One Hole in the Two-Leg t-J Ladder and Adiabatic Continuity to the Noninteracting Limit

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One hole in the two-leg t-J ladder and adiabatic continuity to the non-interacting limit

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We have carried out density-matrix-renormalization group (DMRG) calculations for the problem of one doped hole in a two-leg $t-J$ ladder. Recent studies have concluded that exotic "Mott" physics — arising from the projection onto the space of no double-occupied sites — is manifest in this model system, leading to charge localization and a new mechanism for charge modulation. In contrast, we show that there is no localization and that the charge density modulation arises when the minimum in the quasiparticle dispersion moves away from π. Although singular changes in the quasiparticle dispersion do occur as a function of model parameters, all the DMRG results can be qualitatively understood from a non-interacting "band-structure" perspective.

A strongly correlated quantum system is one in which the interactions are at least comparable to the kinetic energy, so weak-coupling perturbative approaches cannot be justified. However, a key question is – under what circumstances does the behavior of such systems extrapolate smoothly to the weakly interacting limit so that, at least at the phenomenological level, weak coupling intuitions can still be applied? There are certainly forms of broken symmetry, such as charge-density wave order in more than 1D, which are at the very least unnatural at weak coupling, and there can be still more exotic phases, especially those that support topological order and fractionalization, which have no weak-coupling analogues. What about the important case of a doped Mott insulator? It has been argued by many authors that there is an additional quantity, sometimes referred to as "Mottness", which through the effect of the constraint of no double-occupancy produced by a strong local "Hubbard U," can invalidate the quasiparticle picture and preclude the adiabatic continuation to the weakly interacting reference state that underlies Fermi liquid theory.

The idea that the quasiparticle picture fails qualitatively has gained strong support from a set of papers by Zhu *et al*[1–4], in which extensive numerical experiments have been carried out using the density matrix renormalization group (DMRG)[5] on a set of $t-J$ ladders. It has long been thought that the undoped two-leg $t-J$ ladder is adiabatically related to a band insulator, and a number of early exact diagonalization[6] and quantum Monte Carlo[7] studies supported the idea that doped holes form conventional quasiparticles. In striking contrast, Zhu *et al* reported that a doped hole in a two leg ladder *localizes* at large length scales, *a finding that is incompatible with Bloch's theorem for any quasiparticle state.* Similar localization was reported on three and four leg systems, although the data is less extensive. Zhu *et al* proposed an explanation for this behavior based on considerations of "hole phase-strings" and a new type of "Weng statistics." It has been further proposed,[8] that this new paradigm can account for a wide range of phenomena in doped Mott insulators, including stripe formation in the cuprates.

In this paper, we have focussed on the two-leg $t-J$ ladder with one doped hole. We have carried out DMRG calculations to extract the ground-state properties of ladders of length up to $L = 1000$, and time-dependent DMRG[9–11] (tDMRG) calculations on ladders up to $L = 120$ to obtain unprecedentedly complete information concerning the dynamical one-hole Green function, G. Following Zhu *et al* we have considered a range of values of the parameter α, the ratio of the hopping matrix elements and the exchange couplings on the legs and the rungs of the ladder. In contrast to them, we find that the one hole state is never localized. On the other hand, we corroborate their discovery that a notable change in the character of the one-hole state occurs at a critical value of $\alpha = \alpha_c \approx 0.68$; in particular the quasiparticle effective mass diverges as $\alpha \to \alpha_c$. However, this singular behavior does not imply the existence of a phase transition, as changes in the properties of a single doped hole do not reflect changes in the thermodynamic state of the system. Indeed, we show directly from the structure of G that the quasiparticle is well defined for α on both sides of α_c, that there is no "spin-charge separation," and that the quasiparticle weight, $Z(\alpha)$, is always substantial. Indeed, all the properties of the low energy one hole states can be adiabatically related to those of a single hole in a non-interacting "band" insulator – the singular changes reflect a shift of the ground-state sector from a Bloch wave vector $k = \pi$ for $\alpha < \alpha_c$ to $k = k_0(\alpha) < \pi$ for $\alpha > \alpha_c$. The divergent effective mass dramatically reflects a point at which the minimum of the quasihole dispersion, $\varepsilon(k)$, shifts away from π.

