Quasiparticle collapsing in an anisotropic t-J ladder

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Quasiparticle collapsing is a central issue in the study of strongly correlated electron systems. In the one-dimensional case, the quasiparticle collapsing in a form of spin-charge separation has been well established, but the problem remains elusive in dimensions higher than one. By using the density matrix renormalization group (DMRG) algorithm, we show that in an anisotropic two-leg t-J ladder, an injected single hole behaves like a well-defined quasiparticle in the strong rung limit but undergoes a "phase transition" with the effective mass diverging at a quantum critical point (QCP) towards the isotropic limit. After the transition, the quasiparticle collapses into a loosely bound object of a charge (holon) and a spin-1/2 (spinon) accompanied by an unscreened phase string as well as a substantially enhanced binding energy between two doped holes. A phase diagram of multileg ladders is further obtained, which extrapolates the QCP towards the two-dimensional limit. The underlying mechanism generic for any dimensions is also discussed.

The Landau's Fermi liquid theory is characterized by the low-lying quasiparticle excitation that carries well-defined momentum, charge, spin, and a renormalized effective mass. The collapse of such a quasiparticle excitation will be a hallmark of a non-Fermi-liquid state. In particular, the breakdown of the quasiparticle in a form of spin-charge separation has been conjectured in the study of doped Mott insulators, notably the high-T_c cuprates [1–8]. However, no consensus has been reached yet on how a quasiparticle precisely falls into parts in such strongly correlated electron systems.

A t-J square ladder as a quasi-one-dimensional (1D) doped Mott insulator system has been intensively investigated [9–21]. Such systems are beyond a purely 1D system due to the presence of closed loops of various sizes and can be accurately studied by the DMRG numerical method [22]. Experimentally, there are also several available materials with the ladder structure [23]. Because of the peculiar quantum destructive interference in the closed paths, a DMRG study has recently revealed [20] a generic self-localization of a single hole injected into the spin ladders in the isotropic limit. It implies the failure of a conventional quasiparticle picture in a way very distinct from a purely 1D system [24].

In this paper, we focus on a two-leg t-J ladder system in which the undoped spin background remains gapped. By using DMRG, we find that for an injected hole, the quasiparticle description is restored if the ladder is in an anisotropic (strong rung) regime. Then, as the ladder anisotropic parameter is continuously tuned from strong rung coupling towards the isotropic limit, there exists a QCP, at which the quasiparticle collapses with its effective mass diverges. Subsequently the doped hole fractionalizes into a composite structure as a bound state of an incoherent holon and a deconfined spinon. The momentum distribution of the hole also exhibits a qualitative change across the QCP. The underlying microscopic mechanism responsible for the fractionalization of the hole will be discussed. Interestingly the binding energy of two holes also gets substantially enhanced after the quasiparticle collapsing. Such a QCP is further shown to persist with the increase of the leg number of the ladders, which may shed light to the

understanding of the quasiparticle collapsing and pairing in the two-dimensional (2D) doped Mott insulator.

The t-J Hamiltonian $H = H_t + H_J$ for an anisotropic two-leg ladder system is composed of four terms: $H_{t_\perp} + H_{t_\parallel} + H_{J_\perp} + H_{J_\parallel}$ given by

$$
\begin{aligned}
H_{t_\perp} &= -t_\perp \sum_{i,y=0,\sigma} (c_{i,y,\sigma}^\dagger c_{i,y+1,\sigma} + \text{H.c.}), \\
H_{t_\parallel} &= -t_\parallel \sum_{i,y,\sigma} (c_{i,y,\sigma}^\dagger c_{i+1,y,\sigma} + \text{H.c.}), \\
H_{J_\perp} &= J_\perp \sum_{i,y=0} \left(\mathbf{S}_{i,y} \cdot \mathbf{S}_{i,y+1} - \frac{1}{4} n_{i,y} n_{i,y+1} \right), \\
H_{J_\parallel} &= J_\parallel \sum_{i,y} \left(\mathbf{S}_{i,y} \cdot \mathbf{S}_{i+1,y} - \frac{1}{4} n_{i,y} n_{i+1,y} \right),
\end{aligned} \tag{1}
$$

