Localization in a \( t-J \) type ladder with translational symmetry

Rong-Yang Sun,\(^1\) Zheng Zhu,\(^2\) and Zheng-Yu Weng\(^1,3\)

\(^1\)Institute for Advanced Study, Tsinghua University, Beijing, 100084, China
\(^2\)Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
\(^3\)Collaborative Innovation Center of Quantum Matter, Tsinghua University, Beijing 100084, China

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An explicit spatial localization of a hole is shown in a two-leg \( t-J \) ladder in the presence of a staggered chemical potential, which still retains a translational symmetry, by density matrix renormalization group method. Delocalization can be recovered in the following cases, where either the hidden phase string effect is turned off or a finite next-nearest-neighbor hopping \( t' \) is added to sufficiently weaken the phase string effect. In addition, two holes are always delocalized by forming a mobile bound pair, in contrast to the localized single holes, which points to a novel pairing mechanism as one of the essential properties of a doped Mott insulator.

\[ H = H_1 + H_2 + H_{\mu}, \]

where the hopping term \( H_1 = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + h.c. \) and the superexchange term

\[ H_J = J \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j) \]

are the same as the \( t-J \) model, where \( c_{i\sigma} \) is the annihilation operator of the electron, \( S_i \) is the spin operator, and \( n_i \) is the local electron density operator which is always subjected to the no-double-occupation condition, i.e., \( n_i \leq 1 \). The model is defined in a two-leg ladder of square lattice with total number of sites \( N = N_x \times N_y \) (with \( N_y = 2 \) \([20]\)), and is further in the presence of a chemical potential term \( H_{\mu} = \sum_i \mu_i n_i \), with \( \mu_i = \mu_a \) or \( \mu_b \) alternating for the odd and even rungs along the one-dimensional chain direction. In the following, we shall mainly fix \( \mu_a = t \) and \( \mu_b = 0 \) in the most calculations, but a continuous variation of \( \mu_a \) will be also discussed.

As a comparative study, we also modify the above \( t-J \) like model into the so-called \( \sigma \cdot t-J \) like model, in which only the hopping term is changed from \( H_1 \) to \( H_{\sigma-t} = -t \sum_{\langle ij \rangle, \sigma} \sigma c_{i\sigma}^\dagger c_{j\sigma} + h.c. \) by inserting a sign

\[ \sigma = \pm 1 \]
FIG. 1. (Color online) The spatial distribution of the hole density defined on the rung labelled by $x$ in a two-leg ladder of $N = N_x \times 2$ with $N_x = 500$ under an open boundary condition. Main panel: a hole is spatially localized in the central area in a $t$-$J$ model with staggered chemical potentials of $\mu_a = t$ and $\mu_b = 0$, whereas it is always delocalized in the $\sigma \cdot t$-$J$ model with the same chemical potentials. Inset: the delocalized density profiles for two doped holes in both models.

$\sigma = \pm 1$, which can be proven [18, 20] to precisely compensate the phase string sign structure hidden in the original $t$-$J$ model even in the presence of $H_\mu$. The phase string effect is caused by the nearest-neighbor hopping of the hole, but will get “scrambled” by introducing a sufficiently large next-nearest-neighbor hopping term, $H_\mu = -t' \sum_{i} (\langle i \rangle \sigma \langle i+1 \rangle \sigma + h.c.)$, in the $t$-$t'$-$J$ model [25].

In the following DMRG calculation, we fix $t'/J = 3$ as the same in [18, 20, 26] and focus on the $\mu_a = t$ and $\mu_b = 0$ to study the ground states of the one hole and two hole doped cases. At $\mu_a = \mu_b = 0$, we recover the isotropic 2-leg $t$-$J$ ladder results [18, 20, 26]. In the simulation, we choose an open boundary condition (OBC) along the chain direction and keep 300 to 500 states to control the truncation error up to the order of $10^{-11}$ for one hole doped case and $10^{-10}$ for the two hole case with 200 to 3000 sweeps.

**Hole density distribution.**—Define the hole density per rung by summing up two sites of each rung labelled by $x$:

$$n_h^x \equiv \sum_{i \in x} (1 - n_i).$$ (1)

Its distribution is presented in the main panel of Fig. 1 for the single-hole ground states of the $t$-$J$ (red dots) and $\sigma \cdot t$-$J$ (blue dots) ladders in the presence of an alternating chemical potential, $\mu_a = t$ and $\mu_b = 0$, as a function of $x$ along the one-dimensional chain direction.

