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Charge density correlations in t-J ladders investigated by the contractor-renormalization method

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Using four-site plaquette or rung basis decomposition, the contractor-renormalization method is applied to two-leg and four-leg t-J ladders and cylinders. Resulting range-2 effective Hamiltonians are studied numerically on *periodic rings* taking full advantage of the translation symmetry as well as the drastic reduction of the Hilbert space. We investigate the role of magnetic and fermionic degrees of freedom. Spin gaps, pair-binding energies, and charge correlations are computed and compared to available exact-diagonalization and density-matrix renormalization-group data for the full Hamiltonian. Strong evidence for short-range diagonal stripe correlations are found in periodic four-leg t-J ladders.

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Competition between superconducting correlations and charge ordering has long been a challenge to numerical computations[1,2] of low-dimensional strongly correlated electron systems. Spin and hole-doped ladders[3] offer an ideal system to investigate the crossover between one to two dimensions. The two-leg ladder, for example, is known to exhibit a robust spin gap at and close to half filling as well as hole-pair binding.[4,5] Dominant power-law $d_{x^2-y^2}$-like pairing and $4k_F$-charge-density-wave (CDW) correlations at small doping are characteristic of a Luther-Emery (LE) liquid regime.[6,7] However, the spin-gap magnitude drops sharply as the number of legs is increased, e.g., from $0.50J$ in the Heisenberg two-leg ladder to $0.190J$ in the Heisenberg four-leg ladder.[8] Both the increase of the magnetic correlation length (of the undoped ladder) as well as the drastic reduction of the available ladder length for increasing leg number restrict enormously the accuracy of standard numerical techniques such as exact diagonalization (ED) and density matrix renormalization-group (DMRG) techniques. In addition, the DMRG method is limited (in practice) to open boundary conditions (OBC) in the leg direction.

In this Communication, we use the contractor-renormalization (CORE) method[9,10] to investigate hole-doped two-leg and four-leg ladders.[12] Our aim is to get further insights on the issue of pairing and density correlations from the investigation of large enough systems with periodic boundary conditions (PBC) in the ladder direction. Such investigations are greatly needed to complement available DMRG calculations using OBC. Our approach is done in two steps: (i) using an appropriate partition into small subsystems, we use the CORE method to construct an effective Hamiltonian, which integrates out quantum fluctuations at short length scales; (ii) we use ED techniques (supplemented by finite-size analysis) to compute various physical properties (pair binding, spin gaps, etc.) and compare them to those of the original model. The method provides strong evidence for stripe correlations in translationally invariant four-leg ladders.

We shall consider here a generic n-leg t-J ladder,

$$\mathcal{H}=J_{\mathrm{leg}}\sum_{i,a}\vec{S}_{i,a}\cdot\vec{S}_{i+1,a}+J_{\mathrm{rung}}\sum_{i,a}\vec{S}_{i,a}\cdot\vec{S}_{i,a+1}+t_{\mathrm{leg}}\sum_{i,a}(c^{\dagger}_{i,a}c_{i+1,a}+\mathrm{H.c.})+t_{\mathrm{rung}}\sum_{i,a}(c^{\dagger}_{i,a}c_{i,a+1}+\mathrm{H.c.}),\tag{1}$$

where $c_{i,a}$ are projected hole fermionic operators. Open (ladders) or systems closed (cylinders) along the rungs with isotropic coupling, $t_{\mathrm{leg}}=t_{\mathrm{rung}}=1$ and $J_{\mathrm{leg}}=J_{\mathrm{rung}}=J$, will be of interest here.

In order to implement the CORE algorithm the ladders are decomposed in small four-site subunits, as shown in Fig. 1, whose M low-energy states are kept to define a reduced Hilbert space. The full Hamiltonian (1) is then diagonalized on N connected units (with OBC) to retain its M^N low-energy states. These true eigenstates are then projected on the reduced Hilbert space (tensorial product of the M states of each unit) and Gram-Schmidt orthonormalized.[9,10] An effective Hamiltonian containing N-body interactions with an identical low-energy spectrum can then be constructed in terms of the reduced basis by a unitary transformation.[11] For the sake of simplicity, we shall restrict ourselves to the range-2 approximation $(N=2)$.[12]

