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 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 composite object of a self-localized charge (holon) and a deconfined spin-1/2 (spinon), accompanied by a substantially enhanced binding energy between two holes. A phase diagram of multi-leg ladders is further obtained, which extrapolates the QCP towards the two-dimensional limit. The underlying novel mechanism generic for any dimensions is also discussed.

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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$^{9–21}$. Because of the peculiar quantum destructive interference in the closed paths, a DMRG study has recently revealed$^{22}$ 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$^{23}$.

In this Letter, 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 made of a self-localized 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

$$H_{t\perp} = -t_{\perp}\sum_{i,y=0}^{n_y} (c_{i,y,\sigma}^\dagger c_{i+1,y,\sigma} + h.c.),$$
$$H_{t\parallel} = -t_{\parallel}\sum_{i,y=0}^{n_y} (c_{i,y,\sigma}^\dagger c_{i+1,y,\sigma} + h.c.),$$
$$H_{J\perp} = J_{\perp}\sum_{i,y=0}^{n_y} (S_{i,y} \cdot S_{i+1,y+1} - \frac{1}{4} n_{i,y} n_{i+1,y+1}),$$
$$H_{J\parallel} = J_{\parallel}\sum_{i,y=0}^{n_y} (S_{i,y} \cdot S_{i+1,y} - \frac{1}{4} n_{i,y} n_{i+1,y}).$$

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 $\sigma$ are leg and spin indices, respectively. $c_{i,y,\sigma}$ is the electron creation operator and $S_{i,y}$ the spin operator at site $(i,y)$. The Hilbert space is always constrained by the no-double-occupancy condition, i.e., the number operator $n_i \leq 1$. Here, $H_{t\perp}$ ($H_{t\parallel}$) and $H_{J\perp}$ ($H_{J\parallel}$) describe the

![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 inter-chain (intra-chain) hopping and super-exchange couplings, respectively. At $\alpha = 1$, it reduces to the isotropic limit.](image-url)
inter-chain (intra-chain) 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 $t/J = 3$. Then we continuously tune $\alpha$ 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 $\alpha \to 0$.[5]

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 $\langle H_0 \rangle$ over $\alpha$. (Note that the superexchange energy $\langle H_J \rangle$ remains smooth, 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.[25] But beyond the critical point $\alpha_c$, the quasiparticle picture of the single doped hole will break down completely.

By contrast, such a peculiar “phase transition” in the single hole ground state disappears once two holes are injected into the gapped two-leg spin ladder. In the latter case, the bound state is present smoothly in both regimes as shown by the binding energy $E_b$ in Fig. 2 (red circles). However, as clearly shown in Fig. 2 the binding energy gets substantially enhanced in the quasiparticle collapsing regime of $\alpha > \alpha_c$. Here the binding energy is defined by $E_b = E_G^{\text{2-hole}} + E_G^{\text{0-hole}} - 2E_G^{\text{1-hole}}$, where $E_G^{\text{2-hole}}$, $E_G^{\text{1-hole}}$, and $E_G^{\text{0-hole}}$ denote the ground-state energies of the two-hole, one-hole, and undoped states, respectively.

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 $\Phi$ threading through [cf. the inset of of Fig. 3(a)]. Then the ground state energy difference between $\Phi = \pi$ and 0, i.e.,

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

corresponds to the energy difference under the change of the boundary condition from the periodic to anti-periodic one for the charge (hole). If the doped hole behaves like a “Bloch
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\delta E_{E_{\text{G}}}^{1-\text{hole}} = \frac{E_{\text{G}}(1,0,\ldots,1) - E_{\text{G}}(0,1,\ldots,0)}{N_{\alpha}^2} \propto \frac{1}{N_{\alpha}^2} \]

The effective mass \(m_{\alpha}^*\) is expected to be proportional to \(1/N_{\alpha}^2\), with the inverse of the slope \(m_{\alpha}^*\) proportional to the effective mass.

As shown in Fig. 3 (a), a finite \(m_{\alpha}^*\) is indeed obtained at \(0 < \alpha < \alpha_c\) (which diverges at \(\alpha = 0\) because of the vanishing inter-rung hopping). Then \(m_{\alpha}^*\) diverges again approaching the critical point \(\alpha_c\) [cf. the inset of Fig. 3 (a)]. Beyond \(\alpha_c\), \(\delta E_{E_{\text{G}}}^{1-\text{hole}}\) starts to oscillate and decay exponentially as a function of \(N_{\alpha}\) as illustrated in Fig. 3 (b), with the disappearance of the term proportional to \(1/N_{\alpha}^2\). It implies the

self-localization of the doped hole with the effective mass \(m_{\alpha}^* = \infty\) at \(\alpha \geq \alpha_c\).

