Block entropy and quantum phase transition in the anisotropic Kondo necklace model

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We study the von Neumann block entropy in the Kondo necklace model for different anisotropies η in the XY interaction between conduction spins using the density matrix renormalization group method. It was found that the block entropy presents a maximum for each η considered, and, comparing it with the results of the quantum criticality of the model based on the behavior of the energy gap, we observe that the maximum block entropy occurs at the quantum critical point between an antiferromagnetic and a Kondo singlet state, so this measure of entanglement is useful for giving information about where a quantum phase transition occurs in this model. We observe that the block entropy also presents a maximum at the quantum critical points that are obtained when an anisotropy Δ is included in the Kondo exchange between localized and conduction spins; when Δ diminishes for a fixed value of η, the critical point increases, favoring the antiferromagnetic phase.

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I. INTRODUCTION

Quantum phase transitions correspond to a change in the nature of the ground state of a many-body system, driven by parameters different from temperature, like couplings between particles and external fields. In recent years, it has been observed that different measures of entanglement (the quantum property responsible for nonlocal correlations in a system) present a particular behavior at the quantum critical points of various one-dimensional spin models. For example, the concurrence (which measures the entanglement between a pair of qubits [1,2]) presents a singularity in its first derivative at the quantum critical point of the anisotropic XY chain with a transverse magnetic field [3], and a maximum at the antiferromagnetic transition in the XXZ model [4]; the von Neumann block entropy (the entanglement between a block and the rest of the system) diverges with the size of the block at the quantum critical point and saturates near criticality [5], where the form of the divergence in the first case depends on having periodic or open boundary conditions (as in the XXZ model [6]). In spite of the recent advances connecting quantum information elements and properties of many-body systems [7], the relationship between entanglement and quantum criticality is not completely clear. For example, assuming certain conditions it was shown that the concurrence can indicate first- or second-order quantum phase transitions by means of singularities of their values or their derivatives [8] (the XY model corresponds to the second case). On the other hand, in some models in which the previous result is not applicable, the concurrence does not present any special feature at the critical points while the block entropy does (as in dimerized Heisenberg chains and in Heisenberg ladders [9]), or alternatively neither the concurrence nor the block entropy indicates a quantum phase transition (as in the XY chain with three-spin interactions [10], where the derivative of the concurrence presents a discontinuity at a point which does not correspond to a quantum phase transition). So an important effort still has to be made to better understand the connections between quantum criticality in spin systems and entanglement.

In recent years, heavy fermions have become some of the most important materials for studying different types of quantum phase transitions [11]. These systems (intermetallic compounds containing mainly Ce, Yb, and U that possess quasiparticles of large effective mass [12]) present a rich phase diagram which includes magnetic order, superconductivity, and non-Fermi liquid behavior. The quantum phase transition between antiferromagnetic and spin liquid (Kondo singlet) states occurs due to the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions [13]: the first corresponds to the screening of localized moments (in the inner f shell) due to the spins of conduction electrons (in s, p, and d orbitals), forming singlets between them throughout the system, and the second is an indirect coupling between localized moments, mediated by conduction electrons, that favors antiferromagnetic ordering. This interplay has been studied intensely, and one of the models considered for this purpose is the Kondo necklace [14]:

$$H_{\mathrm{KN}} = t\sum_{i=1}^{N}\left(s_i^x s_{i+1}^x + s_i^y s_{i+1}^y\right) + J\sum_{i=1}^{N}\vec{S}_i\cdot\vec{s}_i, \qquad (1)$$

where $\vec{S}_i$ and $\vec{s}_i$ correspond to localized and conduction spins at site i, respectively; J is the Kondo coupling; and t represents the kinetic energy of conduction electrons. This model was proposed in order to focus on the magnetic behavior of heavy fermions, freezing out charge fluctuations but retaining the competition between RKKY interactions and the Kondo effect. In this sense, the first term in the Hamiltonian tends to mimic the hopping of conduction electrons throughout the system (in one dimension, the XY interaction can be mapped to a band of spinless fermions at half filling using a Jordan-Wigner transformation), and the second term corresponds to the Kondo exchange between localized and conduction spins. The ratio of the Kondo coupling and the hopping parameter, J/t, determines the magnetic behavior of the system.

