Orbital polarons versus itinerant $e_g$ electrons in doped manganites

Maria Daghofer, Andrzej M. Oleś, and Wolfgang von der Linden

Institute of Theoretical and Computational Physics,
Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria

Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland

(Dated: March 23, 2022)

We study an effective one-dimensional (1D) orbital $t$-$J$ model derived for strongly correlated $e_g$ electrons in doped manganites. The ferromagnetic spin order at half filling is supported by orbital superexchange $\propto J$ which stabilizes orbital order with alternating $x^2 - y^2$ and $3z^2 - r^2$ orbitals. In a doped system it competes with the kinetic energy $\propto t$. When a single hole is doped to a half-filled chain, its motion is hindered and a localized orbital polaron is formed. An increasing doping generates either separated polarons or phase separation into hole-rich and hole-poor regions, and eventually polarizes the orbitals and gives a metallic phase with occupied $3z^2 - r^2$ orbitals. This crossover, investigated by exact diagonalization at zero temperature, is demonstrated both by the behavior of correlation functions and by spectral properties, showing that the orbital chain with Ising superexchange is more classical and thus radically different from the 1D spin $t$-$J$ model.

At finite temperature we derive and investigate an effective 1D orbital model using a combination of exact diagonalization with classical Monte-Carlo for spin correlations. A competition between the antiferromagnetic and ferromagnetic spin order was established at half filling, and localized polarons were found for antiferromagnetic interactions at low hole doping. Finally, we clarify that the Jahn-Teller alternating potential stabilizes the orbital order with staggered orbitals, inducing the ferromagnetic spin order and enhancing the localized features in the excitation spectra. Implications of these findings for colossal magnetoresistance manganites are discussed.

[Published in Phys. Rev. B 70, 184430 (2004)]

PACS numbers: 75.47.Lx, 71.30.+h, 75.10.Lp, 79.60.-i

I. INTRODUCTION

Doped perovskite manganese oxides $\text{R}_1-x\text{A}_x\text{MnO}_3$, where $\text{R}$ and $\text{A}$ are rare earth and alkaline earth ions, have attracted increasing attention because they show a rich variety of electronic, magnetic and structural phenomena, and several different types of ordered phases. To explain the colossal magnetoresistance (CMR) and metal-insulator transition observed in these compounds as a function of either doping $x$ or temperature $T$, which suggests their potential technological applications, one has to go beyond the simple double exchange model of Zener and investigate a complex interplay between magnetic, orbital, and lattice degrees of freedom, as well as the conditions for the itinerant behavior of strongly correlated $e_g$ electrons.

The theoretical challenge is to understand the properties of doped manganites in terms of the dynamics of correlated $e_g$ electrons which involves their orbital degrees of freedom. Although several features such as the transition to ferromagnetic (FM) order under doping, and the magnetic excitations in the FM phase, were qualitatively reproduced within the Kondo model which assumes a nondegenerate conduction band, it is evident that the degeneracy of $e_g$ orbitals plays a major role in the double exchange model, in the transport properties of doped manganites, and in the CMR effect itself. In the undoped $\text{LaMnO}_3$ charge fluctuations are suppressed by large on-site Coulomb interaction $U$, leading to superexchange which involves both spin and orbital $e_g$ degrees of freedom.

Purely electronic superexchange models describing the orbital order of $e_g$ electrons were suggested early on by Kugel and Khomskii and are of great interest recently. In cuprates, like in $\text{KCuF}_3$, they lead to enhanced quantum effects while in manganites these models, which originate from several charge excitations due to either $e_g$ or $t_{2g}$ electrons, are richer and include interactions between large and more classical spins. These interactions, together with the Jahn-Teller (JT) effect, stabilize $A$-type antiferromagnetic (AF) phase coexisting with orbital order in undoped $\text{LaMnO}_3$. While the shape of the occupied orbitals in the low-temperature phase of $\text{LaMnO}_3$ is still controversial, the two-sublattice orbital alternation in an orbital ordered state within the FM planes of $\text{LaMnO}_3$ is well established. When the spin dynamics in the FM planes of $\text{LaMnO}_3$ is frozen at low temperature, one can constrain an effective model to purely orbital superexchange instead of considering more complex complete spin-orbital model. The superexchange orbital interactions favor then alternating directional ($3z^2 - r^2$-like) and planar ($x^2 - y^2$-like) orbitals along every cubic direction.

A considerable simplification is allowed in the FM phase at finite doping and at $T = 0$, where the spins are aligned and an effective $t$-$J$-like charge-orbital model is sufficient. Experimentally, at doping higher than $x \approx 0.10$ one finds a FM insulating phase, followed by a metallic phase. The microscopic reasons of this behavior are intriguing — it contradicts the usual spin po-
larionic picture of a FM phase. A puzzling competition between the insulating and metallic behavior within the FM phase was also reported for La_{0.88}Sr_{0.12}MnO_{3}.\textsuperscript{25}

Here we will concentrate on the generic behavior due to \( e_g \) orbital degrees of freedom in a FM phase, and we will treat the spin dynamics classically, as usually done in the double exchange model.\textsuperscript{2,3,11} This approach is complementary to focusing on the quantum effects in double exchange, which was presented recently.\textsuperscript{2,3} Our aim is to study the correlation functions and spectral properties of a one-dimensional (1D) orbital t-J model by exact diagonalization at zero temperature \((T = 0)\), and by classical Monte Carlo simulations of spin correlations at finite temperature in order to establish the consequences of orbital order and orbital dynamics in doped manganites. In the strongly correlated regime the charge dynamics couples to orbital excitations and can be described in terms of the orbital t-J model for doped manganites.\textsuperscript{14,27,28} As in the spin t-J model, a doped hole moves in an orbital ordered state by dressing itself with orbital excitations.\textsuperscript{22} However, the structure of the quasiparticle (orbital polaron)\textsuperscript{22} is here quite different from that derived from the t-J model as the orbital model is more classical.

As a reference system we use a 1D spin t-J model for which the behavior of a single hole is well understood. A hole created in a 1D Néel state is mobile and may be thought as decaying into a magnetic domain wall. In fact, it gives a charged domain wall already after a single hop and leaves behind a solitonic defect from which it separates and next propagates independently. This is the simplest visualization of hole-spin separation in a 1D system. The familiar string picture and quasiparticles on the energy scale of \( \sim 2J \) are then recovered when a staggered magnetic field is applied and suppresses domains of reversed spins.\textsuperscript{29,31}

We show below that an analogous phenomenon of hole-orbital separation does not occur for the orbital degrees of freedom, but instead a single hole is trapped in a 1D chain when orbitals alternate. This explains why an insulating behavior may extend to finite doping. A staggered field has a well established physical origin in this case, and could follow from the frozen JT modes with alternating oxygen distortions along the chain itself, and on the bonds perpendicular to its direction, when the chain is embedded within a three-dimensional (3D) crystal. This interaction may play also an important role for the transport properties of lightly doped manganites and is difficult to separate from on-site Coulomb interaction \( U \).\textsuperscript{22} Therefore, it was even suggested that models including Hund’s exchange \( J_H \) between conduction electrons and \( t_{2g} \) spins, but neglecting Coulomb interaction \( U \), could capture the essential physics of manganites.\textsuperscript{32} We will investigate below the JT term which leads to a staggered field acting on the orbitals. Note, however, that the 1D case is special as static JT distortions, preventing fluctuations of occupied orbitals, suppress completely hole motion along the chain, while in a two-dimensional (2D) model they lead instead to an enhanced coherent component in the hole motion mainly due to suppression of incoherent processes.\textsuperscript{25}

Another feature characteristic of the orbital physics and different from spin models is that the lattice responds to the doping. As pointed out by Kilian and Khaliullin,\textsuperscript{34} the breathing motion of the MnO\(_6\) octahedra provides a strong tendency towards hole localization in the presence of singly occupied (almost) degenerate \( e_g \) levels, as shown in a 2D model.\textsuperscript{22} A static hole polarizes then the orbitals occupied by \( e_g \) electrons in its neighborhood, and this polarization is expected to happen in addition to the effects promoted by the orbital superexchange interactions. We also consider this interaction in the present 1D model and show that it simply renormalizes the superexchange interaction, and thus it could lead to qualitatively new features and be of more importance only in higher dimension.

The paper is organized as follows. In Sec. II we present the effective t-J orbital model for \( e_g \) electrons moving along a 1D chain in a FM plane of, e.g., La\(_{1-y}\)Sr\(_y\)MnO\(_3\). In Sec. III this model is analyzed first qualitatively by comparing the energies of two phases: (i) insulating phase with localized \( e_g \) polarons, and (ii) metallic phase with itinerant carriers. Next we analyze the correlation functions and the spectral properties of a finite chain of \( N = 14 \) sites filled by up to five holes, and demonstrate a crossover from the insulating to metallic phase under increasing doping. At finite temperature \( T \) we derive an effective t-J orbital model, with electron hopping and orbital interactions depending on actual configuration of core spins (Sec. IV). The interrelation between spin and orbital order, the correlations around a doped hole, and the evolution of spectral properties under increasing doping are next investigated using a combination of exact diagonalization with Monte Carlo simulations. Finally, we summarize the results and present general conclusions in Sec. V.

