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Kondo necklace model with planar and local anisotropies: entanglement approach

J.J. Mendoza-Arenas, R. Franco, and J. Silva-Valencia
Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia
e-mail: jjmendozaar@unal.edu.co

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We use the density matrix renormalization group to calculate the von Neumann block entropy in the Kondo necklace model. We have included two anisotropies: η in the exchange interaction between conduction spins, and Δ in the coupling between localized and conduction spins. Calculating the energy gap for the one-dimensional model at zero temperature, it was obtained that when $\eta > 0$, a quantum phase transition between Kondo singlet and antiferomagnetic states for finite couplings occurs, and as Δ increases the Kondo singlet phase is favoured. Now we observe that the quantum critical points of the model can be identified by a maximum of the von Neumann block entropy, so entanglement measures can be useful for determining the phase diagram of the anisotropic Kondo necklace model.

Keywords: Anisotropic Kondo necklace; block entropy; quantum phase transition.

Usamos el grupo de renormalización de la matriz densidad para calcular la entropía de von Neumann de bloque en el modelo de Kondo necklace. Hemos incluido dos anisotropías: η en la interacción de intercambio entre espines de conducción, y Δ en el acoplamiento entre los espines localizados y los de conducción. Calculando el gap de energıa para el modelo unidimensional a temperatura cero, se obtuvo que cuando $\eta > 0$, ocurre una transición de fase cuántica entre estados de singlete de Kondo y antiferromagnético para acoplamientos finitos, y cuando Δ aumenta la fase de singletes de Kondo se favorece. Ahora observamos que los puntos críticos cuánticos del modelo pueden ser identificados por un máximo de la entropía de von Neumann de bloque, de manera que medidas de entreveramiento pueden ser útiles para determinar el diagrama de fases del modelo de Kondo necklace anisotrópico.

Descriptores: Kondo necklace anisotrópico; entropía de bloque; transición de fase cuántica.

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1. Introduction

In recent years, a great effort has been done to understand the role of entanglement in the quantum critical behavior of condensed matter systems. At first, it was observed that mesures of entanglement such as the concurrence (entanglement between a pair of qubits [1]) and the von Neumann block entropy (entanglement between blocks in a bipartite system) are useful for identifying the quantum critical points of some spin-1=2 systems, such as the anisotropic XY chain in a transverse magnetic field [2, 3] and the XXZ model [3,4]. The concurrence can indicate a quantum phase transition by a singular behavior of its value or of its derivatives, depending on the order of the transition [5]. The block entropy S, which is given by

$$S(\rho) = -tr(\rho \log_2 \rho) = -\sum_i \lambda_i \log_2 \lambda_i \qquad (1)$$

where ρ is the reduced density matrix of one block of the bipartite system and λ_i are its eigenvalues, can point out a quantum critical point by means of a local maximum or minimum [6], and by its logarithmic scaling [3]: if the bipartite system (with open boundary conditions) has N sites, and one of its parts has x sites, the block entropy S(x) has the following divergent form at criticality:

$$S(x) = \frac{c}{6} log_2 \left(\frac{2N}{\pi} \sin\left(\frac{\pi x}{N}\right)\right) + g + \frac{A}{2} \qquad (2)$$

where c is the central charge of the corresponding conformal field theory, A is a non-universal constant and g is the boundary entropy [7]. Near criticality, S(x) saturates, which is explained by the area law [8]: the block entropy between two regions depends on the extension of their boundary, which in one dimensional chains is independent of their size, so the block entropy saturates to a constant value. Nevertheless, it has been XY observed that in some models, the mentioned entanglement measures do not give any signals of criticality (as in the XY chain with three spin interactions [9]), or the block entropy presents a special property at the critical points while the concurrence does not (as in Heisenberg ladders and dimerized Heisenberg chains [6]), or vice versa (as in the two-impurity Kondo model [10]). Therefore, more analysis of entanglement in condensed matter systems is required to have a better understanding of its connection with quantum phase transitions.

