Study of the 1D anisotropic Kondo necklace model at criticality via an entanglement entropy estimator

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Abstract

We use an estimator of quantum criticality based on the entanglement entropy to discuss the ground state properties of the 1D anisotropic Kondo necklace model. We found that the $T = 0$ phase diagram of the model is described by a critical line separating an antiferromagnetic phase from a Kondo singlet state. Moreover we calculate the conformal anomaly on the critical line and obtained that $c$ tends to 0.5 as the thermodynamic limit is reached. Hence we conclude that these transitions belong to Ising universality class being, therefore, second order transitions instead of infinite order as claimed before.

1. Introduction

Heavy-fermion compounds belong to a class of materials which exhibit many intriguing and anomalous phenomena as, for example, the Kondo effect. In these materials the $f$ shell electrons present an unstable character that oscillates between localized and itinerant. Because of this ambiguous behaviour they can be found in a broad variety of states including metallic, superconducting, insulating and magnetic states [1, 2]. Interestingly, it has been showed that most of the properties of these systems can be attributed to their proximity to a magnetic quantum critical point (QCP) [3], and due to this important characteristic, the study of these system at low temperatures has been of great interest recently (see, for example, Refs. [4, 5]).

A standard Hamiltonian which has been largely used to describe the physical properties of these compounds is the Kondo lattice model [6, 7]. It assumes the presence of one localized impurity spin on each site of the lattice, coupled to the conduction electrons of the metal. The interaction between the magnetic moments of the $f$ electrons of the impurities and those of the conduction electrons, $J$, is responsible for the Kondo effect. This Kondo interaction tends to compensate the local moments, forming singlets, giving rise to a non magnetic...
ground state. At the same time, because of the large concentration of impurities, it appears an interaction between their magnetic moments. This is an inter-site coupling of the Ruderman-Kittel-Kasuya-Yosida (RKKY) type and it is mediated by the conduction electrons. The RKKY interaction tends to establish a long range magnetic order in the system, in general, an antiferromagnetic ground state. This competition induces a magnetic quantum phase transition in this model which is the actual case in most heavy fermions materials. A simplified version of the Kondo lattice Hamiltonian was introduced by Doniach in Ref. [7]. This model, called Kondo necklace (KN), replaces, into the Kondo interaction, the spins of the conduction electrons by a set of pseudo-spins on a linear lattice, the charge degrees of freedom being frozen out. In spite of this approximation, the interplay between the Kondo mechanism and magnetic ordering remains as an essential feature. Although the KN model has been extensively studied over the last decades many questions about the phase diagram and magnetic properties of intricate versions of this model still remain open and we believe it will still be necessary some effort to be completely understood.

Among the recently studied systems is the one-dimensional KN model in the presence of an Ising-like anisotropy. The general Hamiltonian that describes the system is given by

$$H = \sum_{i=1}^{N-1} W (\sigma_i^x \sigma_{i+1}^x + (1-\delta)\sigma_i^y \sigma_{i+1}^y) + \sum_{i=1}^{N} J \vec{S}_i \cdot \vec{\sigma}_i,$$  \hspace{1cm} (1)

where $\sigma^\mu$ and $S^\mu$, $\mu = x, y, z$, are spin-1/2 Pauli matrices denoting the spin of the conduction electrons and those of the local moments, respectively. $J$ is the intra-site exchange interaction between them. The indices $i$ and $i + 1$ denote nearest neighbors on a chain of $N$ sites and $W$ is an antiferromagnetic coupling which represents the hopping of the conduction electrons between neighboring sites (see in Fig. 4 a schematic representation of the chain with $N = 6$ sites, i.e, 12 spins). The Ising like anisotropy parameter ($\delta$) varies from zero to one.