The most striking feature illustrated in Fig. 1 is that the single hole is clearly localized in the central area of the ladder in the staggered $t$-$J$ model (red dots). Here an exponential fall off by six orders of magnitude in the hole density away from the central region merely spanned by about 150 rungs is shown. This is in sharp contrast to the delocalization profile of the single hole in the $\sigma \cdot t$-$J$ model, which only differs from the $t$-$J$ model by a sign $\sigma$ in the hopping term, with the same superexchange term and staggered chemical potentials.

Furthermore, the density distributions of two doped holes are presented in the inset of Fig. 1 where the charge density profiles become delocalized in both models. This is in sharp contrast to the single-hole case of the staggered $t$-$J$ model, where the hole is well localized spatially in the main panel. It implies that two holes must form a new object to become mobile, which is to be further examined below.

**Inverse participation ratio for the one hole case.**—A useful quantity to measure the localization in the single particle theory is the inverse participation ratio (IPR) defined by

$$\text{IPR} = \frac{1}{\sum_i p_i^2},$$ (2)

where $p_i$ is the probability that the single particle is located at site $i$ satisfying $\sum_i p_i = 1$. To generalize this concept to a many-body system with one doped hole, we
may define \( p_i \) as the probability that the hole is at site \( i \) by tracing out the spin background. The single hole ground state can be expressed as

\[
|\Psi_G\rangle = \sum_{i,\{\sigma\}_i} C_{i,\{\sigma\}_i} |i,\{\sigma\}_i\rangle ,
\]

where \( |i,\{\sigma\}_i\rangle \) denotes the Ising basis \( \{\sigma\}_i \) with one hole at site \( i \). Then \( p_i = \sum_{\{\sigma\}_i} |C_{i,\{\sigma\}_i}|^2 = 1 - n_i \).

If the hole is localized at one site \( p_i = 1 \), one finds IPR = 1 according to Eq. (2). In the opposite limit that the hole is uniformly distributed over \( N \) sites of the lattice in a delocalized state, \( n_i^0 = 1/N \) or IPR = \( N \), which is linearly scaling with \( N \). The IPR versus \( N \) in the present staggered \( t-J \) and staggered \( \sigma \cdot t-J \) ladders are shown in the main panel of Fig. 2. For the staggered \( t-J \) model, initially IPR increases linearly with smaller \( N \) but then quickly saturates to a constant as \( N = N_x \times 2 \) becomes larger than 400 (red dots). Such a scaling behavior is consistent with the localization picture previously found in Fig. 1. On the other hand, IPR remains linearly proportional to \( N \) for the \( \sigma \cdot t-J \) model (blue open circles), also consistent with the delocalization behavior in Fig. 1.

Furthermore, later we shall discuss a localization-delocalization transition by adding a next-nearest-neighbor hopping \( t' \) at a critical point \( t'/t = t'_c/t \sim 0.15 \), and in Fig. 2 the corresponding IPR clearly exhibits a linear \( N \) or delocalized behavior (black triangles) at \( t'/t = 0.3 > t'_c/t \).

In the inset of Fig. 2 the IPRs for the two hole cases of the staggered \( t-J \) (red full circles) and staggered \( \sigma \cdot t-J \) (blue open circles) models indicate linear-\( N \) scaling behaviors, which support the delocalization picture of two holes in both cases. Here the probability for finding a hole at site \( i, p_i \equiv (1-n_i)/2 \), is defined for a two hole case.

**Equal-time one-hole propagator.**—The equal-time hole propagation in the single-hole ground state \( |\Psi_G\rangle \) is defined as

\[
G_{\sigma}(i,j) \equiv \langle \Psi_G\rangle c^\dagger_{i \sigma} c_{j \sigma} |\Psi_G\rangle .
\]

Note that this is not a conventional equal-time Green’s function in which \( |\Psi_G\rangle \) is taken as the half-filling ground state. The quantity defined in Eq. (4) tracks the motion of the hole in its true ground state. Define the distance between site \( i \) and \( j \) on the same chain of the leg by \( r \equiv |i-j| \), with the reference point \( j = j_0 \) fixed at the central site, the calculated quantity is shown in Fig. 3.

\[G_{t}(j_0, j_0 + r)\text{ indicates an exponential decay at large } r \text{ in the staggered } t-J \text{ model (red full circles), but it remains finite in the staggered } \sigma \cdot t-J \text{ system (blue open circles). It is consistent with the previous results indicating that the hole is localized in the former as opposed to its delocalization behavior in the latter.}

**Localizaiton-delocalization transitions.**—So far we have established by the DMRG calculation that a single hole doped into a two-leg quantum spin ladder will be spatially localized in the \( t-J \) model in the presence of a staggered chemical potential, \( \mu_a = t \) and \( \mu_b = 0 \), along the chain (\( x \)) direction of the ladder. Note that the latter has doubled the unit cell along the \( x \)-direction but does not truly break the translational symmetry. By contrast, by turning off the phase string effect with inserting a sign factor \( \sigma = \pm 1 \) into the hopping term of the staggered \( t-J \) model, one obtains the so-called staggered \( \sigma \cdot t-J \) model, in which the localization of the hole is immediately removed to result in a delocalized single hole ground state.

