Pairing tendencies in a two-orbital Hubbard model in one dimension

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The recent discovery of superconductivity under high pressure in the ladder compound BaFe$_2$S$_3$ has opened a new field of research in iron-based superconductors with focus on quasi-one-dimensional geometries. In this publication, using the density matrix renormalization group technique, we study a two-orbital Hubbard model defined in one-dimensional chains. Our main result is the presence of hole binding tendencies at intermediate Hubbard $U$ repulsion and robust Hund coupling $J_H/U = 0.25$. Binding does not occur either in weak coupling or at very strong coupling. The pair-pair correlations that are dominant near half-filling, or of similar strength as the charge and spin correlation channels, involve hole-pair operators that are spin singlets, use nearest-neighbor interactions for the charge and spin correlation channels, involve hole-pair operators that are spin singlets, use nearest-neighbor interactions.

I. INTRODUCTION

High critical temperature superconductors based on iron represent one of the most important open problems in condensed matter physics [1–7]. Early considerations based on Fermi surface nesting provided a robust starting point to rationalize their properties. However, the effect of repulsion between electrons cannot be neglected [6] as exemplified by the existence of large magnetic moments at room temperature [8,9], superconducting materials without hole pockets [10], as well as unexpectedly complex spin arrangements [7]. Electronic correlation effects must be incorporated to understand the plethora of challenging results that experiments are rapidly unveiling.

A new avenue of research for progress in the iron superconductors family has recently opened. It has been shown experimentally that BaFe$_2$S$_3$ [11–13] becomes superconducting at pressures above 10 GPa with an optimal critical temperature $T_c = 24$ K. What is remarkable is that this material is not layered, like all other iron-based superconductors, but instead has the geometry of a two-leg ladder. In other words, they have a dominant crystal structure involving pairs of chains, “legs”, that are coupled via bonds of strength similar to those along the legs, dubbed the “rungs”. This same compound, but at ambient pressure, is a Mott insulator with magnetic order involving ferromagnetic (FM) rungs and antiferromagnetic (AFM) legs [14]. For the case of KFe$_2$Se$_3$, another two-leg ladder material, the magnetic state is as in BaFe$_2$S$_3$ with FM rungs and AFM legs [18]. These same magnetic states were also found theoretically using the Hartree-Fock approximation [20]. Their origin is nontrivial: the 2 × 2 FM iron block patterns arise from frustration effects between fully FM tendencies at very large Hund coupling and AFM tendencies in all directions at small Hund coupling [20]. Hartree-Fock results for layers [24] and chains [25] also revealed a similarly complex landscape of possible competing magnetic states once interactions are incorporated.

For proper context, it is necessary to recall that in the context of the copper-oxide high-$T_c$ superconductors, the theoretical and experimental study of two-leg ladder compounds made a considerable impact. In general, theorists can produce accurate results for quasi-one-dimensional systems and the early predictions of subtle quantum effects, such as spin gaps and superconducting tendencies upon doping [26–28], were later confirmed experimentally. For instance, high-pressure experiments for the two-leg ladder compound Sr$_2$GeCu$_2$O$_6$ reported a superconducting critical temperature of 12 K [29]. A quantitative difference between Cu- and Fe-based ladders is that the bridge between coppers is via an oxygen along the Cu-Cu bond, while in chalcogenides the bridge between irons is via chalcogen atoms located up and down the middle of the iron plaquettes. As a consequence, for the chalcogenides electronic hoppings of similar strength are to be expected along legs, rungs, and also plaquette diagonals.

Although the computational study of two-leg ladder one-orbital Hubbard and $t-J$ models were very successful in the context of the cuprates, the case of the iron superconductors, even restricted to ladders, is more challenging. The reason is that multiorbital Hubbard models are needed and even powerful techniques such as the density matrix renormalization group (DMRG) [30] have difficulty in reaching sufficient accuracy for conclusive results. In spite of these limitations, a recent publication [31] reported progress in the study of a two-orbital model for BaFe$_2$S$_3$. In particular, the magnetic order with FM
experiments showed that indeed pressure transfers charge agreement with the Cu-oxide two-leg ladders context where causes doping of the two-leg ladders, a result supported by it is the Hund coupling even further boosting pairing tendencies by introducing extra varying the many couplings and electronic densities and is presented, with emphasis on pairing and superconducting a systematic study of a two-orbital model defined on chains course, is that much longer systems can be analyzed thus size restrictions. In Ref. [31] it was assumed that high pressure because of the competition between established definitely that pairing of electronic origin is active in two-orbital Hubbard models.