on a two-leg ladder with the total site number $N = N_x \times N_y$ ($N_y = 2$) as sketched in Fig. 1. In Eq. (1), the summation over i along the chain direction runs over all rungs, $y (= 0,1)$ and σ are leg and spin indices, respectively. $c_{i,y,\sigma}^\dagger$ is the electron creation operator, and $\mathbf{S}_{i,y}$ is the spin operator at site (i,y). The Hilbert space is always constrained by the no-double-occupancy condition, i.e., the number operator $n_i \leqslant 1$. Here, $H_{t_\perp}$ ($H_{t_\parallel}$) and $H_{J_\perp}$ ($H_{J_\parallel}$) describe the interchain (intrachain) hole hopping and spin superexchange interaction, respectively. For simplicity, in the following we shall fix $t_\perp/J_\perp = t_\parallel/J_\parallel = 3$, or equivalently, take $t_\perp \equiv t$, $J_\perp \equiv J$, $t_\parallel \equiv \alpha t$, $J_\parallel \equiv \alpha J$ with $t/J = 3$. For the present simulation, we use $U(1)$ invariant code and set J as the unit of energy. We keep up to 4000 states in each DMRG block with around 10 to 50 sweeps, and this is proven to be enough to give excellent convergence when the truncation error is of the order of or less than 10^{-8}. Then we continuously tune α from 0 to 1 between the strong rung and isotropic limits as illustrated in Fig. 1. At half filling, the system remains spin gapped without a phase transition, and in particular, the ground state simply reduces to a direct product of spin-singlet rungs in the strong rung limit of $\alpha \to 0$ [25].
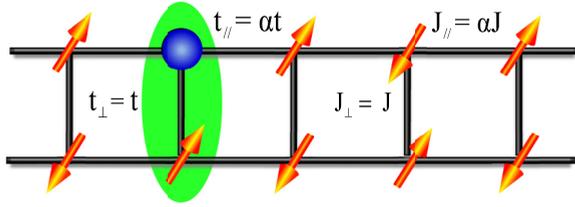
FIG. 1. (Color online) The parameters of the anisotropic t-J model on a two-leg square ladder. Here, $t_\perp = t$ ($t_\parallel = \alpha t$) and $J_\perp = J$ ($J_\parallel = \alpha J$) describe the interchain (intrachain) hopping and superexchange couplings, respectively. At $\alpha = 1$, it reduces to the isotropic limit.

Now consider the one-hole-doped case. As shown in Fig. 2 and the inset, a QCP is clearly indicated at $\alpha = \alpha_c \sim 0.7$ by the first- and second-order derivatives of the kinetic energy $\langle H_t \rangle$ over α. (Note that the derivatives of the superexchange energy $\langle H_J \rangle$ remain smooth without a singularity, which is not shown in the figure.) What we shall establish first below is that at $\alpha < \alpha_c$, the single doped hole behaves like a Bloch quasiparticle, which possesses a well-defined momentum, effective mass, charge, spin, and finite quasiparticle weight. In fact, at strong rung limit $\alpha \ll 1$, the quasiparticle behavior can be well described by a perturbation theory [26]. But beyond the critical point α_c, the quasiparticle picture of the single doped hole will break down completely.

By contrast, when two holes are injected into the gapped two-leg spin ladder, they always form a binding state in the quasiparticle collapsing regime. The pairing even persists into the quasiparticle regime with reducing binding strength, which eventually vanishes around $\alpha \sim 0.6$ as shown by the binding energy E_b in Fig. 2 (red circles). Here the binding energy is defined by $E_b \equiv E_G^{2\text{-hole}} + E_G^0 - 2E_G^{1\text{-hole}}$, where $E_G^{2\text{-hole}}$, $E_G^{1\text{-hole}}$, and E_G^0 denote the ground-state energies of the two-hole, one-hole, and undoped states, respectively.
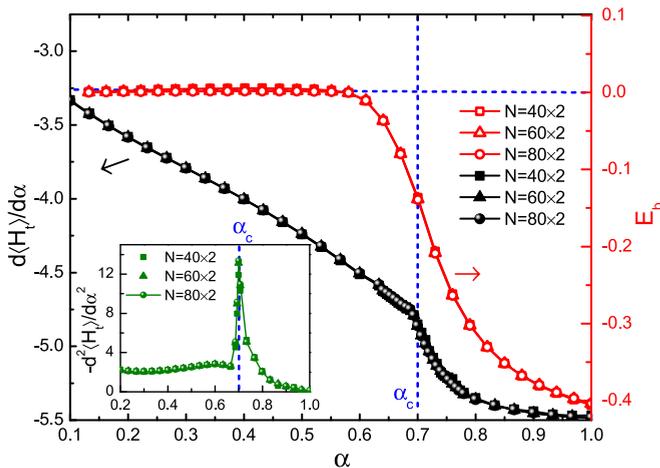