## II. ORBITAL t-J MODEL

We consider the 1D orbital t-J model,

\[
H_0 = H_t + H_J + H_{JT},
\]

obtained for \( e_g \) electrons in FM manganites at \( T = 0 \). The Hamiltonian \( H_t \) acts in the restricted Hilbert space without double occupancies. Due to the absence of the SU(2) symmetry, the kinetic energy in the \( e_g \) band takes a form which depends on the used orbital basis. For the present 1D model it is most convenient to consider a chain along \( c \) axis and to use the usual orbital basis \( \{x^2 - y^2, 3z^2 - r^2\} \), for which we introduce a compact notation,

\[
|x\rangle \equiv \frac{1}{\sqrt{2}}|x^2 - y^2\rangle, \quad |z\rangle \equiv \frac{1}{\sqrt{3}}|3z^2 - r^2\rangle.
\]

A chain along \( a \) or \( b \) axis could also be analyzed using this basis but in each case one obtains a simpler and more
transparent interpretation of the results with a basis consisting of a directional orbital along this particular cubic axis, and an orthogonal to it planar orbital, e.g. $3x^2 - r^2$ and $y^2 - z^2$ for a $a$ axis.

The model given by Eq. (1) stands for a chain composed of $\text{Mn}^{3+}$ and $\text{Mn}^{4+}$ ions coupled by the effective hopping $t$, which originates from the transitions over oxygen. Due to the symmetry, the $|x\rangle$ electrons cannot move, and the hopping term $H_t$ allows only for intersite transitions between a site occupied by a $|z\rangle$ electron and an empty neighboring site,

$$H_t = -t \sum_i (\bar{c}_{i,z}^{\dagger} c_{i+1,z} + \bar{c}_{i+1,z}^{\dagger} \bar{c}_{i,z}),$$

(3)

where an operator $\bar{c}_{i,z}^{\dagger} = c_{i,z}^{\dagger}(1 - n_{ix})$ creates a $|z\rangle$ electron when site $i$ is unoccupied by an $|x\rangle$ electron. The hopping $H_t$ describes thus spinless fermions with an orbital flavor in a restricted Hilbert space, in analogy to the original $t$-$J$ model in spin space, but only one $|z\rangle$ component is here itinerant, while the other $|x\rangle$ one is immobile and hinders the motion of $|z\rangle$ electrons along the chain.

The superexchange in undoped $\text{LaMnO}_3$ is given by a superposition of several terms which originate from charge excitations due to either $e_g$ or $t_{2g}$ electron hopping — they are discussed in Sec. IV.A. While the $t_{2g}$ part is AF, the $e_g$ terms favor either FM or AF spin order on a bond $|ij\rangle$, depending on occupied $e_g$ orbitals at sites $i$ and $j$. For the realistic parameters of $\text{LaMnO}_3$, one finds the $A$-type AF order in the ground state, with FM planes staggered along the third direction. Taking a cubic $c$ direction within a FM plane, the superexchange expression simplifies enormously. Treating large $S = 2$ spins at Mn$^{3+}$ ions classically, all AF terms drop out at $T = 0$, and the remaining orbital superexchange favors alternating $e_g$ orbitals.

Therefore, the superexchange interactions reduce then to the purely orbital interactions which favor alternating directional $(3z^2 - r^2)$-like and planar $(x^2 - y^2)$-like orbitals along every cubic direction. In the present 1D model one finds

$$H_J = 2J \sum_i \left( T_i^z T_{i+1}^z - \frac{1}{2} \bar{n}_i \bar{n}_{i+1} \right),$$

(4)

where operators

$$T_i^z = \frac{1}{2} \sigma_i^z = \frac{1}{2} (n_{ix} - n_{iz}),$$

(5)

stand for orbital pseudospins $T = 1/2$, with two eigenstates defined in Eq. (2), and $\bar{n}_i = \bar{c}_{i,z}^{\dagger} \bar{c}_{i,z} + \bar{c}_{i,z}^{\dagger} \bar{c}_{i,z}$ is an electron number operator in the restricted Hilbert space. The superexchange constant $J = t^2 / \varepsilon (6A_1)$ is then given by the high-spin excitation energy $\varepsilon (6A_1)$.

The last term in Eq. (1) stands for the staggered field induced by the cooperative JT effect,

$$H_{\text{JT}} = 2E_{\text{JT}} \sum_i \exp(i\pi R_i) T_i^z,$$

(6)

considered also in Ref. [37] and supporting the alternating orbital order. It gives an energy gain $E_{\text{JT}}$ per site in the ground state of an undoped 1D chain, and follows from the alternating oxygen distortions around manganese ions in $\text{LaMnO}_3$. The present simplified form [Eq. (6)] of a general expression [38], which depends on the type of oxygen distortion, is sufficient in the 1D model.

At finite doping $x = 1 - n$, where $n$ is an average $e_g$ electron number per site, the present $t$-$J$ model gives an interesting problem, with competing tendencies towards orbital alternation in insulating state on one hand, described by orbital correlations,

$$T(n) = \langle T_i^z T_{i+n}^z \rangle,$$

(7)

and uniform $|z\rangle$ polarization in metallic state on the other. The nature of the ground state obtained at finite doping is best investigated by considering a few characteristic correlation functions, containing information about the orbital state and about the orbital order between two nearest neighbor sites, both at distance $n$ from a hole, and about the orbital correlations across a hole. To optimize them we introduce:

$$P(n) = \langle \bar{n}_i T_{i+n}^z \rangle,$$

(8)

$$R(n) = \langle \bar{n}_i T_{i+n}^z T_{i+n+1}^z \rangle,$$

(9)

$$Z = \langle T_{i-1}^z \bar{n}_i T_{i+1}^z \rangle,$$

(10)

where $\bar{n}_i$ is a hole number operator at site $i$,

$$\bar{n}_i = 1 - \bar{c}_{i,z}^{\dagger} \bar{c}_{i,z} - \bar{c}_{i,x}^{\dagger} \bar{c}_{i,x}.$$

(11)

These correlation functions will be discussed in Secs. III and IV. Note that the kinematical constraint gives $P(0) = R(0) = 0$.

We compare the orbital correlations and the spectral properties obtained for the orbital chain, with these found for a 1D $t$-$J$ spin model for $S = 1/2$ spins,

$$H_{t,\text{JJ}} = -J \sum_{\sigma} (\bar{c}_{i-1,\sigma}^{\dagger} \bar{c}_{i,\sigma} + \bar{c}_{i-1,\sigma} \bar{c}_{i,\sigma})$$

$$+ 2J \sum_i \left( \bar{S}_i^z \bar{S}_{i+1}^z + \frac{1}{2} \bar{n}_i \bar{n}_{i+1} \right)$$

$$+ 2h_s \sum_i \exp(i\pi R_i) S_i^z,$$

(12)

where $\bar{c}_{i,\sigma}^{\dagger} = c_{i,\sigma}^{\dagger}(1 - n_{i,-\sigma})$ is a creation operator of an electron with spin $\sigma$ at site $i$ in the restricted Hilbert space. In contrast to the orbital model, here the electrons with both spin flavors are mobile and exchange between the sites $i$ and $i + 1$, so the interaction is a scalar product $\bar{S}_i^z \bar{S}_{i+1}^z$ instead of the Ising term $T_i^z T_{i+1}^z$. For convenience, we use the same units as in Eqs. (1) and (3); here $J = 2t^2 / U$ with $U$ being the excitation energy. The staggered field $\propto h_s$ simulates the long-range spin order present in a 2D model and plays a similar role to the JT field in the present orbital model. For doped spin chain we consider analogous correlation functions to: orbital-orbital [41], hole-orbital [42], orbital order at distance $n$ from the hole [43], and around a hole [10], with spin operators $S_i^z$ in place of $T_i^z$ [Eq. (12)].
In the next Section we report the results obtained by Lanczos diagonalization of an \( N = 14 \) orbital chain with periodic boundary conditions and different electron filling at \( T = 0 \), and compare them to more familiar spin physics. We have verified that the results concerning the crossover to metallic phase are representative and do not depend on the chain length in any significant way.

## III. NUMERICAL RESULTS AT \( T = 0 \)

### A. Analytic estimation of the crossover from orbital polarons to itinerant electrons

The ground state of the orbital \( t-J \) model depends on two parameters: \( J/t \) and \( E_{\text{IT}}/t \), and on hole doping \( x = 1 - n \). We first investigate the ground state (at \( T = 0 \)) changing these parameters. A realistic value of \( t \sim 0.4 - 0.5 \) eV was estimated for manganites using the charge-transfer model.20 Taking this as an energy unit, and the spectroscopic value for the energy of the high-spin excitation \( \varepsilon (\sigma \uparrow \downarrow) = U - 3J_H \simeq 3.8 \) eV, this leads to \( J/t \simeq 1/8 \). We will consider also \( E_{\text{IT}} > 0 \), which promotes localized behavior of \( e_g \) electrons.