The organization of the manuscript is as follows. Section II provides details of the model, technique used, and observables measured. Section III contains the main results, addressing both magnetic and pairing properties of the model under scrutiny. Section IV contains our main discussion and conclusions.

\section{MODEL AND METHOD}

The multiorbital Hubbard model used in this publication is defined as

\begin{equation}
H = -t \sum_{\langle ij \rangle \gamma \sigma} c_{i \gamma \sigma}^\dagger c_{j \gamma \sigma} + \text{H.c.} + U \sum_{\gamma \gamma'} n_{i \gamma \uparrow} n_{i \gamma' \downarrow} \\
+ \left( U' - \frac{J_H}{2} \right) \sum_{\gamma \gamma'} n_{i \gamma \uparrow} n_{i \gamma' \downarrow} - 2J_H \sum_{\gamma < \gamma'} S_{i \gamma} \cdot S_{i \gamma'} \\
+ J_H \sum_{\gamma < \gamma'} \left( P_{i \gamma \uparrow} P_{i \gamma' \downarrow} + \text{H.c.} \right),
\end{equation}

where $c_{i \gamma \sigma}^\dagger$ ($c_{i \gamma \sigma}$) creates (annihilates) an electron at site $i$ of a chain, with orbital $\gamma$ (either $a$ or $b$), and spin projection along the $z$-axis $\sigma$. The first term represents the kinetic energy of the electrons. Note that for simplicity, the $2 \times 2$ hopping matrix is the unit matrix, i.e., only hoppings between the same orbitals is allowed. Although our overarching goal is the understanding of iron-based superconductors, these hoppings do not intend to represent the tunneling amplitudes of any particular material but they are chosen for simplicity. The second is the standard onsite Hubbard repulsion $U$ between spins $\uparrow$ and $\downarrow$ electrons. The third term is the repulsion between electrons at different orbitals. As shown in many previous publications, besides the canonical $U$ repulsion the coupling strength affecting this term contains a contribution regulated by the Hund coupling $J_H$. Fourth is the portion that explicitly shows the ferromagnetic character of the Hund interaction. The last term is the pair hopping. The number operator is defined as $n_{i \sigma \gamma} = c_{i \gamma \sigma}^\dagger c_{i \gamma \sigma}$ and the pair as $P_{i \gamma} = c_{i \gamma \uparrow}^\dagger c_{i \gamma \downarrow}$. The standard relation $U' = U - 2J_H$ is assumed. While many of the results are for $J_H/U = 0.25$, considered realistic and used in the previous publication for ladders [31], in some of the results below the Hund coupling is varied. The bandwidth corresponding to the kinetic energy portion is $W = 4t$ and the Hubbard strength will be provided primarily as $U/W$. The hopping is the unit of energy $t = 1.0$, unless stated otherwise.

To obtain our results we use the DMRG technique with open boundary conditions with focus on the ground-state of the two-orbital chain, employing at least 1600 states. Most of the results are for a 32 sites two-orbital chain, unless stated otherwise, while some of the results were confirmed using up to 64 sites. Truncation error remain below $\sim 10^{-6}$ for all of our results [35].
We have measured several observables. The binding energy that is an indicator for pairing tendencies [36] is defined as
\[ \Delta E = E_N + E_{N-2} - 2E_{N-1}, \]
where \( E_N \), \( E_{N-1} \), and \( E_{N-2} \) are the total ground state energy of the half-filled, 1-hole doped, and 2-hole doped systems. Here, \( N = 2L \) with \( L \) the length of the chain. The real space charge and spin correlations are
\[ N(R) = \frac{1}{N_R} \sum_{|i-j|=R} \langle (n_i n_j) - \langle n_i \rangle \langle n_j \rangle \rangle, \]
\[ \text{Sp}(R) = \frac{1}{N_R} \sum_{|i-j|=R} \langle S_i \cdot S_j \rangle, \]
where \( N_R \) is the number of neighbours at distance \( R \) from site \( i \) (namely, averages over pairs of sites at equal distance are performed). The Fourier transform of \( \text{Sp}(R) \) is the spin structure factor \( \text{Sp}(k) \).

