Magnetic order in ferromagnetically coupled spin ladders

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A model of coupled antiferromagnetic spin-1/2 Heisenberg ladders is studied with numerical techniques. In the case of ferromagnetic interladder coupling, we find that the dynamic and static structure factor have a peak at $(\pi, \pi/2)$ where the first (second) direction is along (transversal) to the ladders. Besides, we suggest that the intensity of this peak and the spin-spin correlation at the maximum distance along the ladder direction remain finite in the bulk limit for strong enough interladder coupling. We discuss the relevance of these results for magnetic compounds containing ladders coupled in a trellis lattice and for the stripe scenario in high-Tc superconducting cuprates.

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I. INTRODUCTION

One of the main topics in condensed matter physics in recent years has been the study of low-dimensional antiferromagnetic spin systems. The strong interest in this field has been sparked by the realization that CuO$_2$ planes play an essential role in high-Tc superconductors, which was followed by the appearance of several compounds characterized by the presence of strong electronic correlations. These compounds include many cuprates, nickelates, vanadates and manganites, and are characterized by important and unique properties. In most of them the proximity of low-dimensional antiferromagnetic (AF) phases are the key to understand these properties.

At the same time, the concept of spin ladder originally introduced to explain the presence of a spin gap in $(VO)_2P_2O_7$ and later in layered cuprates like Sr$_{n-1}$Cu$_n$O$_{2n}$ (Refs. 2,3) became an important theoretical tool to understand the behavior of strongly correlated systems. The physics of the two-leg spin ladder is characterized by the existence of a singlet-triplet spin gap and an exponential decay of correlation functions. The ground state which can be thought to a good approximation as a product of singlets living on the rungs is well understood. However, the above-mentioned cuprates, the important case of Sr$_4$Cu$_2$O$_{4+1}$, as well as many other compounds like CaV$_2$O$_5$, actually contain layers of coupled two-leg ladders. These ladders are coupled by frustrated interactions in a trellis lattice which make its study with analytical or numerical techniques quite difficult. In principle, in the absence of frustration, a reduction of the gap as the interladder coupling increases is expected. Eventually, the system becomes gapless at a quantum critical point (QCP) and for larger coupling it behaves essentially as a two-dimensional (2D) spin-1/2 square antiferromagnet. Much less is known for the trellis lattice, although a Schwinger boson study suggests the transition from a spin liquid to a possible spiral order as the interladder coupling (ILC) increases. Quantum Monte Carlo (QMC) studies of this frustrated system are hampered by the “minus sign problem” and the possibility of using this powerful technique is severely reduced. In this sense, one of the objectives of the present work is to study a model in which the frustrated AF interladder couplings of the trellis lattice are replaced by much simpler ferromagnetic (FM) couplings in a square lattice. We expect that some of the physics of the frustrated system can be captured by this effective simplified model.

Besides, there are compounds which consist of FM coupled ladders like SrCu$_2$O$_3$. The results of the present work could be relevant to other FM coupled gapped systems like the dimerized chains in $(VO)_2P_2O_7$. Previous studies have compared the behavior of AF and FM frustrated and unfrustrated coupled gapless spin systems (spin chains).

Alternatively, a renewed interest in coupled ladders comes from the high-T$_c$ cuprate superconductors themselves. A number of recent experiments, mainly neutron scattering studies, indicate the presence of incommensurate spin correlations which in turn have been interpreted as coming from the segregation of charge carriers into 1D domain walls or “stripes” leaving the regions between them as undoped antiferromagnets. There are several theoretical scenarios that have predicted or that attempt to explain this stripe order but the origin of this order and its relation to superconductivity is still controversial. In particular, the problem of stripe formation in a 2D microscopic model like the t-J or Hubbard models is extremely difficult to study with analytical or numerical techniques. In principle, the inclusion of charge and spin degrees of freedom is essential for the understanding of this problem. However, it has been suggested that assuming the presence of a stripe structure it is very instructive to study its magnetic properties by using a model with spin degrees of freedom only. In this simplified model, the AF insulating regions between the charged stripes are considered as n-leg isotropic ladders coupled by an effective interaction. In one such study, following the initial picture from Ref. the insulating regions were considered as 3-leg ladders coupled by AF interactions. However, a numerical study of the 2D t-J model as well as early studies of charge in-
homogeneities in Hubbard and t-J models\cite{11}, indicate the formation of “bond-centered” stripes, i.e. doped two-leg ladders alternating with undoped two-leg ladders. Coupled spin two-leg ladders were also studied\cite{14} but its relevance to the physics of Cu-O planes is relative since they miss the essential ingredient that the magnetic order of the AF slices is $\pi$-phase shifted as emphasized in Ref.\cite{16}. Hence, the second motivation for the present work comes from the assumption that this $\pi$-phase-shift between ladders can be modeled by taking a ferromagnetic coupling between them.