FIG. 2. (Color online) The first-order derivative of the kinetic energy $\langle H_t \rangle$ and the second-order derivative (the inset) indicate the presence of a quantum critical point at $\alpha (\equiv t_\parallel / t_\perp) = \alpha_c \sim 0.7$ (with $t_\perp / J_\perp = t/J = 3$). The two-leg ladder is also substantially enhanced at $\alpha > \alpha_c$ as shown by the binding energy E_b.

For the single hole case, a finite effective mass at $\alpha < \alpha_c$ is identified in the inset of Fig. 3(a). Here, to determine the effective mass of the charge, the two-leg ladder is made of a loop along the long chain direction with a magnetic flux Φ threading through [cf. the inset of of Fig. 3(a)]. Then the ground state energy difference between $\Phi = \pi$ and 0, i.e.,

$$\Delta E_G^{1\text{-hole}} \equiv E_G^{1\text{-hole}}(\Phi = \pi) - E_G^{1\text{-hole}}(\Phi = 0), \quad (2)$$

corresponds to the energy difference under the change of the boundary condition from the periodic to antiperiodic one for the charge (hole). If the doped hole behaves like a "Bloch quasiparticle," $\Delta E_G^{1\text{-hole}}$ is expected to be proportional to $1/N_x^2$, with the inverse of the slope m_c^* proportional to the effective mass.

As shown in Fig. 3(a), a finite m_c^* is indeed obtained at $0 < \alpha < \alpha_c$ (which diverges at $\alpha = 0$ because of the vanishing inter-rung hopping). Then m_c^* diverges again approaching the critical point α_c [cf. the inset of Fig. 3(a)]. Beyond α_c, $\Delta E_G^{1\text{-hole}}$ starts to oscillate and decay exponentially as a function of N_x as illustrated in Fig. 3(b), with the disappearance of the term proportional to $1/N_x^2$. It implies the self-localization of the doped hole [20] with the effective mass $m_c^* = \infty$ at $\alpha \geqslant \alpha_c$.

On the other hand, the effective mass can also be determined alternatively. Figure 3(c) shows the one-hole ground state energy $E_G^{1\text{-hole}}$ calculated under the fully open boundary condition. Besides a constant term, $E_G^{1\text{-hole}}$ can also be well fitted by m_s^{*-1}/N_x^2, with m_s^* essentially the same as m_c^* at $\alpha < \alpha_c$ as shown in the inset of Fig. 3(c). One finds that m_s^* also diverges at α_c. However, in contrast to m_c^*, m_s^* becomes finite again at $\alpha > \alpha_c$. Namely, in opposition to the charge part of the doped hole (holon) being localized at $\alpha > \alpha_c$, a charge-neutral gapless excitation (spinon) is still present in this regime.

The sharp contrast between m_c^* and m_s^* suggests that the quasiparticle collapses at $\alpha > \alpha_c$ by a specific form of the electron fractionalization. One may directly measure the spin-charge separation by calculating the spin-charge correlator $\langle n_i^h \cdot S_{i+r}^z \rangle$. As shown in Fig. 4(a) ($\alpha = 0.4 < \alpha_c$), the spin and charge are tightly bound together at a length scale of one lattice constant. Such a stable hole object has a well-defined mass m^* and behaves like a Bloch wave with a definite momentum. The momentum distribution 1-$n(\mathbf{k})$ of the hole is presented in the inset of Fig. 4(a). Here $n(\mathbf{k}) \equiv \sum_\sigma \langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \rangle$, which can be obtained by a Fourier transformation of $\sum_\sigma \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle$. The inset of Fig. 4(a) shows that the hole momentum distribution as a universal curve after the rescaling $k_x - k_0 \to N_x \cdot (k_x - k_0)$ with $k_0 = \pi$, indicating that the hole in the ground state possesses a well-defined momentum $(k_0, k_y = 0)$ with a finite quasiparticle spectral weight Z_0 in the thermodynamic limit.