In one dimension at zero temperature, the Kondo necklace model is well understood: most studies, such as quantum Monte Carlo simulations [15], bosonization [16,17], density matrix renormalization group (DMRG) [16,18], and bond operator mean field theory [19,20], showed that no phase transition at a finite value of J/t occurs between

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antiferromagnetic and Kondo singlet states. Recently, an anisotropy η in the XY interaction of conduction spins has been included, which takes values from $\eta = 0$ [isotropic case (1)] to $\eta = 1$ (Ising limit). This parameter defines the following anisotropic Kondo necklace model:

$$H_{\mathrm{AKN}} = t \sum_{i=1}^{N} \left[s_i^x s_{i+1}^x + (1-\eta) s_i^y s_{i+1}^y \right] + J \sum_{i=1}^{N} (\vec{S}_i \cdot \vec{s}_i). \quad (2)$$

The critical behavior of this Hamiltonian is not completely understood; a quantum phase transition for some values of η [21], for every $\eta > 0$ [22] and no phase transition [23], have been obtained using different approaches (real-space renormalization group, Lanczos, and bond-operator methods, respectively). Our previous results with DMRG analysis [24,25], in which the energy gap, correlation functions, and structure factors were calculated, give strong evidence that supports the second possibility. If the effect of the crystalline electric field on the system is considered, an anisotropy Δ should be included in the Kondo exchange [20], so that we replace

$$\vec{S}_i \cdot \vec{s}_i \rightarrow S_i^x s_i^x + S_i^y s_i^y + \Delta S_i^z s_i^z. \quad (3)$$

Our DMRG study of this situation suggests that, when $\eta = 0$, the system remains in the Kondo singlet state regardless of the value of Δ, but when $\eta \neq 0$, Δ notably affects the position of the quantum critical point, favoring the antiferromagnetic phase as Δ decreases [26].

The entanglement in impurity systems that present the competition between the Kondo effect and the RKKY interactions has been analyzed several times. In elliptical quantum corrals with impurities in the foci, the von Neumann entropy between the conduction electrons in the ellipse and the impurities allows one to identify the Kondo and the RKKY regimes [27]; for the two-impurity Kondo model it was found that a minimum nonzero correlation between both impurities is needed for them to create an entangled state (concurrence different from zero), and this correlation occurs at the quantum critical point [28]. Nevertheless, the von Neumann entropy between the conduction electrons and the impurities does not show any particular behavior at the quantum phase transition; when spin-orbit interactions of conduction electrons are included, the concurrence between the impurities can be severely affected, to the point of driving them between maximally entangled and nonentangled configurations through different experimental conditions [29]. For the Kondo necklace model, where instead of having a few impurities (as in the systems mentioned above) a localized magnetic moment at each site of a chain is considered, the entanglement has been analyzed for small lattices. The concurrence between different pairs of spins was calculated for the cases $\eta = 0$ and $\eta = 1$, for two and four sites with periodic boundary conditions, with ferromagnetic and antiferromagnetic couplings, and including magnetic field and finite temperature [30]. The quantum critical point $J = 0$ for the Ising case was identified by means of the single-qubit concurrence (our DMRG results indicate that this conclusion is not correct [24,25]). The more general model (2) was considered for larger chains (up to eight sites) using exact diagonalization [26], where the concurrence between different pairs was also obtained. It was observed that, when the Kondo coupling J increases, the localized and conduction spins at the same site become more entangled, since the Kondo effect tends to generate singlets along the chain while neighboring conduction spins diminish their entanglement; however, unlike the work of Saguia and Sarandy [30], it was found that the concurrence between localized spins is not equal to that between conduction spins, and that a finite amount of the second quantity is required to entangle localized spins. Also, we observed that, as the anisotropy η increases from the isotropic limit $\eta = 0$ to the Ising limit $\eta = 1$, the neighboring spins diminish their concurrence while localized and conduction spins of the same site get more entangled, and the concurrence does not seem to give any information about the position of the quantum critical points of the model.