In this paper we will study the 2-leg $t-J-\alpha$ model

$$H = -\sum_{\langle i,j\rangle,\sigma} t_{ij} c^\dagger_{i,\sigma} c_{j\sigma} + \sum_{\langle i,j\rangle} J_{ij}(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j). \quad (1)$$

Here $\langle ij\rangle$ indicates nearest-neighbor sites with $t_{ij} = t$ and $J_{ij} = J$ on the rungs, and $t_{ij} = \alpha t$ and $J_{ij} = \alpha J$ on the legs, $c^\dagger_{j,\sigma}$ creates an electron on site j with spin polarization σ, the spin operator on site j is $\mathbf{S}_j$, the charge is $n_j = \sum_\sigma c^\dagger_{j,\sigma} c_{j,\sigma}$, and the action of the Hamiltonian is restricted to the Hilbert space with no doubly occupied sites, $n_j = 0$, 1. The index $i = (l_x, l_y)$ with $l_y = 1$ and 2 denoting the two legs and l_x runs from 1 to L. Here we set $J/t = 1/3$ and study a range of α values. This is the same realization of the $t - J$ model that was studied by Zhu *et al.*. They gave a quasiparticle interpretation to their results for $\alpha < \alpha_c \approx 0.7$, but they identified a transition at $\alpha = \alpha_c$, such that, among other anomalies, for $\alpha > \alpha_c$ and ladders of length $L > 100$, they reported localization of the charge in a region of width $\xi \sim 100 < L$.

Our ground state DMRG calculations were fairly standard, the main exception being that an unusually large number of sweeps were needed for the one hole ground states. All the calculations reported here were performed using the ITensor library (http://itensor.org). A sufficient number of states, roughly 200-400 for the one hole case, were kept to limit the truncation error per step to $\sim 10^{-10}$. For each system, first the ground state for the undoped system was obtained, with four sweeps giving high-accuracy convergence, and this matrix product state $|\phi\rangle$ was stored. We then applied the operator $c_{j_0\downarrow}$, where j_0 is a site at the center of the system, creating a one hole state with the hole localized in the center. Sweeps were then carried out, resulting in a set of ever better approximate one-hole groundstates, $|\psi(s)\rangle$, where s indicates the number of sweeps. At each sweep we made diagonal measurements of the energy and the density on each site, as well as off-diagonal measurements of the hole amplitude, $F(j,s) = \langle\phi|c^\dagger_{j\downarrow}|\psi(s)\rangle$.

Figure 1(a) shows the spreading of the density in a 1000×2 system versus sweep with $\alpha = 1$. Here the hole density for site j is $n_h(j) \equiv 1 - n_j$; the figure shows the rung hole density $\bar{n}_h(l_x) = \sum_{l_y} n_h(l_x, l_y)$. The density continues to spread out as the sweeps progress. (Note, to facilitate comparisons with previous results, we have eschewed tricks that could be used to accelerate convergence to the true ground state, such as starting with a delocalized hole as the initial state.) The inset in Fig. 1(a) shows the full width at half-maximum (FWHM) of the charge density profile for $\alpha = 1$ ladders of different lengths L. This value of α is greater than α_c and places the system in the region where Zhu *et al.* reported localization. However, as seen in the inset, we find that the FWHM scales as L. The saturation of the FMHW reported by Zhu *et al.* in Fig. 2c of Ref [4] appears to be an artifact of their calculation which arises from limiting the number of DMRG sweeps. In fact, as shown in Fig. 4c of [4], they, too, find the charge density extends over a 200x2 ladder when the sweep number is increased.