The zero temperature phase diagram of this model in the ($\delta$, $K$) plane, with $K = J/W$, has been studied by different methods as renormalization group [8], Lanczos [9], and DMRG [10]. The main results found in the literature can be summarized as follows. The line $K = 0$ corresponds to the one-dimensional (1D), purely anisotropic XY model which is ordered at $T = 0$ [23]. For $K \neq 0$ and $\delta = 0$ case, the original KN model is recovered and it is already well established that any finite value of the interaction $J$ give rise to a non-magnetic Kondo state [12, 13, 14]. In the full anisotropic case ($\delta = 1$), there is an unstable fixed point separating an antiferromagnetic phase for small values of $K$ from a spin compensated, Kondo-like phase, reached in the strong $J$ interaction regime. The exact value of $K_c$ is not known but there is a consensus that this transition is in the same class of universality of the 1D quantum Ising model [12]. The great controversy arises when we consider the anisotropy parameter in the region $0 < \delta < 1$. In this case the two phases described above are still present but it is on debate if a critical value of anisotropy is required for the appearance of long-range magnetic order, as predicted in Ref. [8], or if it is present for
any value of anisotropy, as reported in Refs. [9, 10]. Other important point of
discussion is the class of universality of the ordered-disordered transition. RG
calculation indicates it is a second order phase transition but the authors of
Ref. [10] proposed it is of Kosterlitz-Thouless type.

To investigate the critical behaviour of the 1D anisotropic KN model at zero
temperature we use an estimator of quantum criticality based on the behaviour
of the entanglement entropy in gapless and gapfull systems. This method has
proved to be a powerful numerical tool to precisely locate quantum critical points
and calculate the central charge with low computational cost (small lattice sizes)
in a large variety of 1D quantum systems [15, 16]. By considering systems
with sizes of up to 24 spins, we found that the T=0 phase diagram of this
model is described by a critical line separating an antiferromagnetic long range
order, which is present for any finite value of anisotropy, from a non-magnetic
Kondo singlet phase. This general result is in accordance to Lanczos and DMRG
calculations. However, we have calculated the conformal anomaly on the critical
line and obtained that $c$ tends to 0.5 as the system size increases. Hence we
conclude that the transitions for any $\delta \neq 0$ belong to Ising universality class
and, therefore, they are of the second order kind instead of infinite order as
claimed in Ref. [10].

The paper is organized as follows: In the next section we outline the formal-
ism adopted and, in the last section, we present and discuss our results.

2. Formalism

In this work we present a systematic study of the quantum behaviour of the
model described by Eq. 1 at $T = 0$. To identify the critical coupling ($K = J/W$)
and anisotropy ($\delta$) separating the various quantal phases of the system we
employ an estimator of quantum criticality based on the von Neumann entangle-
ment entropy. It works in the following way. Let us consider a quantum system
of $L$ spins in a pure state $|\psi\rangle$ and a bipartition of the system into two blocks:
a block of $l$ contiguous spins and other containing the spins of the rest of the
chain ($L - l$ spins). The entanglement entropy between $l$ and $L - l$ is given by

$$S(L, l) = -\text{Tr} (\rho_l \ln \rho_l)$$

(2)

where $\rho_l = \text{Tr}_{L-l}\rho$ denote the reduced density matrix for block $l$, with $\rho =
|\psi\rangle\langle\psi|$. As it has been shown in Refs. [17, 18, 19, 20, 21] the quantity defined
in Eq. 2 presents a very interesting scaling behaviour in 1D systems. Suppose
this system is dependent of a given parameter, let us say $\lambda$, and at $\lambda = \lambda_c$ it
presents a QCP. In the critical point, conformal invariance implies a diverging
logarithmic scaling which can be written as

$$S(L, l) = \gamma \ln \left[ \frac{L}{\pi} \sin \left( \frac{\pi l}{L} \right) \right] + \beta$$

(3)

where $\beta$ is a nonuniversal constant and $\gamma$ is a constant related to the central
charge, namely $\gamma = c/3$ when periodic boundary conditions are adopted in the
chain. If $\lambda \neq \lambda_c$ and $(l, L - l) \rightarrow \infty$, then the entanglement entropy $S(L, l)$ is not only independent of $l$ but also independent of $L$. There is entanglement only between sites separated by a distance of the order of the correlation length ($\xi$), and this quantity of entanglement is unchanged by a variation of either $L$ or $l$ when both $l$ and $L - l$ are very large.