In summary, the purpose of the present work is to study ferromagnetically coupled two-leg ladders and compare their behavior with the case of AF coupling. If this model is considered as an approximation of AF systems in the trellis lattice, the FM coupling is an effective interaction coming from the frustrated interactions between ladders. If this model is considered as an approach to the stripe phase of the cuprates, the FM interaction comes from a collective effect determined from the competition of charge and spin degrees of freedom. In both cases, the results of the present study lead to predictions which can be tested experimentally. We use essentially numerical techniques like QMC (world-line algorithm) which allows us to reach low enough temperatures so as to capture ground state properties, and exact diagonalization with the Lanczos algorithm (LD), complemented by the continued fraction formalism to compute dynamical properties.

II. QUASI-ONE DIMENSIONAL STUDY.

To gain insight about the effects of FM interladder couplings we start from the case of FM coupled AF dimers which are the simplest systems with a spin gap. We are thus led to 1D or quasi-1D systems which are much easier to study from the numerical point of view. Besides, systems with a random distribution of AF and FM couplings have received some theoretical attention and their possible physical realization in SrCuPt$_{1-x}$Ir$_x$O$_6$ has been discussed\cite{17}. The Hamiltonian is given by:

$$
\mathcal{H} = \mathcal{H}_{\text{dimer}} + \mathcal{H}_{\text{inter}}
$$

where:

$$
\mathcal{H}_{\text{dimer}} = J \sum_a \mathbf{S}_a;1 \cdot \mathbf{S}_a;2,
$$

$$
\mathcal{H}_{\text{inter}} = \sum_{a,b,i,j} J_{\text{inter},a,b,i,j} \mathbf{S}_{a;i} \cdot \mathbf{S}_{b;j},
$$

where $a$ is a dimer index and $i = 1, 2$ labels the sites in a dimer. $J = 1$ for simplicity. Periodic boundary conditions are imposed in the longitudinal direction. There are several ways of coupling dimers. We consider here the simplest case of dimers forming a FM-AF alternating chain (Fig. 1(a)). Another possibility is that of dimers forming a two-leg ladder with FM leg and AF rung interactions. This second case has already been studied numerically\cite{18} but it is not relevant for the problems we wish to address. Besides, we consider the case of FM-coupled AF plaquettes instead of dimers in which case we have a two-leg ladder with FM-AF alternating interactions along the legs (Fig. 1(b)).

Our first concern in this section is the behavior of the spin gap starting from the situation of isolated dimers or plaquettes. Using exact diagonalization we computed the spin gap $\Delta$ by subtracting the energies in the $S = 0$ and $S = 1$ subspaces on finite clusters with up to 24 sites. The extrapolation to the bulk limit was done using the law $\Delta_\infty + b \exp(-L/L_0)/L$. The final result is shown in Fig. 2. We notice that in the limit $J_{\text{inter}} \to -\infty$ we

$$
\Delta = \frac{41}{4} \Delta_\infty \text{ divided by } 4 \text{ (from Ref. (19)).}
$$

![FIG. 1.](image.png)