Instead of inserting a sign factor to switch off the phase string in the \( t-J \) model, one may add the next-nearest-neighbor hopping \( t' \) to the model, which can also suppress the phase string effect. It is expected that when the ratio \( |t'/t| \) is large enough, the phase string gets sufficiently reduced to restore the delocalization in such a translationally invariant system. Indeed in Fig. 4\( a \), a “second-order-like” phase transition as clearly indicated by a discontinuity in the first-order derivative and a divergent-like sharp peak in the second-order derivative of the ground state energy versus \( t' \) at a critical point \( t'_c/t \sim 0.15 \) (we focus on \( t'/t > 0 \) side). Correspondingly the delocalization as IPR \( \sim N \) is indeed shown in the main panel of Fig. 2 at \( t'/t = 0.3 > t'_c/t \) (black triangles).

On the other hand, if we focus on the staggered \( t-J \) ladder and continuously reduce \( \mu_a \) from \( \mu_a = t \) to the uniform limit: \( \mu_a = \mu_b = 0 \), there is no phase transition as shown in Fig. 4\( b \), with the continuous and smooth
behavior in the first and second order derivatives of the ground state energy versus $\mu_a$. It implies that at least in finite-size systems with $N \sim 40 \times 2$, which are much larger than the internal size $20$ of the doped hole, the single hole state in the uniform $t$-$J$ ladder with $\mu_a = \mu_b = 0$ is in the same phase as that of the staggered $t$-$J$ ladder. Note that in the uniform $t$-$J$ ladder, although the single hole density profile has been previously shown to be extended in finite-size calculations $15, 22$, the charge response to a magnetic flux inserting into the ring formed by the ladder has been indeed shown to vanish exponentially with the circumference of the ring or the ladder length $N_x$ $15, 20$. Furthermore, the ground state is shown $21$ to have an intrinsic translational symmetry breaking as composed of two components, with a Bloch-like standing wave superposed on top of an incoherent component induced by the randomness of the phase string. Thus, the strong staggered chemical potential in the present case may significantly enhance the scattering between the two components to result in a true spatial self-localization.

Pairing mechanism.—In contrast to the localization of a single hole in the staggered $t$-$J$ model, two holes have exhibited delocalization behavior in the density profile and IPR scaling, as shown in the insets of Figs. $1$ and $2$ respectively. In the following, we show that such two doped holes are actually paired up to become a mobile object freely moving on a gapped spin background just like the case at $\mu_a = \mu_b = 0$ $26$.

Define the binding energy of two injected holes by $20$

$$E_b \equiv (E_{0}^{2h} - E_{0}^{0h}) - 2(E_{0}^{1h} - E_{0}^{0h}),$$

where $E_{0}^{0h}$ is the ground state energy of the undoped spin ladder at half-filling, $E_{0}^{1h}$ is the ground state energy of the one hole doped system and $E_{0}^{2h}$ is the ground state energy of the two hole doped system. If $E_b < 0$, two doped holes will form a bound pair to lower the total energy.

The binding energies for the staggered $t$-$J$ (full red circles) and staggered $\sigma$-$t$-$J$ (open blue circles) models as a function of the length $N_x$ of the two-leg ladder are shown in Fig. $5$ respectively. One sees a negative $E_b$ in the staggered $t$-$J$ case, clearly indicating that the two holes are paired up with $E_b \sim -0.12 J$ at large $N_x$. In contrast, the positive binding energy $E_b$ is shown in the staggered $\sigma$-$t$-$J$ model at finite $N_x$, which is expected to be extrapolated to $0$ as $N_x \rightarrow \infty$. Namely, despite that two holes are always delocalized in both models (cf. the insets of Figs. $1$ and $2$), they must form a bound pair in the staggered $t$-$J$ model in order to overcome the tendency of localization for the individual holes in this model. It therefore points to a novel pairing mechanism of kinetic-energy-driven $26$, which is however not present in the staggered $\sigma$-$t$-$J$ model even though the superexchange term $H_J$ remains the same.

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