

Hole-doped Hubbard ladders

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Abstract

The formation of stripes in six-leg Hubbard ladders with cylindrical boundary conditions is investigated for two different hole dopings, where the amplitude of the hole-density modulation is determined in the limits of vanishing density-matrix renormalisation group truncation errors 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.

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PACS: 71.27.+a; 71.10.Fd; 71.10.Pm; 74.20.Mn

Keywords: Two-dimensional Hubbard model; Stripe formation

There is an ongoing controversial discussion about whether the ground state of interacting doped lattice models in two dimensions like the t - J and the Hubbard model shows a charge modulation when subjected to particular, e.g., cylindrical boundary conditions.

Recently, attention has turned to the two-dimensional Hubbard model on $R \times L$ -site ladders with local electron–electron repulsion U and electron hopping t ,

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

where $x = 1, \dots, R$ is the rung index and $y = 1, \dots, L$ is the leg index. Cylindrical boundary conditions (closed in the rung y -direction and open in the leg x -direction) are assumed. For $U = 0$, this model describes a Fermi gas, obviously without stripes in the ground state. Moreover, using renormalization group techniques, no instability toward stripe formation has been found in the weak-coupling limit $U \ll t$ [1]. In the strong-coupling limit $U \gg t$, the Hubbard model can be mapped onto a t - J model

with $J = 4t^2/U \ll t$, which exhibits stripes in the ground state, at least on narrow ladders with $J \approx 0.35t$ [2, and references therein]. An investigation of stripe formation in the Hubbard model at different couplings and fillings could thus significantly improve our understanding of these structures.

In a recent density-matrix renormalization group (DMRG) calculation White and Scalapino [2] have shown that a narrow stripe appears in the ground state of a 7×6 -site cluster for $U \geq 6t$. For weaker couplings, the hole and spin densities were interpreted as a broad stripe. 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.

In this work, we exclusively consider 6-leg ladders ($L = 6$) with $R = 7r$ rungs for $r = 1, \dots, 4$. Since we are interested in the ground state of the hole-doped regime, we consider a system with $N_1 = 4r$ or $N_2 = 8r$ holes doped in the half-filled band, corresponding to $RL - N_1 = 38r$ or $RL - N_2 = 34r$ electrons. The average hole density is thus $n_1 = N_1/RL = 4/42 \approx 0.095$ or $n_2 = N_2/RL = 8/42 \approx 0.190$, respectively.

We employ a recently developed parallelised DMRG code [3], keeping up to $m = 8000$ density-matrix eigenstates

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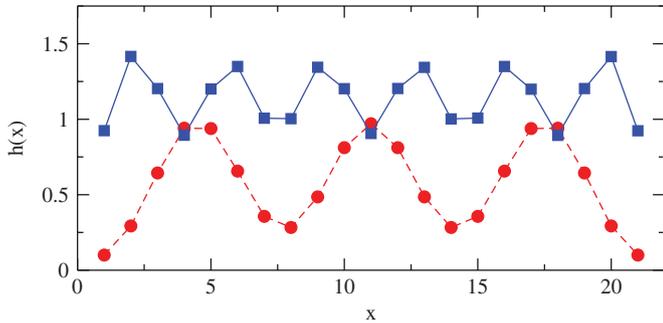


Fig. 1. y -integrated hole density versus x for $N_1 = 4r$ (circles) and $N_2 = 8r$ (squares) on a 21×6 ladder at $U = 12t$.

per block for systems with up to $R \times L = 126$ sites. We focus on the hole density $h(x, y) = 1 - \langle \hat{n}_{x,y,\uparrow} + \hat{n}_{x,y,\downarrow} \rangle$, where $\langle \dots \rangle$ represents the (DMRG) ground-state expectation value. A stripe is related to a hole density modulation in the leg direction,

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

Stripe “signatures” derived from the staggered spin density are artifacts of the method and can be identified as such [4].