In the present paper we study the entanglement in the anisotropic Kondo necklace model (2) for large chains using the density matrix renormalization group [31,32]. We focus on the calculation of the von Neumann block entropy for different anisotropies η and its behavior near the quantum critical points obtained in previous papers [24,25], looking for a special characteristic of this quantity at the quantum phase transition.

II. BLOCK ENTROPY AT CRITICALITY

First, we review the results obtained previously for model (2) with the density matrix renormalization group method [25]. We considered systems of 100 sites with open boundary conditions, implemented the finite-system method with five sweeps, and set the energy scale by taking $t = 1$; the diagonalization of the renormalized Hamiltonian was made using the Davidson algorithm. We calculated the gap between the energies of the ground state and the first excited state (E_g) as a function of J for many anisotropies η and took the quantum critical point J_c as the point at which the gap became zero. In Fig. 1, the decay of the gap is shown for the case $\eta = 0.8$, where it is observed that J_c is finite. To obtain the value of J_c, we fitted the gap to a Kosterlitz-Thouless tendency:

$$E_g = A \exp[-b/(J - J_c)^{0.5}]. \quad (4)$$

We made this assumption because it was proposed for the isotropic Kondo necklace model [16,18]; for the present case we obtained $J_c = 0.4668(7)$. In the inset of Fig. 1, we plot $\ln E_g$ as a function of $1/\sqrt{J - J_c}$ for points near J_c with small

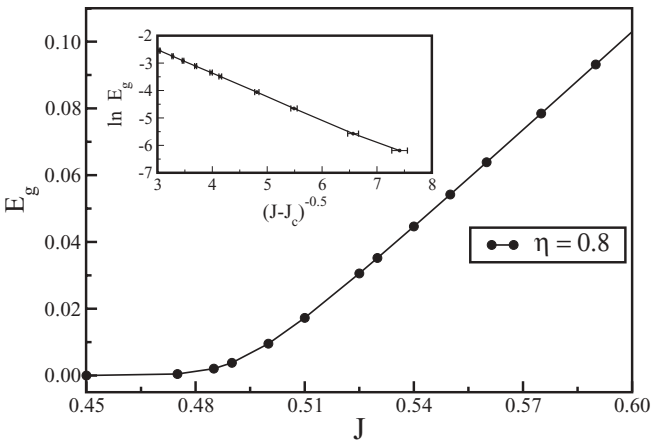

FIG. 1. Energy gap E_g as a function of J for 100 sites and $\eta = 0.8$. The inset shows its logarithmic tendency near J_c.

errors, where the linear tendency indicates that the Kosterlitz-Thouless behavior is suitable for describing the closing of the gap. We also calculated different correlation functions and structure factors, which support the assumption that for $J > J_c$ there is no magnetic order in the system (but rather RKKY oscillations), while for $J < J_c$ an antiferromagnetic order has been established. We observed that even for very small anisotropies η a quantum phase transition takes place at a finite value of J.

Our main goal in this paper is to find out if entanglement measures can indicate the quantum critical points of the anisotropic Kondo necklace model, obtained as explained above. As mentioned before, our results for small chains suggest that the concurrence does not show any particular behavior for the values of J considered, which could be related to a quantum phase transition [26], so we do not calculate it for larger chains. Instead, we focus on the von Neumann block entropy S. In general, the system of study can be divided into two sub-blocks, and the block entropy S is calculated using the expression

$$S(\rho) = -\mathrm{tr}(\rho \log_2 \rho) = -\sum_i \lambda_i \log_2 \lambda_i, \tag{5}$$

