Coexistence of pairing tendencies and ferromagnetism in a doped two-orbital Hubbard model on two-leg ladders

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Using the Density Matrix Renormalization Group and two-leg ladders, we investigate an electronic two-orbital Hubbard model including plaquette-diagonal hopping amplitudes. Our goal is to search for regimes where charges added to the undoped state form pairs, presumably a precursor of a superconducting state. For the electronic density $\rho=2$, i.e., the undoped limit, our investigations show a robust $(\pi,0)$ antiferromagnetic ground state, as in previous investigations. Doping away from $\rho=2$ and for large values of the Hund coupling J, a ferromagnetic region is found to be stable. Moreover, when the interorbital on-site Hubbard repulsion is smaller than the Hund coupling, i.e., for $U'<J$ in the standard notation of multiorbital Hubbard models, our results indicate the coexistence of pairing tendencies and ferromagnetism close to $\rho=2$. These results are compatible with previous investigations using one-dimensional systems. Although further research is needed to clarify if the range of couplings used here is of relevance for real materials, such as superconducting heavy fermions or pnictides, our theoretical results address a possible mechanism for pairing that may be active in the presence of short-range ferromagnetic fluctuations.

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I. INTRODUCTION

It is widely believed that magnetism is a fundamental ingredient to explain the origin of high-temperature superconductivity in several materials. In fact, there is experimental evidence that the superconductivity in many heavy fermion (HF) compounds is mediated by spin fluctuations.[1–4] Mechanisms for superconductivity based on antiferromagnetism have been extensively discussed for the Cu-based high-temperature superconductors as well.[5] Recently, considerable excitement has been generated by the discovery of high-temperature superconductivity in the iron pnictides.[6] Except for the cuprates, the iron-based superconductors now have the highest superconducting (SC) critical temperature T_c of any material (see, for example, Ref. 7). As in HF systems and cuprate superconductors, in the pnictides, there is also evidence that the superconductivity is not mediated by the electron-phonon interaction.[8,9]

Magnetism and superconductivity can appear in different ways. In some HF compounds, superconductivity and antiferromagnetic (AFM) order coexist,[1] while for the cuprates the superconductivity emerges after the long-range AFM order is destroyed by doping.[5] In some HF systems, it is the superconductivity and ferromagnetism (FM) (as opposed to AFM order) that coexist.[10] In this work, we will be interested in detecting a clear evidence of pairing of extra charges that are added to the undoped limit where magnetic order exists. Using a two-orbital model and two-leg ladders, it will be shown that a possible region for the robust coexistence of (spin triplet) pairing together with magnetic order is where ferromagnetism develops. This is in qualitative agreement with previous investigations carried out using one-dimensional systems.[11] Our effort should be considered simply as providing the first steps in relating pairing and magnetism in a complex two-orbital model via computational techniques on ladder geometries. Antiferromagnetic order, as found in the pnictides, could also be favorable for pairing tendencies in the spin singlet channel, as discussed recently.[12,13]

In principle, a theoretical investigation based on model Hamiltonians for strongly correlated materials starts with an effective tight-binding model, containing the minimum ingredients to describe the physics of the materials under investigation. However, even if a well-defined reasonable model is used, it is still highly nontrivial to extract the ground state properties of these effective models in two or three dimensions using unbiased numerical methods. In fact, at present, there are no accurate techniques to study Hubbard-like models in dimensions two and three. Thus, in order to get at least some insight on the ground states properties of theses models, it is common practice to study the model Hamiltonians in quasi-one-dimensional geometries. In particular, a very popular route that has been used for several theoretical investigations is to study strongly correlated electronic systems using "ladder" geometries.[14] The N-leg ladders consist of N chains of length L coupled by some parameter (as, for example, fermionic hopping terms). The two-dimensional system can in principle be obtained by considering the limits of both N and L sent to infinity, although in practice this is difficult to do. This ladder-based procedure has been used to investigate models for the high temperature superconductors[15] and for the HF systems.[4,16] Some important results were obtained with this method. For example, research based on microscopic models for the high T_c superconductors,[5] as well as research on HF models,[4] indicate that superconductivity mediated by antiferromagnetic

fluctuations can be stabilized, in agreement with several experiments. Thus, the use of ladders appears to be an important ingredient to unveil dominant ground state tendencies. Moreover, the hopping amplitudes that will be used in our investigations below include next-nearest-neighbor diagonal hoppings that are only possible when plaquettes exist in the lattice under consideration.

