Hole Doped Hubbard Ladders

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Abstract

The formation of stripes in six-leg Hubbard ladders with cylindrical boundary conditions is investigated using DMRG at two different hole dopings, and the amplitude of the hole density modulation is determined in the limits of vanishing DMRG truncation error and infinitely long ladders. The results give strong evidence that stripes exist in the ground state of these systems for strong but not for weak Hubbard couplings. The doping dependence of these findings is analysed.

Stripes on Hubbard ladders?

Controversial discussion: Does the ground state of interacting doped lattice models in two dimensions like the *t-J* and the Hubbard model show a charge modulation when subjected to particular, e.g., cylindrical boundary conditions?

Here, consider 2-dimensional Hubbard model on $R\times L$–site ladder with cylindrical boundary conditions,

$$H = -t\sum_{xy\sigma}\left(c^\dagger_{x,y,\sigma}c_{x,y+1,\sigma} + c^\dagger_{x,y,\sigma}c_{x+1,y,\sigma} + \text{h.c.}\right) + U\sum_{xy} n_{x,y,\uparrow}n_{x,y,\downarrow}\ , \qquad (1)$$

with R rungs and L legs.

Known analytical results: No stripe-forming instability for $U \ll t$ [1], but stripes on narrow ladders for $U \gg t$. In between, numerical (DMRG) results only available for a 7×6 ladder [2] with no finite-size scaling.

Stripe signatures: Focus on hole density $h(x,y) = 1-\langle \hat n_{x,y,\uparrow}+\hat n_{x,y,\downarrow}\rangle$, where $\langle\ldots\rangle$ is the DMRG ground-state expectation value.

"Stripe" = density modulation in the leg direction,

$$h(x) = \sum_{y=1}^{L} h(x,y)\ . \qquad (2)$$

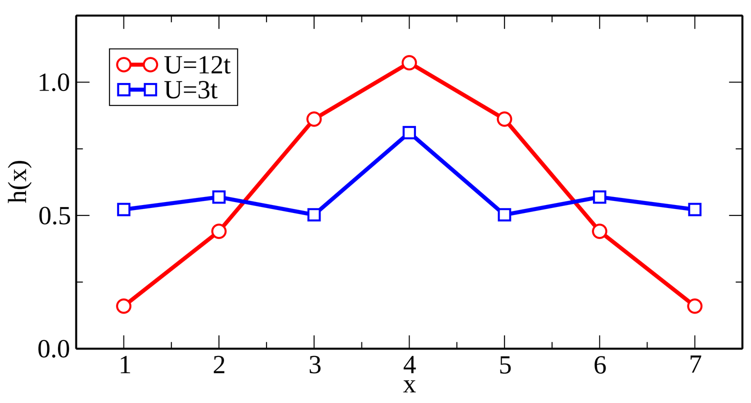

Fig. 1: *y-integrated hole density for a 7×6 ladder with 4 holes at $U=12t$ and $U=3t$.*

Questions:

- What is the exact U dependence?
- Is the stripe formation an artefact of the boundary conditions?
- What happens at larger ladder length?
- How does the stripe depend on the doping?
- Is there really a stripe at $U=3t$?

In this work we consider

- 6-leg ladders ($L=6$) with $R=7r$ rungs for $r=1,\ldots,4$ (up to 168 sites).
- Hole counts of $N_1=4r$ or $N_2=8r$, respectively, in the half-filled band (i.e. $RL-N_1=38r$ or $RL-N_2=34r$ electrons, average hole density $n_1=N_1/RL=4/42\approx 0.095$ or $n_2=N_2/RL=8/42\approx 0.190$).

⇒ Major computational task (cost at least an order of magnitude beyond previous studies). Exact diagonalization ruled out for resource requirements (6×6 out of reach), QMC for the sign problem.

Method of choice: DMRG

- "Optimal" truncated Hilbert basis for ground state (here) but also dynamical calculations.
- Number of density matrix eigenstates kept (m) determines accuracy of ground state.
- Variational method, measure for convergence: Discarded weight $W_m=\sum_{i=m+1}^{d} w_i$, the sum over all discarded reduced DM eigenvalues.
- Extremely low CPU time and memory requirements compared to exact diagonalization.