At half-filling one finds alternating \( |x\rangle/|z\rangle \) orbitals in the ground state at \( J > 0 \), with classical intersite correlations \( T(n) = (-1)^n/4 \). If a single hole is then doped to orbitally ordered state at an \( |x\rangle \) site, it can delocalize within a box consisting of three sites, as each neighboring \( |z\rangle \) electron can interchange with the hole [see Fig. 1(a)]. This state is therefore favored over doping at \( |z\rangle \) site, and one can easily determine the energies of a doped hole in an antibonding and bonding state,

\[
E_{1h,\pm} = \frac{1}{2} \bar{J} \pm \frac{1}{2} \left( J^2 + 8t^2 \right)^{1/2},
\]

with \( \bar{J} = J + 2E_{\text{IT}} \) standing for an excitation energy of the configuration with a hole moved to a left (right) site within a three-site cluster shown in Fig. 1(a).

As long as the holes may be doped into separated three-site units (for \( x \leq 0.25 \)), the total energy (per site) of an insulating phase follows from the weighted contributions of the undoped orbital ordered regions, and doped holes occupying the bonding states of individual clusters, with energy \( E_{1h,-} \),

\[
E_1 = -(1-x)E_{\text{IT}} - (1-2x)J + xE_{1h,-}.
\]

The energy of a metallic phase, which contains only itinerant \( |z\rangle \) electrons for \( n > 0.5 \) [see Fig. 1(b)],

\[
E_M = \frac{1}{\pi} \int_{k<\pi/2} \varepsilon_{k,-} + \frac{1}{\pi} \int_{k<k_F} \varepsilon_{k,+},
\]

is obtained by integrating over the occupied one-particle band states \( \varepsilon_{k,\pm} \). At finite \( E_{\text{IT}} \) one finds,

\[
\varepsilon_{k,\pm} = \pm \sqrt{E_{\text{IT}}^2 + 4t^2 \cos^2 k}.
\]

The superexchange \( xJ \) does not contribute to \( E_M \).

It is now of interest to compare the energy of two extreme situations: (i) an insulating phase with holes localized within three-site clusters, [Eq. 14], with (ii) a metallic (itinerant) phase [Eq. 15]. One finds that at fixed \( J \) and \( E_{\text{IT}} = 0 \), an insulator-metal transition takes place when the hole concentration \( x \) increases. A critical concentration for this transition increases with increasing \( J/t \) [Fig. 1(c)]. The data points obtained from the exact diagonalization of an \( N = 14 \) chain agree with the analytic estimate at \( J/t = 1/12 \) and \( 1/8 \), while for a larger value of \( J/t = 1/4 \) the region of the insulating AO phase is more extended in the chain. Note, however, that the present analytic estimate is anyway only qualitative as the energy of the AO phase can be evaluated using a superposition of holes confined to three-site clusters only up...
to \(x = 0.25\). An extended region of stability of the AO phase results here from larger clusters of the itinerant phase which are still separated by immobile \(|x|\) states; such larger itinerant units occur already for \(x < 0.25\) at low values of \(J/t\), as the gain in the kinetic energy for a hole moving within a larger cluster approaches fast the metallic limit with increasing cluster size, and may be easily compensated when a few exchange bonds are created. Indeed, the data show [see Fig. 1(c)] that the ground state for \(x = 1/14\) remains insulating with two \(|x|\) electrons at \(J = 0.02t\), and becomes metallic only for \(J < 0.02t\).

A simple estimation of the metal-insulator transition is also possible when a polaronic polarization around a hole is included in Eq. (1),

\[
H_D = -\Delta \sum_i \tilde{n}_i (\tilde{n}_{i-1,z} + \tilde{n}_{i+1,z}),
\]

(17)

where \(\tilde{n}_{ij} = \tilde{c}_i^{\dagger} \tilde{c}_{i+1,\pm} \tilde{c}_{i+1,\pm} \) is the electron number operator in the restricted space without double occupancies, and \(\tilde{n}_i\) is a hole number operator. At \(E_{JT} = 0\) a similar expression to Eq. (13) is then obtained, with \(\tilde{J} = J + \Delta\), and the range of an insulating AO phase shrinks in the phase diagram of Fig. 1(c). In fact, the polarization around doped holes is optimized in a metallic phase, and this result is special to the 1D model. Therefore, we shall not consider this interaction further, as it gives qualitatively the same results as the orbital \(t-J\) model at \(\Delta = 0\), but with a somewhat reduced value of \(J\).

At finite JT energy \(E_{JT}\) the situation changes in a drastic way. Even for relatively small \(E_{JT} \approx 0.25t\) the AO phase is stabilized in the entire range of doping shown in Fig. 1(c). Note that even somewhat higher values could be more appropriate for realistic 3D manganites. This suggests that the JT effect may indeed play a very important role in manganites and stabilize an insulating phase with orbital order in a broad regime of doping; we address this question in Sec. III E.

### B. Orbital order at half filling

The superexchange interaction in the orbital model \(4\) is Ising-type, and therefore the orbital order in the undoped system at finite \(J\) is perfect, with alternating occupied \(|x|\) and \(|z|\) orbitals along the chain, and \(\langle T_0^z T_{1+}^z \rangle = -0.25\). The classical character of this ground state is reflected in the one-hole excitation spectra. If a single hole is added at half filling \((n = 1)\), it may be doped either at an \(|x|\) or at a \(|z|\) site. A hole doped at a \(|z|\) site is immobile and the energy of the final state is higher by \(2J\) than that of the initial state, as two exchange bonds are removed. This excitation appears as a localized peak at hole binding energy \(-2J\) in Fig. 2(a).

In contrast, when a hole replaces an \(|x|\) electron at site \(i\), the resulting state is not an eigenstate of \(H_0\), the hole delocalizes over a three-site cluster including also occupied \(|z|\) orbitals at neighboring sites \(i - 1\) and \(i + 1\) [Fig. 2(a)], and the bonding and antibonding hole states \(|34,39|\) contribute. They give two maxima in the excitation spectrum of Fig. 2(a), with energies \(E_{1h, \pm} = 2J\). As the hole cannot hop over the sites occupied by \(|x|\) electrons, these two states are again localized within a cluster, and lead to \(k\)-independent maxima in the spectral function.

Strictly speaking, three-site terms, similar to those known from the derivation of the spin \(t-J\) model, occur as well in the orbital model. One might expect that such terms, \(\propto J \tilde{c}_i^{\dagger} \tilde{c}_{i+1,\pm} \tilde{n}_{ix} \tilde{c}_{i+1,\pm}\), would change the spectral functions as a hole created at \(|z|\) site could then hop to its second neighbors and interchange with immobile electrons in \(|x|\) orbitals. However, we have verified that these processes are of importance only for \(J \sim t\), but do not lead to any significant changes of the spectral properties in the physically interesting regime of \(J \lesssim 0.25t\). Therefore, they are neglected in what follows.

In contrast, the spectral functions obtained with the usual spin \(t-J\) model show a dispersive feature at the highest energy, a similar weaker dispersive feature at low...
energy, and incoherent spectral intensity between them [Fig. 2(b)]. The two dispersive features have a periodicity of π instead of 2π obtained for free electrons, are broadened and rather incoherent. Unlike in the 2D case where a hole is trapped and can move only by its coupling to quantum fluctuations in the spin background, leading to a quasiparticle behavior with a dispersion on the energy scale \( \propto J \), the string potential is absent in a 1D chain. The 1D model shows spin-charge separation, because a hole may propagate after creating and leaving behind a single solitonic defect with two spins of the same direction next to each other.\(^{41,42,43}\) However, the chain used in our case is too small for the spin-charge separation to be clearly visible. A more coherent component can be induced by introducing the coupling between the moving charge and spin fluctuations, which occurs in the presence of an external staggered field generating the string potential.\(^{30,31}\) We address this issue in Sec. III E.

The present \( N = 14 \) spin chain gives at half filling \( \langle S_i^x S_{i+1}^x \rangle = -0.1491 \), a value being already quite close to the exact result \(-0.1477\) for an infinite Heisenberg chain. Therefore, we expect that the results presented for the more classical orbital chain with partly localized wavefunctions are at least of the same quality, and suffer even less from finite size effects.

FIG. 3: Ground state energy \( E_0 \) as a function of the number of itinerant electrons \( N_z \) for 0 up to 5 holes (from top to bottom) added to a half-filled \( N = 14 \) orbital chain, for \( E_{1T} = 0 \), and for: (a) \( J = 0.25t \), and (b) \( J = 0.125t \).

C. Correlation functions at finite doping

First we consider the total energy \( E_0 = \langle H_0 \rangle \) as a function of the number of \( |z\) electrons \( N_z \) at each doping \( x \), and determine the actual distribution of \( e_g \) electrons in the ground state. The density of \( e_g \) electrons in two orbitals, \( n_x \) and \( n_z \), depends on the ratio \( j/t \). At half filling \( (x = 0) \) one finds \( n_x = n_z = 0.5 \), and the occupied orbitals alternate. At large \( j/t \approx 1 \) one expects that the orbital order is still close to perfect in the regions which separate orbital polaron, with the densities \( n_z \approx 0.5 \) and \( n_x \approx 0.5 - x \). On the contrary, in the limit of \( j/t \to 0 \) a single hole (in a finite chain) suffices to destabilize the orbital order, causing a transition to an itinerant (FO) state with \( n_z = 1 - x \), and \( n_x = 0 \).