Recently, a huge theoretical and experimental research has been carried out on the properties of heavy fermion materials. These systems (intermetallic compounds that contain rare-earth or actinide elements such as Ce, Yb and U) have become some of the most valuable strongly correlated systems to study quantum criticality, since they present a great variety of ground states which can be obtained experimentally with equipment available in many laboratories[11]. The magnetic phase diagram of heavy fermions arises due to the competition between the Kondo effect, which corresponds to the screening of localized magnetic moments (in f orbitals) by conduction electrons (in s, p and d orbitals), and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, which is an indirect exchange between localized spins with mediation of conduction electrons [12]. The first effect strengthens the Kondo singlet state, in which the screening is achieved by the formation of singlets between localized and conduction spins, while the secong favours the antiferromagnetic order along the system. One of the models used to study this competition is the Kondo necklace [13], whose anisotropic Hamiltonian is given by:

$$H_{AKN} = t\sum_{i=1}^{N}\left(s_i^x s_{i+1}^x + (1-\eta)\, s_i^y s_{i+1}^y\right) + J\sum_{i=1}^{N}\left((S_i^x s_i^x + S_i^y s_i^y) + \Delta S_i^z s_i^z\right). \qquad (3)$$

$\vec{S}_i$ and $\vec{s}_i$ correspond to localized and conduction spins, respectively, J is the Kondo coupling and t is the Exchange that represents the hopping of conduction electrons (the energy scale is set by taking t = 1). This model considers spin degrees of freedom only, retaining the interplay between the Kondo effect and the RKKY interactions. For the isotropic case ($\eta = 0$, $\Delta = 1$), different methods, such as density matrix renormalization group [14, 15], bosonization [15] and bond-operator mean field theory [21] obtained that in one dimension at T = 0 the system remains in a Kondo singlet state for finite couplings (the quantum critical point is $J_c = 0$). The planar anisotropy η has been included due to the highly anisotropic nature of heavy fermions [16, 17], and as a symmetry problem [18]. Our density matrix renormalization group (DMRG) analysis shows that for $\eta > 0$, a quantum phase transition from a Kondo singlet to an antiferromagnetic state occurs at a finite value of J [19,20]. The local anisotropy Δ is included to take into account the effect of the crystalline electric field on the system [21]; examples of heavy fermions which present it are the hexagonal YbPtIn ($\Delta \ll 1$) and the orthorhombic YbNiGa ($\Delta \gg 1$)22. Δ does not cause a phase transition when $\eta =$ [21, 23], but when $\eta \neq 0$ the critical point J_c increases as Δ diminishes, favouring the antiferromagnetic state [23, 24]. The use of entanglement measures has been considered to study properties of the Kondo necklace model. The concurrence between different pairs of spins was calculated for systems of 2 and 4 sites for the cases $\eta = 0$ and $\eta = 1$ (with Δ = 1) [25]. A subsequent study with exact diagonalization for chains up to 8 sites and the range $0 \leq \eta \leq 1$ (Δ = 1) showed that the concurrence between different pairs of spins presents the competition between the Kondo effect and the RKKY interactions, but does not indicate the critical points [26]. Then, the block entropy was calculated for chains of 100 sites using DMRG [27], and it was observed that it presents a maximum at the quantum critical point J_c for every anisotropy $\eta > 0$ considered; so the block entropy is an appropriate quantity to identify the quantum phase transition of the Kondo necklace with planar anisotropy. In the present work we use the DMRG method to calcúlate the block entropy when the anisotropies η and Δ take different values, to observe if in those cases it indicates where the quantum phase transition takes place.

2. Results and discusion

First we show how the phase diagram of the anisotropic Kondo necklace was obtained [20, 26]. Using the DMRG method [28] for systems of 100 sites with open boundary condicions, we calculated the energy gap between the ground and the lowest excited state as a function of J for different values of η and Δ; the quantum critical point J_c that separates an antiferromagnetic state from a Kondo singlet is the point in which the gap vanishes. As an example, the decay of the gap for η = 0.4 and Δ = 0.3 is presented in Fig. 1. To obtain J_c, we fitted the gap to a Kosterlitz-Thouless tendency, which was also proposed for the isotropic Kondo necklace[14, 15]:

$$Gap = A\exp\left(-b = (J - Jc)^{0.5}\right) \qquad (4)$$

For the case of Fig. 1, we obtained J_c = 0.673(1). In the inset of Fig. 1 we show ln Gap as a function of $1/\sqrt{J - J_c}$, where the linear behaviour indicates that the Kosterlitz-Thouless tendency is appropriate to describe the closing of the gap. Various correlation functions and structure factors supported that for $J < J_c$ the system has antiferromagnetic order, while for $J > J_c$ the system is in a Kondo singlet state [20,26]. Now we present the results of the block entropy. We used the finite-system DMRG algorithm for chains of 100 sites, with open boundary conditions and maximum truncation errors on the order of 10-9, and calculated S(ϱ) using the reduced density matrix of the system block (that is, of half of the chain), so S(ϱ) measures the entanglement between the system and the environment blocks. In Fig. 2 we take a fixed Δ value (Δ = 0.0) and consider different planar anisotropies. For each case, a máximum block entropy Smax appears at a J value very close to the quantum critical point obtained with the gap (J(Gap = 0)), as shown in Table I. For the cases

