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Spin and charge modulations in a single-hole-doped Hubbard ladder: Verification with optical lattice experiments

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We show that pronounced modulations in spin and charge densities can be induced by the insertion of a single hole in an otherwise half-filled two-leg Hubbard ladder. Accompanied with these modulations is a loosely bound structure of the doped charge with a spin-1/2, in contrast to the tightly bound case where such modulations are absent. These behaviors are caused by the interference of the Berry phases associated with a string of flipped spins (or “phase strings”) left behind as a hole travels through a spin bath with a short-range antiferromagnetic order. The key role of the phase strings is also reflected in how the system responds to increasing spin polarization and the on-site repulsion, addition of a second hole, and increasing asymmetry between intra- and interchain hopping. Remarkably, all these properties persist down to ladders as short as ~ 10 sites, as the smoking gun of the phase-string effect. They can therefore be studied in cold-atom experiments using the recently developed fermion microscope.

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I. INTRODUCTION

The Hubbard model is a prime example of a strongly correlated system. It has a deceptively simple appearance: a system of spin-1/2 fermions in a tight binding lattice with onsite repulsion U . Yet despite decades of studies, the problem remains unsolved except in the one-dimensional (1D) case. Of particular interest is the 2D Hubbard model, for it is believed that it captures the key physics of high T_c superconductivity. At half filling, the ground state of a 2D Hubbard model with strong repulsion is an antiferromagnet. There is the expectation that the ground state will become a d -wave superfluid when sufficiently many holes are added. The nature of the ground state as the system is doped away from half filling has been the central question.

In solid-state experiments, it is difficult to change the density of electrons continuously, nor is it possible to remove completely the disordered effects that entangle with strong correlation. As a result, comparison between theory and experiment is not straightforward at times. On the other hand, Hubbard models can now be engineered in cold-atom experiments, with easy control of density and interaction [1–6]. In principle, one can obtain the solution of the Hubbard model by quantum simulation, i.e., finding the nature of the ground state directly from experiments. Unfortunately, current experiments have not reached temperatures low enough to study strongly correlated effects due to the heating caused by spontaneous emission. On the other hand, heating effects can be reduced in small samples, as the low-energy excitations in bulk are gapped out. In addition, the extraordinary development of the atom microscope allows one to image specific atomic species with single site resolution [7–11] making quantum simulations with

small systems a powerful way to explore strong correlation effects.

In this paper, we point out some unusual properties of a two-leg Hubbard ladder that reflect the underlying mechanism controlling the motion of charge and spin, and explain why quantum simulation with small cold-atom systems is a powerful tool for exploration of strong correlation effects. In particular, we show the following:

(i) *Spin and charge modulations.* Pronounced modulations in the spin and particle densities can be triggered by the introduction of a single hole into a half-filled system. These modulations persist as the length of the ladder is reduced. They remain significant for ladders as short as containing eight sites along the chain direction.

(ii) *Spin-charge separation.* Accompanied with the appearance of these modulations is a loosely bound or composite structure of the charge and spin associated with the doped hole. In fact, the modulations disappear once the spin and charge become tightly bound in an asymmetric limit to be detailed in the paper.

(iii) *Phase-string effects.* These phenomena are caused by the interference of the Berry phases associated with the strings left behind by the hole (or phase strings) as it moves through the spin bath of the half-filled system [13]. We point out a number of experimental methods to turn off the phase-string effects. Experimental verification of these phenomena will provide a smoking gun confirming the key role of the phase strings.

Similar density modulations were previously found by two of us (Z.Z. and Z.W.) in a two-leg ladder of the t - J model [14]. Our key results (i) to (iii) for the Hubbard model, however, were not contained in Ref. [14]. The fact that density modulations of bulk samples also occur in small samples means that strong correlations operate within a relatively short range. Such strong correlations can be thoroughly explored by performing quantum simulations on small cold-atom systems.