Parallel DMRG

Lattices significantly larger than 7×6 can only be studied numerically on parallel computers. Up to $m=8000$ and $R=28$ were possible with a shared-memory parallel DMRG algorithm [3]:

Parallelize sparse matrix-vector multiplication in superblock diagonalization step,

$$H\psi = \sum_\alpha\sum_k (H\psi)^\alpha_{L(k)} = \sum_\alpha\sum_k A^\alpha_k \psi_{R(k)}\left[B^T\right]^\alpha_k\ , \qquad (3)$$

and some other loops. Speedups of 5–6 on 8 CPUs can be expected [3]. Large shared memory nodes (e.g., IBM p690, SGI Altix) are the ideal architecture and reach approximately half-peak performance with this code.

Accessible system sizes up to 28×6, but: Carefully check convergence!

Stripes: Raw DMRG data

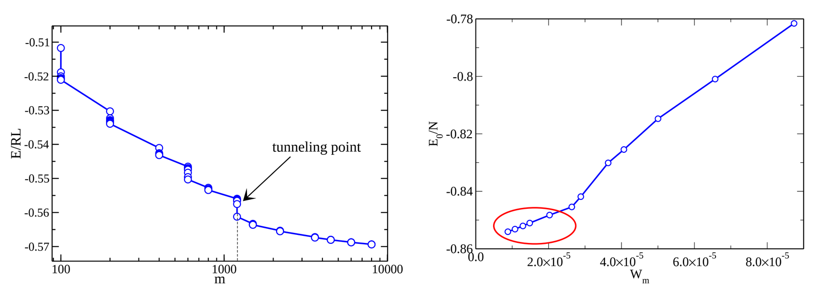

Fig. 2: *Left: "Tunneling" into striped state for 21×6 ladder at small doping and $U=12t$. Right: Energy per site vs. W_m.*

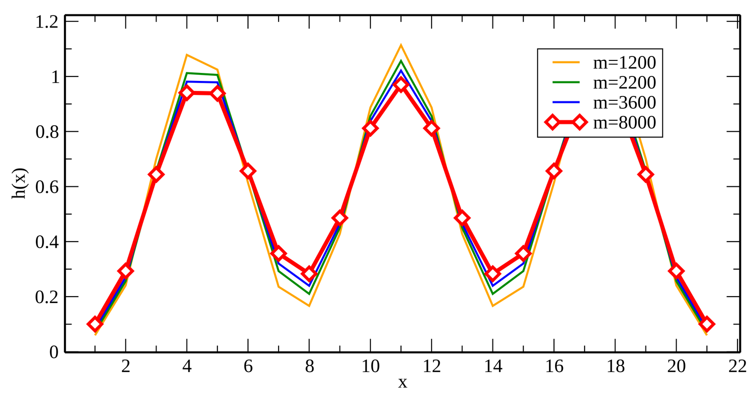

Fig. 3: *m dependence of hole structures, parameters as above.*

Peculiarities:

- Stripe(s) form(s) at certain m_c; the larger the lattice, the larger m_c.
- Well-known linear behaviour of E_0 vs. W_m ⇒ extrapolation sensible also for other observables?
- Amplitude decreases with rising m after stripe has formed. Is there a limit?

⇒ Study spectral analysis of hole density with respect to DMRG truncation errors and finite-size effects. Spectral transform:

$$H(k_x,k_y) = \sqrt{\frac{2}{L(R+1)}}\sum_{x,y}\sin(k_x x)e^{ik_y y}h(x,y) \qquad (4)$$

with $k_x = z_x\pi/(R+1)$ for $z_x=1,\ldots,R$ and $k_y=2\pi z_y/L$ for $-L/2<z_y\le L/2$.