Figure 1(b) shows a correlation function $\langle S^z(l_x, l_y) n_h(j_0)\rangle$ which measures the spin profile when a dynamic hole is on site j_0; here $j_0 = (200, 2)$ on a 400×2 ladder. With this correlation function shown on a log scale as a function of distance l_x along the ladder, the exponential confinement of the spin and charge is apparent in the linear l_x dependence. A linear fit gives a decay length of $\xi = 3.14$ for $\alpha = 1$; this matches closely with previous results of 3.19(1) for the spin-spin correlation length in the undoped ladder.[12] (In contrast, Zhu *et al.* reported that a similar correlation function decayed as a power law for $\alpha > \alpha_c$.)

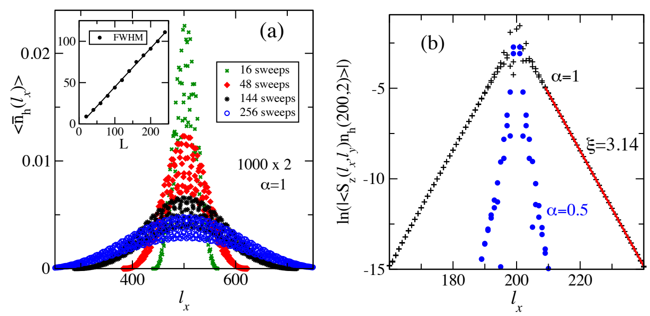

FIG. 1: (a) The density on each site for $\alpha = 1$ on the central portion of a 1000×2 system for the indicated number of sweeps. The inset shows the full width at half maximum of the density on a set of smaller lattices which were converged in the number of sweeps. (b) A correlation function which measures spin-charge correlations, showing that the spin degrees of freedom are exponentially localized close to a dynamic hole, for $\alpha = 0.5$ and $\alpha = 1$. For $\alpha = 1$, the red line shows a linear fit to the data.

To obtain the one particle spectral function, instead of evolving $|\psi\rangle$ with DMRG sweeps, we evolve it in real time, obtaining the state

$$|\psi(t)\rangle = \exp(-itH)c_{j_0,\downarrow}|\phi\rangle \quad (2)$$

After each time-step, the Green function,

$$G(j,t) = \langle\phi|c^\dagger_{j\downarrow}|\psi(t)\rangle e^{iE_0 t} \ , \quad (3)$$

(defined here without the usual i prefactor) was measured for all sites j, where E_0 is the ground-state energy of the undoped ladder. As time evolves, the wavepacket spreads out. We always stop the simulation at a time t_{max} before the packet reaches the edges of the system. Thus any finite size effects are completely negligible, arising only from the undoped state, which has a correlation length that is very small compared to L. Other sources of error are the finite t_{max}, finite truncation error, and finite size of the time steps. Using time steps $\tau = 0.05 - 0.1$, we found the time step error was small enough to have no visible effects on any of the figures below. To measure and control the other two errors, we varied the number of states kept (up to $m = 2000$) and the maximum time (up to $t_{\max} = 100$). Any errors in the results we show primarily appear as slight broadenings of the spectra, and have no impact on our conclusions. Very high quality spectral functions have been obtained with tDMRG on long spin chains[13], and tDMRG has been used for short times on 10×2 ladders[14]; our high-resolution spectra for long ladders appear to set a new benchmark.

The ladder is symmetric under reflection symmetry which interchanges the two legs; correspondingly, the one-hole states can be classified by their symmetry, $\Lambda = \pm 1$, under reflection. Similarly, the Bloch wave-number is a good quantum number. Thus, to interpret the results physically, we perform the Fourier transform of $G(j,t)$

with respect to time (using $G(j,-t) = G(j,t)^*$) and position along the ladder, projected onto the space of states of a given reflection symmetry using both linear prediction[13] and windowing to deal with a finite $t_{\max}$. The real part of this quantity is the spectral function $A(k,\omega)$, which is shown for $\Lambda = +1$ in Fig. 2(a) for the case $\alpha = 1$. The Supplementary Information section contains a further discussion of the tDMRG and figures of $A(k,\omega)$ for more values of α[15].