The study of stripe structures requires a spectral analysis of the hole density with respect to DMRG truncation errors and finite-size effects. The spectral transform is defined as

$$H(k_x, k_y) = \sqrt{\frac{2}{L(R+1)}} \sum_{x,y} \sin(k_x x) e^{ik_y y} h(x, y) \quad (3)$$

with $k_x = z_x \pi / (R+1)$ for integers $z_x = 1, \dots, R$ and $k_y = 2\pi z_y / L$ for integers $-L/2 < z_y \leq L/2$. In the converged DMRG ground state we observe uniform behaviour of $h(x, y)$ along the rungs. This implies that the spectral weight is concentrated at $k_y = 0$. Stripes appear as hole concentrations which are translationally invariant along the rung (y) direction. At a hole doping of $N_1 = 4r$, r stripes show up in a $7r \times 6$ ladder. When the doping is increased to $N_2 = 8r$, the number of stripes doubles (see Fig. 1) and the structures become much less pronounced.

The height and position of the maximum of the power spectrum (squared norm of Eq. (3)), i.e., the dominant harmonic can be extrapolated to the limit of vanishing DMRG truncation error (discarded weight W_m). This is possible because for small W_m , expectation values of operators are polynomials in $\sqrt{W_m}$. Indeed, we find a linear scaling of $H_{\max} = \max_{k_x} |H(k_x, 0)|$ as $\sqrt{W_m} \rightarrow 0$ once the transition to a striped state has occurred. For $U = 12t$, the extrapolated values of H_{\max} are finite. 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 $U = 12t$.

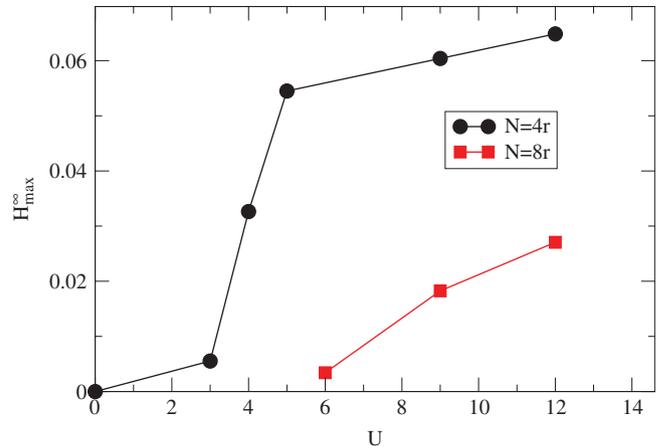


Fig. 2. Amplitude of the dominant harmonic in the hole density modulation versus U , extrapolated to vanishing DMRG error and infinitely long ladders. Circles: $N = 4r$, squares: $N = 8r$.

For smaller values of U , the fluctuation amplitude decreases until $U \lesssim 4t$, and then stays close to zero if U is further reduced.

Eq. (3) implies that when the limit $R \rightarrow \infty$ is taken, the amplitude of the dominant Fourier component in the hole density modulation (2) diverges linearly with \sqrt{R} . Consequently, results for infinite ladder length can be obtained by extrapolating H_{\max} / \sqrt{R} as $R^{-1} \rightarrow 0$. Fig. 2 shows this limit for $N = N_1$ (circles) and $N = N_2$ (squares).

The following conclusions can be drawn from the data. For small U , stripe signatures observed in numerically determined ground states are artifacts of the method 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 $N_1 = 4r$, the transition occurs with a rather steep slope at $U \approx 4t$. Increasing the doping to $N_2 = 8r$ shifts the transition to larger U and makes it much smoother. Moreover, the number of stripes in the ground state is doubled. The existence of a similar transition in real two-dimensional strongly correlated electron systems would be of vital importance for the physics of layered high- T_c cuprates.

This work was partially funded by the Competence Network for Scientific High Performance Computing in Bavaria (KONWIHR). G.H. is indebted to the HLRN Berlin staff.

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