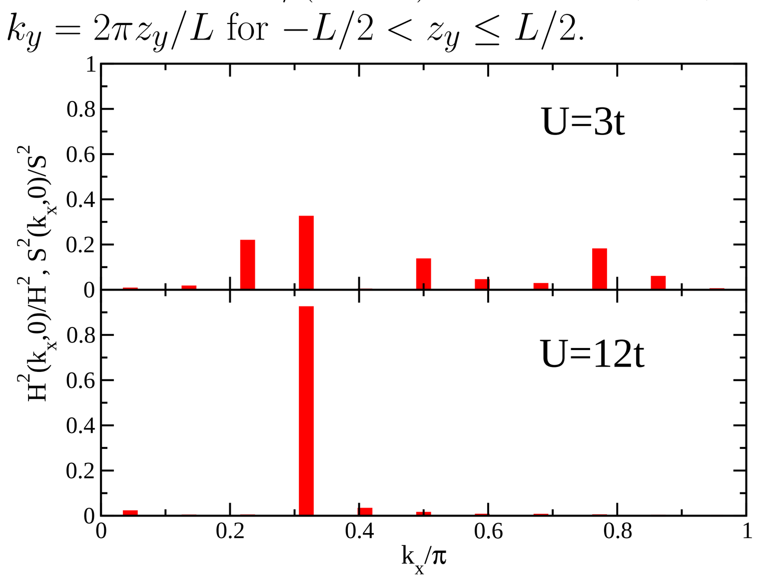

Fig. 4: *Normalized power spectrum of hole density in leg direction for 21×6 ladder at $m=8000$.*

⇒ Doping dependence at finite R and m: r stripes in $7r\times 6$ ladder at doping of $N_1=4r$. Number of stripes doubles with double doping, but stripe amplitude is much smaller.

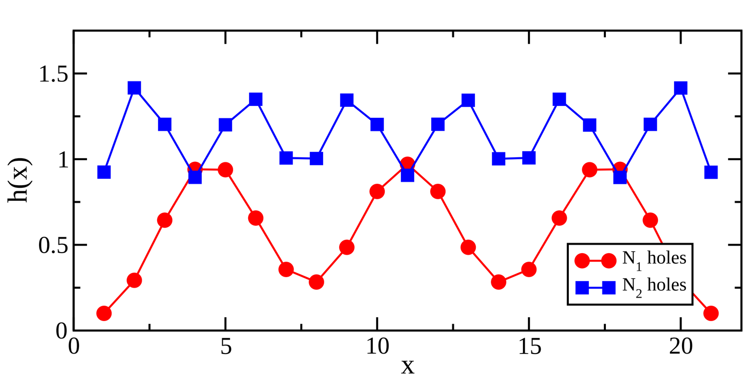

Fig. 5: *y-integrated hole density versus x for two dopings on a 21×6 ladder at $U=12t$ and $m=8000$.*

Real stripes on finite ladders

Extrapolation to vanishing truncation error: Variational DMRG wave function known up to correction ε,

$$|\psi_0\rangle = |\psi_{\text{DMRG}}\rangle + \varepsilon\,|\delta\rangle\ , \qquad (5)$$

so

$$E_{\text{DMRG}} - E_0 \propto \varepsilon^2 \propto W_m\ . \qquad (6)$$

Other observables have errors $\propto\varepsilon\propto\sqrt{W_m}$, including the power spectrum of the hole modulation.

⇒ Extrapolation possible due to known behaviour! Use dominant harmonic of hole modulation power spectrum,

$$H_{\max} = \max_{k_x}|H(k_x,0)| \propto \sqrt{W_m}\ , \qquad (7)$$

for small W_m.

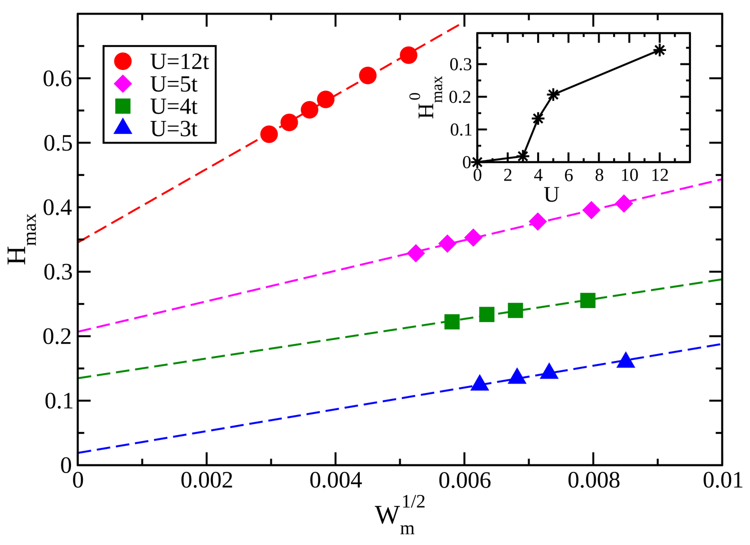

Fig. 6: *Extrapolation of dominant Fourier harmonic of $h(x)$ vs. W_m for a 21×6 ladder at doping N_1.*