The spectral weight is characterized by a sharply defined dispersing pole separated by a gap of order J from a quasi-particle-magnon continuum. For $\alpha = 1$, the minimum in the quasi-particle dispersion occurs at $k_0 \approx 2.01 = 0.640\pi$. A slice of the spectral weight for $\alpha = 0.7$ (just above $\alpha_c \approx 0.68$) at $k_0 \approx 2.85 = 0.907\pi$ is plotted versus ω in Fig. 2(b). The dispersion of the pole in the quasi-particle spectrum versus k for several values of α is shown in Fig. 2(c). As α increases beyond α_c , k_0 moves away from π and at large values of α approaches $\pi/2$.

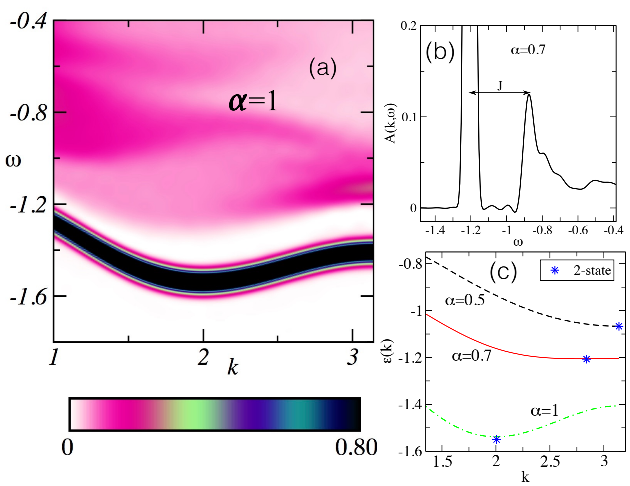

FIG. 2: (a) Spectral weight function $A(k,\omega)$ in the ground-state ($\Lambda = +1$) reflection parity sector for the t-J ladder with $\alpha = 1$, obtained with tDMRG color indicating the value of $A(k,\omega)$. We work in energy units where $t = 1$. (Results for odd reflection parity, $\Lambda = -1$, are shown in the Supplemental Section.) (b) $A(k,\omega)$ near the quasiparticle peak for $\alpha = 0.7$ at $k_0/\pi = 0.907$. The gap to the start of the continuum spectrum is of order J. (c) Quasiparticle dispersions for $\alpha = 0.5, 0.7, 1.0$, obtained from tDMRG. The stars show the values of k_0 and ε_0 obtained from separate ground state DMRG calculations.

For a given value of α, the minimum hole energy ε_0 and the corresponding wave vector k_0 can be determined from the dispersion of the peak in $A(k,\omega)$. Alternatively, for a given value of α, the energy ε_0 and wave vector k_0 can be determined directly from our ground state DMRG calculations. The energy minimum ε_0 for a given value of α is equal to the difference in the one hole and zero hole ground state energies. The wave vector k_0 associated with the one-hole ground state can be determined from the peak in the spatial Fourier transform of $F(j,s)$, which sharpens as the sweep number s increases. Plots of ε_0 and k_0 versus α are shown in Fig. 3.

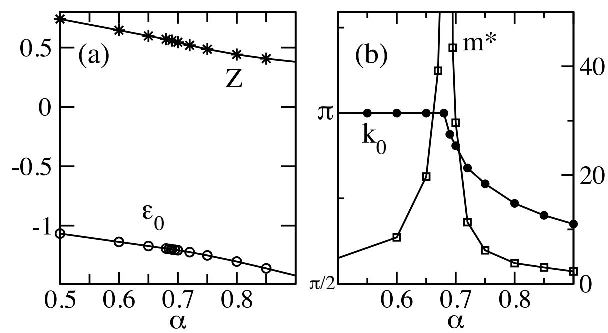

FIG. 3: The one quasi-hole properties as a function of α: The figure shows (a) Z and ε_0, and (b) k_0 and m^*. These results were obtained from 400×2 systems from measurements as the hole spread out with successive sweeps.

