I. INTRODUCTION

The colossal magnetoresistance observed in certain manganites has attracted much attention in condensed matter physics.\cite{1,2,3} Typically perovskite manganites, for example La$_{2/3}$Ca$_{1/3}$MnO$_3$, exhibit this enormous enhancement of the magnetoresistance.\cite{2} It is now generally accepted that the colossal magnetoresistance originates from the strong correlation between electrons, namely, the double exchange and superexchange interactions, Jahn-Teller effect etc. play an important role, although this phenomenon is far from being understood.\cite{4}

In these compounds due to the crystal field, the five-fold degenerate $d$ orbitals are split into two-fold degenerate ($e_g$) and three-fold degenerate ($t_{2g}$) orbitals which are coupled to each other via Hund’s coupling. The electrons in the $e_g$ orbitals are delocalized while the $t_{2g}$ electrons are localized.\cite{5} To understand the compounds in question, it is crucial to investigate models with more than one orbital. Hybridization between different orbitals is claimed to be important also in other compounds like Ca$_{2−x}$Sr$_x$RuO$_3$.\cite{6} This compound exhibits several remarkable phenomena like orbital-selective Mott transition\cite{7} or heavy-fermion\cite{8} behavior as the chemical concentration or temperature is varied. To account for these effects, multiorbital systems have been in the focus of intensive research recently.\cite{9,10} Our purpose here is to consider further the properties of multiorbital systems.

The minimal model with two orbitals per site can be written as:

\[
\mathcal{H} = \sum_{\langle ij \rangle \alpha \sigma} t^{(\alpha)} \hat{c}^\dagger_{i \alpha \sigma} \hat{c}_{j \alpha \sigma} + V \sum_{\langle j \rangle \alpha \sigma} (\hat{c}^\dagger_{j2\sigma} \hat{c}^{}_{j1\sigma} + \hat{c}^\dagger_{j1\sigma} \hat{c}^{}_{j2\sigma}) + U \sum_{j, \alpha \sigma} \hat{n}_{j \alpha \uparrow} \hat{n}_{j \alpha \downarrow} + \sum_{j, \sigma} (U' - J \delta_{\sigma' \sigma}) \hat{n}_{j1\sigma} \hat{n}_{j2\sigma'} - J \sum_j \left[ (\hat{c}^\dagger_{j1\uparrow} \hat{c}^\dagger_{j\uparrow} + \hat{c}^\dagger_{j1\downarrow} \hat{c}^\dagger_{j\downarrow} \hat{c}^{}_{j1\uparrow} \hat{c}^{}_{j\uparrow} + \hat{c}^\dagger_{j1\downarrow} \hat{c}^{}_{j\downarrow} \hat{c}^{}_{j1\uparrow} \hat{c}^{}_{j\uparrow}) + \text{H.c.} \right] \tag{1}
\]

Here $\hat{c}^\dagger_{j \alpha \sigma}$ ($\hat{c}_{j \alpha \sigma}$) creates (annihilates) an electron in orbital $\alpha = 1, 2$, with spin $\sigma$ at site $j$, and the corresponding particle number operator is $\hat{n}_{j \alpha \sigma} = \hat{c}^\dagger_{j \alpha \sigma} \hat{c}_{j \alpha \sigma}$, $\langle ij \rangle$ denotes nearest-neighbor sites. The hopping parameter between orbitals of type $\alpha$ on nearest-neighbor sites is $t^{(\alpha)}$, and $V$ is the onsite hybridization between the two orbitals. The Coulomb interaction within band $\alpha$ is $U_\alpha$, while $U'$ denotes the local interaction between the two orbitals, finally $J$ is the Hund’s coupling. The above model is a special case of the multiorbital Hubbard model derived by Oleš\cite{11,12} if we set $V = 0$.

Note that Eq. (1) can be considered as an extended periodic Anderson model when $t^{(2)} = 0$. In this case the model corresponds to a system containing both localized and itinerant electrons, where the conduction electrons are also correlated and interorbital couplings are taken into account as well. This Hamiltonian has been investigated thoroughly by dynamical mean-field theory (DMFT) in infinite spatial dimensions,\cite{13,14,15} and it was revealed how the Kondo and Mott insulating states compete with the metallic state in the half-filled case if the system is assumed to be paramagnetic.\cite{16} It turned out, however, that magnetic long-range order can also be present in the model, namely two types of antiferromagnetic order emerge beside the Kondo insulating state.\cite{15}

