Stripe formation in doped Hubbard ladders

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We investigate the formation of stripes in $7r \times 6$ Hubbard ladders with $4r$ holes doped away from half filling using the density-matrix renormalization group (DMRG) method. A parallelized code allows us to keep enough density-matrix eigenstates (up to $m=8000$) and to study sufficiently large systems (with up to $7r=21$ rungs) to extrapolate the stripe amplitude to the limits of vanishing DMRG truncation error and infinitely long ladders. Our work gives strong evidence that stripes exist in the ground state for strong coupling ($U=12t$) but that the structures found in the hole density at weaker coupling ($U=3t$) are an artifact of the DMRG approach.

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Two-dimensional lattice models for correlated electrons are often used to describe the properties of layered cuprate compounds.[1] Despite numerous studies there is an ongoing controversy about the existence of stripes in these systems. In a hole doped system a stripe is a domain wall ordering of holes and spins. The wall is made of a narrow hole-rich region. The spins are antiferromagnetically ordered between the walls and are correlated with a π phase shift across a wall. The formation of stripes in the ground state has been demonstrated numerically for the *t-J* model on (narrow) ladders[2,3] using the density-matrix renormalization group (DMRG) method.[4] For square lattices, however, the presence of stripes remains controversial[5–8] because a reliable investigation of the ground state in the thermodynamic limit is not possible with the methods currently available.

Recently, attention has turned to the two-dimensional Hubbard model with a local electron-electron repulsion U and an electron hopping term t. For $U=0$ this model describes a Fermi gas, which obviously has no stripes in the ground state. Moreover, no instability toward the formation of stripes has been found in the weak-coupling limit $U \ll t$ using renormalization group techniques.[9] In the strong-coupling limit $U \gg t$, however, the Hubbard model can be mapped onto a *t-J* model with $J=4t^2/U \ll t$, which does have stripes in the ground state, at least on narrow ladders with $J \approx 0.35t$.[2,3] Therefore, investigating the formation of stripes in the Hubbard model at finite coupling U/t could significantly improve our understanding of these structures. Moreover, such investigations should reveal the true capability of the various methods used to study stripes much better than calculations for the *t-J* model alone.

An early DMRG investigation of three-leg Hubbard ladders[10] found that stripes formed in the ground state only for $U \geqslant 6t$. In a recent DMRG calculation White and Scalapino[2] have shown that a narrow stripe appears in the ground state of six-leg Hubbard ladders (more precisely, 7×6-site clusters) for $U \geqslant 6t$. For weaker couplings the hole and spin densities show structures which are interpreted as a broad stripe. In both works, however, no finite-size scaling has been performed and the amplitude of the hole density modulation has not been investigated systematically as a function of DMRG truncation errors. Thus it is not clear if the observed structures are really the signature of a striped ground state in the limit of infinitely long ladders; they could be finite-size effects or an artifact of the DMRG method.

Here, we report on a DMRG investigation of stripes in six-leg Hubbard ladders with up to 28 rungs. Keeping up to $m=8000$ density-matrix eigenstates the amplitude of the hole density modulation can be extrapolated to the limit of vanishing DMRG truncation errors for systems with up to 21 rungs. This allows us to perform a reliable finite-size scaling analysis of the hole density modulation. Calculations for systems of that size are made possible by a parallelized shared-memory DMRG code which runs efficiently on current supercomputer architectures.[11] We show that the stripes found by White and Scalapino[2] are stable in the limit of an infinitely long ladder for strong coupling $U=12t$. For weak coupling ($U=3t$), however, the hole density fluctuations found in Ref. 2 are an artifact of truncation errors and boundary conditions.