![FIG. 2.](image.png)
recover the cases of a spin-1 chain for the coupled dimer
system and a spin-1 ladder for the coupled plaquette one.
It is easy to realize (by solving a two-dimer system and a
two-site spin-1 system) that the gap for the spin-1 chain is
four times larger than the gap obtained by the coupled
dimer system when \( J_{\text{inter}} \to -\infty \) and the gap for the
spin-1 ladder is twice larger than the coupled plaquette
system in this limit. Thus, in the former case we obtain a
gap \( \Delta_{cd} \times 4 = 0.410 \), coincident with the value already
reported in the literature. For the spin-1 ladder we would
obtain a gap \( \Delta_{cp} \times 2 = 0.290 \pm 0.008 \), smaller than the
gap for the \( S=1 \) chain as predicted theoretically. Qualitatively, the
important feature here is that the gap decreases
monotonically from the isolated dimers (or plaquettes) case as
\( J_{\text{inter}} \to -\infty \). In the case of FM coupled
dimers, a monotonic behavior could be guessed from the
fact that this system continuously evolves towards the
valence-bond-solid picture of a spin-1 chain in that limit.

On the other hand, the behavior of the coupled plaquettes
system is not obviously predictable.

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 Lanczos
methods with the continued fractions formalism, we have computed the
dynamical structure function (\( zz \)-component) \( S(q, \omega) \) which is shown in Fig 3. Already
for the simplest case of coupled dimers (Fig 3(a),(b)) one can see
an interesting feature which we will observe also
for the coupled ladders case in the next section. The
position of the gap which is at \( q = \pi \) for AF dimerized
chains shifts to \( \pi/2 \) for the case of FM coupled dimers
A similar behavior is observed for coupled plaquettes
(Fig 3(c),(d)), where the lowest energy peak changes from
\((q_x, q_y) = (\pi, \pi) \) to \((\pi/2, \pi) \) (\( x \) is the longitudinal
direction) by switching from AF to FM interplaquette
couplings. In both cases, there is a transfer of spectral weight
from the original AF peak to the FM one. This behavior
is independent of the absolute value of \( J_{\text{inter}} \), except for
finite size effects.

III. COUPLED LADDERS.

We have now arrived at the central part of this
work. The Hamiltonian for the system we consider now
(Fig 1(c)) is essentially the same as (1) which we rewrite
here for clarity:

\[
\mathcal{H} = \mathcal{H}_{\text{ladder}} + \mathcal{H}_{\text{inter}}
\]

where:

\[
\mathcal{H}_{\text{ladder}} = J \sum_{a,l,i} S_{a,l,i} \cdot S_{a,l,i+1} + J \sum_{a,l} S_{a,l,1} \cdot S_{a,l,2},
\]

\[
\mathcal{H}_{\text{inter}} = J_{\text{inter}} \sum_{a,l} S_{a,l,2} \cdot S_{a,l+1,1},
\]

where \( a \) stands now for a ladder index and \( l = 1, 2 \) for
the two legs in a ladder. We have taken the case of an
isotropic ladder by simplicity. \( J \) is again taken as the
unit of energy.