The quasiparticle collapsing at $\alpha > \alpha_c$ is in a form of fractionalization as shown in Fig. 4(b) (at $\alpha = 1$), where the spin-charge correlator oscillates and decays much slower. Correspondingly, the quasiparticle weight $Z_0 = 0$ at $k_0 = \pi$ and the hole momentum distribution is qualitatively changed as presented in the inset of Fig. 4(b) with two new peaks emerging at $k_x = k_0 \pm \kappa$ and $k_y = 0$ with κ depending on α and t/J.

Figure 4(c) further illustrates how the quasiparticle fractionalizes. At $\alpha < \alpha_c$, the amplitude for the spin-charge separation
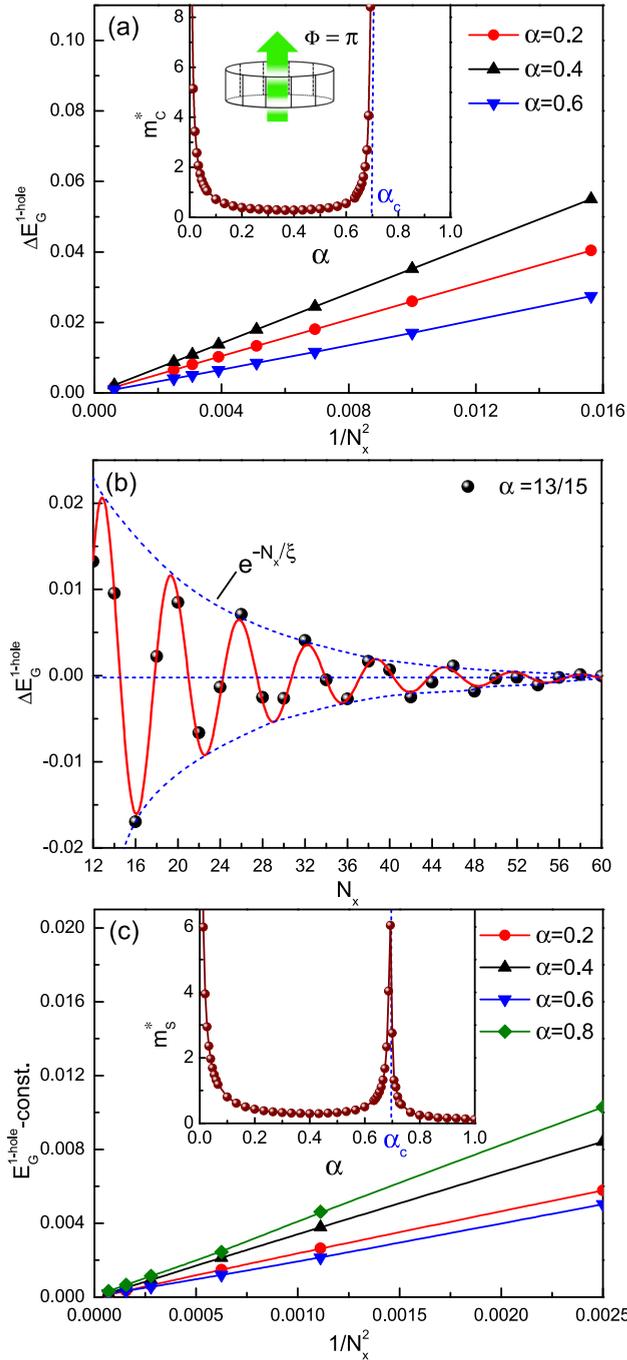
FIG. 3. (Color online) Effective mass of the quasiparticle is well defined at $\alpha < \alpha_c$ but is divergent at the quantum critical point α_c. (a) $\Delta E_G^{\text{1-hole}}$ [defined in Eq. (2)] exhibits a "free particle" behavior: $\Delta E_G^{\text{1-hole}} \propto 1/N_x^2$ in a loop of the circumference N_x (cf. the inset). The effective mass $m^* \propto m_c^*$ with $1/m_c^*$ defined as the slope of $1/N_x^2$ [shown in the inset of (a), in which m_c^* diverges at α_c]; (b) At $\alpha > \alpha_c$, $\Delta E_G^{\text{1-hole}}$ oscillates and decays exponentially