The two-dimensional Hubbard model on a $R \times L$ ladder is defined by the Hamilton operator

$$\hat{H} = -t \sum_{x,y,\sigma} (\hat{c}^{\dagger}_{x,y,\sigma} \hat{c}_{x,y+1,\sigma} + \hat{c}^{\dagger}_{x,y,\sigma} \hat{c}_{x+1,y,\sigma} + \text{H.c.}) + U \sum_{x,y} \hat{n}_{x,y,\uparrow} \hat{n}_{x,y,\downarrow}, \quad (1)$$

where $x=1,\ldots,R$ is the rung index and $y=1,\ldots,L$ is the leg index, $\hat{c}^{\dagger}_{x,y,\sigma}$ and $\hat{c}_{x,y,\sigma}$ are creation and annihilation operators for an electron with spin $\sigma=\uparrow,\downarrow$ at site (x,y), and $\hat{n}_{x,y,\sigma} = \hat{c}^{\dagger}_{x,y,\sigma} \hat{c}_{x,y,\sigma}$ is the corresponding density operator. Here we exclusively consider the Hubbard model on six-leg ladders ($L=6$) with $R=7r$ rungs for $r=1,\ldots,4$. Cylindrical boundary conditions were used (closed in the rung $[y]$ direction

and open in the leg [x] direction), because they are the most favorable ones for DMRG simulations. Moreover, open boundaries break the translational invariance of the system, allowing spin and charge structures to appear as local density variations in a finite ladder. If periodic boundary conditions were used, one would have to analyze correlation functions to detect stripes in finite ladders. Since we are interested in the ground state of the hole-doped regime, we consider a system with $N=4r$ holes doped in the half-filled band, corresponding to $RL-N=38r$ electrons. The average hole density is $n=N/RL=4/42\approx 0.095$ for all cases, as in Ref. 2.

We employ a recently developed parallelized DMRG code[11] to determine the ground-state properties of this Hubbard model. Our DMRG program implements the standard finite-system algorithm[4] for two-dimensional lattices. Parallelization of the most time-consuming tasks allows us to carry out calculations of unprecedented magnitude. For the calculations presented here we have kept up to $m=8000$ density-matrix eigenstates per block for systems with up to $R\times L=168$ sites. This requires up to four weeks walltime and 100 GB of memory per run on eight processors of an IBM p690 node. For comparison, it takes about 6 h to reproduce the results of Ref. 2 for 7×6 clusters with $m=3600$. DMRG calculations have already been performed for the Hubbard model on larger systems (square lattices or ladders) than our 28×6-site clusters but for a significantly smaller number of density matrix eigenstates ($m\leqslant 2000$).[6,12] The computational cost of these simulations was at least an order of magnitude lower than in the present work.

For our six-leg Hubbard ladders, the standard DMRG method yields the ground-state energies and various expectation values for the ground state of the system investigated. Here, we focus on the hole density

$$h(x,y) = 1 - \langle \hat{n}_{x,y,\uparrow} + \hat{n}_{x,y,\downarrow} \rangle \tag{2}$$

and the staggered spin density

$$s(x,y) = (-1)^{x+y} \langle \hat{n}_{x,y,\uparrow} - \hat{n}_{x,y,\downarrow} \rangle, \tag{3}$$

where $\langle \cdots \rangle$ represents the (DMRG) ground-state expectation value. In the first few lattice sweeps of our DMRG calculations or for a small number m of density-matrix eigenstates per block ($m\lesssim 1000$), the DMRG wave function reaches a "metastable" state,[6,10] which depends essentially on the initial conditions, i.e., on the detail of the method used to construct the lattice in the first sweep (for more detail about the DMRG method, see Ref. 4). The hole and staggered spin densities show irregular fluctuations in both the rung and the leg directions at that point of the DMRG calculation.

For all system sizes and coupling strengths investigated, the DMRG wave function "tunnels" to a stable state after several sweeps and for sufficiently large m, as reported in Ref. 2 for 7×6 clusters. We have observed that the larger the system length R, the larger must m be to reach the stable state, ranging, e.g., from $m\approx 600$ at $R=7$ to $m\approx 2200$ at $R=21$ in the $U=12t$ case. This state is then essentially independent of the initial conditions, but it is nevertheless essential to make m as large as feasible in order to get sufficient data for a reliable extrapolation of observables (see below). The tunneling occurs for smaller m when it is possible to utilize the block reflection technique (see Fig. 1). Note, however, that the combination of spin and charge density fluctuations can easily break the symmetry between left and right DMRG blocks and that the block reflection technique should not be used in that case as it can lead to incorrect results.