where ρ is the reduced density matrix of one sub-block and λ_i are its eigenvalues; this quantity measures the amount of entanglement between both sub-blocks. In the DMRG algorithm, where the form of considering entanglement in the renormalization process leads to a successful description of many systems [33], the universe (superblock) is divided into four blocks, where the first two form the system and the other two the environment. For calculating Eq. (5), we took the system block as the sub-block of interest, being ρ, its reduced density matrix. Since we built the phase diagram of the anisotropic Kondo necklace model for systems of 100 sites [25], we first consider chains of the same length to look for special tendencies of the block entropy at the quantum critical points identified previously. Once again, we implemented the finite-system algorithm of the DMRG with five sweeps, taking open boundary conditions and $t = 1$. Since we only need information about the ground state, this was the only target state used in the density matrix projection. We maintained enough states in the truncation process to have maximum truncation errors on the order of 10^{-8}. The necessary number of states m to achieve this varies depending on the values of η and J, since as they diminish (i.e., as we approach the original Kondo necklace model and the RKKY interactions become stronger), the number of maintained states must increase in order to preserve the order of the error (for example, for $J = 0.45$, $m = 40$ gives an error of 10^{-11} when $\eta = 0.8$, but when $\eta = 0.01$ the same order of the error is obtained for $m = 95$). In order to make the calculation more efficient, we implemented the transformation of the wave function of each step in the finite-system algorithm to obtain a good initial guess for the diagonalization of the superblock of the next step [34].

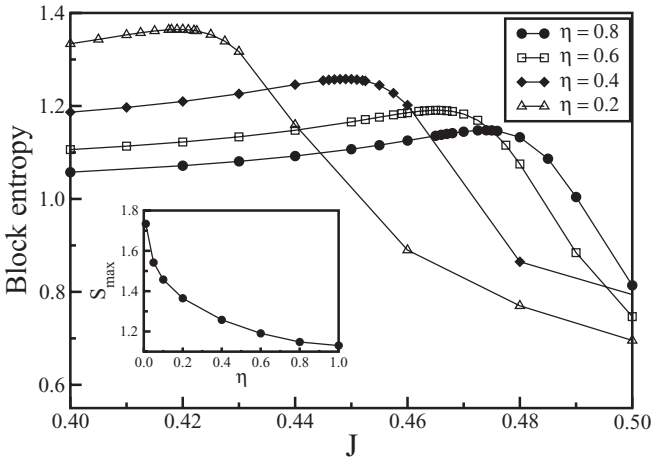

FIG. 2. Block entropy for different anisotropies η and $N = 100$. The lines are guides for the eye. Inset, maximum block entropy for each anisotropy η considered.

In Fig. 2, the block entropy for 100 sites and different anisotropies is shown; the block entropy is calculated in the final step of the DMRG algorithm, when the system and the environment have the same number of sites. For all anisotropies, the qualitative behavior of the entropy is the same: from left to right, it increases slowly as the Kondo coupling J gets larger, presents a maximum ($S_{\max}$), and then decreases rapidly while J keeps increasing. The existence of the maximum can be explained by looking at limit cases of the model: when $J \gg t$, in the Kondo singlet phase, we have nearly independent singlets at each site, so it is expected that different sub-blocks of the systems would be almost nonentangled between them and that the block entropy diminishes as J increases. When $J \ll t$, deep in the antiferromagnetic phase, the state of the superblock can be closely described by a single tensor product of states of the system and environment blocks (each one antiferromagnetic), so the entanglement is small and diminishes as the antiferromagnetic order gets stronger. To go smoothly from one limit to another as the range of J values is swept, a maximum in the block entropy has to appear at an intermediate point. As we argue below, this maximum occurs at the quantum critical points of the model. In the inset of Fig. 2, we show $S_{\max}$ for the anisotropies η considered; we observe that, for large anisotropies, the value of the maximum increases slowly as η diminishes, but as we approach the isotropic case $\eta = 0$, it begins to grow very quickly. In Table I, the values of J for which each maximum is found are presented for each η and are compared to the quantum critical points $J_c = J(E_g = 0)$ obtained in the previous DMRG analysis of

TABLE I. Comparison between critical points obtained with the closing of the gap and the block entropy for $N = 100$.

