Effects of interladder couplings in the trellis lattice

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Strongly correlated models on coupled ladders in the presence of frustration, in particular the trellis lattice, are studied by numerical techniques. For the undoped case, the possibility of incommensurate peaks in the magnetic structure factor at low temperatures is suggested. In the doped case, our main conclusion for the trellis lattice is that by increasing the interladder coupling, the balance between the magnetic energy in the ladders and the kinetic energy in the zig-zag chains is altered leading eventually to the destruction of the hole pairs initially formed and localized in the ladders.

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I. INTRODUCTION

The study of strongly correlated systems in low spatial dimensions is nowadays the center of an intense effort both theoretically and experimentally. Among these low-dimensional systems the ones containing two-leg ladders have received considerable attention. One of the original motivations for the study of ladders was the search for a mechanism for pairing in a strongly correlated model. This possibility was later confirmed by a number of studies and the symmetry of the superconducting order parameter was found to be d_{x^2-y^2} (Refs. 2,3). A considerable interest in these theoretical predictions was renewed by the discovery of superconductivity in the ladder compound Sr_{14}Cu_{24}O_{41} (14-24-41) after being doped with Ca and under a pressure of \approx 3GPa (Ref. 4).

However, the 14-24-41 compound, as well as many other compounds, like another cuprate SrCuO_3 and the vanadates CaV_2O_5 and NaV_2O_5, actually contain layers of two-leg ladders which are coupled by frustrated effective interactions in the so-called trellis lattice. The strength of these frustrating interladder couplings may be weak enough to consider the ladders as essentially isolated or strong enough to change radically the physical behavior of a single ladder.

The original experiments on Sr_{0.4}Ca_{13.6}Cu_{24}O_{41} (Ref. 4) reveal that the superconducting critical temperature reaches its maximum of 12K at a pressure of \approx 3GPa and then decreases as the pressure is further increased. Similar results were obtained for Sr_{2.5}Ca_{11.5}Cu_{24}O_{41} (Ref. 4). The application of pressure to this compound may change the strength of some couplings, or to additionally increase the doping of the ladder layers as holes are transferred from the chain layers also present in this compound. The main purpose of this paper is to analyze the first possibility, neglecting more radical changes in the crystallographic structure. In a highly simplified model for this compound, we consider three sets of couplings: along the ladder legs, along the rungs, and on the “zig-zag” interactions between the ladders. The effect of varying the rung interactions, keeping fixed the leg ones, on a single ladder, has been analyzed extensively. In the present study we will concentrate on the effects of varying the interladder couplings specially on the magnetic and pairing properties.

To this purpose we study the t – J model which is appropriate to describe these cuprates and vanadates characterized by large on-site Coulomb repulsion and close to half-filling. We start our studies with undoped frustrated coupled ladders. For the trellis lattice, it was suggested that it is possible a transition from a spin liquid to a possible spiral order with incommensurate magnetic correlations as the interladder coupling increases. Then, we will consider specially the case of two-hole doping, i.e. the evolution of pairing as the interladder coupling is varied. Preformed hole pairs are already present in the uncoupled ladders and a small ILC could lead to superconductivity (SC) as a proximity effect between the ladders. However, our main concern in this work is not the onset of SC but rather the effect on pairing due to somewhat large ILC.

There are further motivations to study both experimentally the 14-24-41 compound and theoretically the t – J model on the trellis lattice. It is in effect remarkable how a relatively small difference like the one between the square lattice of the Cu–O planes in high-T_c cuprates and the trellis lattice in 14-24-41 leads to such a considerable difference in the superconducting properties of those materials. This difference is even more remarkable if we take into account the presence of stripes in the underdoped regime and (at least) above the superconducting region of the high-T_c cuprates. These stripes can be thought as metallic ladders separated by insulating antiferromagnetic ones, specially in the “bond-centered” stripes, obtained from a numerical study of the 2D t-J model.

In this sense, the t – J model on the trellis lattice is a testing ground for the study of the competition between magnetic and kinetic energies which is at the core of the mechanism of micro-phase separation leading to the formation of stripes in the high-T_c cuprates. Our main conclusion for the trellis lattice is that by increasing the interladder coupling, the balance between the magnetic energy in the ladders and the kinetic energy in the zig-zag
chains in between the ladders is altered leading eventually to the destruction of the hole pairs initially formed and localized in the ladders. We also suggest the possibility that the hole pairs may go to the zig-zag chains in a process which represents a transition from a magnetic to a kinetic mechanism of pair binding.