To study the effects of holes on the magnetic correlations, we define a projector operator \( P_{\gamma \gamma'} \) that projects out the portion of the ground state where site \( i \) and orbital \( \gamma \) are occupied [37]:
\[ P_{\gamma \gamma'} = c_{i,\gamma}^\dagger c_{i,\gamma'}^\dagger c_{i,\gamma'} c_{i,\gamma}^\dagger. \]

To work in the Hilbert space corresponding to \( n_b \) number of holes at specific locations, we apply a product of projectors onto the ground state with \( n_b \) holes. For example, \( P_{\gamma \gamma'} \sum_{\gamma \gamma'} \) projects out the occupied part of the two-hole ground state on orbital \( a \) at site 6, and on orbital \( b \) at site 9. We also calculate the local spin-spin correlations \( \langle \psi | \{ S_{i,\gamma} \cdot S_{j,\gamma'} \} | \psi \rangle \), where the maximum possible magnitude of the correlations is 3/4.

There are many possible superconducting pair correlations that one can explore for this system. Due to the local inter- and intraorbital Coulomb repulsion, onsite pairing is not expected to dominate [36]. Thus, pairing operators for two electrons at nearest-neighbor \( (\gamma \gamma') \) sites \( i \) and \( i+1 \) will be considered in analogy with the approach taken in other purely electronic models where magnetic properties trigger pairing.

An intraorbital nearest neighbor pairing operators is
\[ \Delta_{\gamma \gamma'}^{\gamma \gamma'}(i) = c_{i,\gamma}^\dagger c_{i+1,\gamma}^\dagger - c_{i,\gamma'} c_{i+1,\gamma'}^\dagger, \]
where \( \gamma \) and \( \gamma' \) indicate orbitals \( a \) or \( b \).

The interorbital pairing operator that creates the electrons in a triplet state is given by
\[ \Delta_{\gamma \gamma'}^{ab}(i) = c_{i,\alpha}^\dagger c_{i+1,\delta}^\dagger + c_{i,\delta}^\dagger c_{i+1,\alpha}^\dagger. \]

The pair-pair correlations are given by
\[ \mathcal{O}_{\gamma \gamma'}^{\gamma \gamma'}(R) = \frac{1}{2N_R} \sum_i \langle \Delta_{\gamma \gamma'}^{\gamma \gamma'}(i) \Delta_{\gamma \gamma'}^{\gamma \gamma'}(i + R) \rangle, \]
where \( \pm \) indicates if the pair is a spin triplet or singlet, and \( \gamma \) and \( \gamma' \) indicate orbitals \( a \) or \( b \). Since the results explicitly presented in this manuscript are for the interorbital spin singlet \( \mathcal{O}_{\gamma \gamma'}^{\gamma \gamma'}(R) \) and triplet correlations \( \mathcal{O}_{\gamma \gamma'}^{\gamma \gamma'}(R) \), below we will use the notation \( \mathcal{O}_{\gamma \gamma'}^{\gamma \gamma'}(R) \equiv \mathcal{O}_{\gamma \gamma}^{\gamma \gamma'}(R) \) and \( \mathcal{O}_{\gamma \gamma'}^{\gamma \gamma'}(R) \equiv \mathcal{T}_{\gamma \gamma'}^{\gamma \gamma'}(R) \), respectively. Analogous onsite pairing operators were also considered but their correlations always decayed faster than the dominant NN sites pair-pair correlation \( \mathcal{S}_{\gamma \gamma}(R) \) as shown below. For this reason, the actual expressions for onsite operators are not provided explicitly.

We have measured other observables as well. For example, by averaging the pair correlations over a finite intermediate portion of the chain we can reduce short distance effects, that sometimes lead to believe that pairing is dominant even if the long distance tail is small, and also to reduce boundary effects caused by the open boundary conditions. Here we define the pairing strength as
\[ D = \sum_{R=7}^{12} |\mathcal{S}_{\gamma \gamma}(R)|, \]
where we have used the spin-singlet nearest-neighbor combination explicitly because it will be shown below that it is dominant in our study.

