Doped two-leg ladder with ring exchange: exact diagonalization and density matrix renormalization group computation

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The effect of a ring exchange on doped two-leg ladders is investigated combining exact diagonalization (ED) and density matrix renormalization group (DMRG) computations. We focus on the nature and weights of the low energy magnetic excitations and on superconducting pairing. The stability with respect to this cyclic term of a remarkable resonant mode originating from a hole pair - magnon bound state is examined. We also find that, near the zero-doping critical point separating rung-singlet and dimerized phases, doping reopens a spin gap.

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Two-leg cuprate ladders\(^1\) and two-dimensional (2D) high-temperature (high-\(T_c\)) superconductors seem to surprisingly share many similarities. In addition, ladders exhibit exotic physical behaviors characteristic of one-dimensional systems. Under high hydrostatic pressure, the intrinsically doped Sr\(_2\)Ca\(_2\)Cu\(_4\)O\(_{11.5}\+) ladder material\(^2\) becomes superconducting hence reinforcing the similarity between two-leg ladder and layer-based cuprates. Doped two-leg ladders are also appealing for theorists\(^1\) : its ground state (GS) is believed to be a simple realization of the Resonating Valence Bond (RVB) state proposed by Anderson\(^3\) in the context of high-\(T_c\). In addition, ladders are one of the simplest realistic correlated electron systems to investigate novel mechanisms of superconductivity\(^4\). Interestingly, new low-energy magnetic excitations have been observed by Nuclear Magnetic Resonance (NMR) under pressure, i.e. under doping the ladder planes\(^2\), a finding possibly connected to predicted exotic magnon-hole pair states\(^5\).

Taking into account ring exchange has proven to be essential to understand the spin dynamics of insulating cuprate materials such as both ladders\(^6\) and high-\(T_c\). Ring exchange which permutes cyclically spins on square plaquettes is known to suppress magnetic order in several 2D systems. It naturally appears in a fourth order term of the Hubbard model near half-filling and also in \textit{ab initio} calculations\(^8\). In order to study the properties of lightly doped ladders\(^9\) with ring exchange, we shall use the framework of the \(-J\) Hamiltonian and include a cyclic exchange of magnitude \(K\)

\[
\mathcal{H} = -t \sum_{<ij>,\sigma} \mathcal{P}_G [c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}] \mathcal{P}_G \\
+ \frac{J}{4} \sum_{<ij>} [S_i \cdot S_j - \frac{1}{4} n_i n_j] + K \sum_{ijkl \in \square} [P_{ijkl}^\sigma + P_{ijkl}^\bar{\sigma}]
\]

with \(\mathcal{P}_G\) Gutzwiller projectors. Labels \(i, j, k, l\) of permutation operators \(P_{ijkl}\) stand for the sites encountered along each square plaquette. The expression of the cyclic exchange in terms of spin \(1/2\) operators

\[
\begin{align*}
P_{ijkl}^\sigma & = \frac{1}{4} [S_i \cdot S_j + S_j \cdot S_k + S_k \cdot S_l + S_l \cdot S_i] \\
& + [S_i \cdot S_k + S_j \cdot S_l] + 4 \frac{1}{4} [S_i \cdot S_j] (S_k \cdot S_l) \\
& + (S_i \cdot S_l) (S_j \cdot S_k) - (S_i \cdot S_k) (S_j \cdot S_l)
\end{align*}
\]

includes bilinear frustrating terms and biquadratic terms\(^10\). The \(K\) term leads to a rich phase diagram at half-filling\(^11\). In particular, a phase transition between the RVB rung-singlet phase and a phase with staggered dimer order occurs\(^10\) at the critical point \(K_c/J \approx 0.2\). Experimentally proposed\(^6\) values of \(K/J\) for the insulator ladder material range in a window \(0.025 < K/J < 0.075\). We are also interested here in the proximity of this critical point. Thus, we shall restrict ourselves to parameters \(-0.2 < K/J < 0.2\) and assume a physical value of \(J/t = 0.5\) for which superconducting fluctuations are dominant at low doping\(^9\) when \(K/J < 0\). A similar model has recently been studied on the 2D square lattice\(^14\) in a large \(N\) limit of a derived \(SU(N)\) model.

It is instructive to consider in more detail the effect of the cyclic exchange in terms of the RVB description of ladders\(^15\). Consider a single plaquette. With \(K = 0\), the ground state is exactly described as an RVB state, with the horizontal dimer state added to the vertical dimer state\(^16\). A small nonzero \(K\) rotates between horizontal and vertical valence bond states and acts either to enhance \((K < 0)\) or suppress \((K > 0)\) the resonance. The ground state has energy \(E = -3J + 2K\). For \(K = J/2\), the resonance is destroyed and the singlet ground state is doubly degenerate between linear combinations of the two VB states. On the other hand, a nonzero \(K\) of either sign is frustrating to Néel order. Thus the cyclic term mediates between VB and RVB order.