The t-J model on the trellis lattice is given by the Hamiltonian:

\[ \mathcal{H} = \mathcal{H}_{\text{leg}} + \mathcal{H}_{\text{rung}} + \mathcal{H}_{\text{inter}} \quad (1) \]

where

\[ \mathcal{H}_\alpha = -t_\alpha \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\alpha}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + J_\alpha \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) \]

The couplings are \((t, J),(t', J')\) and \((t_{\text{inter}}, J_{\text{inter}})\) along the legs, along the rungs and between the ladders respectively (Fig. 1). The rest of the notation is standard. Periodic boundary conditions in both directions are considered except otherwise stated. We adopt \(J = 0.4t\), a value usually taken to model high-\(T_c\) cuprates, and in order to reduce the number of independent variables \(J_\alpha = J(t_\alpha/t)^2\). Moreover, we take \(t = 1\). For the undoped compound, neutron scattering experiments for the 14-24-41 compound\(^6\) suggest \(J = 2J'\). However, taking into account the analysis mentioned in Ref. \(^7\) most of our calculations have been done for the isotropic case.

We use various numerical techniques like quantum Monte Carlo (QMC), with a conventional world-line algorithm, and exact diagonalization with the Lanczos algorithm (LD), complemented by the continued fraction formalism to compute dynamical properties.

II. FRUSTRATED COUPLED SPIN LADDERS

The first issue we want to address is the evolution of the magnetic order in the absence of doping as the interladder coupling is increased. To this end we have computed the static magnetic structure factor \(S(q)\) on \(L \times L\) clusters using QMC. Due to the presence of frustration, the minus sign problem prevents us to reach low temperatures and to study larger clusters which would be necessary to perform a finite size scaling. The same problems were already faced in a previous QMC study of the susceptibility of this system\(^8\) in order to reduce the minus sign problem and to take advantage of the simple checkerboard decomposition\(^\text{13}\) we take a slightly modified lattice in which the interladder couplings are “perpendicular” \((J_{\text{perp}})\) and “diagonal” \((J_{\text{diag}})\) as shown in Fig. 1. This lattice contains just half of the diagonal interladder couplings than in the trellis lattice, and we have checked by exact diagonalization on small clusters that this difference does not change qualitatively the results. Even for this modified lattice the minus sign problem is severe as shown in Fig. 2. We recall that the average of any observable \(\mathcal{O}\) in a system which presents this problem is computed as:

\[ \langle \mathcal{O} \rangle = \frac{\langle \mathcal{O}\text{Sign} \rangle}{\langle \text{Sign} \rangle} \]

with respect to a modified partition function of the 2+1-dimensional problem, \(\mathcal{Z}' = \sum_s \exp S(s)\) where \(S(s)\) is an effective action. In particular, the average sign is:

\[ \langle \text{Sign} \rangle = \frac{1}{\mathcal{Z}'} \sum_s \text{Sign}(s) |\exp S(s)|, \]

where \(\text{Sign}(s) = \text{sign}(\exp S(s))\). Then \(\langle \text{Sign} \rangle\) is the ratio of the original partition function \(\mathcal{Z} = \sum_s \exp S(s)\) to \(\mathcal{Z}'\). In practice, at each measurement step, \(\exp S(s)\) is computed as the product of the transition elements of

\[ \text{FIG. 1. Left: trellis lattice. Right: modified trellis lattice. Ladder legs and rungs are indicated with full and dashed lines respectively. In the modified lattice, “perpendicular” and “diagonal” interladder couplings are indicated with dotted and dash-dotted lines respectively.} \]
all the cubes that make up the 2 + 1-dimensional lattice. Nonetheless, although we cannot compute some quantities in the bulk limit, we can indicate qualitatively the behavior of the magnetic order as a function of $J_{\text{inter}}$ (we take $J$ as the unit of energies in this section).