III. RESULTS

In this section, the main results will be described. The language to be used below should always be considered in the framework of one-dimensional systems where long-range order is not possible. For example, expressions such as “staggered AFM order” indicate that staggered spin arrangements decay the slowest with distance as compared with other patterns, but eventually all correlation functions decay to zero with increasing distance in one dimension with short-range interactions.

As expressed before, we remind the readers that experimentally in the Fe-ladders superconductivity appeared with increasing pressure, not with explicit hole doping. However, similarly as in the case of the Cu-ladders, it is believed that pressure may lead to a rearrangement of charge particularly with regards to the average number of electrons at the iron atoms. This perception is supported by recent \textit{ab initio} calculations [33]. As a consequence, in our effort described below we will search for pairing indications by doping with holes the half-filled system, rather than modeling pressure directly.

A. Magnetic order and local moments

Let us start our computational analysis of the two-orbital Hubbard model defined in the previous section by focusing on the magnetic order. Figure 1 contains the spin structure factor
at $U/W = 1.60$, a coupling strength of much importance for pairing as shown below, for different number of holes. For the case of half-filling, $N = 64$ electrons for the 32-sites chain of focus in Fig. 1, the spin order is clearly of the staggered AFM form as expected. In this regime of Hubbard couplings the local spin at every site is already well developed and close to the spin-1 limit, as shown in Fig. 2(a) for most Hund couplings studied, with the exception of $J_H = 0$. Thus, this AFM correlations are compatible with the spin correlations of a Haldane spin-1 chain. Our study of a two-orbital Hubbard model, instead of a Heisenberg model, involves energy scales much higher than those typical of the integer-spin chains and for this reason we will not focus on subtle issues such as spin-gaps in the system. Figure 2(b) shows that together with the development of the spin-1 moments at every site also robust AFM correlations develop at least at short distances, again with the exception of $J_H = 0$.

As the doping of holes increases, Fig. 1 illustrates that spin incommensurate (IC) correlations develop smoothly. While this spin IC order is compatible with spin excitations from the surface characteristics.

### B. Hole pairs and their internal structure

The main result of this publication is that the model studied here presents a regime of hole pair binding that correlates with robust pair-pair correlations in a spin-singlet channel, as will be described below. Figure 3 shows the binding energy $\Delta E$, as defined in Eq. (2), for the case of two holes added to half-filling, varying $U/W$ at a fixed Hund coupling $J_H/U = 0.25$. Starting approximately at $U/W \sim 0.6$ and up to $U/W \sim 3.0$, the binding energy is negative indicative of the formation of a bound state of two holes. Considering recent developments in the study of iron-based superconductors [6], this regime of $U/W$ is realistic. Moreover, the Hund coupling value is also in a reasonable range for pnictides and chalcogenides that are well known for having a robust Hund-driven physics. The results in Fig. 3 were obtained using a 16-sites chain but they appear robust varying the length of the system. For instance, approximately at the minimum of the curve at $U/W = 1.60$ results for 48 sites are only slightly more negative than for 16 sites. Figure 4 contains a size scaling analysis of binding at $U/W = 1.60$ illustrating this conclusion. Our best efforts indicate that size effects are small and moreover with increasing chain length the binding magnitude slightly increases in absolute value. Thus, the bulk-limit binding energy at $U/W = 1.60$ appears to be close to $-0.13$ in hopping units.

Besides the surprising result that binding is possible even in the presence of a strong Hubbard $U$ repulsion, it is interesting to remark the similarity of Fig. 3 with the binding results found

![FIG. 1. Spin structure factor vs. wave vector $k_x$ along the chain direction. Results correspond to $U/W = 1.60$, $J_H/U = 0.25$, various hole dopings as indicated, and employing a 32-sites chain ($N = 64$) and the DMRG technique. In this figure, and others not shown at several values of $U/W$, the peak at $k_x = \pi$ denoting staggered order at half-filling becomes incommensurate upon hole doping.](image1)

![FIG. 2. (a) Spin squared $\langle S^2 \rangle$ and (b) staggered spin structure factor $Sp(\pi)$ vs. $U/W$ for a half-filled 8-sites system using various Hund’s coupling ($J_H/U$) as indicated. At zero $J_H/U$, local moments are not developed up to large $U/W$ and therefore there is no robust magnetic ordering.](image2)