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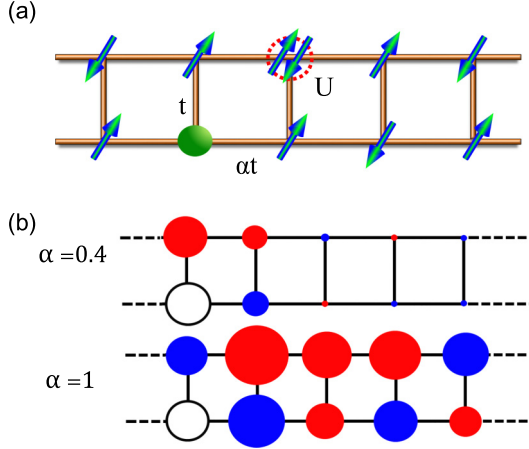


FIG. 1. (a) Structure and parameters of a two-leg Hubbard square ladder. Here, U represents the onsite Coulomb repulsion, and t (αt) describes the interchain (intrachain) hopping. (b) With one hole (open circle) created by removing a down-spin away from the half-filling spin ladder, a total spin $S_z = 1/2$ is found in a spin gapped background in the large U/t (Mott) regime. Such a total $S_z = 1/2$ is found to distribute around the hole at a given site with an alternative distribution of up (red circle) and down (blue circle) spins (with the magnitude represented by the size of each full circle as determined by the hole-spin correlation function [14]). At $\alpha = 0.4$, the doped charge is tightly bound with a spin-1/2; in contrast, the hole and the spin-1/2 are loosely bound at $\alpha = 1$, where the phase string becomes unscreened as previously discussed in the context of the t - J ladder [12] (see text).

II. SPIN AND CHARGE MODULATIONS AS FINGERPRINTS OF STRONG CORRELATIONS

We consider a two-leg Hubbard ladder with size $N = N_x \times 2$ as shown in Fig. 1(a). The Hamiltonian

$$\begin{aligned}
 H = & -\alpha t \sum_{i=1}^{N_x-1} \sum_{j=1,2} c_\sigma^\dagger(i+1, j) c_\sigma(i, j) + \text{H.c.} \\
 & -t \sum_{i=1}^{N_x} c_\sigma^\dagger(i, 1) c_\sigma(i, 2) + \text{H.c.} \\
 & + U \sum_{i=1}^{N_x} \sum_{j=1,2} n_\uparrow(i, j) n_\downarrow(i, j), \quad (1)
 \end{aligned}$$

where αt and t are the hopping integrals along and normal to the chain, respectively, and U is the on-site repulsion. We have studied the case of a single hole injected into the half-filled two-leg ladder using density matrix renormalization group (DMRG) with the numerical details similar to those used in Ref. [14] for the t - J case. Without doping the hole, the density profiles of both spin and charge are simply flat as all the charge and spin fluctuations are gapped in the Mott regime when U is big enough and spins are short-range singlet paired. With inserting a single hole by taking one spin (e.g., down spin) out, as illustrated in Fig. 1(b), a total $S_z = 1/2$ spin will emerge from the gapped spin background, which distributes around the hole with the average on-site up and down spins indicated

by red and blue full circles of varying sizes at $\alpha = 0.4$ and 1, respectively, determined by the hole-spin correlation function.

Figure 2 shows that the hole density exhibits a pronounced modulation for the case $\alpha = 1$, for ladders from 12 to 40 sites. We find that the charge modulations are present in all finite-size ladders, only becoming less visible for ladders shorter than eight sites. Moreover, these modulations remains prominent for smaller U where the system is away from the t - J limit. Similar modulations in spin density have also been found. They are not included in Fig. 2 to avoid over-crowding. The spin modulation is shown in Fig. 3(a) together with the charge modulation for the case $N = 20 \times 2$ and $U/t = 12$. In the same figure the spin and charge modulations for the t - J model case at $t/J = 3$ are also present for comparison. To match quantities that are easily accessible in cold-atom experiments, we plot in Fig. 3(b) the density of both spin components $n_\uparrow(x)$ and $n_\downarrow(x)$, as well as the total density $n(x) = n_\uparrow(x) + n_\downarrow(x)$. Here, in this paper, the charge and spin densities include the summation of two sites in the same rung for each x . The period of the modulation is incommensurate, roughly two lattice sites. Near the center of the chain, the density modulation in each spin component can be as large as 15% of their averaged values, which is detectable with atom microscopes. The fact that Fig. 3 shows a net total spin S_z is because we have removed a spin-down fermion.

