minimize the free energy (10) under the constraints (8) and (9). Our zero-temperature ρ–U phase diagram is shown in figure 2. There are four areas in the phase diagram. But the boundaries are not clearly defined except the paramagnetic edge. In all phases here, spins orient in the xy plane, $\langle S_i \rangle = (s \cos Q \cdot R_i, s \sin Q \cdot R_i, 0)$. The commensurate AFM phase is limited rigorously to $\rho = 1$. Generally we have $Q = (Q_1, Q_2)$. For the ferromagnetic (FM) phase, $Q_1 = Q_2 = 0$. But Q_1 is not rigorously equivalent to Q_2 near the boundary. The (Q, Q) phase exists only when the dopant concentration $\delta = 1 - \rho$ is small enough. We have $Q_1 \simeq Q_2$ near the $(Q, Q)/(Q_1, Q_2)$ boundary. For very large U, the AFM/FM transition takes place at $\delta \sim 0$.

In the (Q_1, Q_2) phase $Q_1 - Q_2$ increases with ρ decreasing for a given U. In the complete phase diagram, s decreases as ρ decreases. If $U > 10$, it is expected that $s = \rho/2$ in the FM area.

As for the electronic structure, it is derived that

$$e^{a,b} = \epsilon + U\rho/2 + \phi_{k+} \pm \sqrt{U^2 s^2 + \phi_{k-}^2} \tag{13}$$

where $\phi_{k+} = -\sin(q_1/2)\cos k'_x - \sin(q_2/2)\cos k'_y$ and $\phi_{k-} = -\cos(q_1/2)\sin k'_x - \cos(q_2/2)\sin k'_y$. Here k' is connected with the original lattice momentum k by $k' = k + Q/2$. $e^{a,b}$ are invariant under transformation of $k' \to -k'$. Since

$$e^b(\pi - k') = \epsilon + U\rho/2 - \phi_{k+} - \sqrt{U^2 s^2 + \phi_{k-}^2} = 2\epsilon + U\rho - e^a(k')$$

the upper band and the lower band are symmetrical with respect to the band centre $\epsilon + U\rho/2$. This means that hole doping and electron doping are symmetrical to each other in our HF theory. It should be pointed out that this hole–electron symmetry results directly from the special $e^{a,b}$ properties based on the 2D square lattice. In our theory, $(\pm q_1, \pm q_2)$ and $(\pm q_2, \pm q_1)$ lead to same free energy. But it is demanded in our HF approximation and diagonalization process that only one of the eight exist in the real system. This resembles ordered FM systems where a ground state of spin $\uparrow$ has same energy as another ground state of spin $\downarrow$ does, but the spin takes only one direction. This is so-called spontaneous breaking of symmetry. It is reasonable for us to confine q_1 and q_2 to region $[0, \pi]$. If q_1 and q_2 are non-zero, the upper band e_a reaches its minimum at $k' = (0, 0)$ and the lower band reaches its maximum at $k' = (\pi, \pi)$. There is an energy gap between the two bands: $g = 2Us - 2\sin(q_1/2) - 2\sin(q_2/2)$. If $g > 0$, the Hall coefficient is determined by one of the two bands so that its Hall concentration scales with the dopant concentration at low temprature. At half-filling the gap is given by $g_0 = 2Us_0$. There are two ways for doped carriers to reduce the gap: the doped carriers can reduce the average spin s; or the doped carriers make q_1 and q_2 non-zero so that the two q terms appear in the gap expression. It is expected that the doped carriers reside in the the half-filling gap.

At half-filling the two energy bands are defined by

$$e^{a,b} = \pm\sqrt{U^2 s^2 + (\cos k_x + \cos k_y)^2}$$

($2t = 1$ in our units). The bandwidth is given by $w_0 = \sqrt{U^2 s^2 + 16t^2} - Us$. When U becomes large, the bandwidth is given by $w_0 \sim 16t^2/U$. There is a great gap $2Us$ between the two bands so that the system is insulating, as it should be. If we took the half-filling bands as bands of the doped system as the rigid-band approximation did, we should obtain too small a band width for heavily doped systems of large U. In contrast, in our theory the large-U bandwidth is $8t$ even for intermediately doped system. Our result is reasonable because it is expected that the effect of the correlation U becomes weak in the heavily doped systems so that its bands ought to be determined mainly by the original t term of Hamiltonian (1). At half-filling the lower band is occupied fully and the upper band is empty so that the system is insulating. This is contrary to the tight-binding band result but is in agreement with the experimental fact of the undoped cuprates. In the lightly doped systems, the gaps between the two bands decrease but still exist. When holes are doped, the upper band is still empty and the holes enter into the lower band. When electrons are doped, the lower band remains full and the electrons enter the upper band. This is different from conventional band-filling. In our theoretical framework, the doped carriers change the band structures when filling the bands. For the lightly electron-doped systems we expect its effective carriers are electron-type. For the lightly hole-doped systems its effective