![FIG. 3. Binding energy ($\Delta E$) vs. $U/W$ at a fixed $J_H/U = 0.25$, and using a 16-sites chain. For intermediate interaction strength, there is a wide range with negative binding energy indicating a region where holes pair.](image3)
before in the context of two-leg ladders (see Fig. 8 of Ref. [31]). In both cases, ladders (short sizes were studied in Ref. [31]) and chains, $\Delta E$ starts positive with increasing $U/W$, drops to negative at intermediate couplings where it remains into the strong coupling regime, and then it becomes positive again at abnormally large $U/W$. Note that the region where $\Delta E$ is positive is not important: in the bulk limit the energy of two holes that do not form a bound state should converge to the energy of two independent holes, rendering $\Delta E$ equal to zero. But the negative region of $\Delta E$ is physically realistic and representative of pair formation: two holes lower the energy of the system by being close to each other.

Figure 5 provides the electronic density using a 32-sites chain, corresponding to the orbital $a$ (the results for $b$ are identical, because the model is invariant if $a$ and $b$ are exchanged). For half-filling, the density is virtually equal to the spin IC tendency in Fig. 1 with increasing doping. What is interesting is that for 2 holes, there is a single minimum indicative of the existence of a hole pair. For 4 holes there are 2 minima, for 6 holes there are 3 minima, and for 8 holes there are 4 minima. All these results are at least compatible with the existence of hole pair formation, as the binding energy indicates.

What is the internal structure of this pair? In Fig. 6 the probability of finding the second hole is shown when the first hole is projected to be at site 16, orbital $a$, of a two-orbital chain with 32 sites, at $U/W = 1.60$ and $J_H/U = 0.25$. The result is normalized to $(P_{16a})$. We find the largest probability of the non-projected hole to be in the other orbital $b$ and at the neighboring site. In the ladder analogy of the two-orbital chain (see Fig. 7), these dominant pairs are equivalent to pairs along the diagonal of effective plaquettes.

Projecting now one or two holes to particular locations and analyzing the spin-spin correlations in that framework leads to interesting conclusions. The results are shown in Fig. 7. First, note that once the two-orbital chain results are displayed representing each of the two orbitals by a chain, then this illustrates that two-orbital chains can be mapped formally into a special case of one-orbital two-leg ladders. This is interesting in several respects, but here we wish to emphasize the resemblance, once again, with the previously published results for two-orbital ladders [31]. Consider Fig. 7(a) for one hole: here the rungs of the effective ladder are ferromagnetic and the legs are AFM. Thus, once the results are plotted as in Fig. 7 the magnetic order resembles the “rung FM - leg AFM” of BaFe$_2$S$_3$ as reported in [31]. Also the AFM spin-spin correlation “across the hole” observed in early studies of models for cuprates [38–40] and also found more recently in models for iron-based ladders [31] is present in Fig. 7(a). From the spin perspective, “across the hole” AFM correlations are effectively equivalent to dropping sites of the chain, explaining the spin IC tendency in Fig. 1 with increasing doping.
The results for two holes are equally interesting and also resemble those of previous investigations for real iron-based ladder models. Figure 7(b) contains the hole arrangement with the largest probability in the two-holes ground state. Similarly as in Fig. 10 of Ref. [31], the plaquette diagonal opposite to the projected holes is FM and the “across the hole” antiferromagnetism is robust. Figure 7(c) shows the case where the two holes are along the rung (i.e., onsite in the real chain). Figures 7(b) and 7(c) are smoothly connected: for instance, by moving the electron at “17b” to “16b” in Fig. 7(c). Fig. 7(b) is recovered if the spin correlations follow as if they were “rubber bands” attached to the electrons. Previous studies in models for cuprates have unveiled similar physics.