III. ORIGIN OF SPIN AND CHARGE MODULATIONS: PHASE-STRING EFFECTS

In the t - J model, it is found that the charge modulation is due to the interference of “phase strings.” A phase string is hidden in a string of flipped spin left behind as a hole moves in a spin bath with antiferromagnetic correlations. Associate with this string is a Berry phase. The total Berry phase accumulated as a hole moves along a closed path C is

$$\tau_C^{\text{ps}} \equiv (-1)^{N_h^\downarrow[C]}, \quad (2)$$

where $N_h^\downarrow[C]$ is the total number of mutual exchanges between the hole and the \downarrow spins as the loop C is traversed. As a hole moves from point a to point b and back, different loops connecting a and b contain different phase-string factors τ_C^{ps} , leading to an oscillator in spatial density [14].

However, for the Hubbard model with reduced U , the general sign structure is different from the t - J model, because holes and doublons can be created through quantum fluctuation. The precise sign structure for the Hubbard model has recently been rigorously worked out [15]. Specifically, the partition function of the Hubbard model can be expressed as [15]

$$\mathcal{Z} = \sum_C \tau_C \mathcal{W}[C], \quad (3)$$

where C denotes the set of closed paths of all particles with a positive weight $\mathcal{W}[C] > 0$. τ_C is the sign function

$$\tau_C = (-1)^{N_h^\downarrow[C]} (-1)^{N_d^\downarrow[C]} (-1)^{N_h^{\text{ex}}[C]} (-1)^{N_d^{\text{ex}}[C]}, \quad (4)$$

where $N_h^\downarrow[C]$ ($N_d^\downarrow[C]$) denotes the total number of mutual exchanges between the \downarrow spins and the holons or empty sites (doublons or double-occupied sites) in a given closed path C ;

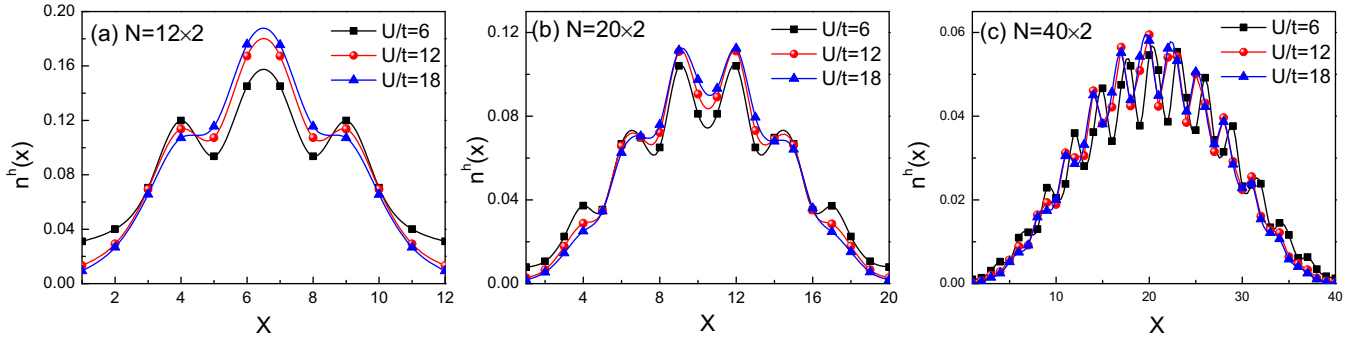


FIG. 2. Real-space charge density distribution along the chain direction of a two-leg Hubbard ladder doped by one hole at various U/t 's. Generically a charge modulation is exhibited in all the sample sizes from (a) $N = 12 \times 2$, (b) $N = 20 \times 2$, and (c) $N = 40 \times 2$. Here the anisotropic parameter is fixed at $\alpha = 1$.

and $N_h^{\text{ex}}[C]$ ($N_d^{\text{ex}}[C]$) denotes the total number of exchanges between the holons (doublons).