Note that microscopic models that may present superconductivity induced by antiferromagnetism, such as the one-orbital Hubbard model and the Kondo Lattice model, have been extensively studied by several authors. However, microscopic models for *superconductivity in a ferromagnetic spin background* have been much less explored, with the exception of studies using one-dimensional chains.[11] This may be caused in part by the perception that superconductivity and ferromagnetism, as opposed to antiferromagnetism, cannot coexist.[17] However, this perception has been challenged by the discovery of superconductivity and FM in the HF compounds UGe_2 (Ref. 10) and URhGe.[18] Moreover, SC and FM were also observed[19] in the *d*-band metal $ZrZn_2$.

Motivated by the discovery of superconductivity in the HF compound UGe_2, a few years ago, Karchev *et al.* proposed a one-band model to study the coexistence of superconductivity and ferromagnetism.[20] However, other researchers have argued that the treatment used to investigate that model, as well as the model itself, were not appropriate to describe the coexistence of these phases.[21–23]

Due to the lack of studies of microscopic models for superconductivity mediated by ferromagnetic fluctuations beyond one-dimensional chains,[11] in this work, we have decided to investigate a microscopic ladder model where the coexistence of superconductivity and ferromagnetism appears possible. In fact, it will be shown below that the two-orbital model that has been originally proposed to describe the low-energy physics of the iron-based superconductors[12,13,24] actually leads to the coexistence of pairing and spin ferromagnetic tendencies. Qualitatively, our results are compatible with those reported using chains.[11] Although the model considered here may not be a proper effective model for superconducting ferromagnets such as UGe_2, we believe that the mechanism that bounds together the charges carriers (see Sec. III B) is so simple and generic that our calculations may also apply in a variety of other models as well.

II. MODEL

In these studies, we have considered the following Hamiltonian defined on a two-leg ladder geometry:

$$
\begin{aligned}
H = & -\sum_{j,\sigma,\gamma,\gamma',\lambda,\lambda'} t^{\lambda,\lambda'}_{\gamma,\gamma'}(d^{\dagger}_{j,\gamma\sigma,\lambda}d_{j+1,\gamma'\sigma,\lambda'} + \text{H.c.}) \\
& - \sum_{j,\sigma,\gamma,\gamma'} \tilde{t}_{\gamma,\gamma'}(d^{\dagger}_{j,\gamma\sigma,1}d_{j,\gamma'\sigma,2} + \text{H.c.}) + U\sum_{j,\gamma,\lambda} \rho_{j,\gamma\uparrow,\lambda}\rho_{j,\gamma\downarrow,\lambda} \\
& + (U' - J/2)\sum_{j,\lambda} \rho_{j,x,\lambda}\rho_{j,y,\lambda} - 2J\sum_{j,\lambda} \mathbf{S}_{j,x,\lambda}\cdot\mathbf{S}_{j,y,\lambda} \\
& + J\sum_{j,\lambda} (d^{\dagger}_{j,x\uparrow,\lambda}d^{\dagger}_{j,x\downarrow,\lambda}d_{j,y\downarrow,\lambda}d_{j,y\uparrow,\lambda} + \text{H.c.}), \qquad (1)
\end{aligned}
$$

where $d^{\dagger}_{j,\gamma\sigma,\lambda}$ creates an electron with spin projection σ in the orbital $\gamma = x, y$ (d_{xz} and d_{yz}, respectively) at the rung j and leg $\lambda = 1, 2$, $\mathbf{S}_{j,\gamma,\lambda}$ is the electron spin density operator, $\rho_{j,\gamma\sigma,\lambda} = d^{\dagger}_{j,\gamma\sigma,\lambda}d_{j,\gamma\sigma,\lambda}$, and $\rho_{j,\gamma,\lambda} = \Sigma_{\sigma} d^{\dagger}_{j,\gamma\sigma,\lambda}d_{j,\gamma\sigma,\lambda}$.

The hopping amplitudes are: $t^{\lambda,\lambda}_{x,x} = \tilde{t}_{y,y} = -t_1$, $t^{\lambda,\lambda}_{y,y} = \tilde{t}_{x,x} = -t_2$, $t^{1,2}_{\gamma,\gamma} = t^{2,1}_{\gamma,\gamma} = -t_3$, and $t^{1,2}_{\gamma,\gamma'} = -t^{2,1}_{\gamma,\gamma'} = -t_4$, if $\gamma \neq \gamma'$, and zero otherwise. To avoid a proliferation of extra parameters in our analysis, we have decided to fix the values of these hoppings from considerations previously used in the pnictide context. Our use of models originally devised for pnictides is simply based on the pragmatic observation that some pairing tendencies and ferromagnetic regions at large J were already observed in those models.[12,13] It should be clear though, that our research is mainly motivated by heavy fermion phenomenology.

