Magnetic Order in the $t$-$J$ and $t$-$t'$-$J$ Models

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The magnetic structure of the $t$-$J$ and $t$-$t'$-$J$ models are investigated. Assuming that the ground state has magnetic long-range order, we calculated the energy of some magnetically ordered states using a simple transformation of the models and the $S \rightarrow \infty$ approximation. The result shows that the Néel state is destroyed by doped holes unless the next-nearest neighbor hopping $t'$ is finite, and that the ferromagnetic phase appears at moderate doping. Mean field analysis shows that the intermediate phase between the Néel and ferromagnetic phase has spiral spin order, although the spiral phase is shown to be unstable against density fluctuations.

KEY WORDS: Magnetic order; $t$-$J$ model; $t$-$t'$-$J$ model.

1. INTRODUCTION

Since the discovery of high-temperature superconductors we have noticed again that there are still lots of rich physics hidden in strongly correlated systems. As well as the Hubbard model, which is one of the simplest models of correlated systems and one of the models with a long history, the $t$-$J$ model has been investigated from various viewpoints by various methods. While, in one dimension, we have an exact solution for the supersymmetric case ($2t = J$) [1] and the Luttinger liquid nature has been explored in the whole phase diagram [2] except for the case of $J >> t$ where phase separation is expected, no exact solution has been obtained for any parameter region of the two-dimensional $t$-$J$ model, and a lot of theoretical works are still being carried out to reveal its nature. Due to the limitations in computer power, numerical works in two dimensions such as Monte Carlo simulation and exact diagonalization are performed only for small system sizes and it is hard to make definite arguments based on the model. Therefore, many theoretical works have taken analytical approaches. There are many problems in the analytical approaches also, however. Since the model has strong correlation (as strong as it could be, in a way), most theoretical approximations would not give correct answers. Unfortunately we do not even know how to check if the obtained result is the right answer or not. So there are a huge number of different results obtained from various approximations, which makes the situation much more complicated. In this situation, we believe that we should use simple and physically transparent approximations when we study such models, because complicated approximations or approximations whose physical meaning is not clear make it vague whether the results are appropriate or not.

In this paper we investigate the magnetic structure of the $t$-$J$ model and the $t$-$t'$-$J$ model using simple approximations. As for the magnetic structure, there are some works which study the existence of magnetic long-range order (LRO) [3–6]. They calculate a wave vector $q$ characterizing magnetic long-range order in the ground state, and they found that $q$ gradually shifts from $Q = (\pi/a, \pi/a)$, where $a$ is the lattice constant, as holes are doped in the half-filled Néel ordered state. As long as the hole fraction $\delta$ is small, $Q - q$ is proportional to $\delta$. If we calculate the compressibility, however, this state, called spiral state, has a negative compressibility, and therefore the spiral state is not stable in the presence of density fluctuations [5].
It is also expected that there is a ferromagnetic phase for the parameters $J \ll t$ and $\delta \ll 1$ [7]. When $J = 0$, namely in the infinite $U$ Hubbard model, we have the Nagaoka theorem that one hole in the half filling would destroy the Néel order and make all the spins up. Although we do not know exactly if this is true when the finite density of holes are doped, some works show that it is.

With these previously obtained results in mind, we derive here similar results on the magnetic LRO using different methods which are simple and physically transparent. In the next section we show the analytical method we employed to study the magnetic structure of the $t$-$J$ model. In Section 3 the effects of spin fluctuations are studied and are shown to give no qualitative change to the mean-field results. The last section is devoted to the summary and discussion.

From now on we use $a = 1$, $\hbar = 1$ as units.