The energy obtained for an \( N = 14 \) chain filled by 9 \( \leq N \leq 14 \) electrons for two values of \( J = 0.25t \) and 0.125\( t \) are shown in Fig. 4. The tendency towards electron delocalization is quite distinct already for a higher value of \( J = 0.25t \), with the minimum of \( E_0 \) moving to \( N_z > 7 \) with increasing doping \( x \). The number of \( |z\) electrons increases\(^{\text{by one}} \) to \( N_z = 8 \) at the electron filling of \( N_e = 12 \) and 11 electrons. At \( N_e = 10 \) there remains just a single \( |x\) electron which still blocks the hopping along the chain, while at \( N_e = 9 \) all electrons are in \( |z\) orbitals, and one obtains a metallic state. This transition to a metallic state is faster at a lower value of \( J = 0.125t \) [see also Fig. 2(c)]. Here adding a hole increases simultaneously the number of \( |z\) electrons by

FIG. 4: Polarization of the orbital (filled circles, full lines) and spin (open circles, dashed lines) background \( P(n) \) at distance \( n \) from a single hole doped to a half-filled \( N = 14 \) chain, as obtained for the ground state of the orbital/spin \( t-J \) model without staggered fields \( (E_{1T} = 0, h_s = 0) \), and for: (a) \( J = 0.25t \) \( (N_z = 7) \), and (b) \( J = 0.125t \) \( (N_z = 8) \).
one, and one finds $N_z = 8$ and $N_z = 9$ for $N_e = 13$ and $N_e = 12$, respectively, while doping by three holes gives already a metallic state with $N_z = N_e = 11$.

The correlation functions in the ground state obtained after doping the chain by a single hole are very transparent at a higher value of $J = 0.25t$, and are easily accessible by looking at the correlation functions (8)–(10). As shown schematically in Fig. 4(a), a hole replacing $|x\rangle$ electron is then confined to a three-site cluster, which can be deduced from the hole-orbital correlation function $P(n)$ [see Fig. 4(a)]. First of all, at the nearest-neighbor of a hole one finds preferably a $|z\rangle$ electron, with $P(1) < -0.25$ indicating that a hole spends more time at a central site than at either outer site of the three-site cluster $|P(1) = -0.25$ would correspond to the bonding state at $J = 0$ and $P(1) = -0.5$ to a static hole at a central site]. This also causes weak alternation of $P(n)$ with increasing $n$ for further neighbors ($n \geq 2$). This result is different again from the spin $t$-$J$ model, where almost no preference for the spin direction is found already at the nearest neighbor of a doped hole. Here the oscillations between even and odd neighbors are also much weaker as a hole is now delocalized, and one is averaging over several different configurations when $P(n)$ is evaluated. They correspond to the domains with opposite spins, and weak oscillations result here only from holon-spinon correlations.

The ground state obtained for one hole at $J = 0.125t$ is qualitatively different, as doping by one hole generates a single orbital flip and the number of itinerant $|z\rangle$ electrons increases to $N_z = 8$. Fig. 4(b) shows that this defect in the otherwise perfect orbital order occurs close to the hole, increasing the island over which the hole can delocalize, extending now over five sites. Hence, one finds $P(1) \simeq -0.44$ and $P(2) \simeq -0.25$, and only starting from the fourth neighbor this correlation is weakly positive. In contrast, decreased value of $J$ does not cause any significant change in the $P(n)$ correlations for the spin $t$-$J$ model — they are only slightly weaker than for $J = 0.25t$.

The orbital order, measured by second correlation function $R(n)$, remains perfect at a sufficient distance from the doped hole, with $R(n) = -0.25$ [Fig. 5(a)]. In case of a higher value of $J = 0.25t$, the order is perfect starting from $n = 2$, while for $J = 0.125t$ with a larger island of the itinerant phase, it starts only at $n = 4$. In addition, the orbital correlation $R(1)$ is here positive [Fig. 5(b)], as two $|z\rangle$ orbitals occur frequently next to each other both at the first and at second neighbor of the hole which polarizes a larger five-site cluster. This behavior shows that phase separation occurs here in the regime of small $J/t$, and its mechanism which originates from orbital physics is completely different from that known from the spin $t$-$J$ model at large $J/t > 1$.

The spin $t$-$J$ model has practically the same spin-spin correlations for both values of $J$. Due to quantum fluctuations in the Heisenberg 1D chain, the correlation function $R(n) \simeq -0.14$ for $n > 1$ [Fig. 5(a)] is much reduced from the classical value $R(n) = -0.25$ found for the orbital model. In fact, the long-range order is absent in the

FIG. 5: Orbital correlations $R(n)$ at distance $n$ from a single hole doped to a half-filled $N = 14$ chain (filled circles, full lines), as obtained for the orbital $t$-$J$ model for $E_{\text{JT}} = 0$, and: (a) $J = 0.25t$, and (b) $J = 0.125t$. Spin correlations obtained in the 1D $t$-$J$ model ($h_Q = 0$) is shown for comparison by open circles and dashed lines.

FIG. 6: Orbital correlations $R(n)$ in a doped $N = 14$ site chain (filled circles, full lines), as obtained for the orbital $t$-$J$ model at $J = 0.125t$, $E_{\text{JT}} = 0$ for doping by: (a) two holes (insulating phase), and (b) three holes (metallic phase). Spin correlations as in Fig. 5.
1D spin chain, and the quantum fluctuations contribute to the energy (per site), which is much lower than in the orbital case, 
\[ e_0 = J\langle S_i^z \cdot S_{i+1}^z \rangle = 3J\langle S_i^z S_{i+1}^z \rangle. \]
The present \( N = 14 \) spin chain gives at doping by one hole \( \langle \tilde{n}_i S_i^z S_{i+1}^z \rangle = -0.1448 \) for \( n = 6, 7 \), a value which is only little reduced from \(-0.1491\) found at half filling, showing that in spite of certain hole delocalization, spin intersite correlations are almost undisturbed by a single doped hole when the distance from it is sufficient.

When doping increases, a gradual crossover in \( R(n) \) correlations towards a metallic chain with \( |z| \) orbitals occupied is found. The region doped by holes extends for two holes over nine sites and gives \( R(n) < 0 \) starting from \( n = 3 \) [Fig. 7(a)]. The correlation function \( R(n) \) is averaged over several bonds, and the values of \( R(n) \) \( \simeq -0.17 \) for \( n = 6, 7 \) result from a superposition of the classical order (\( \langle T_i^z T_{i+1}^z \rangle = -0.25 \)) in the insulating region and a positive value of \( \langle T_i^z T_{i+1}^z \rangle \) correlations within the metallic cluster. When the insulating phase disappears at doping by three holes [Fig. 7(b)], \( R(n) > 0 \) shows that only \( |z| \) orbitals are occupied. Three holes in the metallic phase avoid each other, and one finds a weak local minimum at \( n = 4 \) in \( R(n) \) correlations. The spin system gives instead negative \( R(n) \), as here the hole hopping does not destroy the AF spin order. The correlation functions \( R(n) \) for the spin \( t-J \) model have similar values for either two or three holes, while local minima found at \( n = 7 \) and \( n = 4 \) indicate again characteristic distance between the holes in both cases.

The polaronic character of a doped hole is confirmed by the positive orbital correlation \( Z > 0 \) between its neighbors [10]. At \( J \leq 0.01t \) the ground state is metallic and \( Z = 0.25 \). Next, when \( J/t \) increases, the hole is first trapped in a large metallic cluster (\( Z \simeq 0.22 \)), with its size gradually decreasing down to a five-site cluster when \( J \geq 0.08t \) then a hole is surrounded predominantly by two \(|z|\) electrons [Fig. 7(a)]. This ground state, with \( N_z = 8 \) and \( N_x = 5 \) electrons in the chain remains stable up to \( J = 0.20t \). At \( J/t > 0.20 \) the ground state changes again to \( N_z = 7 \) and \( N_x = 6 \) which gives a small orbital polaron [see Fig. 7(a)]. Due to finite superexchange energy \( J \), the probability that the hole is in the center of a three-site cluster, with two neighboring \(|z|\) electrons, is somewhat higher than that it occupies either of side atoms, with one \(|z|\) and one \(|x|\) occupied orbital next to it. As a result, the correlation function \( Z \simeq 0.02 \) is now weakly positive. For the filling by two holes one has again five different ground states [Fig. 7(b)], with \( Z = 0.25, Z \simeq 0.22, Z \simeq 0.20, Z \simeq 0.16 \), and \( Z \simeq 0.07 \) for increasing \( J/t \). The transition to two separated three-site polarons occurs here at a somewhat higher value of \( J \sim 0.30t \) than the transition to a single three-site polaron for the doping by one hole.

