Copper-oxide ladder compounds are currently under much investigation [4]. Among their interesting properties are a spin-liquid ground state in the undoped limit, and the existence of superconductivity upon hole doping \( \Delta t \). Recently, the first angle-resolved photoemission (ARPES) studies of ladder materials have been reported. Both the doped and undoped ladder \( \text{Sr}_{14}\text{Cu}_{24}\text{O}_{41} \) have been analyzed, finding one-dimensional metallic characteristics [4]. Studies of the ladder compound \( \text{La}_{1-x}\text{Sr}_x\text{CuO}_2 \) found similarities with \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), including a Fermi edge [5]. Core-level photoemission results for the high-Tc cuprates are a spin-liquid ground state in the undoped limit, in spite of the existence of a gap at \((\pi, 0)\) near half-filling (caused by hole pair formation) and flat bands in its vicinity. These features should be observable in ARPES experiments on ladders. The main result of the paper is the nontrivial evolution of the spectral function from a narrow band at \( x = 0 \), to a quasi-noninteracting band at \( x \geq 0.5 \). It was also observed that the low-energy peaks of a cluster spectra acquire finite line-widths as their energies move away from the chemical potential.

Hole-Density Evolution of the One-Particle Spectral Function in Doped Ladders

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The spectral function \( A(q, \omega) \) of doped \( t - J \) ladders is presented on clusters with up to \( 2 \times 20 \) sites at zero temperature applying a recently developed technique that uses up to \( \sim 6 \times 10^6 \) rung-basis states. Similarities with photoemission results for the 2D cuprates are observed, such as the existence of a gap at \((\pi, 0)\) near half-filling (caused by hole pair formation) and flat bands in its vicinity. These features should be observable in ARPES experiments on ladders. The main result of the paper is the nontrivial evolution of the spectral function from a narrow band at \( x = 0 \), to a quasi-noninteracting band at \( x \geq 0.5 \). It was also observed that the low-energy peaks of a cluster spectra acquire finite line-widths as their energies move away from the chemical potential.

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Copper-oxide ladder compounds are currently under much investigation [1]. Among their interesting properties are a spin-liquid ground state in the undoped limit, and the existence of superconductivity upon hole doping \( \Delta t \). Recently, the first angle-resolved photoemission (ARPES) studies of ladder materials have been reported. Both the doped and undoped ladder \( \text{Sr}_{14}\text{Cu}_{24}\text{O}_{41} \) have been analyzed, finding one-dimensional metallic characteristics [4]. Studies of the ladder compound \( \text{La}_{1-x}\text{Sr}_x\text{CuO}_2 \) found similarities with \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), including a Fermi edge [5]. Core-level photoemission experiments for \( (\text{La}, \text{Sr}, \text{Ca})_{14}\text{Cu}_{24}\text{O}_{41} \) documented its chemical shift against hole concentration [6]. Note that the importance of ARPES studies for other materials such as the high-Tc cuprates is by now clearly established [7]. Using this technique the evolution with doping of the Fermi surface has been discussed [8], including the existence of flat bands near momenta \((0, \pi) - (\pi, 0)\) [9]. These plethora of experimental results for the cuprates should be compared against theoretical predictions. However, the calculation of the ARPES response even for simple models is a formidable task. The most reliable computational tools for these calculations are the Exact Diagonalization (ED) method, restricted to small clusters, and the Quantum Monte Carlo (QMC) technique supplemented by Maximum Entropy, limited in doped systems to high temperatures due to the sign problem. Currently, on ladders dynamical properties can be exactly calculated at all densities only on clusters of size \( 2 \times 8 \) [10, 11], while the QMC technique in the realistic regime of large \( U/t \) (Hubbard model) has been applied on \( 2 \times 16 \) lattices only at half-filling [12] and with 1 hole [13], the latter using an anisotropic ladder since for the isotropic case the sign-problem is severe.