The occurrence of these phases originates from the competition between Hund’s coupling and Kondo effect. While the former one aligns the spins of localized and itinerant electrons ferromagnetically at a given site, the latter one tries to screen the localized spins by forming singlets with the itinerant electrons. It has also been discussed how the hybridization affects the orbital-selective Mott localization emerging in two-orbital Hubbard-models.\cite{15}

Since the DMFT approach completely neglects the spatial fluctuations, which is only valid in infinite dimensions, it is necessary to investigate low-dimensional systems where quantum fluctuations are known to be much stronger. Our main goal in this paper is to explore the one-dimensional behavior of the Hamiltonian in Eq. (1).
In earlier papers it has been shown\textsuperscript{17–19} that there is no quantum phase transition in one dimension in the absence of the Hund’s coupling in contrast to the infinite dimensional case. The competition between the Hund’s coupling and the Kondo effect may lead to the appearance of quantum phase transitions and unexpected phases even if true long-range order cannot be present in one dimension.

We apply the density-matrix renormalization-group method\textsuperscript{20–24} (DMRG), which is a powerful tool to find the ground state and to determine the correlation functions. Further advantage of the DMRG method is that we can easily determine the von Neumann entropies\textsuperscript{25–30} of single and multisite subsystems, without the need to calculate excited states, which is in general difficult near a critical point, and their anomalies can be used to detect quantum phase transitions\textsuperscript{31–34}

In our DMRG calculation we applied the dynamic block-state selection algorithm\textsuperscript{35–36} in which the threshold value of the quantum information loss, \( \chi \), is set a priori. We have taken \( \chi = 3 \cdot 10^{-6} \). A maximum of 2000 block states is needed to achieve this accuracy, and the truncation error was in the order of \( 10^{-7} \). Such low value of \( \chi \) is necessary in order to obtain smooth data sets close to critical points. We investigated chains up to a maximum length \( L = 120 \) with open boundary conditions and performed 8 sweeps.

The setup of the paper is as follows. In Sec. II. we define the von Neumann entropies of various subsystems used in our analysis, and the mutual information.\textsuperscript{28,37,38} In Sec. III., A, B and C we discuss the properties of the phases occurring in the model using the mutual information and the eigenvalue spectra of the two-site density matrices. In Sec. III., D we discuss the differences between the phase diagram obtained in the DMFT and for the one-dimensional model. Finally, in Sec. IV. our conclusions are presented.

II. VON NEUMANN ENTROPIES

The von Neumann entropies of different subsystems are known to exhibit anomalies near critical points\textsuperscript{23,31,32} We examined the one-site \( s_i \), two-site \( s_{ij} \) entropies and the block entropy which is the entropy of the subsystem containing sites from 1 to \( \frac{L}{2} \). These quantities can be obtained from the appropriate reduced density matrices\textsuperscript{35,36,38} The entropy of a single site can be obtained as

\[
s_i = -\text{Tr} \rho_i \ln \rho_i,
\]

where \( \rho_i \) is the reduced density matrix of site \( i \), which is derived from the density matrix of the total system by tracing out the configurations of all other sites. We also define the entropies corresponding to the two types of orbitals at a site \((s_i^{(1)}, s_i^{(2)})\) in the following way:

\[
s_i^{(1)} = -\text{Tr} \rho_i^{(1)} \ln \rho_i^{(1)},
\]

\[
s_i^{(2)} = -\text{Tr} \rho_i^{(2)} \ln \rho_i^{(2)},
\]

where \( \rho_i^{\alpha} \) \((\rho_i^{(1)}, \rho_i^{(2)})\) is obtained by performing an additional trace over the remaining "2" ("1") degrees of freedom at site \( i \). The two-site entropy is written as

\[
s_{ij} = -\text{Tr} \rho_{ij} \ln \rho_{ij},
\]

where \( \rho_{ij} \) is the two-site reduced density matrix of sites \( i \) and \( j \). We can also introduce the partial two-site entropies for type \( \alpha \) electrons on site \( i \) and type \( \beta \) electrons on site \( j \):

\[
s_{ij}^{(\alpha\beta)} = -\text{Tr} \rho_{ij}^{(\alpha\beta)} \ln \rho_{ij}^{(\alpha\beta)}, \quad \alpha, \beta \in \{1, 2\}
\]

while the mutual information between \( \alpha \) and \( \beta \) type electrons on sites \( i \) and \( j \) is defined as

\[
I_{ij}^{(\alpha\beta)} = s_i^{(\alpha)} + s_j^{(\beta)} - s_{ij}^{(\alpha\beta)},
\]