In contrast, the spin correlations between two hole neighbors are negative in the spin \( t-J \) model, both for one and for two holes (Fig. 7), showing the solitonic character of charge defect in the spin chain. At low \( J/t \) these correlations are more pronounced, while increasing \( J/t \) leads to more delocalized holes and to weaker correlations \( Z \simeq -0.10 \) and \( Z \simeq -0.12 \) for the states doped either by one or by two holes at \( J/t = 0.1 \). Somewhat stronger AF correlations in two-hole case confirm the solitonic character of charge defects in a 1D spin chain, with a soliton compensated by an antisoliton.

**D. Spectral functions at finite doping**

Next we analyze the spectral functions obtained at finite doping. Starting from the ground state of an orbital chain with a single hole, we found that in the region of very small \( J \) (\( J \sim 0.01t \) for \( N = 14 \) chain) the spectral function of the orbital model shows a free propagation of a hole within the entire chain, and electrons fill \(|z|\) orbitals. This case (not shown) is however only of theoretical interest, and at \( J \simeq 0.125t \), adequate for for LaMnO\(_3\), one finds instead fairly localized spectra [Fig. 8(a)]. One recognizes the maxima which correspond to localized \(|x|\) excitations at \( \omega - \mu \simeq -1.8t \), and the structures corresponding to the bonding and antibonding states of the \(|x|\) excitations at \( \omega - \mu \simeq -3.3t \) and \(-0.3t \). The spectra are \( k\)-dependent and the spectral weight moves to higher energies with increasing momentum \( k \), following the tight-binding dispersion at \( E_{BT} = 0, \varepsilon_{k} = -2t \cos k \). The total widths of the spectrum in Fig. 8(a) is close to \( 4t \), i.e., to full free-electron dispersion obtained for electrons in \(|z|\) orbitals.
FIG. 8: (color online) Spectral functions $A(k, \omega)$ for $N = 14$ chains doped with one hole for $J/t = 0.125$: (a) orbital $t$-$J$ model with $N_z = 8$ and $N_x = 5$ — solid and dashed lines for $|z\rangle$ and $|x\rangle$ excitations; (b) spin $t$-$J$ model with $N_{\uparrow} = 6$ and $N_{\downarrow} = 7$ — solid and dashed lines for hole and electron excitations. Insets show the densities of states $n(\omega)$. Other parameters and peak broadening as in Fig. 2.

The spectrum obtained for spin $t$-$J$ model is drastically different. A broadened quasiparticle band crossing the Fermi energy resembles a tight-binding dispersion with a reduced bandwidth [Fig. 8(b)]. For low momenta $k$, where a larger system would show spin-charge separation, the spectra are especially incoherent. Most of the spectral intensity is in the incoherent part, but one recovers a coherent propagation in the limit of $J \rightarrow 0$, which occurs in this case without polarizing the chain, as both spin flavors are mobile in this limit and the spin direction is irrelevant.

As we have shown in Fig. 3(b), doping $N = 14$ chain by one hole [Fig. 8(b)], but with more weight transferred now to the quasiparticle states above the Fermi energy $\mu$ at $k > \pi/2$. The weight of the quasiparticle states for $\omega > \mu$ is enhanced, while the incoherent spectral weight is decreased for these values of $k$.

The ground state of the orbital chain is insulating at a larger value of $J = 0.25t$ [Fig. 3(a)]. Therefore, the spectral functions consist in this case of several incoherent features for each $k$ value, with the first moment of the spectra following again the single-particle dispersion (Fig. 10). The incoherent feature at $\omega \approx \mu$, originating from excitations within $|x\rangle$ orbitals, is partly below the Fermi energy. This part of the spectral weight follows from $|x\rangle$-hole excitations which are still possible at the filling by $N_z = 9$ and $N_x = 2$ electrons.

### E. Polaron induced by the JT effect

The energies of insulating and metallic phase are close to each other for typical parameters. Therefore, even a moderate JT energy $E_{JT} = 0.25t$ is sufficient to stabilize...
the insulating phase in a broad regime of doping, with occupied $|x\rangle$ orbitals fragmenting the chain into smaller units. When a single hole is doped, the JT field has qualitatively a similar effect as a larger value of $J$ — a hole is then well localized within a three-site cluster, and the hole-orbital correlation $P(n)$ exhibits more pronounced alternation, indicating robust orbital order [Fig. 11(a)], as in Fig. 3(a). The orbital intersite correlations $R(n)$ are perfect already beyond the second nearest neighbor of the hole [Fig. 11(b)].

When more holes are added, the orbital order gradually softens, but a clear tendency towards orbital alternation is observed even for high doping with four holes [Fig. 11(b)]. Note that a second hole may be added at a fourth or sixth site away from the first one. This, together with weak hole hopping within the three-site clusters, weakens both hole-orbital correlations $P(n)$ and the orbital order $R(n)$ at $n = 4$ and (less) at $n = 6$. For the present case of $N = 14$ sites these latter correlations are reduced more for $n \geq 4$ than for $n = 2$. With a third hole added, we found separated holes in three-site clusters, with each hole occupying predominantly the central site of its cluster in order to minimize the JT energy. A typical inter-hole distance is then four lattice constants, and for this reason $P(4)$ becomes negative, and $R(4)$ is reduced stronger than $R(n)$ for any other $n > 0$. The fourth hole is added at one of $|x\rangle$ orbitals within a longer $|z\rangle - |x\rangle - |z\rangle - |x\rangle - |z\rangle$ unit, and makes then the first bigger cluster, with two holes and three mobile $|z\rangle$ electrons. Particularly in this regime of parameters and up to this doping regime, the distribution of holes is reminiscent of doping CuO$_3$ chains in YBa$_2$Cu$_3$O$_{6+\delta}$, where holes are doped first in separated CuO$_2$ units, where they are trapped, generating fragmented units of CuO$_3$ chains and causing jumps and plateaus for the hole counts in the CuO$_2$ planes as a function of doping.

The spectral functions $A(k, \omega)$, presented for two representative doping levels with one and three holes in Fig. 12, show that they are remarkably similar in the entire regime of doping $x < 0.3$. Excitations in $|x\rangle$ orbitals lead to maxima below and above the Fermi energy, with the spectral weight moving gradually to higher energies under increasing doping. For hole excitations in $|z\rangle$ orbitals one finds three nondispersive features: the central peak for doping within the orbital ordered regions, and two side peaks at energies corresponding to the excitations of orbital polarons. The spectral weight of the latter features increases on the cost of the central peak when doping increases, and the spectral weight distribution depends on momentum $k$. At doping increasing up to five holes (not shown) the spectra are still fairly localized, and the $|x\rangle$ spectral weight is further reduced for $\omega < \mu$.

A remarkable change of the spectral functions $A(k, \omega)$ has been found for the spin $t$-$J$ model in presence of a finite staggered field $h_s = 2J$. The field generates a string potential, and simulates thus a 2D model. However, in this quantum model, in contrast to the orbital model shown in Fig. 12(a), a hole is not confined within a polaron but can move coherently when it couples to quantum spin fluctuations, which repair the defects in the spin background generated by a moving hole. As a result, a quasiparticle peak emerges close to the Fermi energy (Fig. 13), indicating a propagation of a hole dressed by spin excitations, with a dispersion $\sim 4J$ [note the units in Eq. 12]. The remaining spectral weight is distributed
over incoherent features at lower energy while the low energy quasiparticle band visible in Fig. 8 has vanished as well as the incoherence of the band for small $k$.

Moreover, the quasiparticle band has lost a simple tight-bindinglike dispersion found before at $h_s = 0$, and instead of crossing the Fermi energy, it has periodicity $\pi$ because of the doubled unit cell and folds back toward lower energies after reaching the Fermi energy at $k = \pi/2$. The peaks are sharpest near this point, confirming the quasiparticle character of this excitation, but have lower spectral weight at $k = \pi$ than at $k = 0$. The quasiparticle band close to the Fermi energy leads to a quite distinct peak in the density of states (see inset of Fig. 13). It is separated by a pseudogap from the electronic excitations at $\omega > \mu$, and also by another pseudogap at $\sim 4J$ below the Fermi energy from the incoherent part of the spectrum at lower energies. Thus, the present case is radically different from the case of $h_s = 0$ [see Fig. 2(b)], and resembles the spectral functions for a 2D model.14

FIG. 12: (color online) Spectral functions $A(k, \omega)$ for an insulating $N = 14$ orbital chain for $J/t = 0.125$ and $E_{\text{JT}} = 0.25t$, obtained for increasing doping by: (a) one hole, and (b) three holes. Solid and dashed lines for $|z\rangle$ and $|x\rangle$ excitations. Insets and peak broadening as in Fig. 2.

FIG. 13: (color online) Spectral functions $A(k, \omega)$ for an $N = 14$ spin $t$-$J$ chain at doping by one hole, as obtained for $J/t = 0.125$ with a staggered field $h_s = 2J$. Solid and dashed lines indicate hole and electron excitations. Inset shows the density of states $n(\omega)$.