with $m_c^* = \infty$ [presented in (b) is the case at $\alpha = 13/15$ with the charge localization length [20] $\xi \sim 12.6$]; (c) The one-hole ground state energy $E_G^{\text{1-hole}}$ calculated under an open boundary of length N_x. Here the slope of $E_G^{\text{1-hole}}$ (subtracted by a constant term) defines another effective mass m_s^* shown in the inset of (c), which is essentially the same as m_c^* at $\alpha < \alpha_c$. But m_c^* and m_s^* differ completely at $\alpha > \alpha_c$, suggesting the charge-spin separation (see the text).
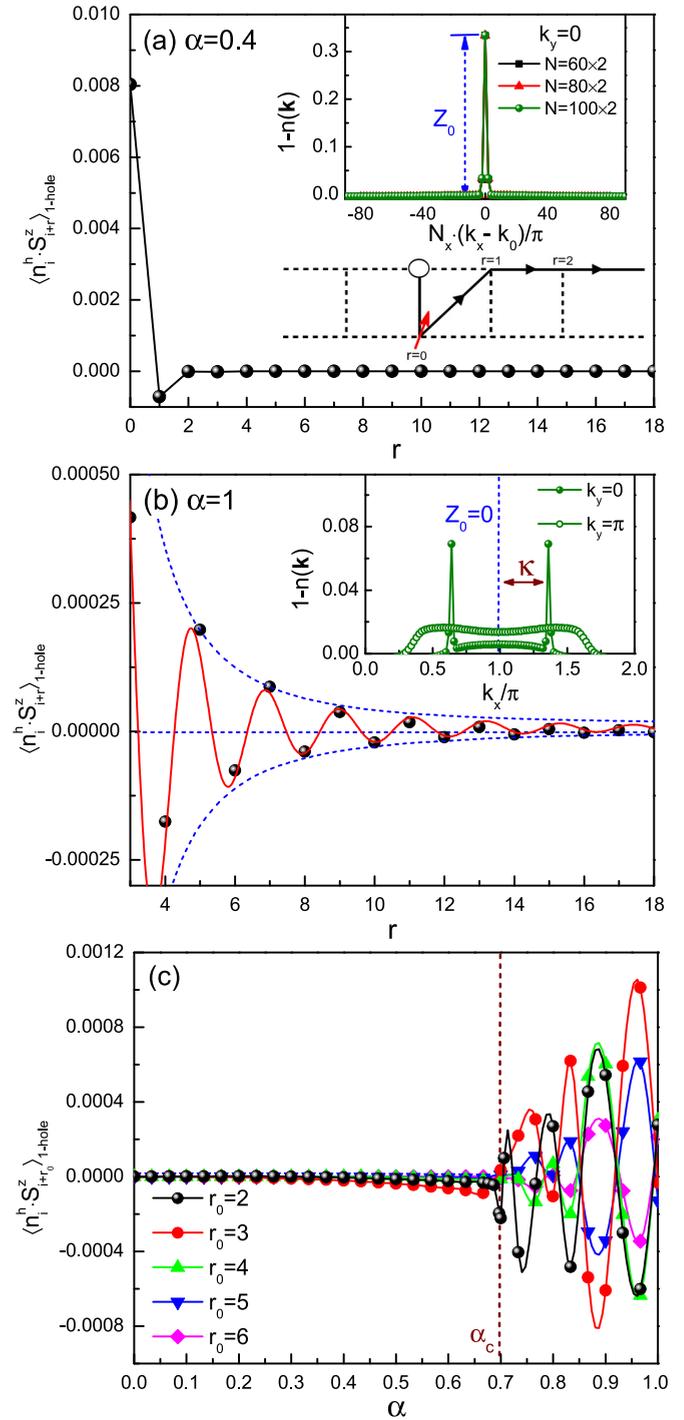
FIG. 4. (Color online) Spin-charge correlator $\langle n_i^h \cdot S_{i+r}^z \rangle$ with the labeling r defined in (a). The tight binding of the holon-spinon inside the quasiparticle is shown in (a) for $\alpha = 0.4 < \alpha_c$ with $N = 60 \times 2$. The inset of (a): the momentum distribution of the hole satisfies a scaling law: $k_x \rightarrow N_x(k_x - k_0)$, indicating a well-defined momentum at $k_0 = \pi$ with a finite spectral weight Z_0 [20]; (b) the fractionalization of the quasiparticle occurs at $\alpha > \alpha_c$ with a composite structure of loosely bound charge and spin as shown by the spin-charge