which measures all correlations both of classical and quantum origin between \( \alpha \) and \( \beta \) type electrons on sites \( i \) and \( j \). In what follows we refer to \( I_{ij}^{(\alpha\beta)} \) as the entanglement between these components. Finally, the block entropy is defined as

\[
s(L/2) = -\text{Tr} \rho_A \ln \rho_A,
\]

where \( A \) denotes the subsystem which contains the sites from 1 to \( L/2 \). In contrast to the one- or two-site entropies, which have a finite upper bound, the block entropy grows as \( \mathcal{O}(\ln L) \) for one-dimensional critical systems\textsuperscript{26,27}

III. RESULTS

In what follows we consider the half-filled case and use the half bandwidth, \( W = 2t^{(1)} \), as the energy scale of the system. For simplicity we assume \( U_1 = U_2 = U \) and \( U = U' + 2J \). In the absence of Hund’s coupling the ground state is either a collective singlet or consists of less entangled local Kondo-singlets depending on the values of Coulomb interactions and the hybridization\textsuperscript{19} There is no quantum phase transition between these phases, just a smooth crossover separates them. To examine the effect of the Hund’s coupling, firstly we consider what happens for a finite Hund’s coupling, namely for \( J/U = 0.1 \) and 0.3, with \( U = 4W \) as the hybridization is varied.
Firstly, we investigate the block entropy of one half of the chain. This quantity is a smooth function of \( V \) for any \( U \) when \( J = 0 \). For any finite \( J \), however, two peaks appear in the block entropy as can be seen in Fig. 1 for different chain lengths for a fixed value of \( J/U = 0.1 \), where the two peaks are around \( V/W = 0.57 \). It is clearly observed that the height of the peaks increases as the chain length is increased. We know that maxima in the block entropy can be attributed to quantum critical points if they evolve into anomalies in the thermodynamic limit. Two peaks may indicate the existence of two phase transitions separating three different phases. To check if it is indeed the case, one has to show that the peaks remain separated and do not merge in the thermodynamic limit. The finite-size scaling of the position of the peaks is shown in Fig. 2. We could treat systems with \( L = 60 \) sites near the critical points due to the high value of the block entropy. To determine the positions of the maxima accurately we used a cubic spline interpolation. Figure 2 shows that the position of the peaks as a function of \( 1/L \) can be fitted well with a linear function.

![FIG. 1. The block entropy, \( s(L/2) \) as a function of hybridization for different chain_lengths and \( J/U = 0.1 \). The lines are guides to the eye.](image)

The distance of the peaks of the block entropy for several chain lengths and \( J/U \) ratios. The extrapolation was performed using chains up to \( L = 60 \).

| \( J/U \) | \( L = 16 \) | \( L = 24 \) | \( L \to \infty \) |
|--------|--------|--------|--------|
| 0.1    | 0.016  | 0.011  | 0.0027(1) |
| 0.3    | 0.040  | 0.028  | 0.006(8)  |

**TABLE I.** The distance of the peaks of the block entropy for several chain lengths and \( J/U \) ratios. The extrapolation was performed using chains up to \( L = 60 \).

**A. The Kondo singlet phase for \( V_2^s < V \)**

Firstly, we consider what happens for large hybridization where the effect of Hund’s coupling is expected to be small compared to that of hybridization and the Coulomb interaction and the properties of the \( J = 0 \) model are expected to be recovered. We examine how the individual system components are entangled to each other using the mutual information. We have seen already in Fig. 1 that for large values of the hybridization the block entropy decreases rapidly, which indicates a less entangled state. This is the case indeed, as is seen in the entanglement map in Fig. 3. We can see that very strong onsite entanglement appear, while the one-particle states on different sites are hardly entangled to each other. To describe the physical origin of this difference in the entanglement within a site and between neighboring sites we calculated the eigenvalues (\( \omega_\gamma, \gamma = 1, \ldots, 16 \)) of the two-site density matrix \( \rho^{(12)}_{ij} \) and the corresponding eigenfunctions.