For large- U and at half-filling, creating a pair of holons and a doublon costs a large energy U , and consequently holons and

doublons must be created and annihilated in tightly bound pairs so that the factor $(-1)^{N_h^{\text{ex}}[C]}(-1)^{N_d^{\text{ex}}[C]}$ becomes $+1$ for most loops. (Their virtual excitations result in a super-exchange coupling $J = 4t^2/U$ between the nearest-neighboring spins.) In this limit, one has $\tau_C \rightarrow +1$ as in the half-filled t - J (i.e., Heisenberg) model. However, with the insertion of a single hole, the phase factor τ_C in Eq. (4) reduces to that of the t - J model [Eq. (2)], $\tau_C \rightarrow \tau_C^{\text{ps}} = (-1)^{N_h^{\text{ex}}[C]}$. The other three factors in Eq. (4) are absent because there is only one hole and there are no doublons in the large U limit.

In the t - J model, one can show mathematically that the phase strings cause the spin and charge modulations by considering an alternate model (referred to as the $\sigma \cdot t$ - J model) which augments the hopping of the particle with a phase factor that cancels the Berry phase [Eq. (2)]. For this model, there are no charge modulations with the doping of a single hole [14]. In the Hubbard case, we are interested in the Mott limit which gives rise to an antiferromagnetic insulating ground state in the half-filled case, but U/t is still not large enough to reach the t - J regime. In this regime, the factor $(-1)^{N_h^{\text{ex}}[C]}(-1)^{N_d^{\text{ex}}[C]}$ is $+1$ for most loops. This is because the doublons and holes generated by quantum fluctuations typically form tightly bound pairs in the Mott regime as discussed before. One can then define an analogous “ σ -Hubbard model” to remove the whole $(-1)^{N_h^{\text{ex}}[C]}(-1)^{N_d^{\text{ex}}[C]}$ by adding a spin-dependent sign σ to the hopping term involving exchanges between a single-occupied site (spin) with either a holon or doublon through a projection operator \hat{P} [16]

$$\begin{aligned}
 H_{\sigma\text{Hub}} = & -\alpha t \sum_{i=1}^{N_x-1} \sum_{j=1,2} c_{\sigma}^{\dagger}(i+1, j) c_{\sigma}(i, j) (\sigma \hat{P} + \hat{Q}) \\
 & - t \sum_{i=1}^{N_x} c_{\sigma}^{\dagger}(i, 1) c_{\sigma}(i, 2) (\sigma \hat{P} + \hat{Q}) + \text{H.c.} \\
 & + U \sum_{i=1}^{N_x} \sum_{j=1,2} n_{\uparrow}(i, j) n_{\downarrow}(i, j)
 \end{aligned} \quad (5)$$

where \hat{Q} is a projection operator such that the corresponding two nearest-neighbor sites are either all singly occupied or involving a pair of empty- doubly occupied sites. Totally one has $\hat{P} + \hat{Q} = 1$. The phase-string effect is therefore removed