Following this strategy, then the hopping amplitudes t_1, t_2, t_3, and t_4 are obtained using the Slater-Koster tight-binding scheme, and they are given by[12,13,25]

$$
\begin{aligned}
t_1 &= -2(b^2 - a^2 + g^2)/\Delta_{pd}, \\
t_2 &= -2(b^2 - a^2 - g^2)/\Delta_{pd}, \\
t_3 &= -(b^2 + a^2 - g^2)/\Delta_{pd}, \\
t_4 &= -(ab - g^2)/\Delta_{pd}, \qquad (2)
\end{aligned}
$$

where the Fe-As hopping amplitudes are $a = 0.324(pd\sigma) - 0.374(pd\pi)$, $b = 0.324(pd\sigma) + 0.123(pd\pi)$, and $g = 0.263(pd\sigma) + 0.31(pd\pi)$. Δ_{pd} is the energy difference between the p and d levels. We have set $(pd\sigma)^2/\Delta_{pd} = 1$ to fix the energy scale, and we use $pd\pi/pd\sigma = -0.2$, as previously discussed.[12,13] Regarding the couplings U, J, and J', note that they are not independent, but they are assumed to satisfy the relation $U = U' + 2J$, which is strictly valid within a cubic environment for the full t_{2g} sector.[26,27] For an explicit derivation of this relation in the case of manganites, see Ref. 28.

We have investigated the model defined above using a two-leg ladder of size $2 \times L$ by means of the Density Matrix Renormalization Group (DMRG) technique,[29] under open boundary conditions (OBC), and keeping up to $m = 1400$ states per block in the final DMRG sweep. We have carried out $\sim 6-13$ sweeps, and the discarded weight was typically $10^{-6}-10^{-9}$ at the final sweep. In our DMRG procedure, the center blocks are composed of 16 states. We have used a FORTRAN DMRG code to calculate most results, and a C++ DMRG code for additional validation.[30] We have also confirmed some of our results against Lanczos Exact Diagonalization techniques, when possible.

In this work, we will focus on the region of Hubbard and Hund parameters where $U_{\text{eff}} \equiv U - 3J = U' - J < 0$, although a few results for positive values of U_{eff} will be presented as well. As shown below, in the region where $U_{\text{eff}} < 0$, there is a robust evidence of binding of holes/electrons close to density $\rho = 2$. In this regime $U' < J$. This inequality may not seem realistic at first sight, since the on-site spin triplet formation favored by J (Hund's rules) has its origin in the alleviation of the Coulombic energy penalization caused by U'. However,

while in the full five-orbital model for Fe-based compounds $U' < J$ is unphysical for the reason stated above, the two-orbital model is an *effective* model and it is unclear how the main parameters are affected by the projection from five to two orbitals. Thus, the regime U' comparable to J may not be unrealistic. Clearly, additional investigations are needed to analyze if this regime of couplings is of relevance for real materials, such as heavy fermions. *Ab initio* calculations are needed for this purpose (beyond the scope of the present analysis).

III. RESULTS

A. Magnetic Properties at $\rho=2$

Let us start our analysis by focusing on the density $\rho=2$. To investigate the magnetic order at this density, the Fourier transform of the real-space spin-spin correlation function was measured

$$S(\mathbf{q}) = \frac{1}{6L} \sum_{j,j',\lambda,\lambda'} e^{iq_x(j-j')} e^{iq_y(\lambda-\lambda')} \langle \mathbf{S}_{j,\lambda} \cdot \mathbf{S}_{j',\lambda'} \rangle, \qquad (3)$$

where $\mathbf{S}_{j,\lambda}=\mathbf{S}_{j,x,\lambda}+\mathbf{S}_{j,y,\lambda}$. In Fig. 1(a), the spin structure factor $S(\mathbf{q})$ of the two-leg model is presented for several system sizes. As can be observed in this figure, there is a robust peak at wavevector $\mathbf{q}=(\pi,0)$, showing the tendency toward a stripelike AFM order. This is the analog of the magnetic order found in pnictides but using a two-leg ladder geometry. Similar results, obtained with Exact Diagonalization on small clusters, were reported before.[12,13] Note that the peak increases with the system size, suggesting the development of a true long-range magnetic order in systems with a higher dimension.