At half filling, retaining in each four-site unit only the lowest singlet and triplet states (four states) gives excellent results.[12] Away from half filling, the simplest truncation, referred to as the ''B'' approximation, is to include, in addition, the lowest singlet hole pair on the four-site unit (of d-wave symmetry in the case of a plaquette). Formally, one can define four hard-core bosonic (plaquette or rung) operators describing the four possible transitions from the singlet half-filled ground state (GS) (vacuum) to one component of the triplet state, $t_{\alpha,i}$, or to the hole-pair state, b_i (Ref. 13). The effective B Hamiltonian $\mathcal{H}^B$ can then be written as a sum of a simple bilinear kinetic term $\mathcal{H}^b+\mathcal{H}^t$ and a quartic interaction $\mathcal{H}^{int}$ (Refs. 10 and 12),

$$\mathcal{H}^b=\epsilon_0+\epsilon_b\sum_i b^{\dagger}_i b_i-J_b\sum_{\langle ij\rangle}(b^{\dagger}_i b_j+\mathrm{H.c.}),\tag{2}$$

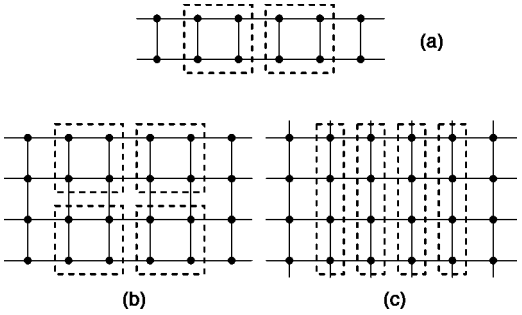

FIG. 1. CORE decomposition in term of plaquette or rung subsystems; (a) two-leg ladder split into plaquettes; (b) four-leg ladder split into 2×2 plaquettes; (c) four-leg cylinder split into four-site rungs.

$$\mathcal{H}^t=\epsilon_t\sum_{i\alpha} t^\dagger_{\alpha i}t_{\alpha i}-\frac{J_t}{2}\sum_{\alpha\langle ij\rangle}(t^\dagger_{\alpha i}t_{\alpha j}+\text{H.c.})$$

$$-\frac{J_{tt}}{2}\sum_{\alpha\langle ij\rangle}(t^\dagger_{\alpha i}t^\dagger_{\alpha j}+\text{H.c.}), \tag{3}$$

$$\mathcal{H}^{int}=V_b\sum_{\langle ij\rangle} n_{bi}n_{bj}+\sum_{\langle ij\rangle}[V_0(t_it_j)^\dagger_0(t_it_j)_0+V_1(t_it_j)^\dagger_1(t_it_j)_1$$

$$+V_2(t_it_j)^\dagger_2(t_it_j)_2]-J_{bt}\sum_{\langle ij\rangle\alpha}(b^\dagger_i b_j t^\dagger_{\alpha j}t_{\alpha i}+\text{H.c.})$$

$$+V_{bt}\sum_{\langle ij\rangle\alpha}(b^\dagger_i b_i t^\dagger_{\alpha j}t_{\alpha j}+b^\dagger_j b_j t^\dagger_{\alpha i}t_{\alpha i}), \tag{4}$$

where $(t_it_j)^\dagger_S$ creates two triplets on plaquettes i and j, which are coupled total spin S. Such an effective Hamiltonian may serve for analytic and numerical treatments. Its parameters listed for $J=0.35$ and $J=0.5$ in Table I are consistent with those found for the Hubbard model.[10] Although, $\mathcal{H}^B$ gives already a faithful description of the physics of the original model, a systematic improvement can be done by adding to the above local basis four extra ''fermionic'' states corresponding to the degenerate ($S_z=\pm1/2$, even and odd chirality or parity) single-hole GS of the four-site unit (hereafter referred to as the ''BF'' approximation).