Similarly, while m^* can be extracted from the curvature of the quasi-particle dispersion around k_0 and Z can be obtained from a frequency integration of $A(k_0,\omega)$, both of these quantities can be directly determined with higher accuracy from the ground state DMRG calculations. An estimate of the quasi-particle spectral weight Z is given by

$$Z(s) = \sum_j |F(j,s)|^2 \qquad (4)$$

We find that this estimate converges very rapidly with the number of sweeps s, much more rapidly than the hole spreads out. As the DMRG sweeps continue, the energy E of $|\psi(s)\rangle$ converges towards that of the one-hole ground state with a correction that varies as $(8m^*\langle x^2\rangle)^{-1}$. Here, $\langle x^2\rangle$ is the variance of the position of the hole, determined from $\langle \bar{n}_h(l_x)\rangle$. By plotting E versus $\langle x^2\rangle^{-1}$, with each point corresponding to a different sweep, one can obtain an estimate of m^*. In addition, one can increase the accuracy of the estimate for Z for the infinite ladder by extrapolating Z versus $\langle x^2\rangle^{-1}$. For $\alpha = 1$, for example, we obtain $Z = 0.34067(1)$. Plots of Z and m^* are shown in Fig. 3. As seen in this figure, there is a sharp change in the quasi-particle character that occurs at $\alpha_c = 0.68$. There are kinks in the slopes of ε_0, k_0 and Z and the curvature of the quasi-particle dispersion vanishes giving rise to a divergence in the effective mass. The shift in k_0 away from π gives rise to the oscillations in the charge density, as has been previously noted by Zhu *et al*, which are found to occur at wave-number $2k_0$.

Since the one hole state has a well defined quasi-particle spectral weight, many properties that are measurable in numerical experiments on systems with large but finite L can be understood in terms of the simpler problem of one-hole on a 2-leg band insulator. Central to this understanding is the quasi-particle dispersion relation which determines the values of $k = \pm k_0$ at which

$\varepsilon(k)$ is minimized, and the dependence of the hole-energy near this point, $\varepsilon(k) = E_0 + \varepsilon_0 + (k-k_0)^2/2m^\star + \ldots$, where $m^\star$ is the effective mass. In order to minimize its zero-point energy on a ladder of large but finite length L, the one-quasiparticle ground-state will always spread to fill the extent of the ladder,

$$\psi_L(n,\tau) \sim \sin(\pi n/L)\cos(k_0 n - \theta), \tag{5}$$

where $\theta = k_0 L/2$. The minimum in the ground state energy of the one hole state is

$$\varepsilon(L) = E_0 + \varepsilon_0 + \pi^2/(2m^\star L^2) + \ldots. \tag{6}$$

Since integrating out the gapped spin degrees of freedom inevitably renormalizes the bare dispersion, for comparison purposes we consider a non-interacting model with band structure

$$E(k) = -\Lambda t_\perp - 2t_\parallel \cos(k) - 2t'_\parallel \cos(2k) \tag{7}$$

in which $\Lambda = \pm 1$ correspond to the valence and conduction bands, respectively, all the t's are assumed non-negative and the rung hopping parameter $t_\perp$ to be sufficiently large compared to the near-neighbor and next-near-neighbor leg hopping parameters $t_\parallel$ and $t'_\parallel$ that the undoped system has an insulating gap. This dispersion is similar to that shown in Fig. 2c. The parameter that plays a role analogous to α is $\tilde\alpha \equiv 4t'_\parallel/t_\parallel$; for $0 \le \tilde\alpha \le 1$, the top of the valence band occurs at $k = \pi$, while for $\tilde\alpha > 1$, the top of the valence band occurs at $k = \pm k_0$ where $\cos(k_0) = -1/\tilde\alpha$. The critical dependences of $\varepsilon_0 = -E(k_0)$, k_0 and m^* on $\tilde\alpha$ can be readily derived from the band dispersion Eq. (7).