Due to the limitations of these techniques an important issue still unclear is the evolution of the one-particle spectral function between the undoped limit, dominated by antiferromagnetic (AF) fluctuations both on ladders and planes, and the high hole-density regime where those fluctuations are negligible. While both extreme cases are properly treated by previously available numerical methods, the transition from one to the other as the hole density \( x \) grows is still unknown. This evolution is expected to be highly nontrivial. For instance, the presence of hole-pairs in lightly doped ladders suggests the opening of a gap in ARPES, similar to the pseudogap of under-doped high-Tc cuprates [13]. Shadow-band features in undoped ladders [1], which are absent at higher hole densities, adds to the complexity of this evolution.

Motivated by this challenging problem, in this paper the density evolution of the spectral function \( A(q, \omega) \) of doped 2-leg \( t - J \) ladders is presented. The calculation is carried out at zero temperature on clusters with up to \( 2 \times 20 \) sites, increasing by a substantial factor the current resolution of the ED techniques. These intermediate size clusters were reached by working with a small fraction of the total Hilbert space of the system [16]. The method is variational, although accurate as shown below. The improvement over previous efforts lies in the procedure used to select the basis states of the problem [17]. The generation of the new basis is in the same spirit as any technique of the renormalization-group (RG) family. If the standard \( S_z \)-basis is used (3 states per site), experience shows that a large number of states is needed to reproduce qualitatively the spin-liquid characteristics of the undoped ladders. The reason is that in the \( S_z \)-basis one of the states with the highest weight in the ground state is still the Néel state, in spite of the existence of a short AF correlation length \( \xi_{AF} \). A small basis built up around the Néel state incorrectly favors long-range spin order. However, if the Hamiltonian of the problem is exactly rewritten in, e.g., the \( \text{rung} \)-basis (9 states/rung for the \( t - J \) model) before the expansion of the Hilbert space is performed, then the tendency to favor a small \( \xi_{AF} \) is natural since one of the dominant states in this basis for the undoped case corresponds to the direct product of singlets in each rung, \( |S\rangle \), which has \( \xi_{AF} = 0 \) along the chains. Fluctuations of the Resonant-Valence-Bond (RVB) variety around \( |S\rangle \) appear naturally in this new representation of the Hamiltonian leading to a finite \( \xi_{AF} \).
FIG. 1. $e_{GS}$ vs $x$ for the $t – J$ model using the method described in this paper for the two clusters indicated ($t = 1$). DMRG results with OBC are also provided for comparison; (b) Ground state hole-hole density correlations vs distance for a variety of clusters and densities as indicated. Some results using DMRG with PBC are also shown; (c) Ground state staggered spin-spin correlations vs distance $d = |i – j|$ along the leg opposite to where site $i$ is located. Number of holes are indicated. Some results with DMRG are also shown. Open (full) symbols are for $2 \times 16$ ($2 \times 20$) clusters.

As a first step, let us compare ORBA predictions for equal-time observables against DMRG results for the same clusters. Here a coupling $J/t = 0.4$ is used. Its particular value is important: if $J/t$ is smaller, then pairs are lost while if it is larger superconducting correlations are important. Only in a small window of $J/t$ is that the ground state can be considered as formed by weakly interacting hole pairs, a regime that we want to investigate in this paper for its possible connection with the phenomenology of high-Tc at finite temperature. Fig.1a contains the ground state energy per site $e_{GS}$ vs $x$ using $\sim 2 – 3 \times 10^6$ states in the rung-basis. The DMRG energies are obtained with $m = 200$ states and open boundary conditions (OBC). Both sets of data are in good agreement [14]. On $2 \times 20$ clusters, the rung-basis approach allowed us to study up to 6 holes [21] which has a full space of $\sim 10^{14}$ states (for zero momentum and total spin), while the largest previously reported exact study on a $2 \times 10$ cluster and 2 holes needs a $\sim 5 \times 10^9$ basis [10,11].