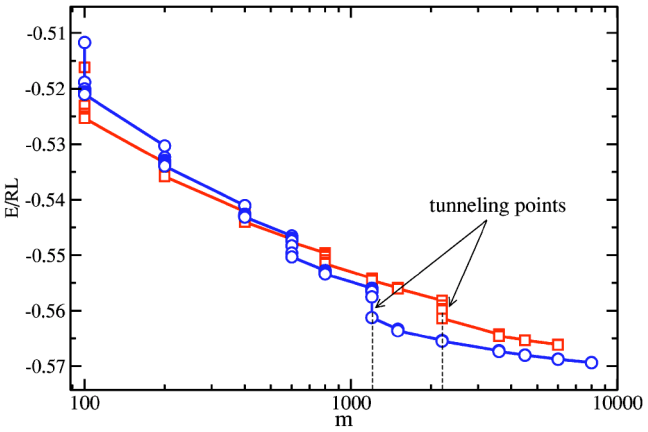

FIG. 1. (Color online) DMRG ground-state energy per site versus m for the 21×6 ladder at $U=12t$, using (circles) and not using (squares) block reflection in the middle of the lattice. Every data point corresponds to one sweep of the DMRG procedure.

For the 7×6 case, it is interesting to note that the transition occurs at a significantly smaller m with our algorithm than in Ref. 2. This may also be attributed to a more favorable choice of initial conditions. Our results for large m are in full agreement with those presented in Ref. 2. The "tunneling" is marked by a sharp drop in energy, while the spin and hole densities become more regular. In particular, the hole density and the staggered spin density are almost constant in the rung direction. The stability of this DMRG "ground state" is demonstrated by the systematic behavior of the energy (for all system sizes) and expectation values (for systems with up to 21 rungs) as a function of the discarded weight (see the discussion below). Some of our results for 28×6 ladders are inconclusive because an insufficient number of sweeps has been performed for the charge and spin density profiles to reach convergence.

On the $7r\times 6$ ladders with $4r$ holes investigated here, r stripes with four holes each appear in the DMRG ground state. These stripes are clearly seen in the hole density modulation in the leg direction

$$h(x) = \sum_{y=1}^{L} h(x,y), \tag{4}$$

which is shown in Fig. 2 for a 21×6 ladder with $U=12t$. In the same figure, one sees that the staggered spin density in the leg direction

$$s(x) = \sum_{y=1}^{L} s(x,y) \tag{5}$$

is finite and changes sign exactly where the hole density $h(x)$ is maximal. Therefore, the specific features of stripes are clearly observed in the DMRG ground state densities. Note,

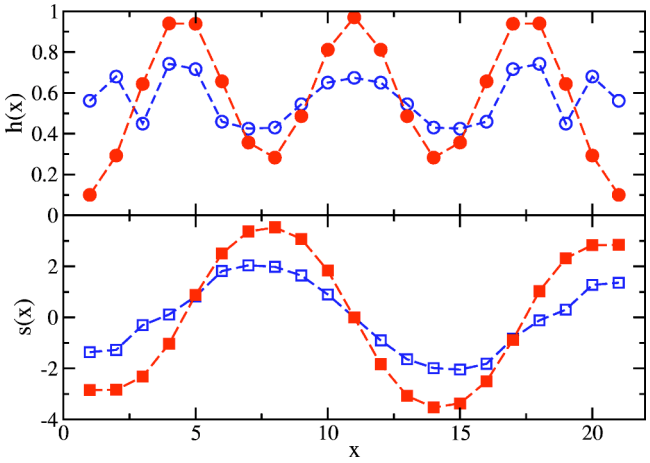

FIG. 2. (Color online) Hole (circle) and staggered spin (square) densities in the leg [x] direction calculated on a 21×6 Hubbard ladder with 12 holes for $U=3t$ (open symbols) and $U=12t$ (solid symbols).

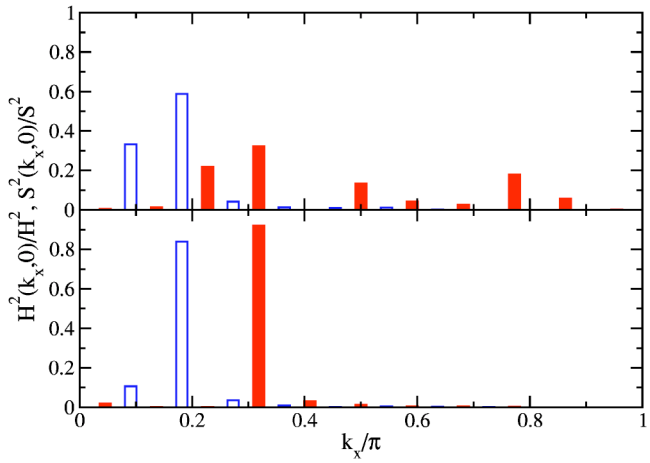

FIG. 3. (Color online) Normalized power spectrum of the hole (solid bar) and staggered spin (open bar) densities presented in Fig. 2 for a 21×6 Hubbard ladder with $U=3t$ (upper panel) and $U=12t$ (lower panel).

