Interorbital interaction in the one-dimensional periodic Anderson model: A density-matrix renormalization-group study

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We investigate the effect of the Coulomb interaction, \(U_{cf}\), between the conduction and \(f\) electrons in the periodic Anderson model using the density-matrix renormalization-group algorithm. We calculate the excitation spectrum of the half-filled symmetric model with an emphasis on the spin and charge excitations. It is found in the one-dimensional version of the model that while the spin gap is smaller – below a certain value of \(U_{cf}\) – than the charge gap, the reversed inequality is valid for stronger \(U_{cf}\). This behavior is also verified by the behavior of the spin and density correlation functions. We also perform a quantum information analysis of the model and determine the entanglement map of the \(f\) and conduction electrons. It is revealed that for a certain \(U_{cf}\) the ground state is dominated by the configuration in which the conduction and \(f\) electrons are strongly entangled, and the ground state is almost a product state. For larger \(U_{cf}\) the sites are occupied alternatively dominantly by two \(f\) electrons or by two conduction electrons.

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I. INTRODUCTION

Kondo insulators are a peculiar group of rare-earth materials, which behave as metals with magnetic moments above a characteristic temperature (\(\sim 100\) K) and become semiconductors at low temperatures due to strong correlations.\textsuperscript{1}\textsuperscript{-}\textsuperscript{3} Gaps are opened in both the spin and charge sectors, and they are in the order of a few meV, which defines the small energy scale of these compounds. These small gaps cannot be understood in a simple band picture, since the strong interaction between the electrons plays a crucial role. Furthermore this is the reason why different energy scales arise in the spin and charge sectors.

The minimal model for the Kondo insulators is the half-filled periodic Anderson model (PAM). In its one-dimensional version the Hamiltonian reads

\[ \mathcal{H}_{\text{PAM}} = -t \sum_{j,\sigma} \left( c_{j\sigma}^{\dagger} c_{j+1\sigma} + c_{j+1\sigma}^{\dagger} c_{j\sigma} \right) + V \sum_{j,\sigma} \left( f_{j\sigma}^{\dagger} f_{j\sigma} + f_{j\sigma}^{\dagger} f_{j\sigma} \right) + \varepsilon_f \sum_{j,\sigma} n_{j\sigma} + U_f \sum_{j} n_{j,\uparrow}^{f} n_{j,\downarrow}^{f} , \]

where the notation is standard and \(W = 4t\) is taken as the energy unit. The spin and charge gaps of the one-dimensional PAM have been studied by several methods in the past decades. The exact diagonalization studies\textsuperscript{3} pointed out that both the charge and spin gaps are finite. This analysis was later confirmed and refined by the density matrix renormalization group calculations.\textsuperscript{4}\textsuperscript{-}\textsuperscript{6} Both methods showed, that the charge gap is always larger than the spin gap, and decreases much more slowly than the spin gap as \(U_f\) is increased and their ratio diverges in the large \(U_f\) limit. Later on, this inequality was rigorously proven for the ordinary periodic Anderson model and it was shown that it remains valid for a \(d\)-dimensional simple cubic lattice as well.\textsuperscript{2}\textsuperscript{-}\textsuperscript{4} The charge and spin gaps are also directly measurable quantities using optical and neutron scattering measurements respectively. It is worth noting that for numerous compounds the experimental ratio of the gaps is less than one, which is in qualitatively good agreement with the theoretical predictions for the one-dimensional PAM, and in some cases, like CeRu\(_4\)Sb\(_{12}\) or CeFe\(_4\)Sb\(_{12}\), even quantitative agreement can be achieved with the theoretical predictions.\textsuperscript{6}\textsuperscript{-}\textsuperscript{8} However for CeRhAs the ratio of the spin\textsuperscript{9} and charge gaps\textsuperscript{10} was found to be greater than one, namely, \(\Delta_s/\Delta_c \approx 1.5\), which cannot be understood at all in the frame of the ordinary periodic Anderson model.\textsuperscript{2}\textsuperscript{-}\textsuperscript{4} One of the major aims of the present paper is to provide a possible explanation to the problem.