We start with the study of the ground state energy of
the system of both FM and AF coupled ladders. To this
purpose we have performed standard QMC simulations
for \( L \times L \) lattices with \( L = 4, 6, 8, 12, \) and 16.
Periodic boundary conditions in both directions are considered.
For each lattice and set of coupling constants, we took
\( T/J = 0.125, 0.100 \) and 0.07, and the Trotter number \( M \)
at each temperature such that the error due to the time
discretization is comparable or smaller than the
statistical error. Typically, \( M = 140 \) for \( T/J = 0.07 \).
We made runs up to \( 10^6 \) MC steps for both thermalization
and measurement. We computed the energy in the total
\( S_z = 0 \) and \( S_z = 1 \) subspaces (\( E_0 \) and \( E_1 \) respectively).
For each set of coupling constants, we extrapolated the
corresponding energies per site $e_0$ and $e_1$ to the bulk limit using the law $e_\infty + b \exp(-(L/L_0)/2)$ in the gaped region and $e_\infty + b/L^3$ in the gapless case. We obtained very close values for $e_{0,0}$ and $e_{\infty,1}$ which gives an indication of the good quality of the fits. The results for the ground state energy for FM and AF ladder couplings are shown in Fig. 4. An interesting feature can be noticed: the energies for both signs of $J_{\text{inter}}$ are degenerate within numerical errors for $|J_{\text{inter}}| < 0.3$. This situation corresponds to a physics governed mainly by singlet dimers on the ladder runs and in this case the sign of the coupling between these relatively isolated dimers is irrelevant. On the other hand, for $|J_{\text{inter}}| > 0.3$, for AF interladder coupling it is possible that the singlets delocalize from a single ladder and finally form a “resonant valence bond” state or that the singlet-triplet excitations be replaced by gapless magnon excitations. Previous numerical studies precisely locate at $J_{\text{inter}} \approx 0.3$ the position of the QCP at which the ladder-like spin liquid is replaced by a long range 2D-like AF order thus choosing the second possibility. The important point we want to suggest is that in both cases the energy of the system would be lower than for the case of FM ILC where the singlets on the ladders still persist. To illustrate this scenario we have computed on the 16 × 16 cluster the spin-spin correlation functions $S(r) = \langle S^z_i S^z_j \rangle$ for $r = (1,0)$ (leg direction), $(0,1)$ (rung), and $(1,1)$, inside a ladder, and $r = (0,1)$ between two ladders. These correlations, normalized in such a way that $S(0) = 1$, are shown in absolute value in the inset of Fig. 4 as a function of $|J_{\text{inter}}|$. The differences between FM and AF ILC appear in the $(0,1)$ (rung) correlations, which remain stronger in the former case, and most importantly, in the interladder $(0,1)$ correlation which increases faster in the latter. Of course, this correlation is negative (positive) in the AF (FM) case.

This indication of a difference between the two ILC cases can be traced to a more intimate level which would also provide experimentally measurable features. To this end, let us examine now the static structure factor $S(q)$ obtained by Fourier transforming the spin-spin correlations obtained by QMC at the lowest temperature attained. In the case of AF ILC the peak is at $(\pi, \pi)$ in all the range from the isolated ladder, which corresponds to the gaped “quantum disordered” region, to the isotropic square lattice, but the extrapolation of its intensity to the bulk limit becomes nonzero only for $J_{\text{inter}} > J_{\text{inter,cr}}$, i.e. in the “renormalized classical” region. For FM ILC, as shown in Fig. 5(a) for $J_{\text{inter}} = -0.2$, the situation is qualitatively different. The peak in $S(q)$ is now at $(\pi, \pi/2)$, a feature which is similar to the one seen in the simpler cases of coupled chains and plaquettes. This behavior has been found for all clusters considered, and for all $J_{\text{inter}} < 0$ except for finite size effects: the smaller $|J_{\text{inter}}|$ the larger the size needed to reach the bulk behavior. This is illustrated for the 4 × 4 cluster.

A highly nontrivial behavior is found if the temperature dependence is analyzed. In Fig. 5(b) the evolution of the structure factor for the 20 × 20 cluster and $J_{\text{inter}} = -0.2$ is shown at $T = 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0, 1.5$ and 2.0. In the high temperature region ($T > 0.8$) the peak is located at $(\pi, \pi)$. As $T$ is lowered the peak starts to shift towards the zero temperature peak $(\pi, \pi/2)$ which is reached at $T = 0.3$. We found almost no variation with cluster size of these two crossover temperatures at this value of $J_{\text{inter}}$. The fact that only at a finite tempera-

![FIG. 4. Ground state energy per site in the bulk limit of AF (open circles) and FM (full circles) coupled ladders as a function of the absolute value of $J_{\text{inter}}$. Error bars are smaller than the symbol size. In the inset, the intraladder (1,0) (circles), (0,1) (squares), (1,1) (triangles), and interladder (0,1) (diamonds) spin-spin correlations are shown as a function of $|J_{\text{inter}}|$ for the 16 × 16 cluster. Open (full) symbols correspond to AF (FM) interladder couplings.](image-url)
ture the peak of the magnetic structure factor starts to be incommensurate is reminiscent to the one first found in La$_{1-x}$Nd$_x$Sr$_2$CuO$_4$ ($x \approx 0.8$) where a charge-stripe order is developed at $T_c = 65K$ followed by a spin-stripe order at a lower temperature $T_s = 50K$.\footnote{23}