Observations:

- At finite R, the data suggests a transition to a striped state at $U\gtrsim 3$, but there might still be a "flat" stripe at $U=3t$.
- Could still be an artifact of DMRG or boundary conditions.
- Data for 28×6 ladders inconclusive (resource limitations).

Does the transition survive the thermodynamic limit?

What about magnetization?

Observe staggered spin density

$$s(x,y) = (-1)^{x+y}\langle \hat n_{x,y,\uparrow} - \hat n_{x,y,\downarrow}\rangle\ , \qquad (8)$$

as a measure for antiferromagnetic order.

Finite antiferromagnetic order is numerically observed.

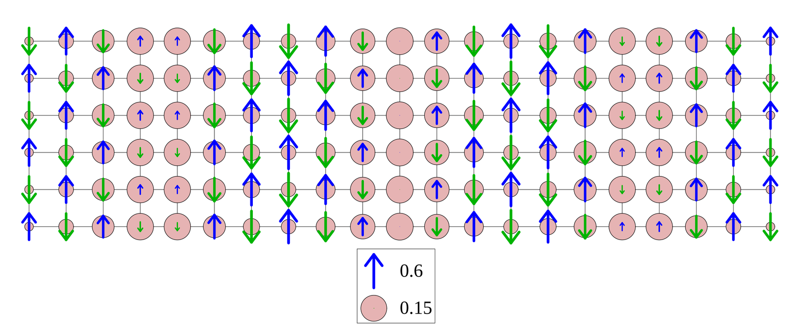

Fig. 7: *Depiction of hole (blobs) and spin (arrows) density for 21×6 at $U=12t$.*

Observations:

- $s(x,y)$ shows "phase slip" across stripe positions.
- Spin structure factor peaked at $k_x=\pi$.
- Extrapolation of dominant harmonic $S_{\max}$ to $W_m\to 0$ compatible with zero magnetization.

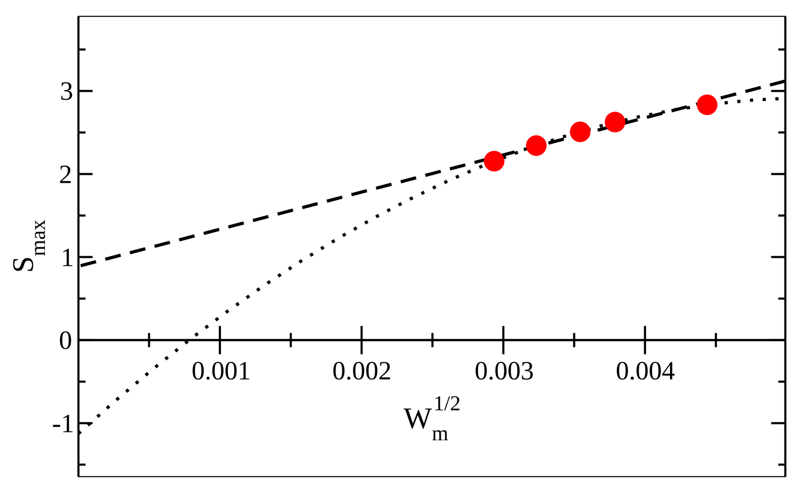

Fig. 8: *Extrapolation of $S_{\max}$ to $W_m=0$ for 7×6 at $U=12t$ using linear and quadratic fits.*

⇒ DMRG describes well charge properties but not spin properties of Hubbard ladders. Finite magnetization may serve as a stripe signature, but is an artifact of the method (not using the spin symmetry).