Several extensions of the PAM have been considered lately, to model the effect of further electron-electron interactions. The role of conduction electron interaction in the Kondo lattice model and PAM has been thoroughly investigated.\textsuperscript{11}\textsuperscript{-}\textsuperscript{13} Recently, the correlations between conduction and \(f\) electrons have been shown to play an important role to understand critical valence fluctuations.\textsuperscript{13} This interaction term leads to the extended PAM (EPAM):

\[ \mathcal{H} = \mathcal{H}_{\text{PAM}} + U_{cf} \sum_{j,\sigma,\sigma'} n_{j\sigma}^{f} \hat{n}_j^{\sigma'}. \]

This model has been investigated by several modern techniques recently\textsuperscript{14}\textsuperscript{-}\textsuperscript{18} and the valence transition has been explained successfully. However, less attention has been paid to the Kondo insulator case.\textsuperscript{15}\textsuperscript{-}\textsuperscript{18} It has been shown recently using dynamical mean-field theory (DMFT), which is exact for infinitely large dimensions that in the symmetric case for small hybridization (\(V \ll W\))
the model displays antiferromagnetic order for small \(U_{cf}\) which, however, disappears for large \(U_{cf}\) and charge order develops. In the charge ordered phase doubly occupied \(c\) and \(f\) sites appear in an alternating fashion, since the \(c\) and \(f\) electrons tend to avoid each other. Since these results were obtained via DMFT, which neglects spatial fluctuations, one can naturally ask what happens in low-dimensional systems, where the fluctuations are more important.

Our purpose in this paper is therefore to examine the one-dimensional EPAM. Naturally, we do not address the possibility of the presence of long-range order that was found in infinite dimensions. We apply the density-matrix renormalization-group method (DMRG), which is a powerful tool to find the ground state and the first few excited states. Further advantage of the DMRG method is that we can determine the von Neumann entropies of single and multisite subsystems, which turned out to be very good indicators of drastic changes in the wavefunction. In Sec. III.B we perform a quantum information analysis and determine the entanglement of the EPAM using the mutual information to get a physical picture for the ground state. Lastly, in Sec. IV, our conclusions are presented.

II. SPIN AND CHARGE GAPS

For convenience the EPAM has been implemented in the DMRG procedure as a generalized Hubbard model with a special topology. The site \(i\) with both \(c\) and \(f\) electrons is replaced by two DMRG sites, one for the conduction electrons, the other for the \(f\) electrons, and therefore instead of working with 16 states per site, only 4 states per DMRG sites have to be considered. These \(\alpha\) states are the empty, singly occupied with up and down spin, and the doubly occupied states, denoted by \(|0\>, |\downarrow\>, |\uparrow\>, |\uparrow\downarrow\>_\), respectively,

\[
\begin{align*}
|1\rangle_c &= |0\rangle, & |1\rangle_f &= |0\rangle, \\
|2\rangle_c &= |\downarrow\rangle_c = \hat{c}_{i\uparrow}^\dagger |0\rangle, & |2\rangle_f &= |\downarrow\rangle_f = \hat{f}_{i\uparrow}^\dagger |0\rangle, \\
|3\rangle_c &= |\uparrow\rangle_c = \hat{c}_{i\downarrow}^\dagger |0\rangle, & |3\rangle_f &= |\uparrow\rangle_f = \hat{f}_{i\downarrow}^\dagger |0\rangle, \\
|4\rangle_c &= |\uparrow\downarrow\rangle_c = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger |0\rangle, & |4\rangle_f &= |\uparrow\downarrow\rangle_f = \hat{f}_{i\uparrow}^\dagger \hat{f}_{i\downarrow}^\dagger |0\rangle.
\end{align*}
\]

The schematic structure is shown in Fig. 1. In what follows the chain length \(N\) is understood as the number of real EPAM sites. In our DMRG calculations, we apply the dynamic block-state selection algorithm \(^{33,34}\) and keep block states up to 2000, the typical truncation errors are

\[
\text{DMRG chain:} \quad \cdots \quad c \quad \begin{array}{c} V \end{array} \quad f \quad c \quad \begin{array}{c} V \end{array} \quad f \quad \cdots
\]

\[
\text{real chain:} \quad \text{site } i \quad \begin{array}{c} \cdots \end{array} \quad \text{site } i+1
\]

FIG. 1. Sketch of the DMRG implementation of the model Hamiltonian Eq. (2).

\(10^{-6} - 10^{-8}\). Open boundary condition is applied, and we considered chains up to length \(N = 50\) and finite-size scaling is used to extrapolate the quantities to the thermodynamic limit.

