Quasiparticle excitations in the hole-doped Hubbard model with orthogonal-dimer structure

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Abstract

We study the hole-doping effects on the half-filled Hubbard ladder model with the frustrated orthogonal-dimer structure. By using the density matrix renormalization group method, we discuss how strong geometrical frustration affects the nature of spin excitations upon hole doping. We find that for large U with strong frustration, a spin-gap metallic phase appears, for which excitations can be described by two independent quasiparticles.

Key words: Hubbard ; DMRG ; frustration

Strongly correlated electron systems with geometrical frustration have attracted much interest. Prototypical systems are the pyrochlore compounds with the lattice of corner-sharing tetrahedral network. [1–7] Recent researches of the metallic pyrochlore compound LiV_2O_4 [8] pointed out that frustration may be important to understand its heavy-fermion behavior. Another well-known pyrochlore compound $Y(Sc)Mn_2$ [9] with spin-liquid ground state is also in a metallic phase.

In this paper, we study the hole-doping effects on the half-filled Hubbard model with such geometrical frustration. Since it is difficult to precisely treat the hole-doping effects on three-dimensional (3D) frustrated systems, we study a simpler model in 1D, which still possesses the essence of strong frustration in the above systems. This simplification enables us to precisely calculate the physical quantities by the density matrix renormalization group (DMRG) method [10].

To be precise, we investigate the frustrated Hubbard ladder with the orthogonal-dimer structure [11], as illustrated in Fig. 1. Note that this model also has the structure of a tetrahedral network. The Hamiltonian we consider here is

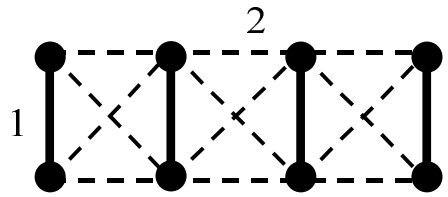

Fig. 1. Hubbard ladder with the orthogonal-dimer structure. The solid and dashed lines correspond to the parameters t_1 and t_2, respectively.

$$H = -\sum_{i,j,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{h.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \qquad (1)$$

where $c_{i\sigma}$ ($c^{\dagger}_{i\sigma}$) annihilates (creates) an electron with spin σ, and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$. Electron hopping takes two different values $t_{ij} = t_1, t_2$ as shown in Fig. 1. We set t_1 to be unity for simplicity. In the noninteracting case ($U = 0$), the model has a dispersionless flat-band mode: two modes are given by $\varepsilon_+(k) = -t_1 - 4t_2\cos(k)$ and $\varepsilon_-(k) = t_1$, reflecting special geometry of the system. Note that similar flat-band mode is also found in the pyrochlore lattice. For $t_2/t_1 = 0.5$, a flat-band ε_- just touches a broad-band ε_+ at $k = \pm\pi$, as shown in the inset of Fig. 2(a), while for $t_2/t_1 > 0.5$ two bands intersect each other as in Fig. 2(b).

In order to discuss spin excitations in a hole-doped

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system near half-filling, we here compute three quantities, i.e. the spin gap Δ_0 at half-filling, the spin gap Δ_2 with two holes and the binding energy Δ_B of two holes,

$$\Delta_0 = E_0(N,1) - E_0(N,0),$$
$$\Delta_2 = E_0(N-2,1) - E_0(N-2,0),$$
$$\Delta_B = 2E_0(N-1,1/2) - E_0(N,0) - E_0(N-2,0),$$

where $E_0(N,S^z)$ is the ground-state energy for the system with N electrons and total spin S^z. We have calculated these quantities up to $N = 96$ by the finite DMRG method, and then performed a finite-size scaling analysis.

Shown in Fig. 2 are the results for (a) $t_2 = 0.5$ and (b) $t_2 = 0.65$. For $t_2 = 0.5$, the spin gap Δ_0 is always finite for any value of $U > 0$. It is seen that hole-doping immediately makes spin excitations gapless, i.e. $\Delta_2 = 0$. The situation is completely different for $t_2 = 0.65$. In this case, for $U < U_c$, doped holes are not mobile because they are accommodated in a flat-band up to a certain critical density of holes. For $U > U_c$, the spin gap Δ_0 shows similar behavior as in the $t_2 = 0.5$ case. In contrast, however, both of Δ_2 and Δ_B are finite for $U > U_c$, implying formation of a bound state of holes with the spin gap. It should be noticed here that the spin gap Δ_2 perfectly coincides with the binding energy Δ_B for both cases of $t_2 = 0.5$ and 0.65. This suggests that the excited states in two holes may be described by two independent quasiparticles.

We recall that the spin-gap Δ_2 in a doped case is totally different from Δ_0 at half-filling. Therefore, the mechanism of spin-gap formation in a hole-doped case is different from that at half filling, and is due to the attractive interaction between holes.

By performing similar calculations for various choices of t_2, we can deduce that the spin gap Δ_2 has a finite value in the region $0.5 < t_2 < 0.84$ when U is sufficiently large, which is indeed consistent with the results of the t-J model with the same ladder structure [12]. This suggests that a flat-band mode, reflecting the frustrated lattice structure, may play an important role to form the spin gap in a metallic phase. We expect that this-type of argument would be also applied to the pyrochlore lattice near half filling.

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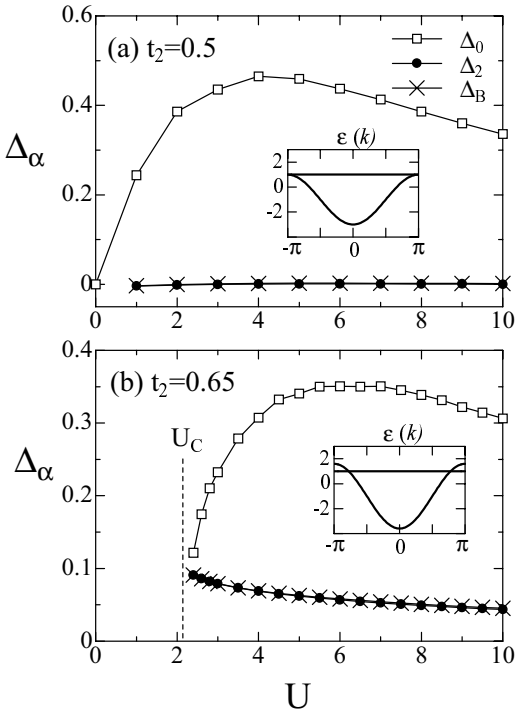

Fig. 2. Spin-gap Δ_0 at half-filling, spin-gap Δ_2 with two holes, and binding energy Δ_B of two holes: (a) $t_2 = 0.5$ and (b) $t_2 = 0.65$. Insets show the energy-momentum dispersion relation at $U = 0$.

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