Typical results are shown in Fig. 2(a) for coupled isotropic ($J' = J$) ladders on the 8 \times 8 cluster. In Fig. 2(a) we show for $J_{\text{perp}} = J_{\text{diag}} = 0.2$ the characteristic structure factor of isolated ladders with a peak at $(q_x, q_y) = (\pi, \pi)$ ($x$ ($y$) is the direction along (transversal) to the ladders). This peak becomes more pronounced as the temperature is lowered. On the other hand, keeping $J_{\text{perp}} = 0.2$ and as $J_{\text{diag}}$ is increased, the peak starts to shift from $(\pi, \pi)$ to $(\pi, \pi/2)$ (Fig. 2(b,c,d)). A second interesting feature should be noticed in Fig. 2(d): the peak of $S(q)$ is located at $(\pi,\pi)$ at high temperature (in this case down to $T \approx 0.8$, in units of $J$) and as the temperature is lowered it starts to shift away from $(\pi,\pi)$. At low temperatures (in this case below $T \approx 0.4$ the peak is located at $(\pi, \pi/2)$. Since it is clear that this behavior is caused by the frustration of the interladder couplings, it will certainly be present in the original trellis lattice. As indicated in Fig. 2(b), it is possible that an incommensurate peak across the ladder direction could be present at intermediate values of $J_{\text{diag}}$ and intermediate temperatures.

The second point we want to examine is the behavior of the excitations of these systems, in particular the $S = 1$ excitations as can be measured by neutron scattering experiments. For this purpose, using conventional LD

FIG. 2. Average sign of the QMC on the modified trellis lattice. (a) at $J = J' = 1$, $J_{\text{perp}} = J_{\text{diag}} = 0.2$ for 4 \times 4 (open circles), 6 \times 6 (full circles), 8 \times 8 (squares), 12 \times 12 (diamonds) and 16 \times 16 (stars) and (b) for the 8 \times 8 lattice, $J = J' = 1$, $J_{\text{perp}} = 0.4$ and $J_{\text{diag}} = 0.4$ (open circles), 0.8 (full circles), 1.2 (squares), 1.6 (diamonds), 2.0 (stars).

with the standard continued fractions formalism we have computed the zero temperature dynamical structure function ($zz$ component) $S(q, \omega)$. In this case, we have to limit ourselves to somewhat smaller clusters but we are confident that the qualitative features we found will survive in the bulk limit.

Results obtained for the 4 \times 4 cluster are shown in Fig. 3. In the absence of frustration (Fig. 3(a)) the peak in $S(q, \omega)$ which corresponds besides to the lowest excitation, is located at $(\pi, \pi)$, as expected in the bulk limit for an AF order. As a frustrating ILC is increased (Fig. 3(b,c,d)) it can be seen that considerable spectral weight is transferred to the peak at $(\pi, \pi/2)$, which becomes finally the lowest energy excitation. Similar results are also shown for the 4 \times 6 cluster for $q = (\pi, \pi)$ and $(\pi, \pi/2)$.

The results shown in Figs. 3 and 4 are unequivocally due to frustration and are qualitatively similar to the ones previously obtained in a system of ferromagnetically (FM) coupled ladders. Similar results have been obtained by LD on the 4 \times 4 and 4 \times 6 clusters of the real trellis lattice. In the case of the trellis lattice, as in the FM ILC case, we expect that the behavior above discussed will be present in the bulk limit for strong enough interladder couplings and low enough temperatures. The impossibility of assessing finite size effects prevents us to determine if this behavior is present for arbitrarily small values of $J_{\text{inter}}$ or, on the contrary, only for values larger than a “critical” one.

FIG. 3. Magnetic static structure factor $S(q)$ obtained by QMC on a 8 \times 8 cluster of the modified trellis lattice, at several temperatures (in units of $J$), $J = J' = 1$, $J_{\text{perp}} = 0.2$ and (a) $J_{\text{diag}} = 0.2$, (b) 0.4, (c) 0.6 and (d) 0.8.

The second point we want to examine is the behavior of the excitations of these systems, in particular the $S = 1$ excitations as can be measured by neutron scattering experiments. For this purpose, using conventional LD

FIG. 4. Dynamical structure factor $S(q, \omega)$ for several momentum for $J$), $J = J' = 1$, $J_{\text{inter}} = 0.8$ and various values of $J_{\text{diag}}$ as indicated in the figures. These results were obtained on a system of two coupled 2 \times 4 (full lines) and 2 \times 6 (dashed lines) ladders.

We have not detected any sign of incommensurability along the ladder direction. Such an incommensurability is expected in principle since a trellis lattice can be also
considered as coupled $J_1 - J_2$ chains ($J_1 = J_{inter}$, $J_2 = J$, in our notation) which are known to present a peak in $S(q)$ at a momentum which continuously varies from $\pi$ to $\pi/2$ (as defined on our modified trellis lattice) as $J_{2}/J_{1}$ goes from $\infty$ to zero. However, notice that, as can be seen in Fig. 3, values of $J_{inter} > 0.6$ at low enough temperatures cannot be reached in our simulations.