In the following, we consider the half-filled symmetric EPAM for moderately large \(U_f\). We address first the effect of \(U_{cf}\) on the spin and charge gaps of the EPAM. The spin gap is defined as

\[
\Delta_s = E_0(S = 1, N_c) - E_0(S = 0, N_c),
\]

where \(E_0(S, N_c)\) denotes the ground-state energy in the given \((S, N_c)\) subspace, where \(S\) and \(N_c\) are the total spin and particle number, respectively. The latter one is \(N_c = 2N\) in the half-filled case. It is known that the ordinary PAM possesses an extra SU(2) symmetry \(^3\) and the charge gap can be calculated from the expression:

\[
\Delta_c = |E_0(S = 0, N_c + 2) + E_0(S = 0, N_c - 2) - 2E_0(S = 0, N_c)|/2.
\]

This extra symmetry, however, is no longer present in the EPAM, and therefore we have to apply the general definition of the charge gap \(^4\):

\[
\Delta_c = E_n(S = 0, N_c) - E_0(S = 0, N_c)
\]

where \(E_n(S = 0, N)\) is the energy of the lowest excited state \(|n\rangle\), for which \(S = 0\) and \(|n\rangle\sum_q \rho_q |0\rangle \neq 0\), where \(\rho_q\) is the \(q\) Fourier component of the charge density operator:

\[
\rho_q = \sum_{i=0}^{N-1} e^{-iqr} \left[ \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} + \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} + \hat{f}_{i\uparrow}^\dagger \hat{f}_{i\uparrow} + \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\downarrow} \right].
\]

This definition of the charge gap is motivated by the fact that in optical measurements this gap is obtained by measuring the conductivity, which is related to the charge density. The spin and charge gaps as a function of \(U_{cf}\) are shown in Fig. 2. The charge gap is not calculated far below the crossing point, since the corresponding charge excitation lies much higher than the spin gap, and it is hard to determine accurately in the DMRG calculations.

It is clearly seen that the system is gapped for any \(U_{cf}\), and in contrast to the DMFT results \(^{33,34}\) as a consequence of the one dimensionality of the model there is no signature of quantum phase transition and the ground state is a spin singlet. We know that \(\Delta_s \sim e^{-\pi U_f/4\alpha V^2}\) for \(U_{cf} = 0\), where \(\alpha\) is a scaling constant. \(^3\) Finite \(U_{cf}\) gives...
rise to an increase of $\Delta_s$, while $\Delta_c$ decreases. They cross at a value $U_{cf}^c \approx U_f/2 + W/4$. It can be seen that this crossing point slightly shifts toward smaller $U_{cf}$ values as $V$ is increased. The sharp increase of the spin gap around and above the crossing point can be understood as follows. Here the $c$ and $f$ electrons try not to occupy the same site. Since the total number of $f$ electrons is $N$ in the symmetric model, and the same holds for the conduction electrons, the two kinds of electrons can best avoid each other by dominantly occupying every second site, the odd sites with two $f$ electrons, the even sites with two conduction electrons, or vice versa. Since the doubly occupied sites are necessarily in a singlet state, a spin flip can be achieved by transferring an electron and one local singlet has to be broken up. As $U_{cf}$ is increased above the crossing point, the first excited state becomes a singlet moreover, this state is the first charge excitation. Surprisingly the charge gap becomes much smaller than the spin gap in this regime in contrast to the usual expectation.

FIG. 2. The spin and charge gaps extrapolated to the thermodynamic limit as a function of $U_{cf}$ for $V/W = 0.1$ (upper panel), $V/W = 0.3$ (lower panel) and $U_f/W = 3$. The lines are guides to the eye.