In this article, after briefly reviewing the undoped case in connection with previous work, we first consider the case of two holes in a ladder, a simple limit where we expect to get physical insight on the various elementary excitations carrying different spin and charge quantum
The effect of doping and connections to experiments.

In a second step, we address the finite doping continuum is located around \( k \) momentum one magnon branch excitation around its minimum at \( \sin / J \approx π/2 \). The dashed line shows \( Δ_s \) which is the spin gap is reduced and vanishes at the critical point \( K/J = 0.25 \). When \( K/J \) does not belong to the Brillouin zone of systems with odd \( L \), \( K/J = 0 \) singlet \( \delta = (\pi,π) \) and that, in the case of two holes under study, \( k_δ \rightarrow (\pi,π) \) in the thermodynamic limit. As \( K/J \) increases, the spin gap is reduced as is the onset of the QP continuum. Lastly, the system with \( K < 0 \) has similar behavior to a two-leg ladder with a rung coupling \( J_⊥ > J_∥ \).

Elementary excitations — The magnetic energy spectrum is shown in FIG. 1 (a). One can distinguish a one magnon branch excitation around its minimum at momentum \( k = (\pi,\pi) \). The bottom of a two-magnon continuum is located around \( k = (0,0) \) with an energy about twice the spin gap. When \( K/J \) increases, the spin gap is reduced and vanishes at the critical point as was previously proposed. There (FIG. 1 (b)), the triplet branch is divided into a symmetric mode \( (k_y = 0, k_x \in [0,\pi/2]) \) reminiscent of the two-magnon continuum, and an antisymmetric mode \( (k_y = \pi, k_x \in [\pi/2,\pi]) \) reminiscent of the one-magnon branch. The doped system (FIG. 1 (c)) is a Luther-Emery liquid provided \( K/J \) remains small enough: a gapless charge mode appears at low momenta, corresponding to the motion of the hole pair, while the one magnon branch remains gapped. A quasiparticle (QP) continuum starts for an energy which equals the pairing energy (computed independently, see after) and larger than the spin gap. Note that the triplet branch has its minimum at an incommensurate momentum \( k_δ = (\pi(1-\delta),\pi) \) and that, in the case of two holes forming a singlet \( d \)-wave bound state when \( L \rightarrow \infty \). Following ref. 6, we define

\[
\Delta_M = E(0h, S = 1) - E(0h, S = 0)
\]

\[
\Delta_S = E(2h, S = 1) - E(2h, S = 0)
\]

\[
\Delta_p = 2E(1h, S = 1/2) - E(2h, S = 0) - E(0h, S = 0)
\]

where \( E(nh, S) \) is the GS energy with \( n \) holes and spin \( S \). \( \Delta_M \) represents the magnon gap, \( \Delta_S \) the spin gap with two holes, and \( \Delta_p \) the pairing energy. Each gap shown on FIG. 2 has been calculated on finite systems with DMRG and then extrapolated to the thermodynamic limit. First, let us make a few general statements on these energies: (i) since a magnon can be created arbitrarily “far away” from the holes, then \( \Delta_S \leq \Delta_M \), (ii) breaking the hole pair creates two quasiparticles so that \( \Delta_S \leq \Delta_p \).

![FIG. 1: (Color online) (a, b) Spectra for undoped ladders from ED calculations on ladders of length \( L = 12, 14 \) and 16. Grey areas are guide to the eyes. (c) Spectra for ladders doped with two holes and \( L = 9, 11, 13 \). Note that \( k_x = π \) does not belong to the Brillouin zone of systems with odd \( L \). The dashed line shows \( Δ_p \) computed independently.](image)

![FIG. 2: (Color online) Comparison between characteristic energies of elementary magnetic excitations in doped ladders. Data are extrapolated from DMRG computations on systems of length up to \( L = 48 \). Proposed experimental values of \( K/J \) for undoped systems are in the Exp. window.](image)
The area of circles is proportional to the correlation value. Up left circle indicates the mean expectation value.

FIG. 3: Hole-hole static correlation functions from ED computations on $L = 13$ ladder with two holes for different $K/J$. Weights $w$ of the projected function are indicated. Lengths of arrows are proportional to the local density values.

These inequalities are well verified in the data. The discontinuity of the spin gap in the infinitesimal doping limit has been attributed to the existence of a bound state between the hole pair and the magnon, responsible for a sharp resonating mode at finite density similar to what can be observed in Inelastic Neutron Scattering (INS) experiments on underdoped cuprates. The binding energy of this bound state can be defined as $\min(\Delta_p, \Delta_M) - \Delta_S$, see FIG. 2. When $\Delta_p < \Delta_M$, the continuum starts at the QP continuum so that the magnon is scattered by QP and acquires a finite life time (dashed part of the $\Delta_M$ line, $K/J \leq -0.04$). When $\Delta_M < \Delta_p$, we expect a continuum of hole pair-magnon scattering states above $\Delta_M$ and below the QP continuum, as shown by the grey dashed area for $-0.04 \leq K/J \leq 0.2$. The binding energy of the bound state is strongly affected by the cyclic exchange with an instability threshold around a value of $K$ significantly smaller than the one of the critical point. Moreover, the pairing energy vanishes simultaneously with the spin gap when $K$ reaches $K_c$.