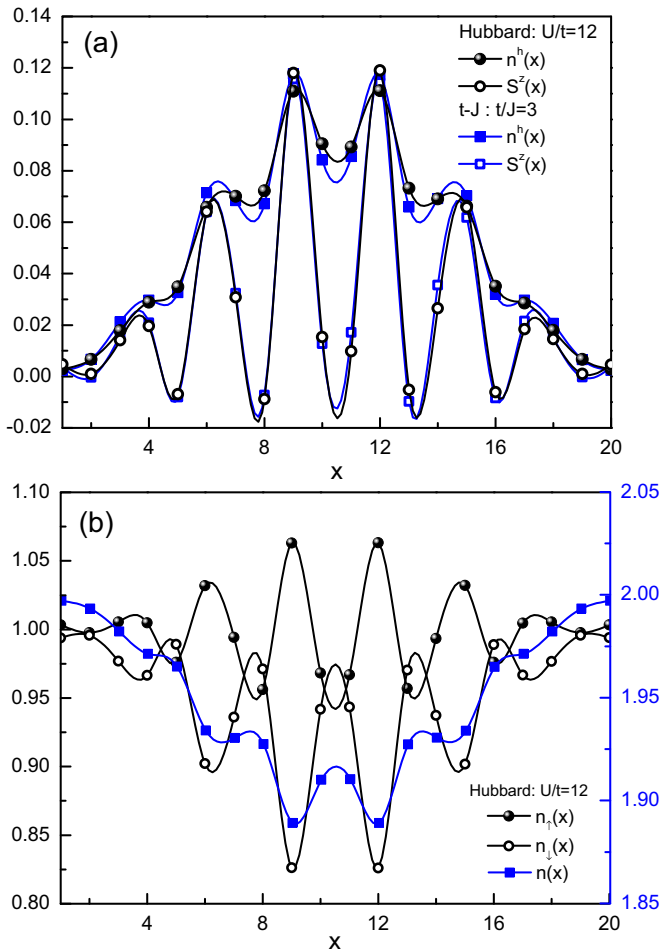


FIG. 3. (a) Both hole density $n^h(x)$ and spin density $S^z(x)$ exhibit modulations as fingerprints of the phase-string effect in the one-hole-doped Hubbard and t - J ladders ($N = 20 \times 2$ with $\alpha = 1$). (b) The total electron density $n(x) \equiv 2 - n^h(x)$ and two spin components, $n_{\uparrow}(x)$ and $n_{\downarrow}(x)$, are shown.

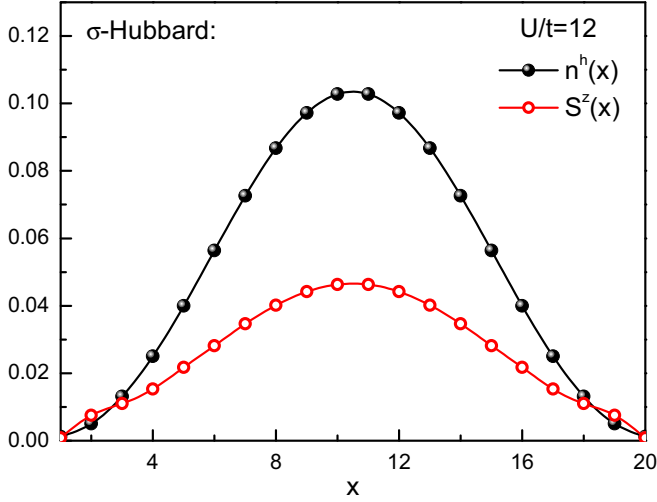


FIG. 4. Both charge and spin modulations are absent in the so-called σ -Hubbard ladders for the single-hole-doped case. The sole distinction between it and the Hubbard model lies in that the nontrivial sign structure in the latter is removed in the former (see text). Here the two-leg ladder in the isotropic case of $\alpha = 1$ is considered ($N = 20 \times 2$ at $U/t = 12$).

completely in the σ -Hubbard model with the sign structure in Eq. (3) reducing to

$$\tau_C \rightarrow (-1)^{N_h^{\text{ex}}[C]} (-1)^{N_d^{\text{ex}}[C]}. \quad (6)$$