The two-leg t-J ladder offers an ideal system to test the efficiency of the CORE method and the choice of the plaquette decomposition. As seen from the behavior of the pair-binding energy $\Delta_P=2E_0(n_h=1)-E_0(n_h=2)-E_0(n_h=0)$ plotted in Fig. 2(a) and from the plaquette charge density-density correlation in the two-hole GS of the BF Hamiltonian plotted in Fig. 3(a), pairs are found to be strongly bound and localized almost on a single plaquette. This confirms *a posteriori* the relevance of CORE and of the local basis. Furthermore, the finite-size scaling of the spin gap for a fixed number of $n_h=2$ holes [see Fig. 2(b)] or at 1/8 hole density [Fig. 2(c)] gives gaps with 10%–20% accuracy in comparison to existing numerical data.[18] Due to the small size of the hole pairs, accurate results are obtained even when fermionic excitations are not included. Note that the effective models lead to a smooth finite-size behavior, in contrast to the original t-J model where ''band-filling'' effects may lead to oscillatory behaviors as seen in Fig. 2.

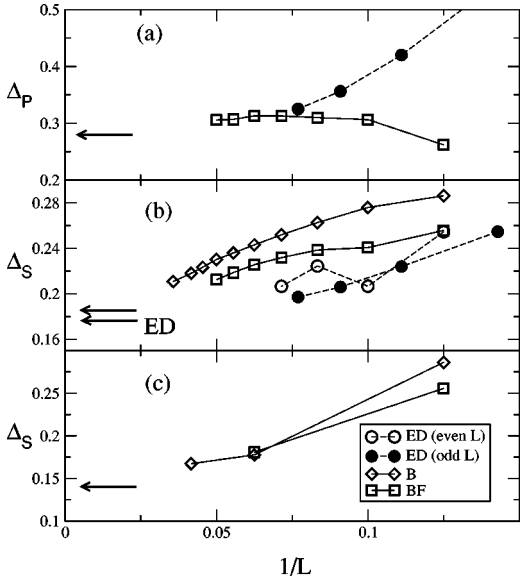

FIG. 2. Finite-size scaling analysis vs $1/L$ for a periodic two-leg $2\times L$ t-J ladder at $J=0.5$ using the decomposition of Fig. 1(a) and the effective B or BF Hamiltonians (as indicated on plot). DMRG and ED data for the original t-J ladder are also shown for comparison. ED data obtained with odd ladder lengths are averaged over boundary conditions (see Ref. 18). DMRG data and $L\to\infty$ ED extrapolations are shown by arrows. (a) Pair-binding energy Δ_P. (b) Spin gap of the two-hole-doped ladder. (c) Spin gap of the $\frac{1}{8}$-doped ladder.

We point out the qualitative agreement between our re-

TABLE I. Parameters of $\mathcal{H}^B$ (in units of t) computed for the t-J ladder model using a range-2 CORE with two plaquettes (row 1 and 2) or two four-site rungs (row 3).

J	ϵ_0	ϵ_b	ϵ_t	J_t	J_{tt}	J_b
0.35	−3.8895	−3.5340	0.1379	0.2128	0.2319	0.2139
0.5	−5.5564	−3.0919	0.1970	0.304	0.3112	0.2174
0.35	−3.5564	−3.6579	0.4733	−0.4836	−0.4336	0.4855
J	J_{bt}	V_b	V_0	V_1	V_2	V_{bt}
0.35	−0.0709	1.0345	−0.1244	−0.0928	0.0412	−0.3298
0.5	−0.1044	0.8326	−0.1777	−0.1326	0.0588	−0.3325
0.35	0.2887	1.4164	−0.2158	−0.0202	0.0149	−0.2489