From \( \rho^{(12)}_{L/2,L/2} \) we found that for \( V/W = 0.8 \) one of its eigenvalues is larger by two orders of magnitude than the others and the corresponding eigenvector is:

\[
\phi^{(12)}_{L/2,L/2} = 0.5574(| \uparrow \rangle_{L/2} | \downarrow \rangle_{L/2} - | \downarrow \rangle_{L/2} | \uparrow \rangle_{L/2}) + 0.4350(| \uparrow \downarrow \rangle_{L/2} + | \downarrow \uparrow \rangle_{L/2}).
\]  

Here \( | \uparrow \rangle_n, | \downarrow \rangle_n \) denote the four possible states of orbital \( \alpha \) on site \( i \). We can see that strong
FIG. 3. Schematic view of all components of the mutual information \( I_{ij}^{(11)}, I_{ij}^{(12)}, I_{ij}^{(22)} \) for \( V/W = 0.8 \) and \( L = 16 \). The numbers are the site indices. The inner and outer circles denote type "2" (localized) and type "1" (itinerant) electrons.

FIG. 4. The same as in Fig. 3 but for \( V/W = 0.3 \).

onsite singlets are formed between localized and delocalized electrons, which we may refer to as Kondo-singlets, since this is the consequence of the enhanced Kondo effect. The entanglement between nearest-neighbor sites is smaller by two orders of magnitude than the onsite entanglement between localized and delocalized electrons. Therefore, the ground state is almost a product state. Since the eigensystem of \( \rho_{L/2,L/2+1}^{(11)} \) and \( \rho_{L/2,L/2+1}^{(22)} \) is quantitatively the same, we consider only the former one. The eigenfunction belonging to the most significant eigenvalue of \( \rho_{L/2,L/2+1}^{(11)} \) reads:

\[
\phi_{L/2,L/2+1}^{(11)} = \begin{align*}
0.6900(|\uparrow\downarrow|L/2\rangle - |\downarrow\uparrow|L/2\rangle) \\
+ 0.1545(|\uparrow\downarrow|L/2\rangle |0\rangle_{L/2+1} - |\downarrow\uparrow|L/2\rangle |1\rangle_{L/2+1})).
\end{align*}
\]

That is, the nearest neighbor coupling between the spins is antiferromagnetic. We checked that the mutual information components have their bulk values at \( L = 16 \) already, which is the consequence of the highly entangled ground state. Indeed, the properties of this phase agree with the known behavior of the conventional periodic Anderson model for large hybridization.

B. The Haldane-like phase for \( V < V_1^{cr} \)

A new phase is expected to appear for small hybridization, where \( J \) dominates. Here we discuss the properties of the phase emerging for \( V < V_1^{cr} \) using the mutual information. The entanglement diagram containing all types of the mutual information is shown in Fig. 4 for \( V/W = 0.3 \). One can see that the strongest entanglement is developed between neighboring delocalized electrons and moderately strong entanglement is present between more distant sites.

Firstly, we consider how the eigenvalue spectrum looks like for \( \rho_{L/2,L/2}^{(12)} \) and \( L = 16 \). We found that one of its eigenvalues is threefold degenerate and larger by an order of magnitude than the others. Its value is very close to 1/3 and the three corresponding eigenfunctions, \( \phi_{L/2,L/2}^{(12)} \gamma \gamma = 1,2,3 \), read:

\[
\begin{align*}
\phi_{L/2,L/2}^{(12),1} &= |\uparrow\rangle_{L/2} |\uparrow\rangle_{L/2} \\
\phi_{L/2,L/2}^{(12),2} &= \frac{1}{\sqrt{2}}(|\uparrow\rangle_{L/2} |\downarrow\rangle_{L/2} + |\downarrow\rangle_{L/2} |\uparrow\rangle_{L/2}) \\
\phi_{L/2,L/2}^{(12),3} &= |\downarrow\rangle_{L/2} |\downarrow\rangle_{L/2}.
\end{align*}
\]

That is, the electrons on the same site are in a state where the S = 1 triplet components have the largest weights.

As a next step we examine the entanglement between nearest neighbor sites. Since the eigensystems of \( \rho_{L/2,L/2+1}^{(11)} \), \( \rho_{L/2,L/2+1}^{(12)} \) and \( \rho_{L/2,L/2+1}^{(22)} \) are quantitatively very similar, we only present results for \( \rho_{L/2,L/2+1}^{(22)} \).

The eigenfunction corresponding to the most significant eigenvalue is:

\[
\begin{align*}
\phi_{L/2,L/2+1}^{(22)} &= 0.7071(|\uparrow\rangle_{L/2} |\downarrow\rangle_{L/2+1} |\uparrow\rangle_{L/2+1} \\
&+ 0.0014(|\uparrow\rangle_{L/2} |\downarrow\rangle_{L/2+1} |\downarrow\rangle_{L/2+1})).
\end{align*}
\]

which means that the entanglement between the neighboring sites results mainly from the singlet formation.