however, that the finite staggered spin density is an artifact of our DMRG method,[2] which does not use the full spin symmetry. In the true ground state of a finite ladder one expects $s(x,y)=0$. In Fig. 2 the results for $U=3t$ appear qualitatively similar to those obtained for $U=12t$ although the amplitudes of the density fluctuations are smaller for the weaker coupling. Nevertheless, one notices that the hole and spin density profiles for $U=3t$ are less regular than for $U=12t$.

To make a quantitative analysis of these structures we have carried out a systematic spectral analysis of the hole and staggered spin densities. The spectral transforms are defined as

$$F(k_x,k_y)=\sqrt{\frac{2}{L(R+1)}}\sum_{x,y}\sin(k_x x)e^{ik_y y}f(x,y) \tag{6}$$

with $k_x=z_x\pi/(R+1)$ for integers $z_x=1,\ldots,R$ and $k_y=2\pi z_y/L$ for integers $-L/2<z_y\leqslant L/2$. Here $f(x,y)$ and $F(k_x,k_y)$ represent either the hole density $h(x,y)$ and its transform $H(k_x,k_y)$ or the staggered spin density $s(x,y)$ and its transform $S(k_x,k_y)$. The transformation in the rung direction (with periodic boundary conditions) is the usual Fourier transform. In the leg direction (with open boundary conditions) we use an expansion in particle-in-the-box eigenstates because this is a natural basis for a finite open system. In the infinite-ladder limit $R\to\infty$ this transformation becomes equivalent to the standard Fourier transformation. As the systems considered have a reflection symmetry $(x\to R+1-x)$, the hole spectral transform $H(k_x,k_y)$ always vanishes for even integers z_x while the spin spectral transform $S(k_x,k_y)$ vanishes for odd z_x if R is odd and for even z_x if R is even. Moreover, in the converged DMRG ground state we observed uniform behavior of $h(x,y)$ and $s(x,y)$ along the rungs. This implies that the spectral weight is concentrated at $k_y=0$ for both densities.

In Fig. 3 we show the power spectrum (squared norm of the spectral transforms) of the hole and staggered spin densities presented in Fig. 2. In both cases, the power spectrum has been normalized by its total weight

$$F^2=\sum_{k_x,k_y}|F(k_x,k_y)|^2, \tag{7}$$

which we denote H^2 and S^2 for the hole and spin power spectrum, respectively. For $U=12t$ one sees that both hole and spin power spectra have a single strong peak containing most of the spectral weight (92 and 84 %, respectively). For $U=3t$, however, we observe a broad distribution without a clearly dominant mode k_x in the hole power spectrum. We find similar results for other ladder lengths $R\leqslant21$. For $R=28$ the power spectra are mostly inconclusive because of the nonconvergence of the hole and spin densities mentioned previously.

For $U=12t$ the observed positions of the dominant peaks in the hole and spin spectral transforms for $r\in\{1,2,3\}$ can be extrapolated to the $R=\infty$ limit, yielding

$$\frac{k_x^H}{\pi}=\frac{2r+1}{R+1}\xrightarrow{R\to\infty}\frac{2}{7} \tag{8}$$

and

$$\frac{k_x^S}{\pi}=\frac{r+1}{R+1}\xrightarrow{R\to\infty}\frac{1}{7}, \tag{9}$$

respectively, which agrees perfectly with the expected values corresponding to one stripe every seven rungs in an infinitely long ladder. For $U=3t$, the position k_x of the maximum in the spectral transforms is not always well defined (for instance, it changes with the number m of density matrix eigenstates kept even for large m) and thus a quantitative analysis of k_x for $R\to\infty$ is not possible.