C. Pair-pair correlations and tendency to superconductivity

The existence of hole binding at half-filling is often a precursor of superconducting tendencies increasing doping. For this reason we have measured the pair-pair correlations in all the channels described in Sec. II, and contrasted their behavior with increasing distance against density-density and spin-spin correlations to find which channel dominates. Representative results are shown in Fig. 8. Figure 8(a) contains results for 2 holes. Here the pair-pair correlations are robust in the spin-singlet channel when involving different orbitals and using nearest-neighbor sites, in agreement with the analysis of the internal structure of the pair in the previous subsection. The analogous spin-triplet pair correlations decay much faster, while spin and charge correlations are in between. However, in spite of the robustness of the singlet pair correlations in Fig. 8(a), the ground state only has two holes and these results, while promising, may be anomalous. More standard and exciting are the results in Fig. 8(b) with 6 holes and a nominal hole doping $x = 6/96 = 0.0625$ ($N = 96$ for a half-filled 48-sites cluster). The same spin-singlet inter-orbital NN-sites pair correlation dominates here as well, as in Fig. 8(a). The decay with distance is similar as in the charge and spin channels but only if the maxima is used for the latter. If, instead, the
minimun in charge and spin correlations are included in finding the
most optimal fits then pair-pair correlations dominate. Note
that the prominent oscillations in charge and spin correlations
have been often reported before (for recent state-of-the-art
efforts, see Ref. [42]), although their origin is not fully
clear; for the pair correlations a smoother behavior is often
observed, as we found. As the number of holes increases, then
the superconducting tendencies remain robust but diminish
compared with spin and charge. In Fig. 8(c) with $x = 8/96$, the
pair-pair decay with distance approximately follows the
average of spin and charge indicating that they compete, while
in Fig. 8(d) with $x = 12/96$, pairing is already less robust
than charge and spin channels. In summary, in a range of
doping near half-filling and for the clusters that we studied,
the superconducting tendencies remain robust but diminish
observed, as we found. As the number of holes increases, then
the superconducting tendencies appear to dominate, or at
the minimum decay at a similar rate as spin and charge.
Thus, the pairing tendencies are robust at intermediate coupling,
compatible with the conclusions regarding hole binding.

In Fig. 9 we show the pairing strength $D$, defined in Eq. (11),
as an indicator of the robustness of pairing correlations
varying $U/W$ for various number of holes. Clearly, it is
the intermediate range of $U/W$ where pairing dominates the
most—as found in the hole binding analysis—and also when
the numbers of holes is small.

Note that the presence of robust superconducting correlations
in Fig. 8 occurs in the region of pair binding shown in
Fig. 3. Away from that region, for example at small Hubbard
coupling such as $U/W = 0.2$ or at very large Hubbard
coupling $U/W = 10$ pairing is not as robust as at intermediate
couplings, as illustrated in Fig. 10. Thus, once again we arrive
to the conclusion that the behavior of the binding energy and
the pair correlation is compatible with one another.

For completeness, note that previous work also unveiled
tendencies towards pairing in electronic two orbitals models
but under rather different circumstances. (i) For instance, in
Ref. [43], Kondo models for Y$_2-x$Ca,BaNiO$_5$ were studied
using Lanczos and DMRG techniques, supplemented by AFM
Heisenberg $J$ terms. The emphasis was on ferromagnetism
and phase separation but tendencies towards hole binding were
also briefly reported. The signal for binding was strongest at
high hole concentration such as $x = 0.4$ and robust values

of $J$ of order one. No pair-pair correlations were calculated,
nor competition triplet versus singlet was studied. (ii) In
Ref. [44], two one-orbital Hubbard chains coupled by an
explicitly ferromagnetic Heisenberg interaction were studied
via bosonization and DMRG/Lanczos methods. Regions of
singlet and triplet superconductivity were reported, but note
that this model has an explicit Heisenberg effective attraction,
without a $U'$ repulsion (similar to our previous effort [45]
to be discussed below). The goal in Ref. [44] was to study
the singlet versus triplet competition in superconductivity,
unlike our efforts that focus on unveiling pairing tendencies
from a complete two-orbital Hubbard model that is explicitly
repulsive. (iii) In Ref. [46] a two-orbital Hubbard model at
$U = \infty$ was studied with emphasis on the influence of the
Hund coupling. When $U'$ was included, charge-density waves
were reported to dominate, while in the absence of $U'$ but
with robust $J_H$ then singlet or triplet pairing dominates.
Our analysis, on the other hand, focuses on a finite intermediate
$U/W$ range where surprisingly we found that singlet pairing
dominate even in the presence of a realistic $U' > J_H$. As
$U/W \to \infty$, we found that hole binding no longer occurs, as
shown in Fig. 3, and the charge or spin channels dominate over
pairing [see Figs. 10(c) and 10(d)] compatible with Ref. [46].
(iv) In Ref. [47], results compatible with ours were produced
via the exact diagonalization of a PBC 6-sites chain with
emphasis on Luttinger liquid parameters using a two-orbital
Hubbard model with a robust band splitting. (v) In Ref. [48],
using the statistically consistent Gutzwiller approximation
for a square lattice, conclusions similar to ours were reached,
reporting a stable spin-triplet $s$-wave superconducting state
for a two-orbital degenerate Hubbard model. This occurs, like
in our case, even in the case $U' > J_H$ and near half-filling.
D. Role of Hund coupling and magnetic moments