According to the above results we can say that the spins are aligned ferromagnetically within a site, but they couple antiferromagnetically between nearest-neighbor sites. The former one is a consequence of the strong Hund’s coupling which prefers parallel alignment of
the physical processes that contribute to the creation of homogeneous, dimerized ground state. Before investigating alternate along the chain, which suggests a spatially inhomogeneous phase. It is clearly seen that strong and weak bonds in Fig. 6, is drastically different from that in the previous phase, whose appearance is indicated by the increased. This is shown in Fig. 5. It is obviously seen that the bonds hardly change as the chain length becomes larger. The extrapolation was performed using a quadratic polynomial:

\[ I_{ij}^{(\alpha\beta)}(L) = I_{ij}^{(\alpha\beta)} + A/L + B/L^2, \]  

where \( I_{ij}^{(\alpha\beta)} \), \( A \) and \( B \) are free parameters.

C. The dimerized phase for \( V_{1}^{cr} < V < V_{2}^{cr} \)

Finally, we examine the properties of the narrow intermediate phase, whose appearance is indicated by the analysis of the block entropy. Using the tools applied in the previous subsections we examine the spatial structure of the ground state. The entanglement map shown in Fig. 6 is drastically different from that in the previous phase. It is clearly seen that strong and weak bonds alternate along the chain, which suggests a spatially inhomogeneous, dimerized ground state. Before investigating the physical processes that contribute to the creation of the strong entanglement, it is important to check if the dimerization remains finite in the thermodynamic limit. We can introduce two types of order parameters for the dimerization:

\[ D_1^{(\alpha)}(V) = \lim_{L \to \infty} \frac{1}{L^2} \left| I_{L/2,L/2+1}^{(\alpha\alpha)}(V) - I_{L/2-1,L/2}^{(\alpha\alpha)}(V) \right|, \]  

\[ D_2(V) = \lim_{L \to \infty} |s(L/2,V) - s(L/2 + 1,V)|. \]  

Since \( D_1^{(\alpha)}(V) \) is a local quantity, we expect that it is less sensitive to the boundary effects. It requires, however, the calculation of several correlation functions, and their computation time scales as \( L^2 \) which can be computationally demanding. The quantity in Eq. (17) is computationally less demanding, but since the block entropy is a non-local quantity its convergence to the bulk value may be slower. Instead of showing \( D_1^{(\alpha)}(V) \) directly, we plot the individual values of the mutual information components \( I_{L/2,L/2+1}^{(\alpha\alpha)} \) and investigate their size-dependence. In this case we could consider chains up to \( L = 120 \), since in the intermediate phase the block entropy has a much lower value than near the critical points and its low value also indicates a less entangled ground state as expected for a dimerized phase. This is shown in Fig. 6. In Fig. 6 we used a quadratic polynomial, Eq. (16) for the extrapolation, which gives an upper bound for the bond strengths. The data can also be fitted using a power-law function:

\[ I_{ij}^{(\alpha\beta)}(L) = I_{ij}^{(\alpha\beta)} + A/L^B, \]  

where \( I_{ij}^{(\alpha\beta)} \), \( A \) and \( B \) are free parameters. The residual sum of squares is roughly of the same order of magnitude for both types of fits, \( O(10^{-6}) \), therefore we give the values of the order parameters for both fits in Table I. The quadratic extrapolation clearly overestimates the order parameters while the polynomial fit underestimates it, since we expect that the order parameter begins to saturate as soon as the bulk limit is achieved.
We consider first the entanglement between localized electrons by examining $\rho_{L/2-1,L/2}^{(22)}$ and $\rho_{L/2,L/2+1}^{(22)}$ for $L = 16$. We have seen that due to the finite-size effects the strengths of the bonds change, but the qualitative picture, which can be obtained from the analysis of the density matrices, remains. For $\rho_{L/2-1,L/2}^{(22)}$ one of the eigenvalues is larger by an order of magnitude than the others, and the corresponding eigenfunction is:

$$\phi_{L/2-1,L/2}^{(22)} = 0.7071(|\uparrow\rangle_{L/2-1}^{(2)} L/2 - |\downarrow\rangle_{L/2}^{(2)} L/2 |\uparrow\rangle_{L/2}^{(2)} - |\downarrow\rangle_{L/2}^{(2)} L/2) \quad (19)$$