Real stripes on infinitely long ladders

Limit $R\to\infty$: Eq. (4) yields linear divergence of $H_{\max}$ for $R^{-1}\to 0$ if modulation amplitude remains finite. ⇒ Extrapolate $H_{\max}/\sqrt{R}$ for each U and N considered, yielding the zero truncation error thermodynamic limit:

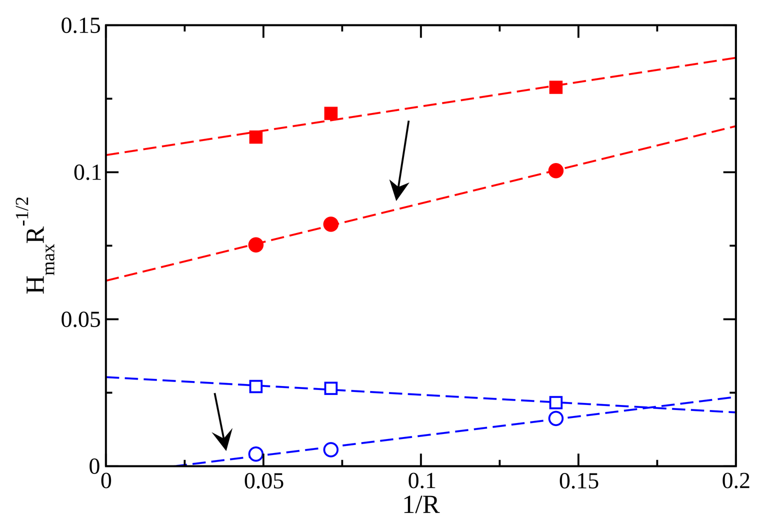

Fig. 9: *Extrapolation of $H_{\max}$ for $R\to\infty$ at small doping. Arrows indicate the previous extrapolation to the $W_m=0$ limit for $U=3t$ (blue) and $U=12t$ (red).*

Observations:

- Stripe signature at $U=3t$ vanishes in the thermodynamic limit.
- Extrapolation has significant impact on hole fluctuation amplitude ⇒ 21×6 is nowhere near the infinite system!
- Resource requirements for parallel DMRG: several hundreds of CPU hours and ≈100 GBytes of memory for largest systems *per run*.

What about doping dependence?

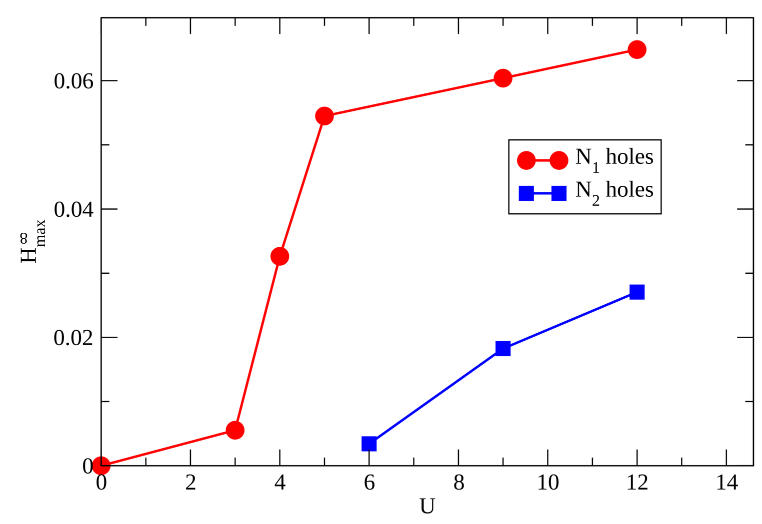

Fig. 10: *Amplitude of dominant harmonic in the hole density modulation versus U for small (red) and large (blue) doping, extrapolated to $W_m\to 0$ and $R\to\infty$.*

No stripes found for doping $N_3=2r$!

Conclusions

For small U, numerical ground state stripe signatures are artifacts of the DMRG method (boundary conditions) and vanish when proper extrapolation procedures are employed. Going from small to large U, there is a crossover from a homogeneous to a striped state. With $N_1=4r$, a steep transition occurs at $U\approx 4t$. At larger doping $N_2=8r$, the transition is shifted to larger U and becomes smoother and the number of stripes is doubled. The existence of a similiar transition in real two-dimensional strongly correlated electron systems would be of vital importance for the physics of layered high-T_c cuprates.

Open question: Is this a phase transition in spite of $R\to\infty$ leading to a quasi-onedimensional system?

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