The origin of the pairing tendencies unveiled here is subtle and in this subsection we report some observations to help clarify this matter. More work is needed to fully comprehend this hole pair formation, so ours are just the first steps in that direction.

One important factor correlated with the pairing we are reporting is the presence of well-formed magnetic moments at every site. This is along the same direction as early studies of the $t-J$ model for cuprates [36], where holes form bound states to reduce the damage that mobile holes induce in an otherwise optimal antiferromagnetic arrangement. Each hole alters the spin order in a finite region, and pairing of holes reduces the size of the regions where spins are not properly arranged. This simple and well-known notion must be at least part of the explanation for our results because pairing in $\Delta E$, as shown in Fig. 3, occurs in regions where moments are well formed, as indicated in Fig. 2.

In addition, we have observed that the Hund coupling in our model clearly is directly related to binding. Figure 11 shows the binding energy in a wide range of $U/W$ parametric with $J_H/U$. At the smallest $J_H/U$ shown, the binding energy is positive and pairs do not have a tendency to form. Consider now the special value $J_H/U = 1/3$. In this case $J_H = U'$ because of the relation $U = U' + 2J_H$. Thus, the natural repulsion $U'$ for two electrons at different orbitals in the same lattice site is compensated by the natural tendency to bind induced by $J_H$. In fact, for $J_H/U = 1/3$, and beyond, i.e., $J_H/U > 1/3$, the binding energy $\Delta E$ is negative at all values of $U/W$.

The reader should note that the connection between the realistic regime $J_H/U < 1/3$ and the unphysical region $J_H/U > 1/3$ is nontrivial. Naively, one may expect $\Delta E$ to be negative for all $U/W$ for $J_H/U > 1/3$, and positive for all $U/W$ for $J_H/U < 1/3$. However, the interpolation, while smooth, is more complex. Figure 11 shows that in the intermediate $U/W$ range, the binding is negative for $J_H/U = 0.20, 0.25$, and $0.30$, with a clear dip in the $U/W \sim 1 - 1/2$ range. This dip, being smoothly connected with the broad negative binding energy region of $J_H/U = 1/3$, must be caused by $J_H$ attraction effects that somehow are not fully compensated by $U'$ at intermediate couplings.

The “earlier” than anticipated attractive effects of $J_H$ at intermediate $U/W$ are explicitly illustrated in Fig. 12 where $\Delta E$ is shown at the optimal $U/W = 1.60$ of our focus, varying $J_H/U$. At least for the small system studied here, $\Delta E$ changes sign before $J_H/U = 0.2$ and it becomes increasingly negative with further increasing $J_H$. While the causal effect of $J_H$ is clear, further work is needed to clarify how can this attraction overcome the $U'$ repulsion in the intermediate coupling range. Moreover, the attraction channel favors spin-singlets involving different orbitals at nearest-neighbor sites. In fact, pairing in the spin-singlet interorbital NN-sites channels is enhanced as $J_H$ increases as shown in Figs. 13(a) and 13(b). Thus, it is a subtle combination of the Hund interaction together with antiferromagnetic short-range order that induces singlet
pairing in this one-dimensional multiorbital model. More work is needed to clarify this interesting effect.

E. Influence of additional interorbital Heisenberg interactions

For completeness, we have also added an extra term to the Hamiltonian in order to boost pairing tendencies. This term is simply a Heisenberg spin-spin interaction with strength $J_D$ defined as

$$H_D = J_D \sum_{ij} S_a^i \cdot S_b^j. \quad (12)$$

The motivation for adding this term is twofolded. First, it plays a role similar to that of “$J$” in the standard $t-J$ model, and we know that increasing $J$ increases pairing tendencies [36]. Second, the new term links the spins of two electrons located at NN sites and at different orbitals [note orbital indexes in Eq. (12)], resembling the structure of the pairs that we have found above. In agreement with these expectations indeed we have observed that pairing tendencies in the dominant spin-singlet NN-sites inter-orbital channel are enhanced as shown in Figs. 13(c) and 13(d). A similar analysis adding instead a NN Heisenberg coupling between electrons in the same orbital only showed minor changes in the decay of the correlations (not shown). Clearly the electrons and holes in the dominant pairs have a preference to be in different orbitals.