$$+ 0.006(|\uparrow\rangle_{L/2-1}^{(2)} 0_{L/2}^{(2)} + |0\rangle_{L/2-1}^{(2)} L/2 |\uparrow\rangle_{L/2}^{(2)}),$$

which means that the origin of the strong entanglement between localized electrons on neighboring sites is the singlet formation. If we consider the neighboring bond, we obtain from $\rho_{L/2,L/2+1}^{(22)}$ that one of the eigenvalues is $\omega_1 = 0.3953$ and there is a threefold degenerate eigenvalue $\omega_2 = 0.1500$. The eigenvector corresponding to the former one is essentially the same as in Eq. (13), while the eigenvectors corresponding to the latter one are the triplet components described in (13). Due to the fact that triplet components are mixed with a larger weight to the singlet component, it destroys the singlet bond between the localized electrons resulting in a much weaker entanglement. Qualitatively the above considerations remain valid for the explanation of entanglement between the itinerant electrons. Lastly we examine the entanglement within a site with the help of $\rho_{L/2,L/2}^{(12)}$. In this case we have again a non-degenerate eigenvalue, $\omega_1 = 0.2467$, and a threefold degenerate one, $\omega_2 = 0.2274$. The eigenvector corresponding to $\omega_1$ is

$$\phi_{L/2,L/2}^{(12)} = 0.5885(|\uparrow\rangle_{L/2}^{(1)} L/2 - |\downarrow\rangle_{L/2}^{(1)} L/2 |\uparrow\rangle_{L/2}^{(2)} - |\downarrow\rangle_{L/2}^{(2)} L/2) \quad (20)$$

$$+ 0.3921(|\uparrow\rangle_{L/2}^{(1)} 0_{L/2}^{(2)} + |0\rangle_{L/2}^{(1)} L/2 |\uparrow\rangle_{L/2}^{(2)}),$$

while the eigenvectors of $\omega_2$ are the triplet states in (13). It can be seen easily, that the onsite spin correlation is still ferromagnetic, but significantly reduced compared to the Haldane-like phase. While the onsite singlet state has negligible weight in the Haldane-like phase, in the dimerized state the onsite triplet and singlet states are mixed with comparable weights.

### D. Discussion

In the light of the above results it is worth examining the nature of the phase transitions and comparing the properties of the phases to what has been obtained in infinite dimensions.

As we mentioned, there is no phase transition when $J = 0$, where the ground state is Kondo-singlet-like discussed in Sec. III A. For any finite $J$ two new phases appear, namely, a Haldane-like and a dimerized phase...
whose properties are discussed below, and they disappear as \( J \to 0 \).

We have seen that for \( V < V_{1}^{cr} \) the ground state is Haldane-like while for \( V > V_{2}^{cr} \) Kondo-singlet-like, and both are gapful and homogeneous. For \( V_{1}^{cr} < V < V_{2}^{cr} \) the translational symmetry is broken due to the dimerization. It is worth noting that similar phase diagram has been obtained in frustrated spin ladders \( ^{23} \) where onsite and nearest-neighbor antiferromagnetic couplings compete with each other.

It is interesting to compare these findings with what has been obtained by DMFT.\(^{24} \) Surprisingly, three distinct phases appear also in the DMFT phase diagram, although their properties are significantly different. In DMFT there is a phase with antiferromagnetic long-range order in which the onsite spins are coupled ferromagnetically while the nearest-neighbor coupling is antiferromagnetic (AF I phase). Further increase of the hybridization drives the system into an intermediate phase \((V_{1}^{cr} < V < V_{2}^{cr})\) where another type of antiferromagnetic order takes place. Here the onsite coupling becomes antiferromagnetic, while the nearest-neighbor coupling remains antiferromagnetic (AF II phase). Finally, for \( V_{2}^{cr} < V \) Kondo-like behavior is realized.

In one dimension we cannot expect true long-range magnetic order, only slow decay of the correlation functions. For \( V < V_{1}^{cr} \) the onsite spins are parallel due to the strong Hund’s coupling. This Haldane-like phase might be the residue of the AF I ordered phase obtained in the DMFT calculation. Above the second critical point, \( V_{2}^{cr} < V \), the ground state is homogeneous, and strong onsite correlations appear, which originate from the enhanced Kondo-effect and the sites are occupied more and more by two localized or delocalized electrons or vice versa. The properties of the Kondo phase are consistent with what has been obtained in DMFT. Both methods exhibit an intermediate phase between them, however, their properties are completely different, which is caused by the enhanced quantum fluctuations.

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