III. CORRELATION FUNCTIONS AND ENTANGLEMENT PATTERNS

A. Correlation functions

As a next step we investigate the correlation functions, which provide a further insight into the effects of the interorbital interaction. The spin and density correlation functions are defined in the usual way:

$$S_{ij}^{(ab)} = \langle \hat{S}_i^{(a)} \hat{S}_j^{(b)} \rangle = \left\langle \frac{1}{2} (a_i^\dagger b_j^\dagger + a_j^\dagger b_i^\dagger) + a_i^\dagger a_j^\dagger b_j^\dagger b_i^\dagger \right\rangle$$

$$N_{ij}^{(ab)} = \langle \hat{n}_i^{(a)} \hat{n}_j^{(b)} \rangle - \langle \hat{n}_i^{(a)} \rangle \langle \hat{n}_j^{(b)} \rangle,$$

where $a$ and $b$ stand for either $f$ or $c$ and $\hat{n}_i^{(a)} = \sum_\sigma \hat{n}_{i\sigma}^{(a)}$. Since the system is gapped for any values of $U_{cf}$, both correlation functions show an exponential decay as can be seen in Fig. 3. The decrease or increase of the gap with $U_{cf}$ is reflected in the variation of the decay length. The large correlation length ($\xi/a \approx 200$, $a$ is the lattice constant) for $U_{cf} \ll U_{cf}^c$ can be explained with the known behavior of the ordinary PAM. It has been pointed

FIG. 3. (color online) The upper and lower panel show the spin and density correlation functions respectively for different values of $U_{cf}$ and $N = 50$ chain length. The other parameters are fixed at $V/W = 0.1$ and $U_f/W = 3$. The lines are guides to the eye.
Knowing that one cannot have true long-periodic oscillation in the f-electron density correlation function, we also observe a peculiar behavior of the charge gap. As long as $U_{cf}$ is below the crossing point the spin correlation function has the longer correlation length which corresponds to the peculiar behavior of the charge gap. We also observe a periodic oscillation in the f-electron density correlation functions in Fig. 4. Knowing that one cannot have true long-periodic oscillation in the f-electron density correlation function increases exponentially by increasing $U_f$.

As long as $U_{cf}$ is below the crossing point the spin correlation function is dominant due to the tiny spin gap. The spin correlation length decreases while the density correlation length increases as $U_{cf}$ is increased. Above the crossing point, the density correlation function has a peak near the threshold which is very reliable tools for detecting drastic changes of the ground state and analyzing its structure. We examined the one-site $s_i$ and two-site entropies $s_{ij}$, which can be obtained from the appropriate reduced density matrices \cite{21,26}. 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 all the other site configurations. We also define the c- and f-parts of the site entropies ($s_i^{(c)}$, $s_i^{(f)}$) in the following way:

$$s_i^{(c)} = -\text{Tr} \rho_i^{(c)} \ln \rho_i^{(c)},$$

$$s_i^{(f)} = -\text{Tr} \rho_i^{(f)} \ln \rho_i^{(f)},$$

where $\rho_i^{(c)}$ ($\rho_i^{(f)}$) is obtained by performing an additional trace over the remaining $f$ ($c$) degree of freedom. 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 the $c$ or $f$ electrons on site $i$ and $c$ or $f$ electrons on site $j$:

$$s_{ij}^{(ab)} = -\text{Tr} \rho_{ij}^{(ab)} \ln \rho_{ij}^{(ab)}, \quad a, b \in \{c, f\}$$

where $\rho_{ij}^{(ab)}$ is derived from $\rho_{ij}$ by tracing out the states of the other electrons. The DMRG implementation described in the beginning of Sec. II. enables us to determine $s_i^{(c)}$, $s_i^{(f)}$ and $s_{ij}^{(ab)}$ separately. The mutual information which measures the entanglement between sites $i$ and $j$ can be obtained from:

$$I_{ij} = -s_{ij} + s_i + s_j,$$

while the mutual information between the $a$ and $b$ type electrons on of sites $i$ and $j$ is defined as

$$I_{ij}^{(ab)} = -s_{ij}^{(ab)} + s_i^{(a)} + s_j^{(b)},$$

out that the correlation length of the spin correlation function increases exponentially by increasing $U_f$.