III. DOPED TRELLIS LATTICE.

We now analyze the hole pairing in the doped trellis lattice as the interladder couplings are increased. To gain some insight in this problem we start by considering an isolated building block of the trellis lattice. This minimal system is a three chain cluster consisting of a ladder and a zig-zag chain, (lines “1”, “2” and ‘3’ in Fig. 1). The Hamiltonian is the one defined in Eq. (1). All the results in this section have been obtained by exact diagonalization. The justification of this study involving somewhat small clusters is based on an extensive body of similar studies of strongly correlated models which shows that an important part of the physics of these models is dominated by short range effects, which are appropriately captured in these small cluster calculations.

In this minimal trellis lattice already appears, upon doping with two holes, the main feature we want to emphasize. In Fig. 3, the relative hole occupancy (or probability of finding a hole) on each chain is shown in the $3 \times 6$ cluster with two holes for $t' = 0.75$, 1.0 and 1.5 as a function of $t_{inter}$. In the three cases, for small $t_{inter}$ the holes are almost completely located in the ladder legs. As $t_{inter}$ increases the probability of finding a hole in the outer ladder leg decreases while increases the occupancy of chain “3” which is connected to the ladder by the zig-zag interaction. There is a neat change of behavior, from a situation in which the occupancy of chain “3” is virtually unoccupied to a situation in which the unoccupied chain is “1”. moreover, this crossover is rather abrupt, specially for $t' = 0.75$.

![FIG. 5. Probability of finding a hole in the outer (circles) and inner (squares) ladder legs, and in the third chain (triangles) of the $3 \times 6$ cluster with two holes for (a) $t' = 0.75$, (b) $t' = 1.0$ and (c) $t' = 1.5$. The probability of finding a hole in chain “1” and the other hole in chain “2”, and the probability of finding a hole in chain “2” and the other in chain “3” are indicated with diamonds and stars respectively.

![FIG. 6. Energy contributions from different terms of the Hamiltonian along the legs (circles), rungs (squares) and zig-zag (triangles). Full (empty) symbols correspond to magnetic (kinetic) energies in absolute value. Results obtained on a $3 \times 6$ cluster for (a) $t' = 0.75$, (b) $t' = 1.0$ and (c) $t' = 1.5$. The gain in kinetic energy on the frustrated chain with respect to the ladder can be explained by qualitative arguments as is shown schematically in Fig 7. In the frustrated chain we have assumed an AF order of the spins along the chains which is expected for $J_2 > J_1$ ($t_2 > t_1$). When the hole moves, as in a simple $t - J$ chain, the]
hole leaves behind just a single frustrated (ferromagnetic) bond. Something similar occurs in the case of AF order along the zigzag chain \((J_1 \geq J_2)\). In the case of ladders, we have assumed a magnetic background formed by spin singlets on the rungs. As a hole moves from its initial position, it leaves behind a string of higher energy singlets on the diagonals of the plaquettes. Hence there is a cost in energy which increases roughly linearly with the distance traveled by the hole.

What are the possible consequences of this behavior found in the three-chain cluster for the trellis lattice? In this case, of course, any chain along the ladder direction belongs at the same time to a ladder and to a frustrated interladder chain. The question is if the holes, initially paired on a plaquette in isolated ladders, would tend to break the pairs and move independently on the frustrated chains as the ILC are increased. There is yet another interesting possibility that is that the holes form pairs on the frustrated chains. These pairs would have more kinetic energy than the ones formed on ladders and this change of pairing would imply a change from a magnetic binding on ladders to a “kinetic binding” on chains. In any case, taking into account the results from the three-chain cluster, we predict a loosening of the pairing on ladders. It is difficult to answer these questions by calculations on finite clusters. Exact diagonalization results for two holes on the 4 × 4 cluster give support to the above mentioned possibilities. In Fig. 5 the hole-hole correlation functions for \(t' = 1.0\) at several distances as a function of \(t_{\text{inter}}\) are shown. At small \(t_{\text{inter}}\), the largest correlation corresponds to a pair of holes along the diagonal of a plaquette, which is typical of isolated ladders. Around \(t_{\text{inter}} = 0.7\) there is an abrupt change to a situation in which the largest correlations correspond to holes belonging to the same frustrated chain. The second hole is slightly more likely to be in the other chain of the same interladder zig-zag chain (site ‘4’ of Fig. 5). Somewhat smaller is the correlation on the same chain but at the largest distance on this cluster (site ‘3’). This behavior is radically different to ladders AF coupled in a square lattice without frustration. In this case, the d-wave pair typical of a ladder evolves smoothly to the rotationally invariant d-wave pair of the square lattice.