All DMRG calculations suffer from truncation errors which are reduced by increasing the number m of retained density matrix eigenstates (for more details, see Refs. 4). The

error in the ground-state energy is proportional to the discarded weight W_m which is defined as the total weight of the discarded density-matrix eigenstates:

$$W_m = \sum_{i=m+1}^{d} w_i. \tag{10}$$

Here, d is the dimension of the density matrix and w_i is its ith eigenvalue. Thus one can achieve a greater accuracy and obtain an estimate of the error with a linear extrapolation of the DMRG energy to the limit of vanishing truncation errors $W_m \to 0$ (for an example of this extrapolation, see Ref. 10). Using this technique we have found that the error in the ground-state energy per site is typically about $4\times10^{-3}t$ ($U=12t$) and $7\times10^{-3}t$ ($U=3t$) for the largest number of density-matrix eigenstates kept ($m=8000$ and $m=6000$, respectively) and $R\leqslant 28$. Consequently, the error in the total energy is of the order of t for the largest system (168 sites). The energy separation between ground state and the lowest excited states, which is of the order of a small fraction of t, is thus significantly smaller than the error in the total energy. Therefore, the DMRG wave functions obtained in our calculations are not accurate descriptions of the true ground states. Although the DMRG wave functions converge systematically to the true ground states (as shown by the linear scaling of the energy with W_m), for $m\leqslant 8000$ they still have significant overlaps with other eigenstates. Expectation values calculated with such a DMRG wave function (i.e., for a given m) could thus be quite inaccurate. In order to get reliable results we will in the following carefully analyze the scaling of observables with increasing m.

If a variational ground-state wave function, as used in the DMRG algorithm, is known up to an error of ε, the corresponding error in the energy is of the order of ε^2. Other observables, whose operators are nondiagonal in the energy basis, converge only with ε. For DMRG we know that $\varepsilon^2 \propto W_m$ (see Ref. 10), thus expectation values of operators are polynomials of $\sqrt{W_m}$ for small discarded weights W_m. For the maximum $H_{\max}$ of the absolute hole spectral transform $|H(k_x,0)|$ we find a linear scaling with $\sqrt{W_m}$ (see Fig. 4). Such a scaling has already been found for other density modulation amplitudes.[13] This allows us to extrapolate $H_{\max}$ to the limit of vanishing truncation errors. We note that $H_{\max}$ decreases with decreasing W_m. This corresponds to a diminution of the stripe amplitude with increasing m (i.e., decreasing W_m) for sufficiently large $m\gtrsim 2000$. This diminution can be seen directly in the hole density profile $h(x)$ [for instance, in Fig. (3b) of Ref. 2]. For $U=12t$ the extrapolated values of $H_{\max}$ are clearly finite as shown in Fig. 4 for a 21×6 ladder. Thus we conclude that the hole density fluctuations found on finite ladders are not an artifact of DMRG truncation errors but a feature of the true ground state for $U=12t$. For $U=3t$, $H_{\max}$ extrapolates to very small values as $W_m \to 0$. Typically, the range of $\sqrt{W_m}$ over which we observe a linear behavior in $\sqrt{W_m}$ is smaller than the smallest value of $\sqrt{W_m}$ used in the extrapolation. This can be seen for the example shown in Fig. 4. The uncertainty in the extrapolated $H_{\max}$ is thus larger than its value for $U=3t$. Therefore, the hole density fluctuations could be the result of DMRG truncation errors and the true ground state could be uniform in that case, i.e., $H_{\max}=0$ for $W_m \to 0$. For intermediate values of U, the extrapolated $H_{\max}$ shows a monotonic increase as U grows, and one sees in the inset of Fig. 4 that the transition from a (probably) uniform state to a striped state occurs between $U=3$ and $U=5$.