η	1.0	0.8	0.6	0.4	0.2	0.1	0.05	0.01
$J(E_g = 0)$	0.4691	0.4668	0.4564	0.439	0.407	0.381	0.3544	0.293
$J(S_{\max})$	0.476	0.474	0.465	0.449	0.419	0.390	0.368	0.323

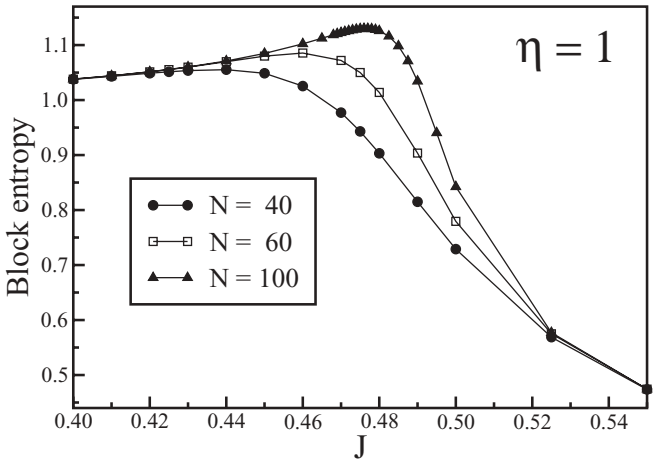

FIG. 3. Block entropy of the full anisotropic case $\eta = 1$ for different sizes of the superblock.

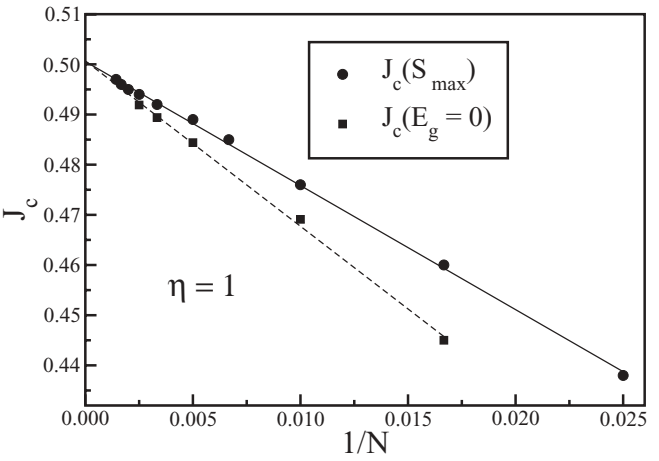

FIG. 4. J_c values of $E_g = 0$ and $S_{\max}$ as a function of $1/N$. The solid and dashed lines are linear regressions of the data obtained from the block entropy and the gap, respectively.

chains of 100 sites, where the Kosterlitz-Thouless decay of the gap was used [25]. The values of J for maximum S are not exactly those where the gap vanishes, but their closeness is very suggestive of a possible relationship between them. The largest difference occurs at $\eta = 0.01$, but in our previous paper it was pointed out that in this case a slightly different decay of the gap, fixing $b = 1$ in Eq. (4) and adding a prefactor J^d, would give a quantum critical point $J_c = 0.318$, much closer to the value of J where $S_{\max}$ appears; nevertheless, it was emphasized that determining the points in which the gap becomes zero can be complicated, and their values cannot be obtained with absolute certainty [25]. To prove that the closing of the gap and the maximum of the block entropy give the same information about the quantum criticality of the system at the thermodynamic limit, we focus on the full anisotropic case $\eta = 1$. In Fig. 3, we show the von Neumann block entropy for $\eta = 1.0$ and different sizes of the superblock as a function of J, where the system has the same length as the environment; for values of J far from the maximum, the entropy S is equal for the different sizes, but near the maximum, the entanglement gets larger as the size increases, making the maximum more pronounced. Also, as the superblock lengthens, the maximum goes to a larger value of J. In Fig. 4 we observe, for systems of different sizes, the critical points obtained with the decaying of the gap (solid squares) and the values of J where $S_{\max}$ occurs (solid circles) as a function of $1/N$. Both curves present a linear behavior; extrapolating to the thermodynamic limit ($1/N \to 0$) we find that $J_c(E_g = 0) = 0.50068(76)$ and that $J_c(S_{\max}) = 0.50056(28)$, which are extremely close. We can even think, within the margin of error, that both values of J are really the same within the thermodynamic limit, and we cannot discard the possibility of having that value equal to 0.5. So we have shown, in the case $\eta = 1$, that the von Neumann block entropy really indicates where the quantum phase transition between antiferromagnetic and Kondo singlet states takes place, giving the same critical point J_c that results from the analysis of the energy gap at the thermodynamic limit and a very similar result in finite systems. The nearness of these values of J for other anisotropies in the chain of 100 sites invites us to propose the same behavior for the entire range of values of η.