![Figure 7](image1.png)

**FIG. 7.** Schematic picture of the movement of a hole (a) in a frustrated \(t - J\) chain and (b) in a \(t - J\) ladder. In each case, the original (final) position of the hole is shown in the top (bottom) panel.

Similar results are obtained for the 6 × 4 cluster with two holes. In Fig. 6 we show pictorially the most likely hole probability for \(t' = t_{\text{inter}} = 1.0\). The area of the circles is proportional to the probability of finding a hole if there is a hole in a given site. In this case the largest probability corresponds to holes located at the maximum distance along the same chain. The next probability in decreasing order also corresponds to a hole in the frustrated zig-zag chain. On this cluster we found that as \(t_{\text{inter}}\) is increased from zero the holes initially at a distance \(\sqrt{2}\) starts to move away on the same ladder and finally they move to the same ILC chain.

![Figure 8](image2.png)

**FIG. 8.** Hole-hole correlation functions vs. \(t_{\text{inter}}\) on the 4 × 4 cluster for \(t' = 1.0\). The relative distances from the reference site are indicated in the plot.

Finally, for the sake of completeness, we show in Fig. 10

![Figure 9](image3.png)

**FIG. 9.** Most likely hole distribution if a hole is located in the position indicated by a solid circle. Results obtained on the 4 × 6 cluster for \(t' = 1.0\) and \(t_{\text{inter}} = 1.0\).
the largest nearest and next nearest neighbor spin-spin correlations for small and large values of $t_{\text{inter}}$ for the most likely position of the holes in each case (see Fig. 8). The structure of these correlations globally agrees with the schematic picture of Fig. 7.

FIG. 10. Largest magnetic correlations for the most likely hole distribution. The line thickness of each segment is proportional to the AF correlation of the connected spins. FM correlations are indicated with dashed lines. Results obtained on the $4 \times 4$ cluster for $t' = 1.0$, (a) $t_{\text{inter}} = 0.4$ and (b) $t_{\text{inter}} = 1.0$.

IV. CONCLUSIONS

In summary, we have performed numerical studies on strongly correlated electron systems, as described by the $t - J$ model, on frustrated coupled ladders, in particular on the trellis lattice. In the undoped case, QMC simulations, although hampered by the minus sign problem, allowed us to reach large enough clusters to detect meaningful changes in the magnetic properties of this system. In this case, for ladders coupled with frustrating interactions, we have shown that the peak of the magnetic structure factor shifts from $(\pi, \pi)$ to $(\pi, \pi/2)$ for low enough temperatures as the ILC is increased. Moreover, the peak at $(\pi, \pi/2)$ becomes also the lowest energy excitation. This behavior is very similar to the one previously found for FM coupled ladders. We have shown also that this behavior appears due to the onset of frustration and hence we expect that it will appear in the trellis lattice as well. This behavior could be detected experimentally on a ladder compound like SrCu$_2$O$_2$Cl$_2$ or Sr$_{1/4}$Cu$_{2/4}$O$_{31/2}$ upon a suitable application of pressure. In fact, after the submission of this manuscript we became aware of an experimental study on the similar ladder compound CaCu$_2$O$_3$. The neutron diffraction results reported in this manuscript indicate that the magnetic structure is incommensurate in the direction of the frustrated interladder interaction in the plane of the ladders, as suggested by the present study (see also Ref. 17). The validity of the simpler FM coupled ladders model also explains the vanishing of the spin gap as due to increasing interladder couplings.

Next, we have analyzed the evolution of pairing when the ILC are increased. In this case the physics is governed by short range effects and so we studied small clusters with exact diagonalization. Our main result is that ILC suppresses pairing in ladders. Results on $4 \times 4$ and $6 \times 4$ clusters indicate that holes move to the chains with first and second neighbor interactions formed by the legs of neighboring ladders and the zig-zag interactions between them. We have identified the mechanism of this suppression of pairing as a gain of kinetic energy of the holes by moving on the frustrated chains. Even for these clusters we have noticed important size effects which unable us to determine if it appears an alternative pairing of holes on the frustrated chains or rather the pairing is completely lost when ILC are large enough and holes begin to move independently from each other. Finally, we would like to stress the radically different behavior found in this case with respect to that found in ladders coupled in a square lattice, where the $d_{x^2-y^2}$ pairing is preserved.

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