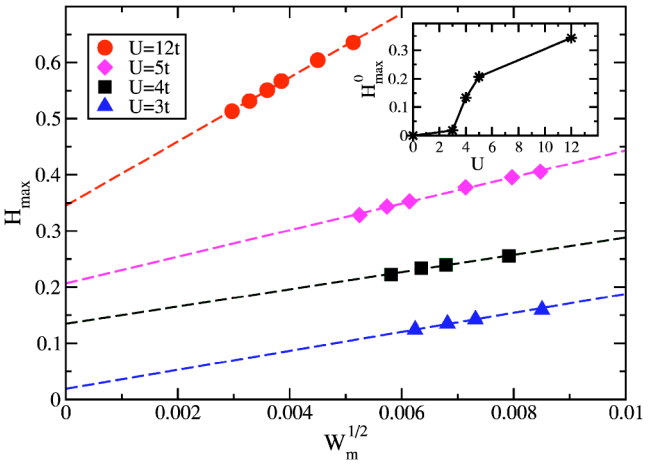

FIG. 4. (Color online) Maximum $H_{\max}$ of $|H(k_x,0)|$ in a 21×6 system between $U=3$ (triangle) and $U=12$ (circle) as a function of the square root of the discarded weight W_m for various numbers of density-matrix eigenstates $1800\leqslant m\leqslant 8000$. Dashed lines are linear fits. Inset: Extrapolation $H^0_{\max}$ of $H_{\max}$ for $\sqrt{W_m}\to 0$ versus U.

Extrapolating the maximum $S_{\max}$ of the absolute spin spectral transform $|S(k_x,0)|$ to the limit $W_m \to 0$ turns out to be more difficult than extrapolating $H_{\max}$. Contrary to $H_{\max}$, $S_{\max}$ has not reached an asymptotic regime (as a function of W_m) for the largest number m of density matrix eigenstates we have used. This difference is probably due to the smaller energy scale of spin excitations compared to that of charge excitations, resulting in a DMRG ground state which describes the charge properties of the true ground state correctly but not its spin properties. Nevertheless, for the smallest (7×6) ladder an extrapolation of $S_{\max}$ to $W_m \to 0$ using linear and quadratic fits suggests that $S_{\max}$ vanishes for $W_m \to 0$ and thus that the true ground state has no spin density fluctuations $s(x,y)=0$ as expected (see Fig. 5).

The artificial breaking of the spin symmetry is similar for all couplings U, indicating that it does not affect the formation of stripes (i.e., the existence of a hole density modulation), which is a strongly U-dependent phenomenon as shown here.

Typically, the discarded weight W_m is about 10^{-5} or smaller for $m=8000$. Although this appears to be a small value, the above discussion shows that errors in the ground-state energy and $H_{\max}$ are still quite large for that number m. This confirms that the absolute value of the discarded weight W_m alone does not give a reliable estimate for errors on physical quantities.

A ladder with a periodic array of stripes has a modulation of the hole density (charge density wave)

$$h(x) = h_0 \sin(k_x^H x), \tag{11}$$

which corresponds to

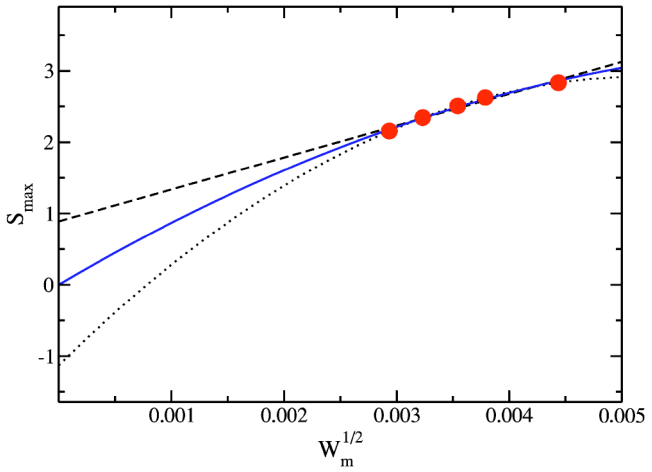

FIG. 5. (Color online) Maximum $S_{\max}$ of $|S(k_x,0)|$ for the 7 $\times 6$ system. Dashed line: linear fit, dotted line: quadratic fit, solid line: quadratic fit with constraint $S_{\max}(0) \geqslant 0$ for $W_m \to 0$.