Calculating the binding energy, or the chemical potential $\mu$ vs $x$, from $e_{GS}$ supplemented by the energies for an odd number of electrons, a tendency to pair formation at low hole-density was observed [10,22]. Fig.1b contains the hole-hole correlations at several densities, compared (in one case) with PBC DMRG results. In Fig.1c spin-spin correlations are shown. The rung-basis properly reproduces the existence of a small $\xi_{AF}$ in the ground state, that decreases as $x$ grows. Size effects are not large for the clusters studied here, and good agreement with DMRG is observed. This technique captures the essence of the ground state behavior [22].

To produce dynamical results Ref. [17] was followed, namely $\sim 10 – 20\%$ states of the reduced basis $N$-holes ground state $|\psi_0\rangle$ were considered [23] and the reduced subspace with, e.g., $N + 1$ holes and $\mathbf{q}$-momentum was obtained through $\hat{O}_\mathbf{q}^\dagger |\psi_0\rangle$ ($\hat{O}_\mathbf{q} = \sum_\mathbf{j} e^{\mathbf{q} \cdot \mathbf{j}} \mathbf{j}^\dagger$, with $\mathbf{j}^\dagger$ the hole creation operator at $\mathbf{j}$, dropping the spin-index, in the rung-basis). All states generated by this procedure were kept, and we worked in such a subspace in the subsequent iterations of the continued fraction expansion [24]. Only the bonding band subspace is discussed here [25].

The $\delta$-functions have a width 0.1$t$ throughout the paper. Fig.2a corresponds to the undoped limit. A sharp peak is observed at the top of the PES spectra, maximized at momenta $q_x = 7\pi/10$, i.e. close to the Fermi momentum for noninteracting electrons $q_x^F = 0.66\pi$. The band defined by those peaks has a small bandwidth, as in 2D models, due to the interaction of the injected holes with the spin background [24,25]. Note that all peaks at momenta $q_x \geq \pi/2$ carry a similar weight and the dispersion is almost negligible. This unusual result is caused by
strong correlation effects. The PES weight above $q_x^F$, e.g. at $q_x = \pi$, is induced by the finite but robust $\xi_{AF}$, and its existence resembles the antiferromagnetically induced “shadow” features discussed before in 2D models [27].

Fig.2b contains results at low but finite hole-density. Several interesting details are observed: (i) the PES band near $\mu$ is flat. This should be an ARPES observable result resembling experiments in 2D cuprates, and it adds to the growing evidence linking the physics of ladders and planes; (ii) $q_x = \pi (\pi/2)$ PES has lost (gained) weight compared with $x = 0$; (iii) the total PES bandwidth has increased; and (iv) the IPES band is intense near $q_x = \pi$, and it is separated from the PES band by a gap. The observed gap is $\Delta \sim 0.4t$ and it is caused by hole pairing. The DMRG/PBC binding energy calculated for the same cluster and density is $\sim 0.32t$ ($m = 200$, truncation error $\sim 10^{-4}$). In the overall energy scale of the ARPES spectra, this difference is small and does not affect the study of the evolution of the dispersion shown here. Note that the results of Fig.2b are similar to those observed near $(\pi,0)$ using ARPES in the 2D cuprates normal state [9][13].

Fig.3. Same as Fig.2 but using a $2 \times 16$ cluster and the hole densities and momenta indicated. In (a) PES, the results are also shown using a width 0.001$t$ (and a different vertical scale) to visualize the individual $\delta$-functions. The number next to each broad peak is the number of poles contributing to it (some are difficult to resolve due to their small weight). In (b) and $q = (\pi/2,0)$ results obtained using 1.1, 2.8, 4.5 million states are shown (dashed lines) from left to right, to illustrate the convergence. The solid lines were obtained with 6.0 million states. At this density the Hilbert space is maximized for the $2 \times 16$ cluster.