IV. ORBITAL POLARONS AT FINITE TEMPERATURE

A. Effective orbital $t$-$J$ model

At increasing temperature the FM spin order assumed in Sec. II is gradually destroyed and AF spin configurations on the bonds occur with finite probability, modifying the form of both $t$ and $J$ terms in Eq. (1). Even when the ground state at $T = 0$ is FM, superexchange interactions which originate from $t_{2g}$ electron excitations play an important role and contribute at finite temperature. These interactions are frequently treated as an effective AF superexchange between core $S = 3/2$ spins, but de facto they depend on the total number of $d$ electrons of two interacting Mn ions. We have verified, however, that the $t_{2g}$ superexchange terms derived for these different configurations are of the same order of magnitude, so it is acceptable to consider their effect as equivalent to a Heisenberg interaction with an average exchange constant $J' > 0$. Therefore, we include in the present 1D model the spin interaction,

$$H_{J'} = J' \sum_i (\vec{S}_i \cdot \vec{S}_{i+1} - S^2). \quad (18)$$

The superexchange due to $e_g$ electron excitations contains spin scalar products multiplied by orbital interactions on the bonds, and the full many-body problem would require treating the coupled spin and orbital dynamics. Here we decouple spins and orbitals in the mean-field approximation, and study the orbital correlations and their consequences for the magnetic order by replacing the scalar products of spin operators on each bond by their average values,

$$\langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle = S^2 (2u_{i,i+1}^2 - 1), \quad (19)$$
where \( u_{i,i+1} = \cos((\theta_{i,i+1}+1)/2) \epsilon_{\chi_i} \), and directions of two classical spins at sites \( i \) and \( i+1 \) differ by angle \( \theta_{i,i+1} \). The complex phase \( \chi_{i,i+1} \) does not have any effect in the present 1D model.

We investigate the effective orbital t-J model,

\[
\mathcal{H}(S) = H_i + H_J + H_F + H_{JT},
\]

(20)

where the AF interactions of core spins \( J_3 \) and the JT field acting on orbital variables are playing the role of external fields. The hopping term \( H_i \) describes the dynamics of \( e_g \) electrons which are locally coupled to \( t_{2g} \) core spins by large Hund’s exchange \( J_H \) element, and have their spins parallel to them in the ground state. In agreement with double exchange mechanism the hopping along each bond \( (i,i+1) \) is then modified by the spin order to

\[
\tilde{t}_{i,i+1} = tu_{i,i+1},
\]

(21)

and vanishes when the spins are antiparallel. This approximation allowed to establish the existence of magnetic polarons in the 1D Kondo model.

The superexchange due to \( e_g \) electrons \( \propto J \) generates orbital interactions in \( H_J \) which follow from virtual charge excitations, either for \( \text{Mn}^{3+} \), or for \( \text{Mn}^{3+} \)-\( \text{Mn}^{4+} \) pairs. Consider first the spin-orbital model of Ref. 21 for an undoped \( \text{LaMnO}_4 \). So far, we included the orbital superexchange [Eq. 4] for a situation when high-spin \( e_g \) excitations dominate, but low-spin excitations would also contribute at finite temperature. Taking realistic parameters for the Coulomb interaction \( U \) and Hund’s exchange \( J_H \), the low-spin \( A_1 \), \( E \), and \( A_2 \) states have the energies: 7.3, 7.8, and 9.6 eV. We keep the relative importance of various excitations and write the terms resulting from various charge excitations to the superexchange, after averaging them over the spin configuration, as follows:

\[
\frac{1}{10} \langle \tilde{S}_i \cdot \tilde{S}_{i+1} + 6 \rangle = \frac{J}{5} \langle 4u_{i,i+1}^2 + 1 \rangle,
\]

(22)

\[
\frac{1}{16} \left[ \frac{t^2}{\epsilon(4A_1)} + \frac{3}{5} \frac{t^2}{\epsilon(4E)} \right] \langle \tilde{S}_i \cdot \tilde{S}_{i+1} - 4 \rangle \approx \frac{2}{J} \langle u_{i,i+1}^2 - 1 \rangle,
\]

\[
\frac{1}{16} \left[ \frac{t^2}{\epsilon(4E)} + \frac{t^2}{\epsilon(4A_2)} \right] \langle \tilde{S}_i \cdot \tilde{S}_{i+1} - 4 \rangle \approx \frac{9J}{20} \langle u_{i,i+1}^2 - 1 \rangle,
\]

(23)

Using the coefficients given in Eqs. 22 and 23, one arrives at the effective orbital t-J model 20, with

\[
H_i = - \sum_i \tilde{t}_{i,i+1} (\tilde{c}_{i+1,z}^\dagger \tilde{c}_{i,z} + \tilde{c}_{i,z}^\dagger \tilde{c}_{i+1,z}),
\]

(24)

\[
H_J = \frac{1}{5} J \sum_i \left[ 2(\tilde{u}_{i,i+1}^2 + 3) \left( 2T_i^2 T_{i+1}^2 - \frac{1}{3} \tilde{n}_i \tilde{n}_{i+1} \right) - \frac{9}{10} \sum_i (1 - \tilde{u}_{i,i+1}^2) \tilde{n}_i \tilde{n}_{i+1} \right],
\]

(25)

The hopping \( (H_i) \) and the interaction \( (H_J) \) terms depend on the actual spin configuration which fixes the bond variables \( \{u_{i,i+1}\} \) [see Eq. 19]. In the FM state at \( T = 0 \) all \( u_{i,i+1} = 1 \), the AF terms vanish, and one recovers the form of \( H_i \) and \( H_J \) used in Sec. 11.

It is a crucial feature of the effective orbital model given by Eq. 20 that spin interactions are influenced by orbital correlations along the chain, and the latter can support either FM (for alternating \( x/z \) orbitals) or AF (for polarized \( z \) orbitals) spin order. At \( T = 0 \) one can find on optimal state by minimizing the total (internal) energy of the system, \( E = \langle \mathcal{H}(S) \rangle \), over the spin and orbital configurations. In fact, at \( T = 0 \) two solutions are possible, depending on the parameters in Eq. 20. Let us consider first a purely electronic model with \( E_{JT} = 0 \) at half filling (we will show below that the situation is similar at \( E_{JT} > 0 \), but the region of stability of the AF states is extended). If \( J' > 0 \), FM order is stable and coexists with alternating orbital order. This situation was discussed in detail in Sec. 111. However, a relatively small value of \( J' = 0.0125t \) is sufficient to compensate the latter energy difference between this state and an AF state with occupied \( \{z\} \) orbitals, and (at \( T = 0 \)) one finds the latter state for \( J' > 0.0125t \). It is interesting to investigate a competition between these magnetic states at finite temperature when the chain is doped.

We investigated the spin and orbital correlations for the effective orbital t-J model 20 at finite temperatures by employing a combination of a Markov chain Monte Carlo (MCMC) algorithm for the core spins, with Lanzos diagonalization for the many-body problem posed by the orbital chain of \( N = 12 \) sites with periodic boundary conditions, at each given distribution of classical variables \( \{u_{i,i+1}\} \) for \( i = 1, \cdots, 12 \), which stands for a particular spin configuration. The partition function to be then evaluated is

\[
Z = \int \mathcal{D}[S] \text{Tr}_{c} e^{-\beta \mathcal{H}(S)},
\]

(26)

where \( \beta = 1/k_B T \) (we adopt the units with \( k_B = 1 \)), and \( \int \mathcal{D}[S] \) denotes the integral over the \( N \)-dimensional space of all core spin configurations for the chain of length \( N \). The core spins \( S \equiv \{\tilde{S}_i\} \) determine the site-dependent hopping parameters \( \{u_{i,i+1}\} \) and thus the fermionic Hamiltonian \( \mathcal{H}(S) \) is fixed.
The trace over the fermionic degrees of freedom, \( \text{Tr}_z e^{-\beta \mathcal{H}(S)} =: w(S) \), gives the statistical weight for \( S \) and is sampled by the MCMC. For independent electrons it can easily be evaluated \( \mathcal{H}(S) \) for interacting electrons one has to use a Lanczos algorithm \( \mathcal{H}(S) \), but as \( w(S) \) is strictly positive, one still has no sign problem. Since the position of the \( |x \rangle \) electrons is conserved, the Hamiltonian \( H \) has a block-diagonal structure, with each block corresponding to one fixed distribution of \( |x \rangle \) electrons along the chain. There are, of course, many such blocks, but their subsequent diagonalization is still much faster than the diagonalization of the complete matrix. For the extreme case of the completely filled chain, each block has dimension one, meaning that the Hamiltonian is already diagonal and no matrix-vector multiplication has to be performed. Furthermore, degenerate eigenvalues can be resolved, if they are in different blocks.

For the MCMC updates, \( w(S) \) was calculated from the lowest few eigenenergies of each block for an \( N = 12 \) chain, until a new Lanczos step did no longer modify the contribution from this block. Observables were only calculated from the lowest 14 eigenstates of the \( \text{whole} \) space. In order to monitor this approximation, the Boltzmann factor of these states was measured. The weight of the highest included state was approximately 1.5 percent for the worst case (filled chain, \( \beta t = 20, J' = 0.02, E_{JT} = 0 \)), 0.3 – 0.5 percent for \( \beta t = 50 \) and the filled chain and negligible for \( \beta = 100 \) or finite doping. This means that for those observables, which are calculated from the eigenstates of the Hamiltonian, at most a few percent of the total weight were missed. For the MCMC updates and for observables which do not need the eigenvectors (core spin correlation and total number of \( |x \rangle \) electrons), the error was even smaller.