The results for the spin structure factor show that along the $y(x)$ axes the spins are aligned following a ferromagnetic (AFM) order, at least at short distances. This stripelike AFM structure is present in a wide range of parameters, as shown in Fig. 1(b) (inset), including $U_{\text{eff}}>0$. Neutron scattering measurements for pnictides also show a similar spin order.[31] We have observed that the stripelike AFM structure appears only when the plaquette-diagonal hopping amplitudes (t_3 and t_4) are of value similar as those of the nearest-neighbor hopping amplitudes. If we force $t_3=t_4=0$, then the peak in the spin structure factor $S(\mathbf{q})$ appears at wavevector $\mathbf{q}=(\pi,\pi)$. Note also that for the two-leg geometry, the $(\pi,0)$ AFM state is not, naturally, degenerate with the $(0,\pi)$ AFM state. Due to this fact, a study in a ladder geometry could make a better connection with the two-dimensional results of the pnictide materials where $(\pi,0)$ is favored over $(0,\pi)$ by a lattice distortion.

For quasi-one-dimensional systems, a true long-range magnetic order is replaced by a power-law decay of the spin-spin correlations. Thus, in order to analyze the range of the magnetic order, we have also investigated the spin-spin correlation function along one of the legs (say, leg 1), defined as

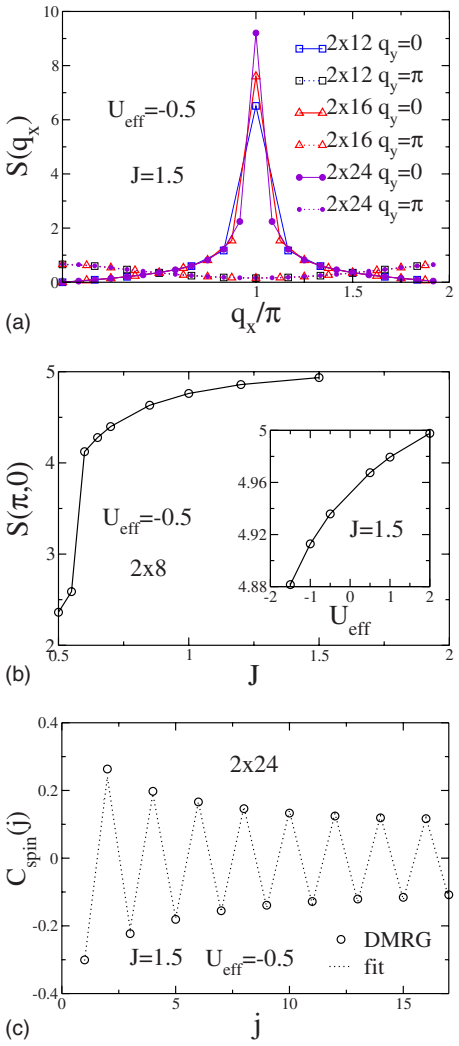

FIG. 1. (Color online) (a) Spin-structure factor $S(q_x)$ vs q_x for the two-leg ladder system with sizes $L=12$, 16, and 24, and for density $\rho=2$, $J=1.5$, and $U_{\text{eff}}=-0.5$. (b) $S(\pi,0)$ as a function of J for ladders with linear sizes $L=8$ and $U_{\text{eff}}=-0.5$. The inset shows the magnitude of this peak as a function of U_{eff}, for the coupling $J=1.5$. (c) Spin-spin correlation $C_{\text{spin}}(j)$ vs j along the long ladder direction, for a system with size $L=24$, and for the couplings $U_{\text{eff}}=-0.5$ and $J=1.5$. The dashed curve is a fit given by Eq. (5).

$$C_{\text{spin}}(l) = \frac{1}{M} \sum_{|i-j|=l} \langle S^z_{i,1} S^z_{j,1} \rangle, \qquad (4)$$

where M is the number of site pairs (i,j) satisfying $l=|i-j|$. In practice, we have averaged over all pairs of sites separated by distance l, in order to minimize boundary effects (a few sites at the edges were also discarded while implementing this averaging procedure).

In Fig. 1(c), the spin correlation function $C_{\text{spin}}(j)$ is shown for the 2×24 cluster and using $U_{\text{eff}}=-0.5$. The dashed line is a fit of the numerical data with the function

$$\tilde{C}_{\text{spin}} = a \frac{\cos(\pi x)}{x^{1/3}}. \qquad (5)$$

Similar results were found for the 2×16 cluster. The observed power-law decay suggests that a two-dimensional

system with the same model and parameters would develop long-range magnetic order at zero temperature.