correlator ($N = 60 \times 2$). The inset of (b): The momentum distribution is fundamentally changed with Z_0 vanishing at k_0 ($N = 100 \times 2$); (c) a sharp increase of the amplitude for the hole-spin separation at $r \geqslant 2$ as $\alpha \geqslant \alpha_c$.
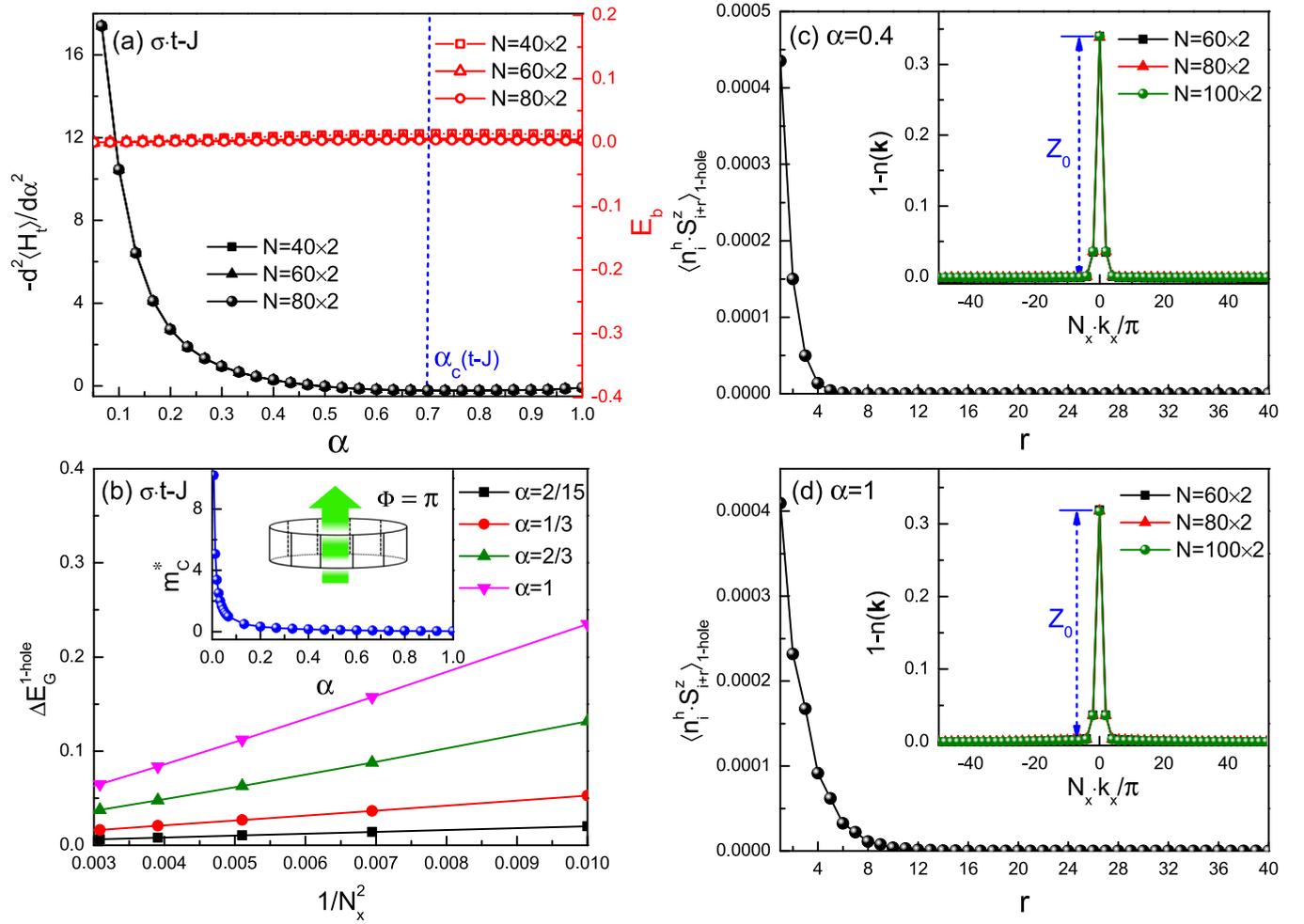
FIG. 5. (Color online) The quantum critical point α_c disappears in the $\sigma \cdot t\text{-}J$ model (see the text) with the quasiparticle description valid throughout the whole regime of α. (a) The second-order derivative of the single hole kinetic energy does not show any singularity at a finite α. Correspondingly, the two-hole binding energy remains weak similar to the quasiparticle regime in Fig. 2; (b) the effective mass determined by the slope of $1/N_x^2$ behavior of $\Delta E_G^{1\text{-hole}}$ remains smooth and finite at $\alpha > 0$ (the inset); (c) and (d): The integrity of the quasiparticle is ensured by the spin-charge binding at different α's ($N = 80 \times 2$). The insets of (c) and (d): The momentum distribution for the single hole is similar to the one in the quasiparticle regime of the $t\text{-}J$ model in Fig. 4(a). The scaling law ensures a well-defined momentum at $k_x = 0$.