An important quantity to compute is the bulk limit of the peak of the structure factor. This quantity is related with the behavior of spin-spin correlations at the maximum distance along the ladder direction ($x$-axis), along the direction transversal to the ladders ($y$-axis) and at the maximum distance of the 2D cluster. In the case of the AF square lattice, this latter quantity is proportional in the bulk limit to the squared staggered magnetization and it should be equal in that limit to the static structure factor at momentum $(\pi, \pi)$\footnote{23}. The finite size scaling of $S(\pi, \pi/2)$ is shown in Fig. 6(a) for $J_{\text{inter}} = -0.2$ and $-0.6$. We have attempted extrapolations to the bulk limit using both exponential and power laws. Due to the fact that clusters with $L = 4, 8, 16$ and $L = 6, 12$ belong to two different sets (which is more noticeable for large values of $|J_{\text{inter}}|$), the extrapolation procedure is not very reliable. However, as shown in Fig. 6(a), one can conclude that $S(\pi, \pi/2)$ is zero for $J_{\text{inter}} = -0.2$ and nonzero for $J_{\text{inter}} = -0.6$. The finite size behavior of the spin-spin correlation at the maximum distance along the ladder direction, $S_{\text{max}, x}$, which is the one with smaller errors in our simulations, is similar to the one for $S(\pi, \pi/2)$ and the extrapolated values are also zero (nonzero) for $J_{\text{inter}} = -0.2$ ($J_{\text{inter}} = -0.6$).

This crossover in the behavior of $S(\pi, \pi/2)$ as a function of $J_{\text{inter}}$ poses us with the question of the existence of a point analogous to the QCP in the AF ILC case. In the limit of $J_{\text{inter}} \to -\infty$ the coupled ladder system becomes equivalent to a system of AF coupled spin-1/2 chains, where a finite coupling is necessary to change to a gapless regime\footnote{23}. To answer this question, let us now examine the behavior of the singlet-triplet spin gap as a function of $J_{\text{inter}}$. Although this is not a convenient quantity to compute with QMC since it involves a difference between absolute values of the energies and then for large clusters the error becomes comparable to its value, we could get an indication of the presence or absence of a gapless region. The gap was computed for finite clusters and then extrapolated to the bulk using the law $\Delta_{\infty} + b\exp(-L/L_0)/L$ (or $a/L^2$ for the gapless case).\footnote{23} The results are depicted in Fig. 6(b). For the AF case, it can be seen a rapid decrease of $\Delta$ as $J_{\text{inter}}$ is increased, confirming earlier predictions and calculations\footnote{23}. The gap vanishes at the QCP, $J_{\text{inter, cr}} \approx 0.3$. For FM ILC we also obtain a monotonically decreasing behavior, similar to the one found in the previous section for coupled dimers and plaquettes. The gap seems larger to that of AF ILC but it could vanish at $J_{\text{inter}} \approx -0.4$ within error bars. The calculation of other quantities like correlation lengths and/or using more powerful techniques should be necessary to obtain a reliable estimation for $J_{\text{inter, cr}}$.

![Fig. 6](https://example.com/fig6.png)

**FIG. 6.** (a) $S(\pi, \pi/2)$ (open symbols) and $S_{\text{max}, x}$ (full symbols) as a function of $1/L$ for $J_{\text{inter}} = -0.2$ (circles) and $-0.6$ (squares). (b) Singlet-triplet spin gap in the bulk limit of FM (open circles) and AF (full circles) coupled ladders as a function of the absolute value of the interladder coupling constant. In the AF case, the value of $J_{\text{inter}}$ at which $\Delta = 0$ is taken from Ref. 23. The lines are guides to the eye.