B. Doping with two holes or electrons

Let us now consider the effect of doping with charges this ladder system. If tendencies toward the pairing of the extra charges are unveiled, they would be an indicator that this model could become superconducting in a two-dimensional geometry, for the couplings here considered.

Let us start with the calculation of the binding energy of two doped holes/electrons. This binding energy is defined as $\Delta_b = E(2) + E(0) - 2E(1)$, where $E(n)$ is the ground state energy with $(4L+n)$ holes/electrons ($4L$ is the number of electrons corresponding to the "undoped" limit where there is an electron per orbital and per site). On a *finite system*, the binding energy $\Delta_b > 0$ is positive if the electrons/holes do not form a bound state,[5] while in the thermodynamic limit Δ_b should vanish in the absence of pairing. On the other hand, if the extra holes/electrons form a bound state, then $\Delta_b < 0$ even on a finite cluster, and this would be indicative that effective attractive forces are present in the system.

Before presenting our numerical results for the binding energies, let us first consider the following strong coupling regime defined by $-U_{\text{eff}} = 3J - U = J - U' \gg 1$. As it will be argued below, and as it was discussed in previous investigations for one-dimensional chains,[11] in this regime, the binding of hole/electrons is clearly present.

For completeness, let us address this limit in detail, although it is clear that large J compared with U' leads to an effective attractive interaction.[11] Let us denote the states of the one-site problem via the symbol $\left(\frac{s_y}{s_x}\right)$, where the "arrows" $s_x(s_y)$ represent the electrons (with their spins projections) at the orbital $x(y)$. For this one-site problem with two electrons and the limit considered here where J is large, the ground state energy is degenerate. Its value is $e_2 = U_{\text{eff}}$, and the three corresponding eigenstates are $\left(\frac{\downarrow}{\downarrow}\right)$, $\left(\frac{\uparrow}{\uparrow}\right)$, and $\left[\left(\frac{\uparrow}{\downarrow}\right) + \left(\frac{\downarrow}{\uparrow}\right)\right]/\sqrt{2}$. Since $-U_{\text{eff}} \gg 1$, we can approximate the Hamiltonian as $H = H_{\text{kinetic}} + H_{\text{int}} \sim H_{\text{int}}$, and the (highly degenerate) ground state energy of the two-leg model becomes $E(0) = 2L \times e_2 = 2L \times U_{\text{eff}}$.

Below, the dominant spin arrangement in the ground state at density $\rho = 2$ is shown to guide the discussion

$$\left(\begin{array}{ccccc} \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow}{\downarrow}\right) \\ \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) \end{array} \right),$$

using only the up and down projections of the spin one states at every site for simplicity. Such a state is to be expected since for $J \gg 1$ the alignment of the two spins at the two orbitals in the same site will occur, and as $U \sim 2J \gg 1$ then having two electrons in the same orbital is not allowed. Of course, any other configuration (such as a fully ferromagnetic state) is also equally likely as the one shown in the figure for $-U_{\text{eff}} \gg 1$. However, the hopping terms will lift the large degeneracy, and our numerical results for the spin-spin correlations presented before indicate that hopping terms favor the $(\pi, 0)$ AFM configuration, for a wide range of couplings in the undoped limit. For this reason, here, we have chosen to present the dominant spin arrangement of the ground state as a stripelike AFM state, but it could be fully FM as well. Regardless of this detail, the arguments we will use below to obtain the energies $E(n)$ will hold true both for a stripelike AFM state, as well as for a FM state.

Let us now add two extra electrons to the undoped system. In the limit being considered here, where the hopping amplitudes are negligible, the best way for the system to minimize its energy is to have the two electrons located on the same site, since in this way less on-site ferromagnetic links are broken. The on-site Hubbard U energy penalization is the same whether the doubly occupied orbitals are at the same site or not, and since U' is negligible with respect to J in the limit considered, then the (effectively attractive) Hund coupling determines the location of the extra charge, leading to the double occupation of both orbitals at the same site.[11] In this case, the dominant spin arrangement of the ground state is

$$\left(\begin{array}{ccccc} \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow\uparrow}{\downarrow\uparrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow}{\downarrow}\right) \\ \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\downarrow}{\downarrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) & \left(\frac{\uparrow}{\uparrow}\right) \end{array} \right).$$

Once again, a stripelike AMF background is used, since for $J \sim 1$ and close to the density $\rho = 2$ our numerical data show [see Fig. 4(a)] that the $(\pi, 0)$ AFM order is the dominant one, but it could have been FM as well.