The binding of holes (and also spinons) in the two-leg ladder can be described as an effect of the resonance in the RVB language: an isolated hole induces a staggered, non-resonating VB state either to the left or the right of the hole, which is only healed by another hole. The destruction of resonance as $K$ is increased towards $K/J \approx 0.2$ should translate directly into weakened and eventual loss of pairing. This effect is clearly evident in FIG. 3. For $K < 0$, the pairing is strengthened both by the enhancement of resonance and by the fact that the cyclic exchange does not act on a plaquette with a hole, favoring states with holes sharing plaquettes.

The pair-magnon binding can be viewed as closely related to ferromagnetic spin polarons. The hopping of holes in a ferromagnetic background is unfrustrated; the magnon produces a small region of enhanced ferromagnetic correlations. In FIG. 4, the bound state has been projected onto the states with two holes on the diagonal of a plaquette (of weights $w$ given on figure) showing indeed a strong ferromagnetic region for $K < 0$. More precisely, the hole pair–magnon binding results from a gain in kinetic energy coming from processes that exchange the triplet and the pair locally on a plaquette. As $K/J$ increases, the “free” magnon excitation lowers its energy while the above resonant processes are less affected.

Finite doping study – We now turn to the more complex case of finite doping. As shown below, we find signatures of the various excitations identified in the previous part. The spin gap for several hole density $\delta$ is displayed in FIG. 5. For $K/J = 0$, we see that it is reduced under doping because holes weaken spin exchange but remains robust. For small magnitude of cyclic exchange (for instance $K/J = 0.06$) this effect is still significant, leading to an appreciable lowering in comparison with the undoped system. As the critical point is approached, the magnetic parent acquires a smaller spin gap but the relative decrease under doping is less and less significant. Interestingly, at the half-filling critical point $K_c/J \approx 0.2$, doping eventually leads to a reopening of the spin gap. Qualitatively, this could be explained by the fact that a hole on a plaquette prevents the action of the ring exchange. Therefore, at sufficiently large doping ($\delta \approx 0.4$), the spin gap depends weakly on $K$ for studied values. Pairing energy also increases at large densities which suggests a deep relation between pairing and spin gap.

We have computed static and dynamic spin structure factor data on $L = 13$ ladder with two holes for different $K/J$. The area of circles is proportional to the correlation value. Up left circle indicates the mean expectation value.

FIG. 4: Spin density around the hole pair in the first triplet state from ED data on $L = 13$ ladder with two holes for different $K/J$. The weights $w$ of the projected function are indicated. Lengths of arrows are proportional to the local density values.

FIG. 5: (Color online) Spin gap for doped two-leg ladders as a function of hole doping $\delta$. Data extrapolated from DMRG computations on systems of length $L = 16$ to 64 and doping $\delta = n/16$, $n = 0, \cdots, 6$, with a number of kept states up to $m = 1600$. The $\delta = 0$ magnon energies are indicated by grey symbols (see arrows). Half the pairing energy for a finite system is also given by dashed lines.
use the standard definitions of excitations that can be detected in INS experiments. We denote poles and their relative weight (see text).

(b) $k$ = (0,0) with $k = (k_x, k_y)$, for a ladder of length 10 with 4 holes. Red dots indicate poles and their relative weight (see text). (b) relative weight of the resonant state at $k_s$.

FIG. 7: (Color online) (a) dynamic structure factor $S(k, \omega)$, with $k = (k_x, k_y)$, for a ladder of length 10 with 4 holes. Red dots indicate poles and their relative weight (see text). (b) relative weight of the resonant state at $k_s$.

Inspecting $S(k, \omega)$ reveals a pole well separated from the rest of the spectrum at momentum $k = k_s$ (FIG. 7 (a)). This peak can be clearly identified as the resonant mode issued from the triplet BS discussed above. Although ED suffers from finite size effects and dynamic spectra are tedious to analyze due to multi-excitation continua, the evolution of its relative weight given by $|\langle \psi_{\text{Res}} | S^z_k | \psi_0 \rangle|^2 / S(k_s)$ (where $| \psi_{\text{Res}} \rangle$ is the resonant state wave function) is still very instructive. Note that in the thermodynamic limit, the resonant mode should not give rise to a single pole but rather a singularity. The evolution of the relative weight is displayed in FIG. 7 (b) and shows that the BS remains robust at finite density and $K > 0$, keeping a sizeable fraction of the total weight. Consequently, we predict that it should be observable in spin dynamics sensitive experiments. This conclusion on the robustness and observability of the Luther-Emery phase is in agreement with recent NMR experiments on doped ladder materials.

Conclusion – In summary, we show that the nature of the Luther-Emery phase and its remarkable resonant mode is preserved for intermediate physical $K/J$ values. In this regime, both spin gap and superconducting pairing energy are very sensitive to the ring exchange. In addition, doping is shown to have a drastic effect at the magnetic critical point of the parent Mott insulator.

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