The estimator used throughout the paper was proposed in Refs. [15, 16] and it is given by the difference of the entanglement entropy obtained for two subsystems of different sizes, for example, $l$ and $l'$, of a system of total size $L$. We write this as:

$$\Delta S = S(L, l) - S(L, l'),$$

where $S(L, l)$ and $S(L, l')$ are the entanglement entropies between $l$ and $(L - l)$ and between $l'$ and $(L - l')$, respectively. From the expressions above, we see that as $(L, l, l') \rightarrow \infty$, $\Delta S \neq 0$ at the critical point while it is zero for any value of $\lambda \neq \lambda_c$. Therefore $\Delta S(\lambda)$ is a good indicator of quantum phase transition in the thermodynamic limit. For a finite size system the scaling of $S(L, l)$ described above is not exact anymore but the result obtained for $\Delta S$ can be easily generalized. In this case, it is expected that $\Delta S \neq 0$ for all values of $\lambda$ but at $\lambda = \lambda_c$ it attains its maximum value. In this way, $\Delta S$ works as an estimator of criticality: to locate a QCP for a fixed finite system size we should look for the value of $\lambda$ for which $\Delta S$ is a maximum. As $L$ increases the peak around $\lambda_c$ should become narrower, so that in the thermodynamic limit it is the only value different from zero. It is important to emphasize that the choice of $l$ and $l'$ for this method is arbitrary but the finite-size effects on $S(L, l)$ are smaller if they are chosen around the middle of the chain.

An interesting characteristic of this method is that it allows to obtain a unique value of the critical parameter and central charge for each $L$, enabling us to estimate their values in the thermodynamic limit by extrapolation. This approach has been tested in different models and the results have shown that this is an excellent numerical method to study quantum criticality in 1D systems [15, 16].

3. Results and discussion

In order to apply the estimator to the KN model we consider subsystems containing $l$ and $l'$ spins of a periodic chain with $L$ spins. Note that, in Eq. 11 $N$ represents the number of sites of the system in an open chain, since there are two spins at each site it implies that $L = 2N$ (As an example, we show in Fig.(1), a schematic representation of the chain with $L = 12$ and $l' = 4$). The adoption of periodic boundary condition in the KN model means that we should take the first sum in Eq. 11 up to $N$, considering $\sigma_{N+1} = \sigma_1$, keeping the second one as it is.

Initially, to test the method, we will discuss the critical point and the central charge of the KN model for the specific case of $\delta = 1$. It is a good starting-point since there is not a great controversy about these results in the literature. To calculate $\Delta S$ we can choose the blocks, $l$ and $l'$, of arbitrary size. In this primary
example, we will use two different bipartitions of the system: (a) \( l = L/2 \) and \( l' = L/4 \) and (b) \( l = L/2 \) and \( l' = L/2 - 2 \). In the first case we take \( l \) and \( l' \) fixed ratios of \( L \) such that the difference between them, \( l - l' = L/4 \), increases with \( L \); for the second bipartition, this difference remains constant, \( l - l' = 2 \). We will compare the accuracy of the numerical results and the optimal bipartition will be used to investigate the critical line in the interval \( 0 < \delta < 1 \).

The basic steps of the approximation, valid for the two bipartitions, are: firstly, we use power method (an iterative eigenvalue algorithm [22]) to obtain the ground state of the chain for a given fixed value of \( L \) up to 24 spins. Then, we calculate \( S(L, l) \) and \( S(L, l') \) as defined in Eq. 2 and subtract them to obtain \( \Delta S \). To locate the QCPs we fix the value of \( \delta = 1 \) and look for the value of \( K \) that gives the maximum value of \( \Delta S \). It is important to emphasize that, due to the geometry of the lattice, we just can choose some specific values of \( L \) to study the correlations along the chain. In fact, the values allowed for \( L \) depend on the bipartition of the system: for the case (a), the chain should contain \( L = 8, 16, \) and 24 spins, while for (b), \( L \) can be equal to 12, 16, 20, and 24 spins.

The critical coupling in the thermodynamic limit is estimated, in both cases, by extrapolating the values of \( K \) found for each spin system size, for larger \( L \). Let us present the results for the two bipartitions separately.