In the limit of couplings considered here, the ground state energy for the doped two-electron system is

$$E(2) = (2L + 5)U_{\text{eff}} + 8J. \tag{6}$$

Note that if the two extra electrons that are in the state $\left(\frac{\downarrow\uparrow}{\downarrow\uparrow}\right)$ were to move in opposite directions (after considering the presence of small but nonzero hopping terms), they would break two ferromagnetic on-site links. Such a state would have a large energy and it is therefore "forbidden" for $-U_{\text{eff}} \gg 1$. However, if the two extra electrons move "together" (i.e., $\left(\frac{\downarrow}{\downarrow}\right)$) in the same direction, forming a spin triplet, then no other on-site FM links are broken. Thus, to minimize the energy, the two-electrons added to the system must form a bound state, at least in the limit where the hoppings amplitudes are very small compared with the Hubbard and Hund couplings (the same spin dominant picture works when instead of adding electrons we remove two electrons, i.e., for the two-hole problem). This argument, known from previous investigations using chains,[11] explains the binding of electrons in the limit $-U_{\text{eff}} \gg 1$. More explicitly, the binding energy of the doped two-electrons/holes system in the limit considered here is given by

$$\Delta_b = -|U_{\text{eff}}|. \tag{7}$$

Based on the discussion above, we conclude that for $-U_{\text{eff}} \gg 1$, there is an indication of pairing, and perhaps superconductivity, in the two-orbital model. In fact, the on-site interorbital pairing state found here in this extreme regime results to be a spin triplet and transforms according to the

irreducible representation A_{2g} of the group D_{4h}.[32] Interestingly, Exact Diagonalization calculations in two-dimensional clusters, still in the FM state of the model but $U' > J$, found indications of a pairing state with the same characteristics and symmetry but with electrons at distance of one lattice spacing from each other.[12,13] The argument presented above for this pairing is actually valid in any dimension, and also it works for the two doped holes case, as already mentioned. To confirm these argumentations, Δ_b was calculated numerically for large values of $-U_{\text{eff}}$. An excellent agreement between the numerical data and the analytic expression [Eq. (7)] was found.

Now, the crucial question is whether there is binding of holes/electrons for values of $-U_{\text{eff}}$ that may be of more relevance for real materials. The answer to this question appears to be positive. In fact, the binding of electrons/holes has been observed numerically for $U_{\text{eff}} \lesssim 0$ and several values of the coupling J, as shown in Fig. 2.[33] More specifically, Figs. 2(a) and 2(b) show the region in the $J-(3J-U)$ plane where the binding energies of electrons [Fig. 2(a)] and holes [Fig. 2(b)] are less than -0.1, for the case of a 2×3 cluster. The region where $\Delta_b < -0.1$ was chosen to be represented, as opposed to $\Delta_b = 0$, since previous experience in the context of the cuprates[5] suggests that this procedure effectively takes into account size effects better. In practice, other values for this "cutoff" do not alter our qualitative conclusions. Similar results were found also for the 2×2 cluster.

Thus far, only small clusters have been considered because the numerical analysis of large clusters would be too time consuming, particularly with regards to calculating the hundreds of points that are required to extract comprehensive phase diagrams. However, larger system sizes were considered for a few selected sets of couplings, as shown in Fig. 2(c). In this figure, Δ_b vs $1/L$ for some couplings is presented. Here, it is clearly observed that in the bulk limit the binding energies of added electrons/holes converge to nonzero values for some coupling sets. Close to $\rho = 2$, these results strongly indicate that there are pairing tendencies for $U_{\text{eff}} \lesssim 0$. Thus, to the extend that future investigations show that J comparable to U' is a realistic regime for effective two-orbital models, this provides a possible mechanism for pairing in real materials.

In Figs. 2(a) and 2(b), the magnetic phase diagram for the case of two doped electrons/holes is also presented. The region above the red (bold) line is a ferromagnetic phase with the maximum total spin $S_{\text{total}} = 2L-1$. Below this line, we have observed that the total spin changes continuously from zero, at $J=0$, up to its maximum value at J_c. As observed in these figures and for a large region of couplings, pairing (and presumably superconductivity) coexists with ferromagnetic tendencies.

C. Phase Diagram

In Fig. 3, the phase diagram (J vs density) of the two-leg ladder for $U_{\text{eff}} = -0.5$ and several system sizes (see legend) is presented. For $\rho = 2$, it was observed that the total spin is zero for L even, and that it can be 0, 1, or 2 for L odd, depending of the values of J. Note that for L odd and $\rho = 2$, the $(\pi, 0)$ AFM configuration $(+-+-+-)$ does not have the same number of + and − spins.