In different models, such as the XY and XXZ models [5] and Heisenberg ladders [35], the divergence of the block entropy $S(x)$ with the size of the system block x for a fixed size N of the superblock at the quantum critical point has been observed. When open boundary conditions are considered [6,35], the divergence has the following logarithmic tendency:

$$S(x) \propto \log_2\left[\frac{2N}{\pi}\sin\left(\frac{\pi x}{N}\right)\right]. \tag{6}$$

The saturation of $S(x)$ away from criticality has also been observed, as described by the area law: the block entropy between two regions depends on the extension of their boundary [36], which in one dimension is independent of the size of the blocks, so the block entropy is a constant for large sizes of the one-dimensional system, and saturates (which means that $\lim_{N\to\infty} S/N = 0$ [37]). In Fig. 5, these

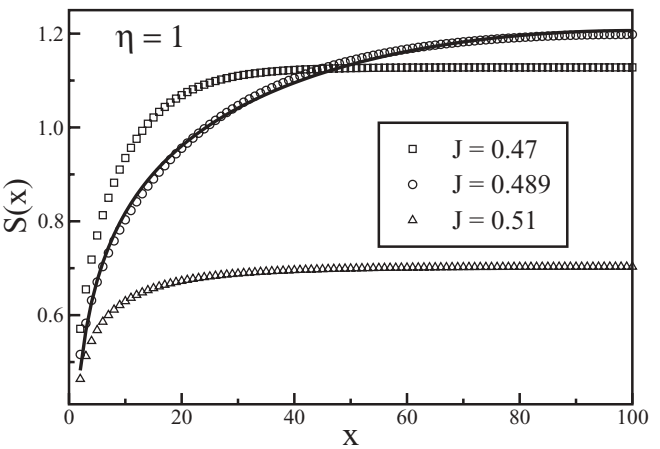

FIG. 5. Block entropy S as a function of the size of the system block x for $N = 200$ and different values of J: it diverges at criticality ($J = 0.489$) and saturates away from criticality.

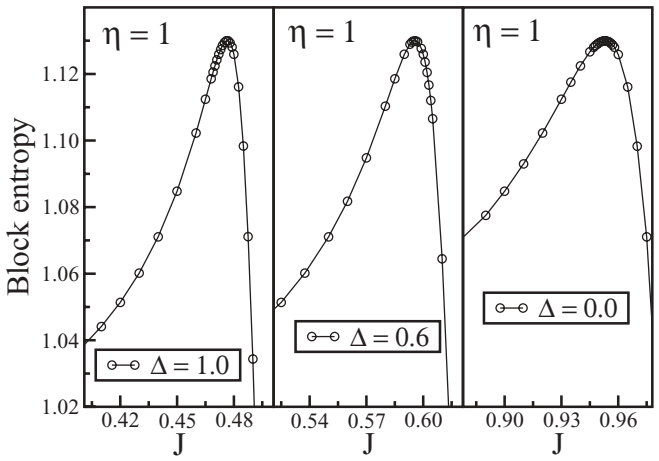

FIG. 6. Block entropy around quantum critical points for $\eta = 1$ and different Δ values, for $N = 100$.

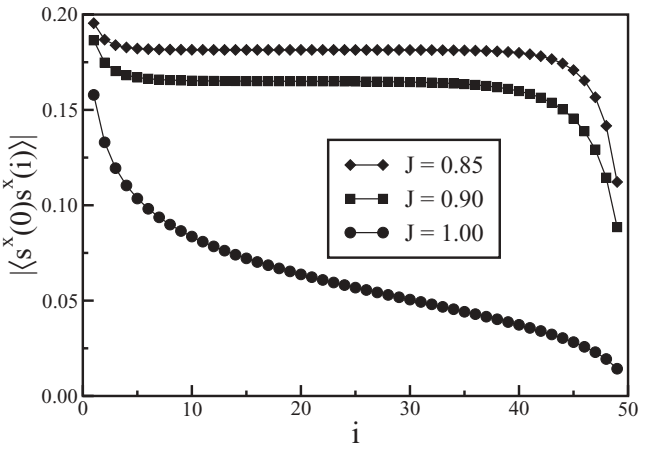

FIG. 7. Absolute value of x correlation functions for $\eta = 1$, $\Delta = 0$, and J values above and below J_c for 100 sites.