In this section we investigate the behavior of the von Neumann entropies of various subsystem configurations, which are very reliable tools for detecting drastic changes of the ground state and analyzing its structure. We examined the one-site $s_i$ and two-site entropies $s_{ij}$, which can be obtained from the appropriate reduced density matrices \cite{21,26}. 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 all the other site configurations. We also define the c- and f-parts of the site entropies ($s_i^{(c)}$, $s_i^{(f)}$) in the following way:

$$s_i^{(c)} = -\text{Tr} \rho_i^{(c)} \ln \rho_i^{(c)},$$

$$s_i^{(f)} = -\text{Tr} \rho_i^{(f)} \ln \rho_i^{(f)},$$

where $\rho_i^{(c)}$ ($\rho_i^{(f)}$) is obtained by performing an additional trace over the remaining $f$ ($c$) degree of freedom. 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 the $c$ or $f$ electrons on site $i$ and $c$ or $f$ electrons on site $j$:

$$s_{ij}^{(ab)} = -\text{Tr} \rho_{ij}^{(ab)} \ln \rho_{ij}^{(ab)}, \quad a, b \in \{c, f\}$$

where $\rho_{ij}^{(ab)}$ is derived from $\rho_{ij}$ by tracing out the states of the other electrons. The DMRG implementation described in the beginning of Sec. II. enables us to determine $s_i^{(c)}$, $s_i^{(f)}$ and $s_{ij}^{(ab)}$ separately. The mutual information which measures the entanglement between sites $i$ and $j$ can be obtained from:

$$I_{ij} = -s_{ij} + s_i + s_j,$$

while the mutual information between the $a$ and $b$ type electrons on of sites $i$ and $j$ is defined as

$$I_{ij}^{(ab)} = -s_{ij}^{(ab)} + s_i^{(a)} + s_j^{(b)},$$

FIG. 4. (color online) The pure density correlation function for different values of $U_{cf}$ and $N = 50$ chain length. The other parameters are fixed at $V/W = 0.1$ and $U_f/W = 3$. The lines are guides to the eye.

FIG. 5. The onsite spin correlation between conduction and f electrons (extrapolated to the thermodynamic limit) for $V = 0.1W$ as a function of $U_{cf}$ and $U_f/W = 3$. The lines are guides to the eye.
which measures the entanglement between the a and b electrons on sites i and j.

At first we consider the single site entropies, which are shown in Fig. 6. For small V the entropy of f electrons starts from slightly above ln 2. When U_{cf} = 0 the f electrons are strongly correlated and since the f-level occupancy must be exactly one (due to the symmetric model), only an electron with up or down spin can occupy the f level. Due to the small c-f hybridization the entropy of f electrons is slightly higher than ln 2, since a small number of doubly occupied levels can also be present. Switching on U_{cf} leads to the appearance of more and more doubly occupied f sites, so the entropy begins to increase. At a certain value of U_{cf}, which is the crossing point defined earlier, a peak is developed, where the entropy of f electrons takes its maximum value, ln 4, then it begins to decrease and approaches ln 2 again, since for large U_{cf} an f site is expected to be either doubly occupied or empty. For larger hybridization this sharp maximum is significantly broadened. Concerning the conduction electrons, their entropy is ln 4 as long as U_{cf} < U_{cf}^{cr}, since they are free particles. Above the crossover value, the probability of finding zero or two c electrons on the same site increases from 1/4 to 1/2, so correlation is developed between c electrons. It is readily observed that there should be a remarkable change in the ground state, where the entropy of f electrons has a maximum. To reveal this behavior we calculated the mutual information between c and f type electrons on sites i and j for several values of U_{cf}. The mutual information for U_{cf} = 0 is shown in Fig. 7 for weak hybridization. It is easy to observe that moderately strong entanglement is developed between f electrons, but much weaker between c and f electrons due to the small hybridization. The former one is the consequence of the strong RKKY-interaction, which results in the antiferromagnetic correlations between the f electrons, the f electrons form a collective singlet. In contrast, only the nearest neighbor entanglement is significant between conduction electrons.

The mutual information diagram has an entirely different structure for U_{cf} = 1.75W ≈ U_{cf}^{cr}, which is shown in Fig. 8. One can see that there is a strong entanglement between the onsite c and f electrons. According to the entanglement map, the ground-state wave function becomes approximately a product state. This observation is also supported by the fact that the entanglement bonds between the sites are much weaker than the onsite bonds. We determine the structure of the onsite state later. Lastly, we consider the case when U_{cf} = 4W > U_{cf}^{cr}. The mutual information is shown in Fig. 9. Here we observe that the strong onsite entanglement remains, however, moderately strong bonds appear between the neighboring c and f sites.