The core spins were rotated for whole sections of the chain at once. Because acceptance for core spin updates was high, we performed two or three such rotations before testing acceptance. Every spin was therefore rotated several times per sweep. The numbers \( N_z \) and \( N_x \) of \( |x \rangle \) and \( |z \rangle \) electrons remained fixed for the evaluation of \( w(S) \), and every five updates we proposed to increase (decrease) \( N_z \) and decrease (increase) \( N_x \), respectively, thereby sampling \( N_z \) and \( N_x \). The total number of electrons \( N_x = N_z \) was kept fixed. Between measurements, 40 to 100 lattice sweeps (depending on temperature) were done in order to decorrelate the samples. We then employed autocorrelation analysis and found the samples to be uncorrelated. To reduce the statistical errors, 200 uncorrelated samples were obtained for each set of parameter values.

**B. Orbital order versus spin order**

In addition to the correlation functions studied in Sec. 13, spin correlations \( \langle S_i^z S_j^z \rangle \) are now investigated by evaluating the spin structure factor,

\[
S(k) = \frac{1}{N^2} \sum_{ij} e^{i k (R_i - R_j)} \langle S_i^z S_j^z \rangle,
\]

which depends on the 1D momentum \( k \), and follows from Monte-Carlo simulations of \( N = 12 \) chains. The averages \( \{ \langle S_i^z S_j^z \rangle \} \) are calculated from the spin configurations \( S \equiv \{ S_i \} \) determined by the MCMC updates for \( \{ u_{i,i+1} \} \).

The interplay between spin and orbital correlations becomes transparent by varying the core spin AF superexchange \( J' \) due to \( t_{2g} \) electrons. We investigated spin and orbital order for two characteristic values of temperature: \( \beta t = 100 \) and \( \beta t = 50 \), each corresponding to \( T \sim 60 \) and \( \sim 120 \) K for \( t \sim 0.5 \) eV, i.e., well below the magnetic transition. First we consider the case of \( J' = 0 \) which reproduces the ground state analyzed in Secs. 13 and 111.

While the orbital alternation, measured by \( T(n) \) correlation function \( 7 \), is perfect at \( T = 0 \), it softens somewhat at higher temperatures, but is still robust at temperature \( \beta t = 50 \), as shown in Fig. 14 (a). Orbital alternation supports the FM spin order at half filling, which gives a distinct maximum at \( k = 0 \) of the spin structure factor \( S(k) \) (see Fig. 15). In the weak doping regime with one or two holes added, the spin correlations \( \langle n_i S_i^z n_{i+n} S_{i+n}^z \rangle \) are driven by superexchange and FM at any distance \( n \) from the hole, and only weakly depend on \( n \). These correlations increase by a factor close to two when the doping changes from two to three holes. This explains why the maximum of \( S(k) \) at \( k = 0 \)
remains almost unchanged in the low doping regime by one or two holes, but is next strongly enhanced when doping increases to three holes. Precisely at this concentration electrons redistribute within the chain and occupy practically only \(|z\rangle\) orbitals, giving a metallic state. This demonstrates that double exchange plays a primary role in the observed insulator-metal transition and significantly enhances the stability of the FM order in the metallic phase.

At \(J' = 0.02t\) the orbital correlations found in the half-filled chain are markedly different [Fig. 15(b)]. At low temperature \((\beta t = 100)\) they indicate that primarily (but not only) \(|z\rangle\) orbitals are occupied, while no \(|x\rangle\) electrons were found in the ground state at \(T = 0\). This orbital state is induced by finite \(J'\), and supports the AF spin interactions due to \(e_g\) excitations which select then low-spin states in the \(e_g\) excitations along \(|z\rangle - |z\rangle\) bonds. When a single hole is doped, the spin correlations remain still AF at low temperature [Fig. 15(a)], except for the spin-spin correlation between the site occupied by the hole and its nearest neighbor, giving rise to a small FM polaron. Therefore, the value of \(S(0)\) increases already at this low doping, and the electron density in \(|z\rangle\) orbitals is enhanced close to the hole itself.

When temperature increases, it becomes clear that the orbital \(|x\rangle/|z\rangle\) alternation, supporting the FM spin interactions, competes at half filling with the above uniformly polarized chain with occupied \(|z\rangle\) orbitals, supporting the AF spin order. A clear tendency towards orbital alternation is detected by a negative nearest-neighbor orbital correlation \(T(1) \simeq -0.10\) [Fig. 16(b)] at higher temperature \((\beta t = 50)\). Although the value of \(S(\pi)\) is still larger than \(S(0)\) at half filling, both (weak) maxima, corresponding to FM and AF order, become almost equal already for doping with one hole [Fig. 16(b)]. This case is qualitatively similar to a chain doped by two holes at \(\beta t = 100\) [Fig. 15(b)], where also two (stronger) maxima of \(S(\pi)\) indicate coexisting islands of FM and AF spin correlations along the chain. Thus, we found that the AF correlations are gradually changed into FM ones with increasing temperature. This trend follows from the difference in the energy scales — when the thermal magnetic excitations destroy the energy gains due to \(J\) and \(J'\), the kinetic energy \(\propto t\) is a dominating energy which can be optimized by selecting \(|z\rangle\) occupied orbitals and FM spin correlations.

At doping by three holes the spin correlations are FM, both at low \((\beta t = 100)\) and at higher temperature \((\beta t = 50)\), showing that the double exchange enhances the effective FM interactions and changes the characteristic temperature at which the spin correlations weaken — thus the Curie temperature \(T_C\) would increase in a 3D case. This agrees with the experimental observations — indeed, the Curie temperature increases with hole doping in the metallic regime.\(^{24,45}\)

Although at \(T = 0\) one finds indeed the AF ground state with \(N_z = 12\) for a half-filled \(N = 12\) chain, many excited states with a few \(|x\rangle\) orbitals occupied are found at low energy and contribute already at \(\beta t = 100\). As a result, electrons are redistributed over \(e_g\) orbitals.
TABLE I: Total number of electrons in itinerant orbitals $N_x$ (top part) and in localized orbitals $N_z$ (bottom part) for different doping level $x$ and for increasing temperature $\beta t$, as obtained in the Monte-Carlo simulations for an $N = 12$ orbital chain [Eq. (20)] (statistical errors are also given). Parameters: $J = 0.125t$, $J' = 0.02t$, $E_{J\Gamma} = 0$.

| $\beta t$ | $x = 0$  | $x = 1/12$ | $x = 1/6$ | $x = 1/4$ |
|----------|----------|------------|-----------|-----------|
| 100      | 9.97 ± 0.09 | 9.80 ± 0.06 | 9.64 ± 0.04 | 9.0 ± 0.0  |
| 50       | 7.85 ± 0.07 | 8.51 ± 0.06 | 8.81 ± 0.04 | 8.98 ± 0.01|
| 30       | 7.47 ± 0.07 | 8.05 ± 0.06 | 8.53 ± 0.05 | 8.88 ± 0.03|
| 20       | 7.34 ± 0.07 | 7.85 ± 0.06 | 8.18 ± 0.06 | 8.55 ± 0.04|

| $\beta t$ | $x = 0$  | $x = 1/12$ | $x = 1/6$ | $x = 1/4$ |
|----------|----------|------------|-----------|-----------|
| 100      | 2.03 ± 0.09 | 1.20 ± 0.06 | 0.36 ± 0.04 | 0.0 ± 0.0  |
| 50       | 4.15 ± 0.07 | 2.49 ± 0.06 | 1.19 ± 0.04 | 0.02 ± 0.01|
| 30       | 4.53 ± 0.07 | 2.95 ± 0.06 | 1.47 ± 0.05 | 0.12 ± 0.03|
| 20       | 4.66 ± 0.07 | 3.15 ± 0.06 | 1.82 ± 0.06 | 0.45 ± 0.04|

by thermal excitations, and the orbital polarization at $\beta t = 100$ is far from complete, with $N_z \simeq 10$ and $N_z \simeq 2$ (Table I). When temperature increases further to $\beta t = 50$ ($\beta t = 20$), orbital disorder increases and one finds $N_z \simeq 7.8$ and $N_z \simeq 4.2$ ($N_z \simeq 7.3$ and $N_z \simeq 4.7$). This demonstrates that the balance between FM and AF terms realized at half filling is rather subtle — increasing temperature favors more disorder in the chain which destroys a uniform AF phase, supported by charge excitations along $|z\rangle - |z\rangle$ bonds.

The population of localized $|x\rangle$ states in the chain decreases quite fast with doping, particularly in the regime of $\beta t \leq 100$. At $x = 1/4$ one finds almost no $|x\rangle$ defects in the metallic chains, except at rather high temperature $\beta t = 20$. Increasing electron density in $|x\rangle$ orbitals with increasing temperature may be seen as a precursor effect for the metal-insulator transition at $T_C$ in the intermediate doping regime.