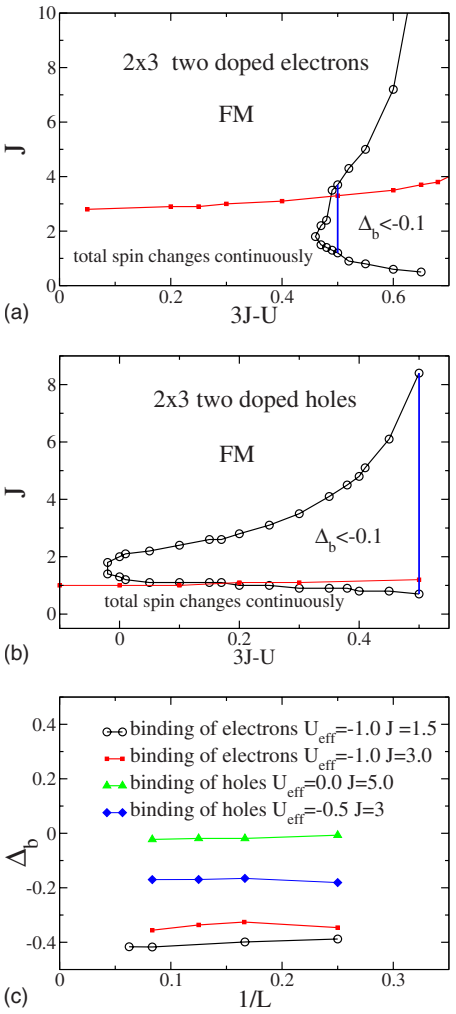

FIG. 2. (Color online) (a)–(b) Phase diagram (J vs $-U_{\text{eff}} = 3J - U$) for the 2×3 cluster showing the region where the binding energies of electrons (a) and holes (b) is smaller than $\Delta_b < -0.1$, indicative of pairing. Above the red line, the total spin saturates to its maximum value. Below this line, the total spin changes continuously from the maximum value to zero at $J=0$. The blue lines show the region of J where $\Delta_b < -0.1$ for $U_{\text{eff}} = -0.5$. These lines are the same as presented in Fig. 3. (c) Δ_b vs $1/L$ for some couplings (see legend).

For $2 < \rho < 2.5 (1 < \rho < 2)$, a ferromagnetic phase was found (the region above the symbols) with magnetic moment per site given by $m = 2 - \rho/2 (m = \rho/2)$. The symbols indicate the value of J_c where the total spin saturates. The critical value J_c was determined by the level crossing of the energies in the sector with $S^z = S^{\max}_{\text{total}}$ and $S^z = S^{\max}_{\text{total}} - 1$. Using this procedure, we were able to obtain J_c for large systems. For densities in the ranges $\rho \lesssim 1.25$ and $\rho \gtrsim 2.5$, we have not found any trace of ferromagnetism. Below the FM region, it is very hard numerically to determine the total spin with good accuracy for large systems. However, our results for the 2×2 and 2×3 clusters with two doped electrons/holes suggest that the total spin changes continuously, from maximum value at J_c to zero at $J=0$. The total spin can be extracted

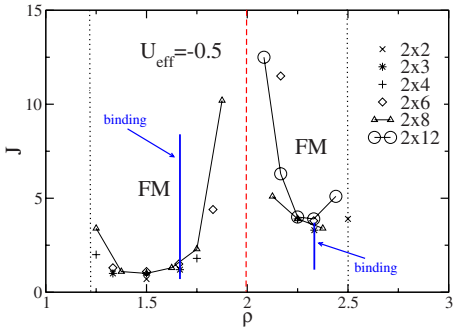

FIG. 3. (Color online) (a) Phase diagram of the two-leg ladder model Hamiltonian defined in Eq. (1). The region above the symbols is a fully saturated ferromagnetic phase (see text). The blue lines correspond to regions where $\Delta_b < -0.1$ for the cluster 2×3 with two doped electrons/holes, as presented in Figs. 2(a) and 2(b).

from the spin structure factor at $\mathbf{q}=(0,0)$. For a few sets of couplings, we also observed, through the value of $S[\mathbf{q}=(0,0)]$, that in fact, the total spin of the ground state changes continuously for the 2×8 cluster as well. These results suggest that the total spin varies continuously below the FM region present in Fig. 3 for any cluster sizes. Overall, our results are qualitatively compatible with those found in one-dimensional systems.[11] Note also that tendencies to FM states at robust J were also reported via Exact Diagonalization methods on small clusters.[12,13]

We believe the FM phase is stabilized by a mechanism that has the same characteristics as the Double Exchange (DE) mechanism.[34] In the original DE scenario, there are mobile and localized degrees of freedom. In the DE mechanism, these degrees of freedom are separated and well-defined. Although we do not have localized degrees of freedom in our model, from the perspective of one electron at a given orbital an electron at the same site but the other orbital behaves in some respects as a localized spin. For doped systems, when an electron moves from one site to the other, in order to minimize the kinetic energy and the energy related with the Hund coupling, all spins have to be aligned.