On the other hand, the effective mass can be also determined alternatively. Fig. 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 be also well fitted by \(m_{\alpha}^*-1/N_{\alpha}^2\), with \(m_{\alpha}^*\) essentially the same as \(m_{\alpha}^*\) at \(\alpha < \alpha_c\) as shown in the inset of Fig. 3 (c). One finds that \(m_{\alpha}^*\) also diverges at \(\alpha_c\). However, in contrast to \(m_{\alpha}^*\), \(m_{\alpha}^*\) becomes finite again at \(\alpha > \alpha_c\). Namely, in opposite 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 \(m_{\alpha}^*\) and \(m_{\alpha}^*\) 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 \(\langle n_i^h \cdot S_j^z \rangle\). 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 \(1-n(k)\) of the hole is presented in the inset of Fig. 4 (a). Here \(n(k) \equiv \sum_{\langle i,j \rangle} \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle \), which can be obtained by a Fourier transformation of \(\sum_{\langle i,j \rangle} \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle \). The inset of Fig. 4 (a) shows that the hole momentum distribution as a universal curve after the rescaling \(k_{x} \rightarrow k_{x} - k_{0} \rightarrow N_{\alpha} (k_{x} - k_{0})\) 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 clearly shown in Fig. 4 (b) (at \(\alpha = 1\)), where the spin-charge correlator oscillates and decays in a power law fashion. Corresponding, the quasiparticle weight \(Z_{0} = 0\) 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 \(\kappa\) depending on \(\alpha\) and \(t/J\).

Figure 4 (c) further illustrates how the quasiparticle fractionalizes. At \(\alpha < \alpha_c\), the amplitude for the spin-charge separation distance \(r \geq 2\) is exponentially small, implying the tight-binding of the holon-spinon within the quasiparticle at \(r < 2\) in Fig. 4 (a). But at \(\alpha \geq \alpha_c\), a sharp arise of the amplitude at \(r \geq 2\) indicate the emergence of a composite structure for the quasiparticle as the spin partner can now move away from the holon, albeit in a power-law fashion as shown in Fig. 4 (b).

To understand the underlying physics of the quasiparticle collapsing, we slightly modify the hopping terms \(H_{1\alpha}\) and \(H_{\text{tr}}\) in Eq. (1) by introducing a sign prefactor \(\sigma = \pm\) such that \(c_{i\sigma}^\dagger c_{j\sigma} \rightarrow \sigma c_{i\sigma}^\dagger c_{j\sigma}\). This is a generalization of the so-called \(\sigma-t-J\) model in the isotropic limit, where the hopping term \(H_{\text{tr}}\) is replaced by \(H_{\text{tr}, \sigma} = -t \sum_{\langle i,j \rangle} \sigma \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle + h.c.\). Then we can carry out the same DMRG calculation, and as clearly indicated in Fig. 5 (a), the QCP \(\alpha_c\) 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 \( t-J \) ladder case) with a finite spectral weight, a finite effective mass \( m^* \), 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 \( t-J \) ladder case.

Previously it has been demonstrated\(^{20} \) that the sole distinction between the isotropic \( t-J \) and \( \sigma-t-J \) models lies in the so-called phase string\(^{22,23} \) 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\(^{22,23} \) for general dimensions of the 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 \( t-J \) ladder with the leg-number \( N_y > 100 \). The phase 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\(^{20} \) before.

Finally, the QCP \( \alpha_c \) is systematically calculated for the multi-leg \( t-J \) ladders as shown in Fig. 6. Here \( \alpha_c \) sep-
arates the non-degenerate quasiparticle state and the spin-charge composite state with infinite degeneracy associated with spontaneous translational-symmetry breaking, i.e., the charge (hole) self-localizing. 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. 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. In fact, a finite $\alpha_c$ does persist in all the even-leg ladders shown in Fig. 6 which monotonically decreases with the increase of the leg numbers up to $N_y = 6$. With the reducing spin gap by increasing $\alpha$ or leg-number $N_y$, the confinement between the holon and its backflow spinon gets weakened, eventually resulting in quasiparticle collapsing at some $\alpha_c$, where an unscreened and irreparable phase string reemerges to accompany the motion of holon. A microscopic wave function approach to this problem will be presented elsewhere.

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