The above statements can be quantified if we introduce the following quantity:

$$I_{\text{dist}} = \sum_{ab} \sum_{ij} I_{ij}^{(ab)} |i - j|^2. \quad (20)$$

$I_{\text{dist}}$ measures the localization of the entanglement. Its values for different values of U_{cf} are shown in Table I. It is easily seen that the entanglement is the most lo-
FIG. 8. (color online) Schematic view of all components of the mutual information \( I_{ij}^{(cc)} \), \( I_{ij}^{(cf)} \), \( I_{ij}^{(ff)} \) for \( U_{cf} = 1.75W \), \( V/W = 0.1 \), \( U_f/W = 3 \) and \( N = 16 \). The inner and outer circles denote \( f \) and \( c \) sites respectively. The numbers denote the real EPAM sites.

FIG. 9. (color online) Schematic view of all components of the mutual information \( I_{ij}^{(cc)} \), \( I_{ij}^{(cf)} \), \( I_{ij}^{(ff)} \) for \( U_{cf} = 4W \), \( V/W = 0.1 \), \( U_f/W = 3 \) and \( N = 16 \). The inner and outer circles denote \( f \) and \( c \) sites respectively. The numbers denote the real EPAM sites.

delocalized when \( U_{cf} = 1.75W \). In the other two cases the entanglement is much more delocalized.

These conclusions have been obtained for finite systems, therefore we have to investigate the finite-size effects. For \( U_{cf} = 0 \) the entanglement bonds show strong dependence on the chain length, while for \( U_{cf} = 1.75W \) and \( 4W \) the above results are very close the bulk limit for \( N = 16 \) already. The size dependence of the bonds for \( U_{cf} = 0 \) is shown in Fig. 10.

We also examined the one-site entropy of the EPAM, and it is shown in Fig. 11. For weak hybridization it drops rather drastically around \( U_{cf} \) corresponding to the crossover point and then starts to increase slowly, while for stronger hybridization the decrease of the site entropy is less drastic. But in both cases \( s_i \) is much smaller above \( U_{cf}^{cr} \) than below this value. A nearly vanishing \( s_i \) is indication that the wave function is dominated by terms localized to this site. It is worth noting, that the magnitude of the entanglement of the onsite bonds is \( O(1) \), while it is \( O(10^{-3}) \) for the next largest entanglement bond when \( U_{cf} = 3W \), \( V = 0.3W \) and \( U_f = 3W \), that is, every other bond is smaller by two orders of magnitude.

One can naturally ask what the relevant physical process is in creating the strong onsite bonds for \( U_{cf} = \)}
1.75W and $U_{c,f} = 4W$. The former one is partially understood from Fig. 5 where the onsite spin correlation is enhanced at $U_{c,f} \approx 1.75W$. To answer this question we examined the eigenvalues ($\omega_{ij}$, $\alpha = 1, \ldots, 16$) of the two-site density matrix $\rho_{ij}^{(ab)}$. For $U_{c,f} = 0$ we found that several eigenvalues of $\rho_{ij}^{N/2N/2}$ are in the same order of magnitude and the eigenvectors contain all basis states $|\alpha_c, \alpha_f\rangle$, except for $|0,0\rangle$ and $|\uparrow\downarrow, \uparrow\downarrow\rangle$. However, for $U_{c,f} = 1.75W$ one of the eigenvalues of $\rho_{ij}^{cf}$ becomes almost two order of magnitude larger than the others. The corresponding eigenfunction reads:

$$
\phi^{(cf)}_{N/2N/2} = -0.5798(|\uparrow\downarrow, 0 \rangle + |0, \uparrow\downarrow\rangle) 
- 0.4048(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle).
$$

(21)

It is revealed that there is a strong resonance between the doubly occupied and empty c and f configurations besides the spin singlet component. The latter one was observed in the spin correlation function in Fig. 5 and corresponds to the enhanced spin Kondo-effect. The former one describes the fluctuations between the doubly occupied and empty c-f configurations. Further increase of $U_{c,f}$ results in the suppression of the singlet part in Eq. (21) and the eigenfunction corresponding to the most significant eigenvalue is for $U_{c,f} = 4W$:

$$
\phi^{(cf)}_{N/2N/2} = 0.7049(|\uparrow\downarrow, 0 \rangle + |0, \uparrow\downarrow\rangle) 
- 0.0561(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle).
$$

(22)

Although the spin singlet part is suppressed, the resonance between the doubly occupied and empty c-f configurations is enhanced. This is the reason why strong onsite entanglement bonds appear in Fig. 5.