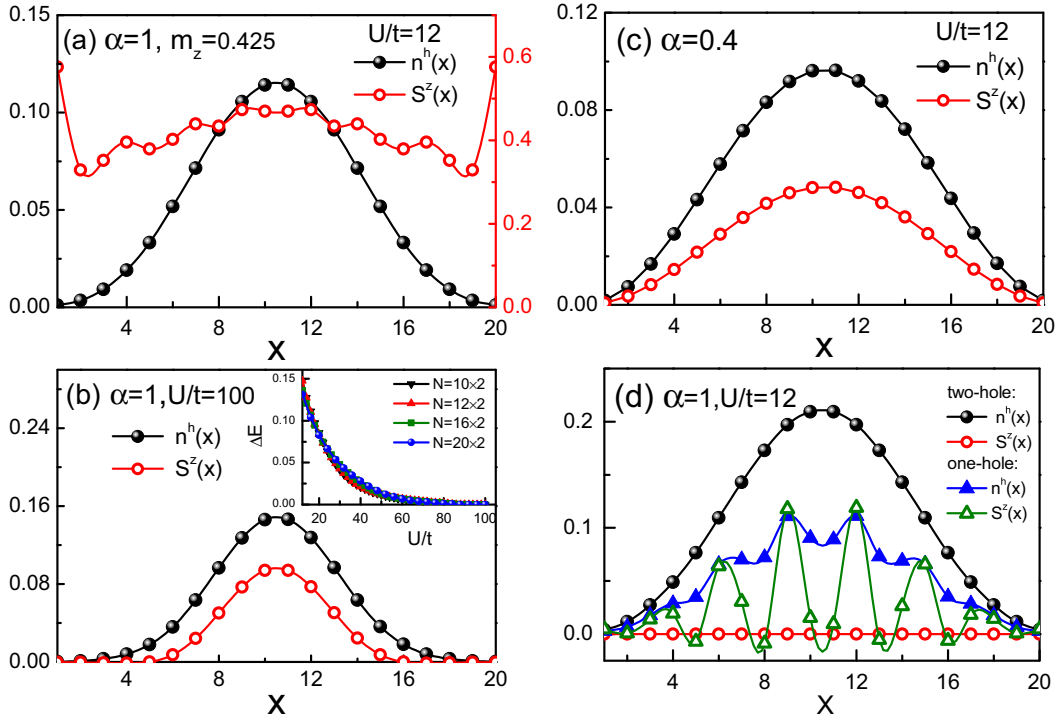


FIG. 5. (a) By polarizing the spin background, the charge modulation can be tuned to vanish. Here $m_z \equiv 2S_z/N$. (b) The charge and spin modulations diminish when the spin singlet-triplet gap ΔE vanishes at large U/t (inset); the case of $U/t = 100$ is shown in the main panel. (c) The charge modulation as the fingerprint of the phase string at $\alpha = 1$ is removed in the strong rung case $\alpha = 0.4$. (d) The charge modulation seen in the single-hole case can be eliminated by the second hole doped into the system, which forms a bound state with the first hole to remove the phase-string effect. Here $U/t = 12$ and $N = 20 \times 2$.

Consequently, the charge and spin modulations are indeed absent upon addition of a hole as shown in Fig. 4, which also has been found recently by Liu and Jiang [16] using DMRG.

IV. OTHER WAYS TO REMOVE SPIN AND CHARGE MODULATIONS

In the following, we point out a number of physical effects that show the phase-string mechanism to be the origin for the spin and charge modulations. The idea is to find ways to diminish the phase-string effects, and verify that the spin and charge modulations will disappear in the process.

A. Spin polarization

Since the phase-string effects are due to the motion of holes in an antiferromagnetic spin background, they can be manipulated by tuning the spin correlation of the background. This may be achieved by increasing spin polarization of the system. Indeed the charge modulation gets continuously weakened with the increase of total spin S_z as shown in Fig. 5(a).

Considering the conservation of total spin S_z in the Hubbard model, we can target a different S_z sector to perform the DMRG simulation. Note that the single-hole ground state corresponds to $S_z = 1/2$, with the magnetization $m_z \equiv 2S_z/N = 0.025$ (with $N = 20 \times 2$). The corresponding charge modulation [cf. Fig. 3] eventually disappears as S_z is increased to, say, $17/2$ or $m_z = 0.425$ as shown in Fig. 5(a). This disappearance of the charge modulation as the number of down spins

are reduced can again be traced back to the phase-string effects. In particular, in the limit of fully polarized spins, the phase-string effect precisely disappears in τ_C [Eq. (4)], where $N_h^\downarrow[c]$ and $N_d^\downarrow[c]$ are always zero or parity even for any closed path C . Without the phase string, here τ_C reduces to simple fermion statistical signs of the holons and doublons, $(-1)^{N_h^\uparrow[c]}(-1)^{N_d^\uparrow[c]}$. Note that the corresponding spin modulation is also diminished in Fig. 5(a).