distance $r \geqslant 2$ is exponentially small, implying the tight binding of the holon spinon within the quasiparticle at $r < 2$ in Fig. 4(a). But at $\alpha \geqslant \alpha_c$ a sharp rise of the amplitude at $r \geqslant 2$ indicates the emergence of a composite structure for the quasiparticle as the spin partner can now move away from the holon over a larger distance as shown in Fig. 4(b).

To understand the underlying physics of the quasiparticle collapsing, we slightly modify the hopping terms $H_{t_\perp}$ and $H_{t_\parallel}$ in Eq. (1) by introducing a sign prefactor $\sigma = \pm$ such that $c_{i\sigma}^\dagger c_{j\sigma} \to \sigma c_{i\sigma}^\dagger c_{j\sigma}$. This is a generalization of the so-called $\sigma \cdot t\text{-}J$ model in the isotropic limit, where the hopping term H_t is replaced by [20]: $H_{\sigma \cdot t} = -t \sum_{\langle ij \rangle \sigma} \sigma (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.})$. Then we can carry out the same DMRG calculation, and as clearly indicated in Fig. 5(a), the QCP α_c simply disappears. Namely, there is no more quasiparticle collapsing, and there exists only one phase continuously interpolating between the isotropic and strong rung limits. Figure 5 illustrates that the single hole moving in the gapped spin background always keeps its quasiparticle identity with a well-defined momentum at $k_x = 0$ (note that it is different from k_0 in the $t\text{-}J$ ladder case)

with a finite spectral weight, a finite effective mass m_c^*, and the spin-charge confinement. As one can see from Fig. 5(c), even in the isotropic limit of $\alpha = 1$, the hole still keeps the integrity of a Bloch quasiparticle with charge and spin tightly bound. As a matter of fact, we have checked that the same phase still persists at $\alpha \gg 1$. Furthermore, the binding energy is also substantially weakened in the whole regime [cf. Fig. 5(a)], similar to the quasiparticle regime in the $t\text{-}J$ ladder case.

