Effect of a geometrical frustration in the doped Mott insulator

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Abstract

The two-dimensional t-J model on the triangular lattice has been studied using high temperature expansions. By calculating the entropy and the spin-spin correlation function through twelfth order in inverse temperature, we revealed that hole doping favors a nearest-neighbor singlet formation, indicating that the resonating valence bond state is stabilized in low temperatures. On the contrary, with electron doping, we find that there exists a wide ferromagnetic region in the phase diagram, which is related to the Nagaoka's ferromagnetism, the flat band ferromagnetism and the Kanamori's ferromagnetism. It is also found that the competition between this ferromagnetic behavior and the antiferromagnetic coupling results in the large effective mass near half filling.

Key words: frustration; RVB; ferromagnetism

1. Introduction

Quantum systems with geometrical frustration have attracted much interest recently. There are a number of typical materials, such as pyrochlore compound LiV_2O_4 which shows a heavy fermion behavior[1] and κ-(BEDT-TTF)$_2$X which has an almost triangular lattice and exhibits superconductivity.

Furthermore, it is expected that the frustration causes fascinating states. One of the examples is a resonating valence bond(RVB) state which is first pointed out by Anderson[2] on the triangular Heisenberg model. From the discovery of high-T_c superconductivity, RVB state in the doped Mott insulator is discussed extensively[3]. However, there is no conclusive result about the appearance of RVB state in high-T_c compound as far as we know. Thus, it is interesting to study the possibility of RVB state in the frustrated lattice where the RVB state seems to be favorable. On the other hand, it is proved rigorously that the ground state is ferromagnet on the kagomé lattice and other line graph with finite electron density[4,5]. Thus, it is also important to investigate a region of ferromagnetism in a general frustrated lattice.

Considering these facts, we study the t-J model on the triangular lattice to investigate the effect of geometrical frustration in the strongly correlated system. Hamiltonian is given as

$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma} P\left(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.\right)P + J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j, \quad (1)$$

where the summation is taken over nearest neighbor pairs and P ensures no double occupancy. For this model, we calculate high temperature series of the entropy, S and spin-spin correlation function, $S(q)$ through twelfth order in inverse temperature. Padè approximation is used for extrapolating the obtained series to low temperatures.

2. Result and Discussion

In the case of $t > 0$, there is nothing particular when $J = 0$. However, when J is induced, we found that the entropy, S, decreases rapidly with decreasing temperature around $0.4 < n < 1$. In addition, the spin

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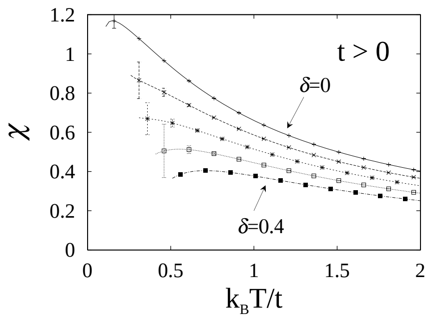

Fig. 1. The spin susceptibility, χ, at $J/t = 0.3$ and $n = 0, 0.1, 0.2, 0.3, 0.4$. Errorbars indicate the scattering of various Padè approximation.

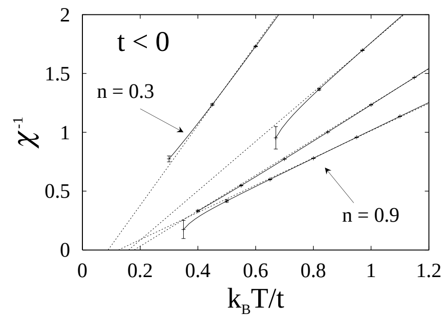

Fig. 2. The inverse spin susceptibility, χ^{-1}, for $J = 0$ and $n = 0.3, 0.5, 0.7, 0.9$. Dotted lines indicate the fitting of data as $\chi^{-1} \sim a(T - \Theta)$.

susceptibility, χ, starts to decrease in similar temperature region as shown in Fig. 1. The peak in χ, which is around $k_BT \simeq 0.1\text{-}0.4J$ at $\delta = 0$, shifts to higher temperatures with hole doping. This behavior is opposite from the case of square lattice[6] where the peak in χ shifts to lower temperature with doping.

The above features of S and χ can be understood as follows. Since the large entropy at $\delta = 0$ in low temperature is due to frustration, we consider that the frustration is released by doping. Simultaneously the behavior of χ suggests that the antiferromagnetic correlation grows with doping. The long-range Néel order, however, is not expected. In fact, the peak of spin-spin correlation function $S(q)$ at $q = Q = (4/3\pi, 0)$ corresponding to the Néel order does not grow with hole doping and no other peak appears. Therefore, we consider that the suppression of χ is due to the formation of nearest-neighbor singlet pairs or the RVB state. This is consistent with the entropy's behavior, since the formation of singlet causes the entropy to decrease around $k_BT = J$.

In the case of $t < 0$, there exists the Nagaoka's ferromagnetism in the limit of $n \to 1$ when $J = 0$. In addition, the ferromagnetism appears in the two electron case with arbitrary positive U since the bottom of the band degenerates. Thus, the problem is whether the ferromagnetic region continues from $n = 0$ to $n = 1$. Figure 2 shows the inverse spin susceptibility χ^{-1} at $J = 0$ with various n. It is found that χ^{-1} behaves as if there exists a finite Weiss temperature $\Theta(> 0)$ which suggest the occurrence of ferromagnetism not only around $n = 1$ but for all region of $0 < n < 1$.

This ferromagnetic region is considered as follows. In the case of $t < 0$, there exist the Nagaoka's ferromagnetism on arbitrary lattices with one hole[7–9]. On the bipartite lattices such as square lattice, it is expected that this Nagaoka's ferromagnetism is easily destroyed with hole doping[10]. However, for the non-bipartite lattices, the ferromagnetism is expected with hole doping when there is a flat band as in the kagomé lattice with $t < 0$. In general, in the case of $t < 0$, the bottom of the band is not at Γ point ($k = 0$) and thus the density of states is large compared with the case of $t > 0$, except for the bipartite case where the case of $t < 0$ is transformed to $t > 0$ by a simple unitary transformation: $c_i \to -c_i$ on the B sublattice. Due to this large density of states, there is a possibility of ferromagnetism in low density region[11]. The flat band ferromagnetism is the special case, i.e. the density of states $D(\epsilon_F) \to \infty$. Note that the triangular lattice is very similar to the kagomé lattice and the density of states is large for $t < 0$.

To summarize, we have studied the effect of hole doping in the triangular Heisenberg model as a typical frustrated Mott insulator. In the case with $t > 0$, we have concluded that the hole doping induces the RVB state, since the entropy and the spin susceptibility starts to decrease in high temperature region. In this case, we expect that the ground state can be a superconducting state, which exactly corresponds to what Anderson speculated as RVB[2,3]. In contrast, for $t < 0$ we found that there exists a wide ferromagnetic region in the phase diagram.

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