2. CLASSICAL SPIN APPROXIMATION

The $t$-$J$ model is usually written in the form

$$H_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (1)$$

where $\hat{c}_{i\sigma} = c_{i\sigma}(1 - n_{i\sigma})$. The second term is just the well-known Heisenberg antiferromagnetic term, and the first term represents particle hopping with a constraint of no double occupancy at each site. The $t$-$t'$-$J$ model contains additional hopping between next-nearest neighbors with energy $t'$. Since the nearest-neighbor hopping on a square lattice is a hopping between different sublattices, the hole motion tends to create some quantum spin fluctuations and to destroy the Néel ordered spin structure, while the next-nearest neighbor hopping can preserve Néel order. The $t$ term in Eq. (1) contains implicitly this sort of coupling between the hole motion and spin flipping. It is much more convenient to analyze the model if we rewrite the $t$ term in a form which shows the coupling more explicitly. For this purpose, we use the following operator algebra, $\hat{c}_\sigma = c_{\sigma} S^{-\sigma}$, $\sigma \hat{c}_\sigma = 2 c_{\sigma} S^\sigma$, and $0 = c_{\sigma} S^{-\sigma}$, where $S^\sigma$ is defined by $S^+ = c^\dagger \hat{c}^\dagger$ when $\sigma = +1$ and $S^- = c^\dagger \hat{c}^\dagger$ when $\sigma = -1$. Inserting these into Eq. (1), we obtain

$$H_{t,J} = -\frac{4}{3} t \sum_{\langle i,j \rangle, \sigma} S^\dagger_{i\sigma} c_{i\sigma} S_{j\sigma} + \text{h.c.} + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (2)$$

Xu et al. [8] obtained a similar form, but our form is rotationally symmetric while their form is not. So the Hamiltonian (2) is an extension of that of Xu et al. In order to study the wave vector of magnetic LRO which gives the lowest energy, we first assume that some sort of magnetic LRO exists in the ground state. For simplicity we also assume that the spins rotate confined in the $x$-$z$ plane. Then it is useful to rotate the coordinates at each site, so that the spins should order ferromagnetically in the new coordinates. We rotate the coordinates at the $\ell$-site about the $y$-axis by an angle $\theta_\ell = \mathbf{q} \cdot \mathbf{r}_\ell$. In the new frame we assume ferromagnetic long-range order (LRO), which corresponds in the original frame to LRO with wave vector $\mathbf{q}$. For the moment, we omit the degrees of freedom of the particles with down spin in the rotated coordinates, and no spin fluctuation is considered at this stage. The effects of spin fluctuations will be studied later. This is nothing but the $S \to \infty$ limit approximation. Consequently, the $t$-$J$ Hamiltonian is written as

$$H = -\frac{4}{3} t S^2 \cos \mathbf{q} \cdot \mathbf{r}_\ell \cos \frac{\mathbf{q} \cdot (\mathbf{r}_\ell - \mathbf{r}_\ell')}{2} d^\dagger_{\ell\uparrow} d_{\ell\downarrow} + \text{h.c.} + J \sum_{\langle i,j \rangle} S^2 \cos \mathbf{q} \cdot \mathbf{r}_\ell \quad (3)$$

where $d$ represents the up-spin particle operator $d_{\uparrow}$ defined in the rotated coordinates, and $d_{\downarrow}$ is omitted. Now the Hamiltonian has a one-body tight-binding form. Notice that the Hamiltonian (3) is valid only in the low doping limit, since the $J$-term must be modified if the moderate density of holes are doped. Transforming Eq. (3) into momentum space to diagonalize, we obtain

$$H = -\frac{4}{3} t S^2 \sum_{\ell \mathbf{q}} \left( C_{\uparrow} C_{\uparrow,\mathbf{q} / 2} C_{\uparrow} + C_{\uparrow} C_{\uparrow,\mathbf{q} / 2} C_{\uparrow} \right) d^\dagger_{\ell\uparrow} d_{\ell\uparrow} + \text{h.c.} + JS^2 N(C_{\uparrow} + C_{\uparrow}) \quad (4)$$

where, for brevity, we have written $\cos q$ as $C_q$. In the half-filled case, $\langle d^\dagger_{\ell} d_{\ell} \rangle = 1$, the hopping term does not contribute to the energy, and the total energy has a minimum at $\mathbf{q} = (\pm \pi, \pm \pi)$. This is simply a classical result for the Heisenberg antiferromagnet. In the finite-doping case, $\langle d^\dagger_{\ell} d_{\ell} \rangle = 1 - \delta$, the optimal $\mathbf{q}$ must change with the hole density $\delta$ because the $t$ term favors $\mathbf{q} = 0$ as seen in Eq. (4).

Using this approximated Hamiltonian, we calculated the energy as a function of $\mathbf{q}$ and look for the optimal $\mathbf{q}$ which gives the lowest energy. For simplicity, let us investigate two types of spin ordering; diagonal $(q_x = q_y = q)$ and stripe $(q_x = \pi, q_y = q)$. 

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