B. Large U/t

At $U/t = 12$, the spin background is a spin singlet with an extra $1/2$ -spin loosely bound to the hole [cf. Fig. 1(b)], while at $U/t = \infty$, the ground state becomes spin fully polarized known as the Nagaoka state [17,18]. As pointed out above, the phase-string effect totally disappears in this limit. One can expect that in a sufficiently large but finite U/t , the spins surrounding the doped hole may still remain polarized, whereas the spin background tends to become a singlet, which may be called a Nagaoka polaron state with a finite total spin $S_z > 1/2$ [19,20]. In Fig. 5(b), the charge and spin modulations are shown to disappear in a Nagaoka polaron state at $U/t = 100$, where the spin singlet-triplet gap [$\Delta E \equiv E_0(S_z = 3/2) - E_0(S_z = 1/2)$] vanishes as shown in the inset. Thus if one tunes U/t experimentally, the spin and charge modulations can also get removed beyond a critical ratio.

C. Large hopping asymmetry

Spin and charge modulations can also be removed by increasing the asymmetry in the hopping integral. In the limit of $\alpha \gg 1$, the ladder reduces to two 1D chains. Since phase-string interference is absent because there are no closed loops that enclose nonzero areas in 1D, there are no spin and charge density modulations in the one-hole case. In the opposite limit where $\alpha \ll 1$, the half-filled case corresponds to a singlet pair on every two sites connected vertically $c_\uparrow^\dagger(i,1)c_\uparrow^\dagger(i,2) - c_\downarrow^\dagger(i,1)c_\downarrow^\dagger(i,2)$. The removal of one fermion will create a localized spin mainly on a vertical rung as indicated in Fig. 1(b) for $\alpha = 0.4$ in the case of $U/t = 12$. Figure 5(c) shows that the charge and spin modulations indeed disappear for $\alpha = 0.4$, which has been also seen in the t - J model case [14]. From the view point of the structure of the partition function in Eq. (3), changing α will change the weight $\mathcal{W}[C]$, making them only significant if the loops are along the chain ($\alpha \gg 1$) limit or to a single rung ($\alpha \ll 1$). Physically, these two limits correspond to the total spin-charge separation (1D) and the tightly bound spin-charge inside a quasiparticle [cf. Fig. 1(b)]. In either case, the loop interference

of phase-string factors becomes trivial and will not cause density and spin modulations.

D. Adding another hole

Figure 5(d) shows that the charge distribution for the two-hole-doped Hubbard ladder (at $U/t = 12$) is smooth, in sharp contrast to the modulation found in the single-hole case. This looks as if the phase-string effects of these two holes cancel each other, which will be impossible unless the two holes are bound together (but distributed all over the sample). For a bound pair, the nontrivial sign of the fluctuating phase string associated with each of these two holes is the same. The total phase-string factors then becomes trivial (i.e., $+1$), leading to a smooth density profile. This cancellation of the phase-string factor has also been observed previously for the t - J model [21]. We have verified here that the cancellation persists away from the t - J limit. The disappearance of the spin and charge modulations therefore reflects the binding of holes through phase strings, which is a non-BCS pairing force. Note that the pairing of the two holes could be in either a singlet or triplet channel, but the former with total spin $S = 0$ is generally lower in energy.

V. CONCLUDING REMARKS

The mechanism that controls the nature of the ground state of the Hubbard model in the Mott regime has been a question of central interests. Our studies of the two-leg Hubbard ladder show that the phase-string effect is central to the organization of spin and charge degrees of freedom. It is truly timely that cold experiments have advanced to the point at which the physical conditions discussed here can be engineered, and all the phenomena discussed here can be studied with the newly developed fermion microscope. Not only will these experiments verify the dramatic spin and density modulations triggered by a single doped hole, but also verify the key role of phase strings. It is conceivable that other strongly correlated effects will persist down to a small sample. Quantum simulation of small cold-atom systems can be a new powerful way to study strongly correlated phenomena of bulk systems.

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