The final part of our study which can eventually lead to a deeper understanding of the excitations involved in this system is the analysis of the dynamical structure factor $S(q, \omega)$ which has been done with LD as in the previous section. In this case, we have to limit ourselves to somewhat smaller clusters but we hope that the qualitative features we found will survive in the bulk limit. Results obtained for the $4 \times 4$ cluster are shown in Fig. 7. For AF ILC (Fig. 7(a)) the peak in $S(q, \omega)$ is located at $(\pi, \pi)$, as expected in the bulk limit for an AF order. When a FM

![Fig. 7](https://example.com/fig7.png)

**FIG. 7.** Dynamical structure factor obtained by LD on the $4 \times 4$ cluster vs. frequency at several momenta $q$ for (a) AF and (b) FM interladder couplings. From bottom to top the values of $q$ are $(\pi/2, \pi/2)$, $(\pi, \pi)$, $(\pi, \pi/2)$, $(\pi, 0)$, $(\pi/2, 0)$, $(\pi/2, \pi)$, $(0, \pi)$ and $(0, \pi/2)$.
ILC is involved (Fig. 4(b)) it can be seen that considerable spectral weight is transferred to the peak at \((\pi, \pi/2)\), which becomes also the lowest energy excitation. Results for the \(6 \times 4\) cluster are quite similar and it is quite reassuring that these results are consistent with the ones obtained with QMC and shown in Fig. 4.

IV. CONCLUSIONS

In summary, we have numerically obtained some exact (except for extrapolation procedures) results for ferromagnetically coupled systems, in particular two-leg ladders. Our main results are embodied in Fig. 4 and Fig. 7, i.e. at zero temperature the structure factor is located at \((\pi, \pi/2)\) and it corresponds to the lowest energy excitation. Fig. 4(a) also suggests finite values of this peak of the structure factor and the spin-spin correlation at the maximum distance along the ladder axis in the bulk limit for strong \(J_{\text{inter}}\). There also two crossover temperatures, a higher one at which the peak starts to shift away from \((\pi, \pi)\) and a lower one at which the peak reaches its zero temperature position. Besides the intrinsic interest for the theoretical understanding of spin-1/2 ladder systems, we will try to emphasize in this section their possible relevance for realistic compounds containing ladders. As mentioned in the introduction, we should consider in the first place ladder compounds like \(\text{SrCu}_2\text{O}_2\) (which upon \(\text{Ca}\)-doping and under pressure becomes superconducting) and \(\text{CaV}_2\text{O}_5\). In these compounds, the ladders are coupled forming a trellis lattice. In the former case the interladder couplings are actually ferromagnetic. In the others, due to the frustrated nature of the AF ILC one could speculate that to some extent they could be modeled effectively by FM couplings. For all these compounds, then we predict that neutron scattering experiments would show peaks at \((q_x, q_y) = (\pi, \pi/2)\), where the \(x\) (\(y\)) axis is in the direction parallel (perpendicular) to the ladders. As also suggested in the introduction, our results could be related to the striped structure which dynamically appears in the \(\text{Cu-O}\) planes of high-\(T_c\) cuprates. In this case we are able to trace the origin of the neutron scattering peaks observed away from \((\pi, \pi)\) to an effective ferromagnetic interaction between \(\pi\)-shifted insulating spin ladders. In fact, this behavior can be observed already for the simplest case of ferromagnetically coupled AF dimers as shown in Section I. In this case, it is easy to verify on small chains by LD or QMC that the peak moves continuously from \(q = \pi/2\) to \(\pi\) as some of the FM couplings are replaced by AF ones. If this picture could translate to coupled ladders, then one would be lead to the conclusion that some of the spin two-leg ladders are \(\pi\)-shifted while others are in phase in order to reproduce the experimentally observed incommensurate peaks. Another feature we want to emphasize is the temperature evolution of the structure factor (Fig. 5(b)): the peak at \((\pi, \pi/2)\) is reached at a finite temperature and there is a range of temperatures in which an incommensurate peak is present. As mentioned in the previous section, this is reminiscent of the order in which charge and the spin stripes appear in the cuprates as the temperature is decreased. The fact that the spin gap possibly remains finite for somewhat strong values of \(|J_{\text{inter}}|\) is also interesting for the stripe scenario of cuprates although in this case our results for the bulk limit are affected by large error bars. Of course, the question of to what extent this model of FM coupled ladders could apply to this scenario should come of detailed comparison with more realistic models like 2D t-J or Hubbard models.

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