In addition, as has been shown in Ref. [32] one can also analyze the sources of entanglement encoded in $I_{ij}^{(ab)}$ by studying the behavior of the matrix elements of $\rho_{ij}^{(ab)}$. They can be expressed in terms of the generalized correlation functions of the transition operators $T_i^{\alpha'\alpha(a)}$ and $T_j^{\beta\beta(b)}$, where $T_i^{\alpha'\alpha(a)}$ describes the transition from state $|\alpha\rangle^{(a)}$ ($\alpha = 1 \ldots 4$ defined in Eqs. (22)-(24)) of the a type electrons on site i into state $|\alpha'\rangle^{(a)}$, while it annihilates all other states. For example

$$
T_i^{(2,3)(c)}|3\rangle^{(c)} = T_i^{(2,3)(c)}|3\rangle^{(c)} = c_{i3}^{\dagger} |0\rangle
$$

(23)

and

$$
T_i^{(3,4)(f)}|4\rangle^{(f)} = T_i^{(3,4)(f)}|4\rangle^{(f)} = f_{i4}^{\dagger} |0\rangle.
$$

(24)

We study the connected part of the generalized correlation functions, $\langle T_i^{\alpha'\alpha(a)}T_j^{\beta\beta(b)} \rangle_C = \langle T_i^{\alpha'\alpha(a)}T_j^{\beta\beta(b)} \rangle - \langle T_i^{\alpha'\alpha(a)} \rangle \langle T_j^{\beta\beta(b)} \rangle$, where the disconnected part, given by the product of the expectation values of local transition operators, is substracted. We demonstrate here, that these can be used to identify the relevant physical processes that lead to the generation of entanglement. Namely, we show the matrix elements of two different transition operators giving the largest contribution in $\rho_{ij}^{(ab)}$. One of them describes the hopping of a down- and up-spin electron pair, the other one is a spin-flip. The matrix elements of these operators are shown in Fig. 12. It is clearly seen that the magnitude of spin-flip process matrix elements is significantly reduced as $U_{c,f}$ is increased. At the same time the fluctuations of the up- and down-spin electron pairs is enhanced. These results support our previous findings derived from the analysis of the eigensystem of the two-site density matrix $\rho_{ij}^{(ab)}$.

The decay of the sorted values of the mutual information is governed by the smallest gap in the model. We found that for $U_{c,f} \approx U_{c,f}^{*}$ it exhibits the fastest decay, where both the spin and charge gaps are large. For other $U_{c,f}$ values we observed a slower decay, which is in agreement with the behavior of the gaps.

IV. CONCLUSIONS

In this paper we investigated an extended periodic Anderson model, where the interaction between conduction and f electrons has been included. Our aim was to examine the properties of the model in one dimension by applying the density matrix renormalization group algorithm. As a first step, we investigated the spin and charge excitations of the model. It turned out that the model
is always gapped and the spin gap is much smaller than the charge gap below a certain value of the c-f interaction. At the crossing point the spin and charge gap coincides, and the charge gap becomes much smaller above this value. This result may give a possible explanation for the anomalous behavior of the gaps observed in CeRhAs, where $\Delta_s/\Delta_c > 1$ was measured.

As a next step, the spin and density correlation functions have been determined. Below the crossing point the spin correlation function is dominant due to strong antiferromagnetic coupling mediated by the RKKY interaction. As $U_{cf}$ is increased the spin correlation length decreases, while the density correlation length increases and becomes dominant above the crossing point. In contrast to the DMFT results, where an antiferromagnetic-charge order transition was found, no phase transition occurs in one dimension, however, the behavior of the correlation functions supports this scenario.

Finally, we performed a quantum information analysis to reveal the structural changes in the ground state wave function. The one-site entropy of c and f electrons varies rapidly around the point where the spin and charge gaps are equal. The entropy of f electrons has a maximum there, while the entropy of c electrons starts to decrease rapidly. We calculated the mutual information for several c-f interaction strength, which measures the entanglement between different sites. It turned out that for small hybridization the wave function is approximately a product state consisting of strongly localized states at the sites. For larger $U_{cf}$ the strong onsite entanglement remains, which originates from the tendency of charge ordering, the preference of having two electrons on even sites and two c electrons on odd sites or vice versa.

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