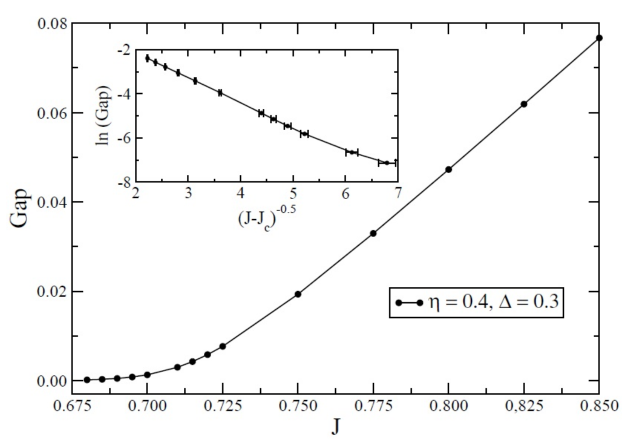

FIGURE 1. Energy gap as a function of J for 100 sites, η = 0:4 and Δ = 0:3. The inset shows its logarithmic decay near Jc.

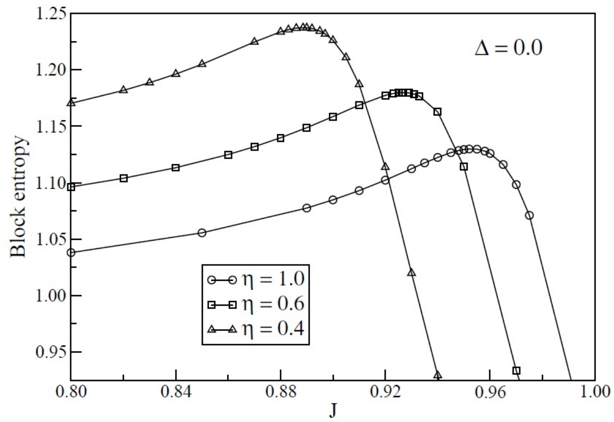

FIGURE 2. Block entropy for Δ = 0:0 and different η values, for N = 100-

TABLE I. Comparison between critical points obtained from

η	1.0	0.6	0.4
$J(Gap = 0)$	0.9358	0.9102	0.8728
$J(S_{max})$	0.9360	0.9267	0.8887

considered here, the largest difference between both values of J is of 1.8%. The values are not exactly the same, since it is very dificult to obtain the quantum critical points from the gap with complete certainty [20, 26], and finite-size effect are important [27]; nevertheless, the proximity between the values of J in which Smax takes place and the critical points obtained from the gap suggest that the block entropy is an useful quantity to identify the quantum phase the gap and the block entropy transition in the anisotropic Kondo necklace model, when both planar and local anisotropies are considered. It is worth noting that, as in the case of Δ =1.027, S_{max} increases as η decreases (that is, as we move away from the Ising limit η = 1.0).

Now we observe the block entropy for fixed η values and different local anisotropies Δ. In Figs. 3 and 4 the results for η = 0.8 and η = 0.4 are show, respectively. Again, a maximum appears very near the quantum critical points of the model, so that for the present cases, the largest difference between the value of J in which the máximum appears and that in which the gap vanishes is of 2.1%. We observe that as Δ decreases, J(Smax) increases (the antiferromagnetic phase is favoured, a larger value of J is needed to create the Kondo singlet state), and the peak widens, so the entanglement gets larger around the critical point. We also appreciate that for large η values, S_{max} decreases only slightly as Δ diminishes: for the case $\eta = 0.8$, the difference between the maximum of $\Delta = 0.8$ and Δ = 0.0 is of 0.2%; a smaller difference is observed in the case η = 1.027. On the other hand, for smaller planar anisotropies, S_{max} decreases more appreciably as Δ diminishes: for the case η = 0.4, the difference between the maximum of Δ = 0.9 and Δ = 0.1 is of 1.3%. So as η decreases, more importance it has in determining the maximum entanglement as Δ varies. Finally, we show the logarithmic divergence of the block entropy S(x), as a function of the size of the system block x, at the quantum critical point J_c of a specific case, namely η = 0.8 and Δ = 0.8, in which J_c = 0.5264 (where S_{max} takes place, see left side of Fig. 3). The calculation was done in the last sweep of the finite-system DMRG algorithm, where the system block lengthens until being of the same size of the environment [28]. The logarithmic tendency is presented in Fig. 5, where the solid line corresponds to the fitting of S(x) to Eq. 2, which follows very closely the results obtained with the DMRG (solid circles). The obtained value of the central charge of the conformal field theory is c= 0.881(8); comparing this value with that of the case η = 1.0 and $\Delta = 1.0^{27}$ (c = 0:870(5)), we can expect that, within the limits of the errors, both values of c are equal, so in both cases the critical universality class is the same. For points outside criticality, such as J = 0:49 and J = 0:57, the block entropy saturates, as shown in Fig. 5 block x for N = 100, η = 0:8, Δ = 0:8 and different J values.