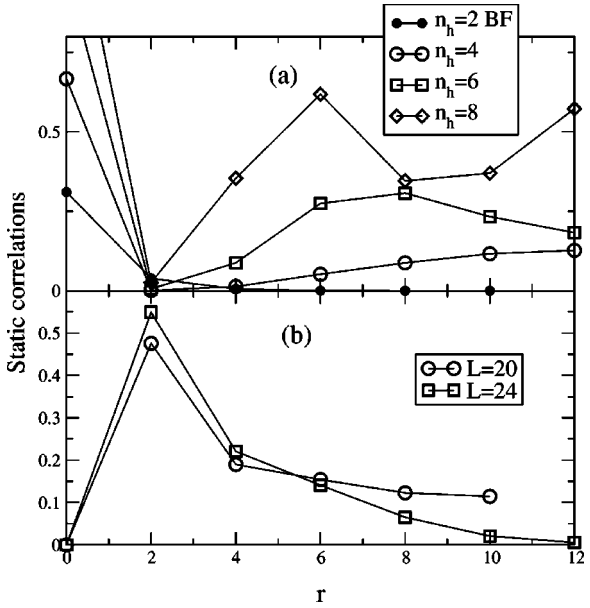

FIG. 3. Correlations as a function of distance (in units of the original bond length) up to $r=L/2$ in $2\times L$ t-J ladder at $J=0.5$. (a) Plaquette charge-density correlations for $L=24$. The BF Hamiltonian (B Hamiltonian) is used for $n_h=2$ holes (otherwise). (b) Hole-pair density-S_z correlation in the lowest triplet excited state of 2×20 and 2×24 two hole-doped ladders using the B Hamiltonian.

sults and those of Siller *et al.*[17] who used a more involved hard-core charged boson model with longer-range repulsive interactions (giving rise to a Luttinger liquid behavior), but neglected both fermionic and gapped triplet excitations.[17] Our more systematic and general treatment using the B Hamiltonian gives a similar qualitative picture as can be seen from the charge correlations shown in Fig. 3(a); we observe the characteristic $4k_F$-CDW spatial oscillations of the LE phase showing the same number of maxima as the number of hole pairs. Let us emphasize that this is also in agreement with DMRG calculations.[17] Our approach performed on finite homogeneous systems is then complementary to the DMRG technique using OBC.

Although the agreement with the hard-core charged boson model is qualitatively good, we believe that including magnetic triplet excitations in the local basis is nevertheless important to describe interplay between magnetic and pairing correlations. For example, it is known that the lowest triplet excitation in a two-hole-doped (or very weakly doped) t-J ladder consists of a hole-pair-magnon bound state.[18] Indeed, the extrapolated value of the spin gap in the presence of two holes [see Fig. 2(b)] is lower than that of the undoped ladder ($0.5J$) and the hole-pair binding energy [shown in Fig. 2(a)]. Moreover, as seen in Fig. 3(b), the correlation between the hole-pair density and the plaquette S_z component clearly shows an enhancement at short distance.[14]

We finish the investigation of the two-leg ladder by using the effective Hamiltonian to calculate the Luttinger liquid parameter K_ρ which governs the long-distance power-law behavior of the charge correlations related to the unique massless charge mode. Some values of K_ρ obtained from the Drude weight D and the compressibility κ (Ref. 15) as $K_\rho = \pi\sqrt{D\kappa/2}$ are listed in Table II. In addition, we also list here the charge velocity u_ρ obtained from the relation $u_\rho = \pi D/K_\rho$ which agrees within a few percent to the values obtained directly from the linear dispersion of the charge mode. Note also that these values compare very well to existing ED (Ref. 7) and DMRG (Ref. 17) data.

TABLE II. Parameters K_ρ and u_ρ as a function of doping computed on 2×24 (12.5%,8.3%,4.2%) and 2×28 (14.3%,10.7%,7.1%,3.6%) ladders with B Hamiltonian and $J/t=0.5$.

Doping	14.3%	12.5%	10.7%	8.3%	7.1%	4.2%	3.6%
K_ρ	0.559	0.602	0.668	0.753	0.798	0.914	0.920
u_ρ	0.881	0.779	0.652	0.445	0.399	0.188	0.180

We now turn to the investigation of the four-leg t-J ladder (with OBC along rungs) or cylinder (with PBC along rungs), for which the best choices of unit decomposition are depicted in Fig. 1(b) and Fig. 1(c), respectively. Results for pair-binding energies and spin gaps are shown in Fig. 4(a)–4(c). Results for ladders and cylinders are similar although the hole-pair binding is much stronger in cylinders where hole pairs are preferably formed on cross-sectional plaquettes (periodic rungs) rather than on ''surface'' plaquettes. Generically we found that the pair-binding energy is larger than the spin gap of the undoped (Heisenberg) system ($0.190J$ for the $4\times L$ ladder). Therefore, the lowest triplet state in the two-hole-doped (or very lightly doped) four-leg ladder is similar to a Heisenberg ladder magnon, which may be (or may not be) loosely bound to a hole pair depending on whether its