(a) \( l = L/2 \) and \( l' = L/4 \)

As discussed in the last section, as \((l, l', L)\) increases, \( \Delta S \rightarrow 0 \), except in the critical point where it tends to:

\[
\Delta S = S(L, \frac{L}{2}) - S(L, \frac{L}{4}) = \frac{\gamma}{2} \ln(2).
\]

This result can also be written as:

\[
c = \frac{6 \Delta S}{\ln(2)}.
\]

From this expression we see that, just like \( \Delta S \), \( c \) is a maximum at the critical point. Thus, once we have localized \( K_c \) we use the corresponding maximum
value of $\Delta S$ to calculate $c$ in Eq. 6 for each $L$. The value of $c$ in the thermodynamic limit is estimated by extrapolation.

In Fig. 2 we show the evolution of $\Delta S$ as a function of $K$ for $\delta = 1$. As we can see, the maximum of $\Delta S$ occurs in $K = 0.5$ and, as $L$ increases, the peak becomes narrower around this value. With the value of $K_c$ in hands, the calculation of the central charge is a simple application of Eq. 6. In Table 1 we show the values of $K_c$ and $c$ as a function of $L$. See that these parameters converge fastly to the values $K_c = 0.5$ and $c = 0.5$, as $L$ increases. Therefore we believe that they are good numerical approximation to the true values of the quantum critical point, which are reached only in the thermodynamic limit. Based on this approximation, we conclude that $K = 0.5$ corresponds to the QCP of the system for $\delta = 1$ and that, this transition, characterized by $c = 0.5$, belongs to the Ising universality class.

Figure 2: Dependence of the difference of entropy $\Delta S$ with $K$ for various values of $L$, taking the bipartition as defined in (a). See that, as $L$ increases, the maximum value of $\Delta S$ tends to $K = 0.5$ and the peak around $K_c$ become narrower. These characteristics lead us to conclude that $K = 0.5$ corresponds to the QCP of model for $\delta = 1$.

| $L$ | $K_c$  | $c$   |
|-----|--------|-------|
| 8   | 0.48   | 0.5273|
| 16  | 0.50   | 0.5035|
| 24  | 0.50   | 0.5013|

Table 1: System size dependence of the critical coupling, $K_c$, and the central charge, $c$, at the QCP of the anisotropic KN model for $\delta = 1$, by considering the bipartition (a). The values of these parameters in the thermodynamic limit are estimated by extrapolation.

b) $l = L/2$ and $l' = L/2 - 2$

By using this bipartition we obtain that, as $(l, l', L)$ increases:

$$\Delta S = S(L, \frac{L}{2}) - S(L, \frac{L}{2} - 2) = \begin{cases} -\gamma \ln[\cos(\frac{2\pi}{L})], & K = K_c \\ 0, & K \neq K_c \end{cases}$$

(7)
From this expression we can see that, for $K = K_c$, $\Delta S \sim L^{-2}$, which tends to zero as $L \to \infty$. However, we should point out that $\Delta S$ is still a maximum at the critical point because the vanishing of $\Delta S$ for $K \neq K_c$ is much faster (exponential) than for $K = K_c$ (power law). Therefore, $\Delta S$ still works as an estimator of quantum criticality and the method can be used as before. The central charge at the critical point can be obtained by:

$$c = \frac{-3\Delta S}{\ln(\cos(2\pi/L))}. \quad (8)$$

In Fig. 3 we show the evolution of $\Delta S$ as a function of $K$ for $\delta = 1$. As already expected, the height of $\Delta S^{\text{max}}$ decreases as $L$ increases. However, as discussed above, the position of the maximum value of $\Delta S$ still indicates the critical point. As it can be seen, $\Delta S$ presents a peak increasingly narrow around $K = 0.5$ as $L$ increases. To calculate the central charge and discuss the class of universality of the transition we use Eq. 8. We show in Table 2 the finite size values of $K_c$ and $c$ as a function of $L$. See that, as $L$ increases, $c \to 0.5$. The fast convergence of $c$ leads to the conclusion that this is a good approximation to the value of the central charge in the thermodynamic limit for the model with $\delta = 1$.