The blue lines in Fig. 3 are the same that were presented in Figs. 2(a) and 2(b). We expect that the region of binding extends beyond these lines up to the density $\rho=2$, forming regions in parameter space where superconductivity exists inside the phase diagram.

We have also measured the spin structure factor $S(\mathbf{q})$ away from the undoped density $\rho=2$. In Fig. 4, $S(\mathbf{q})$ is presented for some particular densities for the two-leg ladder model with size $L=16$, $J=1.5$, and $U_{\text{eff}}=-0.5$. As can be observed in Fig. 4(a), there is still a peak at $\mathbf{q}=(\pi,0)$ for densities close to $\rho=2$. Note that these peaks have smaller intensity than those found for $\rho=2$ in Fig. 4(a), for the system with size $L=16$. We have also observed that the height of the peak at $\mathbf{q}=(\pi,0)$ increases with the system sizes for the densities close to $\rho=2$. These results indicate that a stripelike AFM magnetic order also exists for densities close to $\rho=2$. As shown in Fig. 4(b), this order does not exist anymore for $\rho\gtrsim 2.2$ and $\rho\lesssim 1.7$, at least within the precision of our calculations, and it is replaced by ferromagnetic tendencies. Note that for the electron doped case, there is a small peak at $\mathbf{q}=(0,\pi)$ for densities $\rho\gtrsim 2.2$.

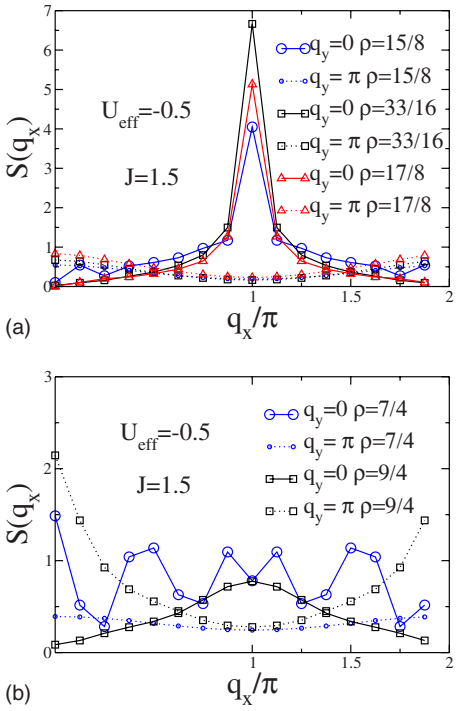

FIG. 4. (Color online) Spin-structure factor $S(q_x)$ vs q_x for the two-leg ladder system with size $L=16$, $J=1.5$, and $U_{\text{eff}}=-0.5$. (a) $S(q_x)$ for the densities $\rho=15/8$, $\rho=33/16$, and $\rho=17/8$ (see legend). (b) $S(q_x)$ for the densities $\rho=7/4$ and $\rho=9/4$.

IV. CONCLUSION

Using ladders, we have studied analytically and numerically a two-orbital Hubbard model. Via the DMRG technique, we were able to investigate the model defined on a two-leg ladder geometry for systems with linear sizes up to $L=24$. Our spin structure factor data show that for the "undoped" density $\rho=2$, a stripelike AFM order is present, as observed in previous Exact Diagonalization studies.[12,13] We have also presented evidence for triplet pairing tendencies of added electrons/holes close to the density $\rho=2$, in some range of couplings, in qualitative agreement with previous investigations using chains,[11] and with Exact Diagonalization calculations in a less extreme FM regime of models for pnictides.[12,13] More precisely, we have found that pairing (and presumably superconductivity) and ferromagnetism coexist for a large region of parameters in the regime $U'<J$. Even for U' comparable to J, our results still indicate a (mild) tendency to pairing. Whether this range of couplings for U' and J is realized in real materials, such as heavy fermions or pnictides, is a matter to be decided via experiments, or with the help of *ab initio* computer simulations.

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