Fig.3a contains results at $x = 0.1875$. The trends observed at $x = 0.1$ continue, the more dramatic being the reduction of the $q_x = \pi$ PES weight caused by the decrease in $\xi_{AF}$. The lost weight appears in the $q_x = \pi$ IPES signal. The gap is still observed in the spectrum. Weak BCS-like features both in PES and IPES near $q_x^F$ can be seen. Fig.3b contains data at $x = 0.3125$, and up to $6 \times 10^6$ states. The Hilbert space is maximized at this density for the $2 \times 16$ cluster. Now the result resembles more a noninteracting system on a discrete lattice. The IPES signal is no longer very flat, and the IPES band now has a clear energy minimum near the momentum where PES is maximized. Fig.3c contains results for $x = 0.5$ where a quasi-non-interacting dispersion is obtained using about $3 \times 10^6$ states in $|\psi_0\rangle$. The inset shows that the trend continues at lower electronic densities. The bandwidth evolves from being dominated by $J$ near half-filling, to having $t$ as natural scale at $x \sim 0.3$ or larger. This evolution is smooth, yet nontrivial, following the reduction of $\xi_{AF}$ with doping.

A conceptually interesting issue in the context of finite-cluster spectra of electronic models is whether finite line-widths for the dominant peaks can be obtained by such a procedure. Studying the small clusters reached by ED techniques it naively seems that those peaks are usually generated by just one $\delta$-function (one pole). However, in the bulk limit, peaks away from the Fermi level should have an intrinsic width. How can we reach such a limit from finite clusters? One possibility is that as the cluster grows, the number of poles $N_p$ in a small energy window centered at the expected peak position must grow also, with their individual intensities becoming smaller such that the combined strength remains approximately constant. While this idea seems reasonable, it still has no explicit verification, but the intermediate size clusters reached in this study allow us to test it. Consider as an example Fig.3a where the actual energy and intensity of the poles contributing to the main features are shown explicitly. As the peaks move away from the top of the PES band, $N_p$ was indeed found to increase providing evidence compatible with the conjecture made above [28].

Fig.4a contains the main-peak weights in the PES band vs density. Size effects are small. The weight at $q_x = \pi$ diminishes rapidly with $x$, following the strength of the spin correlations of Fig.1c. Overall the region affected the most by spin correlations is approximately $x \leq 0.25$. Fig.4b summarizes the main result of the paper, providing to the reader the evolution with $x$ of the ladder dominant peaks in $A(q,\omega)$. The area of the circles are proportional to the peak intensities. At small $x$ a hole-pairing-induced gap centered at $\mu$ is present in the spectrum, both the PES and IPES spectra are flat near $(\pi,0)$, and the band is narrow. The PES flat regions at high momenta exist also in the undoped limit, where they are caused by the short-range spin correlations. Actually the resolution in densities and momenta achieved in this study allow us to reach the conclusion that the undoped and lightly doped regimes are smoothly connected. As $x$ grows to $\sim 0.3$, the flat regions rapidly loose intensity near $(\pi,0)$, and the gap collapses.
Summarizing, the bonding-band spectral function of the 2-leg $t - J$ model has been calculated, and results can be used to guide future ARPES experiments for ladder compounds. These experiments should observe flat bands and gap features near $(\pi, 0)$ in the normal state. The data was found to be remarkably similar to experimental results for the 2D cuprates along the $(0, 0) - (\pi, 0)$ line. A common explanation for these features was proposed. Finally, note that the ORBA method discussed here introduces a new way to calculate dynamical properties of spin and hole models on intermediate size clusters. The method can be applied to a variety of strongly correlated electronic models.

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![FIG. 4. (a) Weight of the low-energy dominant feature in $A(q_x, \omega)$ for two momenta $q_x$ in the bonding band vs. $x$. Cluster sizes are indicated; (b) Evolution with doping of the dominant feature band ($t = 1$). The open (full) circles are centered at the peak energies $\epsilon_{QP}$ below (above) $\mu$. The hole densities are indicated. The area of the dots is proportional to the weight of the peak. The results can apply to 2D systems along the $(\pi, 0) - (0, 0)$ line.](image)
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