![Figure 3: Dependence of the difference of entropy $\Delta S$ with $K$ for various values of $L$, by considering the bipartition (b). See that, although the height of $\Delta S^{\text{max}}$ decreases as $L$ increases, $\Delta S$ presents a peak increasingly narrow around $K = 0.5$ indicating that this is the critical point in the model for $\delta = 1$.](image)

Based on the results showed above we can conclude that the two bipartitions used in this first analysis are equivalent and that there is not a real advantage in one choice over the other. Independently of the bipartition used, the estimated value for $K_c$ and $c$, in the thermodynamic limit, are the same. Moreover, in both cases, $c$ is expressed with high precision (the uncertainty is in the third decimal place) even in a very small chain (just 16 spins). Therefore, as the results seem to be not affected by the choice of one of the bipartitions, we will choose to continue our investigation by taking only the bipartition (b) from now on.
Table 2: System size dependence of the critical coupling $K_c$ and the central charge $c$ at the QCP of the anisotropic KN model for $\delta = 1$, by considering the bipartition (b). The values of these parameters in the thermodynamic limit are estimated by extrapolation.

| $L$  | $K_c$  | $c$   |
|------|--------|-------|
| 12   | 0.49   | 0.5054|
| 16   | 0.50   | 0.5023|
| 20   | 0.50   | 0.5011|
| 24   | 0.50   | 0.5009|
| Estimate to $L \to \infty$ | 0.50 | 0.5 |

Table 3: The critical coupling, $K_c$, of the KN model for different values anisotropy ($\delta$).

| $\delta$ | 0.0 | 0.1 | 0.3 | 0.5 | 0.7 | 1.0 |
|----------|-----|-----|-----|-----|-----|-----|
| $K_c$    | 0.0 | 0.40| 0.46| 0.48| 0.49| 0.50|

Following the procedure described above, we have calculated the central charge at the critical point for several values of $\delta$. Our results show that the estimated value for $c$ is 0.5 for the entire line. As an example of our calculations, we show in Fig. 5 the values of $c$ as a function of $L$ obtained for $\delta = 0.4$ and $\delta = 0.7$. We see clearly that $c$ tends to 0.5, as $L$ increases, for both values of anisotropy. Therefore, we conclude that the transitions along the line belong to the quantum 1D Ising model universality class and they are of the second order type.

4. Summary and Conclusion

In summary, we have examined the QPTs of the 1D Kondo necklace model in the presence of an Ising-like anisotropy. The model is suitable to describe heavy fermion systems and emphasizes magnetic degrees of freedom neglecting
charge fluctuations. By using an estimator of quantum criticality based on the behaviour of the entanglement entropy \[13, 15\], we found that the T=0 phase diagram of this model is described by a critical line separating an antiferromagnetic long range order, which is present for any finite value of anisotropy, from a non-magnetic Kondo singlet phase. This general result is in accordance to Lanczos and DMRG calculation. However we have calculated the central charge on the critical line and obtained that $c \to 0.5$, as $L$ increases, for any $\delta \neq 0$. Hence we conclude that these transitions along the line belong to the Ising universality class and, therefore, they are of the second order type instead of infinite order as claimed in Ref. [10].

It is very interesting to note the similarity between the phases diagrams of the anisotropic KN model, as obtained here, and that of the $XY$ model in a transverse field ($\lambda$) obtained by Barouch and McCoy in Ref. [23]. The isotropic ($\delta = 0$) version of both systems presents an infinite order critical point ($J = 0$ for the KN model and $\lambda = 1$ for the $XY$ Hamiltonian), however, any perturbation in the anisotropic parameter (any $\delta > 0$) turns the critical behaviour of the spin chains from the universality class of the $XX$ model into that of the Ising model. In the KN model, the $RKKY$ ($J$) interaction plays the role of the transverse field in the $XY$ model: it destroys the correlations along the chain leading the system to a paramagnetic phase. We leave this point to be further explored in future works.

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Figure 5: Dependence of the central charge with the system size at the critical points of $\delta = 0.4$ and $\delta = 0.7$. The dotted line denotes the value $c = 0.5$ corresponding to estimate of $c$ in the $L \to \infty$ limit.

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