Previously it has been demonstrated [20] that the sole distinction between the isotropic $t\text{-}J$ and $\sigma \cdot t\text{-}J$ models lies in the so-called phase string [27,28] associated with each path of the hole motion, which is present in the former but is precisely removed in the latter. The same proof remains true in the present anisotropic ladder case. Such a phase string represents a singular phase shift produced by the scattering between the spin background and doped charge [7,27–29] for general dimensions of bipartite lattice. Its destructive quantum interference has been previously found to lead to the localization of the doped hole in the isotropic limit $\alpha = 1$ of the $t\text{-}J$ ladder with the leg-number $N_y > 1$ [20]. The phase
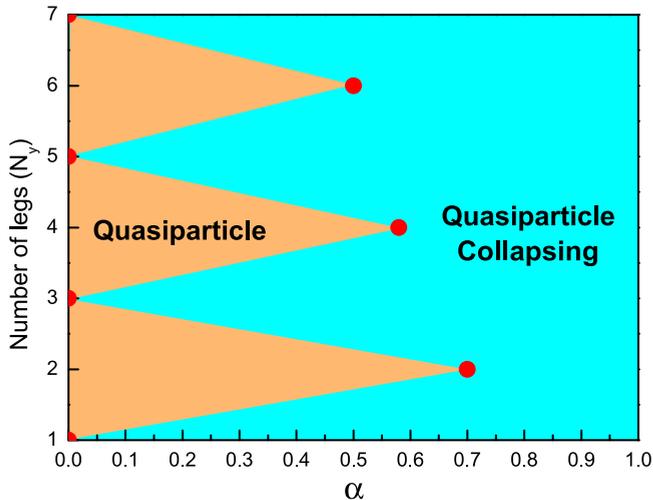
FIG. 6. (Color online) The QCP (red dot) separating the quasiparticle (orange-colored) and quasiparticle collapsing (blue-colored) regimes is shown as a function of the anisotropy parameter α for the t-J ladders of the leg number N_y from 1 to 7 (with $t/J = 3$).

string is also responsible for the strong binding found in the quasiparticle collapsing regime of the t-J model (cf. Fig. 2), as has been carefully examined in the isotropic case [21] before.

Finally, the QCP α_c is systematically calculated for the multileg t-J ladders as shown in Fig. 6. Here α_c is determined by the singularity in the ground state energy similar to that for the two-leg ladder shown in the inset of Fig. 2. Similar to the two-leg case, in the multileg ladders the horizontal chains are glued by a fixed hopping integral t and a superexchange coupling J perpendicular to the chain direction. Physically, α_c separates the nondegenerate quasiparticle state from a quasiparticle collapsing state. For an odd-leg spin ladder, the spin background always remains gapless at half filling, and generally $\alpha_c = 0^+$ is found in the single-hole state where a true spin-charge separation persists. By contrast, as our above study of the two-leg ladder has clearly shown, in the presence of a spin gap in an even-leg ladder, the singular phase string effect may get "screened" via a tight binding of the charge and spin partners to form a coherent Bloch-type quasiparticle, at least in the strong rung limit of $\alpha \ll 1$. With the reducing spin gap by increasing α or leg-number N_y, the tight binding between the holon and its backflow spinon gets weakened, eventually resulting in quasiparticle collapsing at some α_c, where the holon and spinon form a *loosely bound state* (instead of a simple spin-charge separation in the odd-leg cases) with an unscreened and irreparable phase string reemerging to accompany the motion of the hole. In fact, a finite α_c does persist in all the even-leg ladders shown in Fig. 6, which monotonically decreases with the increase of the leg numbers up to $N_y = 6$. A microscopic wave function approach to this problem will be presented elsewhere.

Note added. After the submission of the present paper, we became aware of a DMRG study of the same two-leg t-J ladder doped by one hole [30], in which the authors have confirmed the existence of $\alpha_c \sim 0.7$, the divergence of the effective mass m_s^* at α_c, and the incommensurate momentum split together with the enlarged spin-charge separation at $\alpha > \alpha_c$ found in this paper. However, we notice that the physical interpretation of the nature at $\alpha > \alpha_c$ in that paper is different from the current picture of Bloch quasiparticle collapsing. We point out that our interpretation is further supported based on some additional DMRG probes including the charge response to the inserting flux and the $\sigma \cdot t$-J model without the phase string effect, etc., which are absent in that paper.

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