features are shown for the anisotropic Kondo necklace model, considering a superblock of 200 sites. At the quantum critical point ($J_c = 0.489$ for 200 sites, where the entropy presents the maximum), $S(x)$ diverges with x [the solid line in Fig. 5 corresponding to the fitting of $S(x)$ to Eq. (6), which follows very closely the values obtained with the DMRG]; the factor of term 6 is $c/6$, so the obtained central charge c of the conformal field theory would be $c = 0.870(5)$. For points below and above the critical point ($J = 0.47$ and 0.51, respectively), the block entropy saturates, in accordance with the area law.

Now we consider the case when the local anisotropy Δ is included in the Hamiltonian [see Eq. (3)], taking $\eta = 1$. With the same analysis of the energy gap described above for a system of 100 sites, we found that, for $\Delta = 0.6$ and $\Delta = 0$, $J_c = 0.5859$ and $J_c = 0.936$, respectively, which means that as Δ decreases the antiferromangnetic phase is favored and the formation of Kondo singlets is harder to achieve [38]. As before, the maximum values of the block entropy S occur very near these values, as shown in Fig. 6 [$J_c(S_{\max}) = 0.596$ for $\Delta = 0.6$ and $J_c(S_{\max}) = 0.953$ for $\Delta = 0$; the case $\Delta = 1$ corresponds to Hamiltonian (2)], so S seems to be an appropriate quantity for identifying the quantum phase transition even in this situation. It is interesting to observe that, in contrast to the case when η varies, $S_{\max}$ has the same value for a fixed η and the different Δ considered, and that as Δ diminishes, the peak broadens, increasing the entanglement around $S_{\max}$.

For a specific case, namely $\eta = 1$ and $\Delta = 0$, we present x correlation functions $|\langle s_0^x s_i^x \rangle|$ for a superblock of 100 sites, where s_0 is a conduction spin at the middle of the chain and s_i is a conduction spin separated from the latter i sites, to show that, indeed, we have magnetic and nonmagnetic states for points below and above the critical point, respectively (see Fig. 7). At $J = 0.85$ and $J = 0.9$, the correlations remain constant for a large part of the chain, so there is magnetic order (the decay at the end is due to the open boundary conditions), while at $J = 1.0$ the correlations decay quickly with the distance, which means that the magnetic order no longer exists.

III. CONCLUSIONS

We have calculated the von Neumann block entropy between the system and its environment for the anisotropic Kondo necklace model, using the density matrix renormalization group. Having previous knowledge of the quantum critical points J_c that separate an antiferromagnetic and a Kondo singlet state for different anisotropies η of the model, obtained from the analysis of the energy gap for chains of 100 sites, we computed the block entropy around these points and observed that a maximum appears very close to them. Taking the full anisotropic case $\eta = 1$, we found that the critical point obtained from the gap and the value of J where the maximum occurs vary linearly with $1/N$, and that at the thermodynamic limit ($N \to \infty$) both tend to the same value, so the block entropy is truly useful for giving information about the localization of the quantum phase transition of the model. A similar relationship between the energy gap and entanglement is obtained when an anisotropy Δ, which takes into account the effect of the crystalline electric field, is included: Δ affects the phase diagram, helping to stabilize the antiferromagnetic state as it diminishes, and for a system of 100 sites the block entropy also presents a maximum very near the quantum critical points. A calculation of correlation functions for a specific case ($\eta = 1$, $\Delta = 0$) shows that we really have magnetic and nonmagnetic configurations below and above the identified quantum critical point.

The presented results can be useful for gaining a better understanding of the relationship between entanglement and quantum phase transitions and for helping to elucidate which measures of entanglement can give information about the critical behavior of determined types of microscopic models.

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