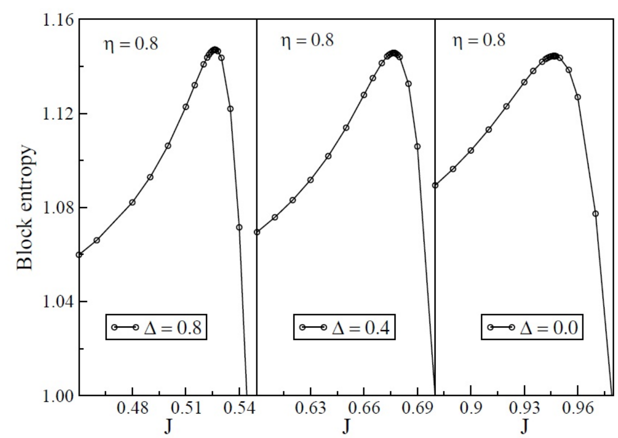

FIGURE 3. Block entropy for η = 0:8 and different Δ values, for N = 100.

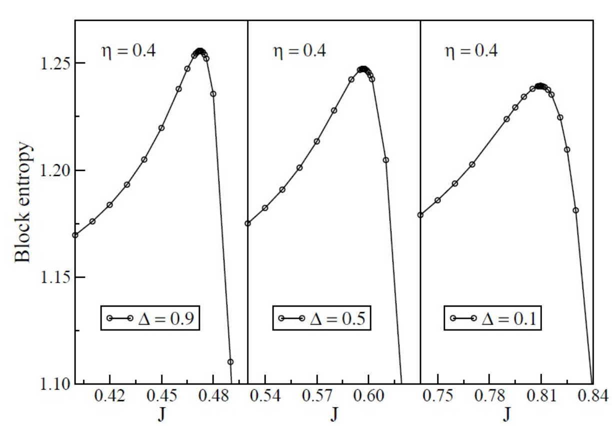

FIGURE 4. Block entropy for η = 0.4 and different Δ values, for N = 100.

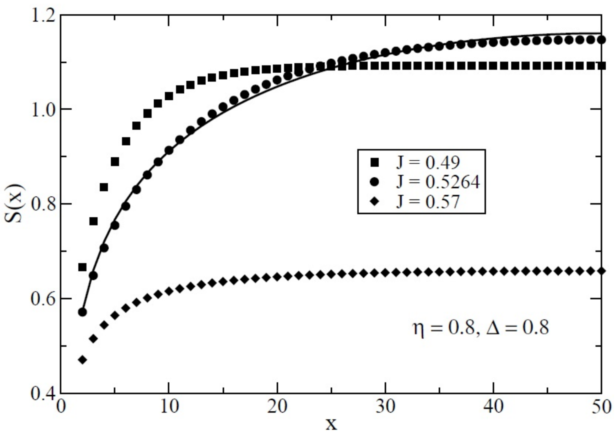

FIGURE 5. Block entropy as a function of the size of the system.

3. Conclusions

We have used the density matrix renormalization group method to calculate the von Neumann block entropy of the Kondo necklace model with planar and local anisotropies. We have shown how the phase diagram of the model was obtained from the analysis of the energy gap, where the quantum critical points that separate a Kondo singlet from an antiferromagnetic state correspond to the values of J where the gap vanishes. Calculating the block entropy for various combinations of planar and local anisotropies, we obtained that it presents a maximum very near the corresponding quantum critical points J_c, so we can think that the block entropy is an adequate quantity to identify where the quantum phase transitions of the Kondo necklace model take place, when both planar and local anisotropy are considered. The logarithmic scaling of the entanglement with the size of the system at the critical point was also observed for a particular case, as its saturation away from criticality. We expect that these results can be valuable to help elucídate the relation between entanglement and quantum phase transitions in condensed matter systems.

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