$$\frac{[\varepsilon_0 + t_\perp]}{t_\parallel} = \begin{cases} -(4-\tilde\alpha)/2 & \text{for } \tilde\alpha < 1 \\ -(2+\tilde\alpha^2)/2\tilde\alpha & \text{for } \tilde\alpha > 1 \end{cases} \tag{8}$$

$$\frac{1}{t_\parallel}\frac{d\varepsilon_0}{d\tilde\alpha} = \begin{cases} 1/2 & \text{for } \tilde\alpha < 1 \\ (2-\tilde\alpha^2)/2\tilde\alpha^2 & \text{for } \tilde\alpha > 1 \end{cases} \tag{9}$$

$$\pi - k_0 = \begin{cases} 0 & \text{for} \quad \tilde\alpha < 1 \\ \sqrt{2(\tilde\alpha-1)/\tilde\alpha} & \text{for} \quad 1 \gg (\tilde\alpha - 1) > 0 \\ \pi/2 - 1/\tilde\alpha & \text{for} \quad \tilde\alpha \gg 1 \end{cases} \tag{10}$$

and

$$m^* = \frac{1}{2t_\parallel}\begin{cases} [1-\tilde\alpha]^{-1} & \text{for } \tilde\alpha < 1 \\ \tilde\alpha(\tilde\alpha^2-1)^{-1} & \text{for } \tilde\alpha > 1 \end{cases} \tag{11}$$

The qualitative features observed in the evolution of the one-hole state of the $t-J-\alpha$ model as a function of α are reflected in the band model as a function of $\tilde\alpha$. i) The one-hole energy ε_0 has a non-analytic change in slope at $\tilde\alpha = \tilde\alpha_c$ given by Eq. [9]. ii) The vector $k_0(\tilde\alpha)$ has a square-root singularity at $\tilde\alpha = \tilde\alpha_c$ as given by Eq. [10], and $2k_0$ determines the oscillations of the charge density. iii) The effective mass $m^*(\tilde\alpha)$ diverges linearly upon approaching $\tilde\alpha_c$ from both sides as given in Eq. [11].

A formal relation between the strongly and weakly interacting models can be established through adiabatic continuation. Here, we define a multi-parameter $t-J$-Hubbard model Hamiltonian (given explicitly in Eq. (1) of the Supplemental material) that in one limit is equivalent to the $t-J-\alpha$ model of Eq. 1, and in another limit represents a non-interacting band-insulator, with the band structure given in Eq. (7). For all values of parameters, this Hamiltonian respects all the symmetries of the problem, including time-reversal, lattice translational, and mirror symmetries. Adiabtic continuity is established between the two limiting models if there exists a path in parameter space such that the gap (at least within subspaces defined by irreducible representations of the symmetry group) is everywhere non-zero. Our DMRG results establish that there is no gap-closing and so no barrier to adiabatic continuity upon reducing the model to one of decoupled rungs in the $\alpha = 0$ limit. In this limit the interactions can be adiabatically set to 0, again without any gap closures. Finally, in the solvable non-interacting limit, we restore the hopping matrix elements along the ladder, $t_\parallel$ and $t'_\parallel$, still without encountering any gap closures. (The final two steps are readily studied analytically.) This analysis constitutes a proof that the low energy one-hole states of the $t-J-\alpha$ model are adiabatically connected to those of a non-interacting band insulator which holds regardless of the value of α in the entire range we have studied.

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