$$H_{\max} = |H(k_x^H,0)| = \sqrt{\frac{(R+1)L}{2}} h_0. \qquad (12)$$

If the amplitude h_0 of the hole density modulation is finite in the limit of an infinitely long ladder ($R \to \infty$), the maximum $H_{\max}$ of the spectral transform must diverge as $\sqrt{R}$ for $R \to \infty$. In Fig. 6 we show the finite-size scaling of $H_{\max}/\sqrt{R} \sim h_0$ as a function of the inverse ladder length for $U=3t$ and $U=12t$. The values of $H_{\max}/\sqrt{R}$ obtained for a fixed number m of density matrix eigenstates converge to finite values for $R \to \infty$, suggesting the existence of stripes in this limit for both couplings U. After extrapolation to the limit of vanishing DMRG truncation errors, however, $H_{\max}/\sqrt{R}$ seems to vanish for large R in the case $U=3t$ while it still converges to a finite value for $U=12t$ (see Fig. 6). This indicates that stripes exist in the ground state of infinitely long ladders for sufficiently strong coupling such as $U=12t$ but that the hole and spin structures found in finite ladders for weak couplings such as $U=3t$ are artifacts of open boundaries and DMRG truncation errors. It has already been observed in other problems[13] that DMRG truncation errors can result in an artificial broken symmetry ground state after extrapolation to infinite system sizes, while extrapolating first to the limit of vanishing truncation errors restores the true ground-state symmetry in the thermodynamic limit.

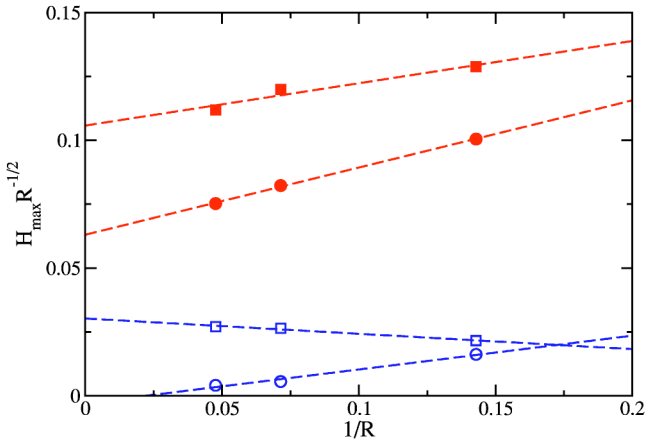

FIG. 6. (Color online) Amplitude $H_{\max}/\sqrt{R} \propto h_0$ of the hole density modulation for a fixed number ($6000 \leqslant m \leqslant 8000$) of density-matrix eigenstates (square) and extrapolated to the limit $W_m \to 0$ (circle) as a function of the inverse ladder length $1/R$ for $U=12t$ (solid symbols) and $U=3t$ (open symbols). Dashed lines are linear fits.

Our study shows the presence of stripes in the ground state of infinitely long ladders for $U=12t$ but a uniform ground state for $U=3t$. Therefore, there is a quantum phase transition at a critical value U_c between a uniform phase (for $U<U_c$) and a phase in which the translation symmetry is broken by the formation of stripes (for $U>U_c$). The amplitude $h_0 \sim H_{\max}/\sqrt{R}$ of the hole density modulation can be seen as the order parameter of the stripe phase. The results for finite ladder lengths show that the critical coupling U_c probably lies between $U=3t$ and $U=5t$ (see the data for 21 $\times 6$ ladders in the inset of Fig. 4). Extensive calculations for various values of U and a systematic extrapolation of the order parameter $h_0 \sim H_{\max}/\sqrt{R}$ to the limit of infinite ladder length will be necessary to calculate U_c more precisely and to determine the nature of the phase transition.

Our conclusions for ladders of finite width cannot be extended to a two-dimensional lattice with $L=R \to \infty$. Nevetheless, combined with other results for two-dimensional systems[1,5–9] our findings suggest that a similar transition between a uniform ground state (possibly with off-diagonal superconducting correlations) and a stripe ground state could occur at finite coupling U in the two-dimensional Hubbard model close to half filling. The existence of such a transition in two-dimensional strongly correlated electron systems could play a significant role in the physics of layered cuprate compounds.

In conclusion, we have investigated the formation of stripes in six-leg Hubbard ladders at a hole doping of 9.5%. Using a parallelized DMRG code we have been able to determine the amplitude of the hole density modulation in the limits of vanishing DMRG truncation errors and infinitely long ladders. Our results show that stripes exist in the ground state of these systems for strong but not for weak couplings.

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