Future studies of superconductivity in the two-orbital Hubbard model analyzed here can benefit from enhanced pairing effects by including $J_D$.

IV. CONCLUSIONS

In this publication we have investigated the magnetic, hole pairing, and superconducting properties of a two-orbital Hubbard model defined on a chain. The primary motivation is the recent report of hole binding tendencies in a similar model but defined on a two-leg ladder geometry [31], motivated by the discovery of superconductivity under high pressure in the ladder compound BaFe$_2$S$_3$ [11]. In that previous computational effort, the binding tendency was found to be negative, thus signaling pairing, but the results could not be confirmed beyond small systems $2 \times 8$. In addition pair-pair correlations were not measured in that early effort. In the present work much longer chains can be studied and a variety of correlation functions were measured and their decay with distance compared to decide which is dominant. In the same spirit as in Ref. [31], here our search for superconducting tendencies was based on hole doping while the experimental setup relied on pressure. The \textit{ab initio} calculations in Ref. [33] justify our theoretical approach because they reported that pressure leads to modifications in the average electronic density at the iron atoms.

Our results are interesting for several reasons. The data reported here for the binding energy resemble those of the ladder, but on chain sizes up to 64 sites. Size scaling shows that the results survive the bulk limit. Qualitatively both for ladders and chains it is the intermediate region of $U/W$ where binding does occur. Having almost saturated magnetic moments is important together with a robust Hund coupling. Neither very weak nor very strong $U/W$ coupling seem suitable for pairing, a conceptually interesting result. The absence of pairing at very large $U/W$ may be related with competing ferromagnetic tendencies when holes are added, as in double exchange models. This line of research is being investigated at present.

Moreover, by measuring pair-pair correlations in the spin singlet channel, and using pair operators involving different orbitals and nearest-neighbor sites, a region of hole density and couplings was identified where superconducting correlations decay slower, or at least at the same rate, than spin and charge correlations. Having different orbitals and nearest-neighbor sites is compatible with the internal structure of the pair.

By varying the Hund coupling into the region believed to be unphysical where $J_H$ becomes as large as $U^*$ (this occurs at $J_H/U = 1/3$ if the standard relation $U = U^* + 2J_H$ is assumed [45,49]), then an unexpected smooth continuity was observed between $J_H/U > 1/3$, where binding occurs at all values of $U/W$ because $J_H$ becomes an effective attraction when it overcomes $U^*$, and the region widely believed to be realistic $J_H/U \sim 0.25$. This smooth continuity occurs primarily at intermediate $U/W$ couplings. Thus, for reasons that still need better clarification the effective $J_H$ attraction at $J_H/U > 1/3$ can become operative even at smaller Hund couplings in a reduced $U/W$ range. The chosen dominant channel involves holes in different orbitals, a spin-singlet combination, and nearest-neighbors sites.

The observation that pairing, charge, and spin correlations are sometimes of similar strength, as in Fig. 8(c) for $N = 8$ electrons (48 sites), suggests that future work should also address the possible formation of “pair density waves”. These are subtle broken-symmetry states that intertwine charge density waves, spin density waves, and superconducting orders. In this state the superconducting order parameter is spatially modulated in such a way that the uniform component is zero or very small, but it has a strong oscillatory component [50–52].

In summary, these results contribute towards understanding pairing tendencies in quasi-one-dimensional iron-based superconductors. Binding was found to occur at intermediate couplings, a regime that previous studies showed to be realistic for chalcogenides [6,7]. There is plenty of work ahead. While superconducting correlations already appear to dominate at low hole doping, these results must be confirmed using even longer chains. Moreover, although it seems clear that a robust Hund coupling and robust magnetic moments are needed, developing an even more detailed qualitative understanding of the origin of pairing is important. Our group will continue working along these lines in the near future.

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