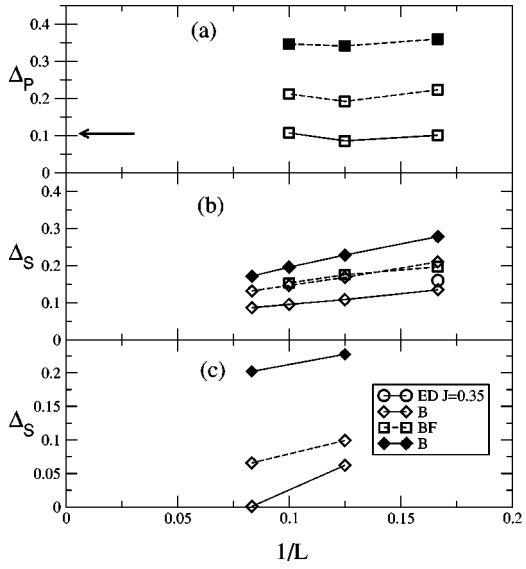

FIG. 4. Finite-size scaling analysis vs $1/L$ for a periodic four-leg $4\times L$ t-J ladder (open symbols) using the decomposition of Fig. 1(b) for $J=0.35$ (full lines) and $J=0.5$ (dashed lines). Data are also shown in the case of a periodic *cylinder* (filled symbols) for $J=0.35$ using the decomposition of Symbols and Fig. 1(c). notations and similar to Figs. 2(a)–2(c). (a) Pair-binding energy Δ_P. (b) Spin gap of the two-hole-doped system. (c) Spin gap of the $\frac{1}{8}$-doped system.

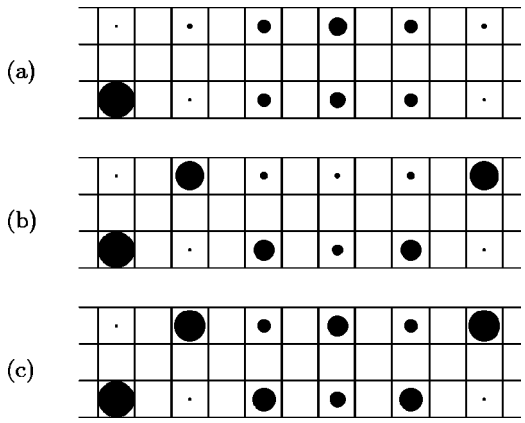

FIG. 5. Hole-pair density-density correlation on a 4×12 ladder at $J/t=0.35$. PBC are used in the leg direction and correlations are measured from the reference plaquette on the lower left corner. From top to bottom, $n_h=4,6,8$. The surfaces of the dots are proportional to the values of the correlations.

excitation energy is lower or equals the magnon energy of the undoped system. Since the data shown in Fig. 4(b) are not fully conclusive we have computed in addition the hole-pair density-S_z correlation and found, as for the two-leg ladder case, an enhancement of the spin density on the neighboring sites of the hole pair suggesting, indeed, the existence of a hole-pair-magnon bound state.

Upon increased doping, as seen from the hole-pair density-density correlation shown in Fig. 5, we observe a clear tendency of the hole pairs to align along the diagonal $(1,\pm1)$ directions with a periodicity corresponding to one pair for every two plaquettes, a behavior also reported in DMRG calculations[16,19] and reminiscent of the picture of diagonal stripes. Note that real-space charge correlations are fully consistent with the power-law decay found in the effective charge boson model.[19]

To conclude, the CORE method is a powerful method to extract effective Hamiltonians for strongly correlated models. It allows numerical simulations on significantly larger systems than those available for the original model. We show that including charge *and* spin bosonic excitations gives reliable results as long as the hole-pair-binding energy is not too small. Results for the effective model of the two-leg t-J ladder are in excellent agreement with known analytic and numerical data. Within the effective models hole-pair triplet bound states form for both two-leg and four-leg ladders, a key feature to be compared to SO(5) phenomenological theories.[20] In addition, the method enables unbiased (since calculated on translationaly invariant clusters) analysis of hole-pair density correlations. While $4k_F$-CDW correlations are found in two-leg ladders, our computations provide clear evidence in favor of short-range diagonal stripes in four-leg ladders.

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[14] Within the two-site rung decoupling scheme no hole-pair-magnon bound state is found (Ref. 13) in contradiction with numerical results (Ref. 18). However, this result might apply to *anisotropic* ladders [J. Riera (private communication)].

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