carriers ought to be hole-type. In both cases, effective carriers are proportional to the dopant concentrations. This is in agreement with the Hall-effect experiments on the doped superconducting cuprates [7, 9]. If we make use of the usual energy-band-theoretical results for the doped cuprates, we should obtain wrong conclusions about the Hall concentrations.

To make our discussion more quantitative, we take a set of typical parameters to show our results. We let $U = 3$ and $\delta = 0.15$. Minimizing the zero-temperature free energy, we obtain $\epsilon = -0.8769$, $s = 0.3720$, $q = (1.934, 1.571)$, and $f = -0.1896$. The corresponding Fermi surface is shown in figure 3. The half-filling energy gap is given by $g_0 = 2Us_0 = 2.482$. For our present system we derive $g = -0.8290$. This is to say that no gap is present for $\rho = 0.85$. Due to $e^a(0, 0) = -0.0164$, carriers have been doped partially into the upper band. Therefore, there are electrons in the upper band and holes in the lower band. The system consists of a nearly filled band and a nearly empty band. There are two types of carriers in the system. The Hall concentrations will deviate from the dopant-scaling behaviour in heavily doped systems such as the $\rho = 0.85$ system, being in agreement with the experiments of the superconducting cuprates. On the other hand, its Fermi surface become more complex. It consists of two parts: the major part around the corners of the Brillouin zone and the minor part around the centre, as shown in figure 3. When $\rho = 0.95$, we obtain $\epsilon = -0.9465$, $s = 0.3998$, $q = (1.050, 1.000)$, and $f = -0.08665$. The corresponding gap is given by 0.4378. The minimum of the upper band is $e_d^a = 0.6975$ and maximum of the lower band is $e_t^b = 0.2597$. The centre of the two bands is at $e_c = 0.4786$. In other words, the Fermi level is at -0.4786 away from the band centre. The distance between the band centre and the top of the lower band is 0.2189, but there is a distance of 1.241 between the half-filling band centre and the top of the half-filling lower band. Its Hall concentration should exhibit a good dopant-scaling behaviour. It is obvious that the Fermi levels of $\delta = 0.05$ and 0.15 reside in the half-filling energy gap, being in agreement with the experimental results [7, 9].

As for the shape of the Fermi surfaces, they are peculiar and very different from the tight-binding Fermi surfaces and the rigid-approximation Fermi surfaces. For lightly doped systems, $q_1 \simeq q_2$ are small so that their Fermi surfaces are ellipses centred at $k = (\pi/2, \pi/2) + (q_1, q_2)$ or $k' = (\pi, \pi)$. The Fermi surface in the $\delta = 0.15$ system is shown in figure 3. The tight-binding Fermi surface is shown, too, to compare with our theoretical result. It is obvious that the Fermi surface is asymmetrical, as explained above. This asymmetry has been observed in photoemission experiments on the cuprate materials [9]. Considering the symmetry of the two bands, our Fermi surface of $\delta = 0.15$, pocketing mainly around the centre of Brillouin zone and having a smaller part around the corners of Brillouin zone, is consistent with the experimental Fermi surface of $YBa_2Cu_3O_{6.9}$ [9].

In summary, we propose a Hartree–Fock theory of the standard Hubbard model. Commensurate antiferromagnetic order exists only at half-filling. Upon doping, incommensurate magnetic orders appear and electronic states build into the half-filling gap. Fermi surfaces, locating mainly around the corners of Brillouin zone and having a minor part around the Brillouin-zone centre, contain areas proportional to the dopant concentration so that the Hall concentrations scale with the dopant concentrations. These results are in agreement with the recent transport, neutron-scattering, and photoelectron experiments on the high-temperature cuprates.

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