C. Polaronic features at finite doping

The spectral functions $A(k, \omega)$ obtained for the FM phase at half filling for $J = 0$ (not shown) are similar to those discussed in Sec. IIIA. Apart from some broadening due to finite $T$, the one-hole excitations are again fairly localized, similar to those shown in Fig. 2. In the doped regime one finds first the localized spectra at low doping, similar to those of Fig. 3(a), with a distinct pseudogap at the Fermi energy $\mu$. As found before at $T = 0$, doping by three holes suffices for the crossover to the metallic phase, with somewhat broadened peaks in $A(k, \omega)$, following the one-particle dispersion due to the hopping within $|z\rangle$ orbitals, like in Fig. 3(a).

In contrast, the spectral properties obtained for the AF phase found at half filling with $J' = 0.02t$ are quite different (Fig. 17). First of all, there are predominantly $|z\rangle$ electrons at low temperature $\beta t = 50$, and still more so at $\beta t = 100$, so the spectral weight of the localized $|x\rangle$ hole excitations, found at energies $\omega \approx -1.3t$ and $\sim t$ [Fig. 13(b)], appears to be very low. The $|z\rangle$ excitations have insulating character and are incoherent. They are given by a superposition of two features, namely a dispersionless peak at the hole binding energy $\omega \approx -2J$ and a weakly dispersive band with bandwidth $\approx 0.5t$. The first feature stems from the few $|z\rangle$ electrons which are surrounded by $|x\rangle$ electrons and is similar to that discussed in Sec. IIIA. The second feature comes from electrons moving within the $|z\rangle$ polarized parts, with the strongly renormalized hopping $\propto t_{i,i+1}$ 24 for aligned $|z\rangle$ orbitals along an almost perfect AF bond. If the AF order were perfect, the bandwidth would vanish, because no hopping would then be possible. Both the dispersive and the dispersionless structures are broadened owing to thermal fluctuations of the core spins. The superposition of these two bands yields a single peak with large intensity for $k = 0$, because the bandwidth is approximately $\sim 0.5t = 4J$ and the both bands therefore coincide at this point. For the same reason, the spectral weight at $k = \pi$ consists of two almost symmetric maxima. This interpretation is corroborated by the results for $\beta t = 50$ (not shown), where (i) the dispersionless feature has a higher weight, because the population of $|x\rangle$ orbitals increases with increasing temperature (see Table I), and (ii) the structures in $A(k, \omega)$ are still more broadened because of the larger thermal fluctuations.

The spectrum changes rapidly when doping increases. At doping of $x = 1/12$ (one hole in an $N = 12$ chain) a polaronic peak is found above $\mu$, while below $\mu$ the spectrum separates into a broad incoherent part at intermediate energies, and a low-energy peak with large intensity for low values of $k = 0$ and $k = \pi/6$, being a symmet-
FIG. 18: (color online) Spectral functions $A(k, \omega)$ for an $N = 12$ orbital chain at temperature $\beta t = 100$ doped by: (a) two holes, and (b) three holes. Solid and dashed lines, inset and parameters as in Fig. 17.

FIG. 19: (color online) Spin structure factor $S(k)$ as in Fig. 15, but for up to four holes. Parameters: $J = 0.125t$, $J' = 0.02t$, $E_{JT} = 0.25t$.

We have shown above that the orbital and magnetic order are interrelated and influence each other. Therefore, as pointed out before, not only the superexchange, but also purely orbital interactions which follow from the JT effect are of importance for the observed magnetic AF order in LaMnO$_3$. Now we will show that also in the present 1D model the JT effect may modify the magnetic order. This is particularly transparent by considering a uniformly polarized insulating state with occupied $|z\rangle$ orbitals, coexisting with an AF order, and stabilized by weak superexchange $J' = 0.02t$ (Fig. 17). If an alternating JT potential, given by Eq. (6), increases, the AF order is easily destabilized — already at $E_{JT} = 0.25t$ we found an almost perfect orbital staggering in the broad temperature regime at half filling [Fig. 14(c)], which induces instead the FM spin order, visible as a broad maximum in $S(k)$ centered at $k = 0$ (Fig. 19). However, this maximum is less pronounced and other correlations $S(k)$ with $k > 0$ are also present, unlike for $J' = E_{JT} = 0$, showing that the FM order induced by the JT potential is definitely much weaker.

Even for moderate JT potential $E_{JT} = 0.25t$, increas-
and inset as in Fig. 17. Parameters: $\beta t = 12$, orbital chain (20), as obtained at temperature $E_t = 0$ and one expects that also spin stiffness should be reduced by the JT coupling in CMR manganites.

The transition to metallic phase is damped by the JT distortions, and although the FM correlations increase significantly at doping $x = 1/3$ (Fig. 19), the chain remains insulating. Only for as high doping as $x = 5/12$, the $|x\rangle$ electrons are practically eliminated in the considered temperature range $\beta t \geq 50$, and a metallic behavior takes over. This metallic state gives almost free dispersion of $|z\rangle$ states in $A(k, \omega)$, while $|x\rangle$ (electron) excitations are again localized [Fig. 20(b)]).

V. SUMMARY AND CONCLUSIONS

The present study clarifies that orbital degrees of freedom are of crucial importance for the understanding of magnetic correlations in CMR manganites. First of all, for the realistic parameters of manganites the FM and AF state are nearly degenerate at half filling. In both cases the decisive term stabilizing the magnetic order originates from the $e_g$ superexchange. Although the ground state at $T = 0$ would be FM in the absence of the AF superexchange between core spins, is is easy to flip the balance of magnetic (and orbital) interactions and stabilize instead the AF order in a purely electronic model. Here we adopted the AF interaction $J' = 0.02t$ between core spins in order to stabilize the AF spin order in an undoped chain (the true value of $J' \simeq 0.004t$ in LaMnO$_3$, estimated from the value of Néel temperature of CaMnO$_3$, is smaller by a factor close to five$^{20}$), and to demonstrate a gradual crossover from an AF insulator to a FM metal under increasing doping. In this regime of parameters the present 1D chain stands for the AF order along c axis in the A-AF phase realized in LaMnO$_3$.

We have shown that even in the 1D model the magnetic interactions are internally frustrated, with competing FM and AF terms in the superexchange. A delicate balance between these terms is easily disturbed by the JT potential originating from the lattice. This allows one to investigate within the same framework both types of magnetic order which coexist in the $e_g$ superexchange. Note, however, that the FM correlations are weakly reduced from their values found in the absence of the JT interactions ($J' = 0$ and $E_{JT} = 0$), demonstrating that the FM interactions do not depend explicitly on the JT terms, but are only induced by a given type of orbital order. In this way the

![FIG. 20: (color online) Spectral functions $A(k, \omega)$ for an $N = 12$ orbital chain (20), as obtained at temperature $\beta t = 100$ for: (a) three holes, and (b) five holes. Solid/dashed lines and inset as in Fig. 17 Parameters: $J = 0.125t$, $J' = 0.02t$, $E_{JT} = 0.25t$.](image)
JT coupling to the lattice helps to remove the frustration of magnetic interactions in CMR manganites.

The evolution of spin correlations for increasing doping showed that indeed two mechanisms are responsible for ferromagnetism: when the weakly doped 1D chain is insulating, the FM interactions are induced both by the superexchange terms following from the high-spin excited states, and by the local double exchange within polaronic states around single holes trapped in the insulating phase. The double exchange interactions is much stronger than the superexchange, and it fully takes over and operates in the metallic phase at higher doping. The difference between these two mechanisms is reflected by a fast increase of FM correlations at the insulator-metal transition which was investigated both within a purely electronic model, and including the JT potential induced by the lattice.

It is quite remarkable that orbital polarons found in the present model with orbital degeneracy in the regime of AF spin correlations resemble FM polarons which occur in the Kondo model. This provides some support to a simplified picture of a nondegenerate conduction band which is able to capture the essential physics when the orbitals are polarized, and the orbital degrees of freedom are quenched and do not contribute in any significant way. A conservative point of view, based on double exchange mechanism, is that the FM polarons compete with the AF order and cause a transition to the metallic FM phase. Yet, this is not the only possibility — we have shown that the FM phase at low doping could be insulating due to immobile orbital polarons, which allow to understand why this phase could be FM and insulating at the same time. Such polarons are expected to play an essential role in the insulator-metal transition within the FM phase in manganites.

We believe that many qualitative features found in the present 1D study are generic for the interplay between orbital and magnetic order in CMR manganites. Work is in progress on higher dimensional systems. Among others, an interesting question is to what extent the orbital order is modified when two $e_g$ orbitals start to fluctuate more strongly in either 2D or 3D systems, both due to quantum effects and due to increasing doping.

Acknowledgments

We thank E. Arrigoni and A. Prüll for valuable discussions. This work has been supported by the Austrian Science Fund (FWF), Project No. P15834-PHY. A. M. Oleś would like to acknowledge the kind hospitality of Institute of Theoretical and Computational Physics, Graz University of Technology, and support by the Polish State Committee of Scientific Research (KBN) under Project No. 1 P03B 068 26.

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