Entanglement in the 1D Kondo Necklace Spin System

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Abstract

We discuss the thermal and magnetic entanglement in the one-dimensional Kondo necklace model. First, we show how the entanglement naturally present at zero temperature is distributed among pairs of spins according to the strength of the two couplings of the chain, namely, the Kondo exchange interaction and the hopping energy. The effect of temperature and the presence of an external magnetic field are then investigated, being discussed the adjustment of these variables in order to control the entanglement available in the system. In particular, it is indicated the existence of a critical magnetic field above which the entanglement undergoes a sharp variation, leading the ground state to a completely unentangled phase.

Recently, investigations towards a general theory of entanglement and the search for experimental proposals for the implementation of a quantum computer have strongly motivated the discussion of the content of entanglement present in condensed matter systems as, for instance, interacting spin chains (See, for example, refs. [1, 2]). In this work, we study the thermal and magnetic entanglement in the one-dimensional Kondo necklace (KN) model, which was proposed in ref. [3] to study heavy fermions emphasizing the magnetic degrees of freedom of the system. Heavy fermion compounds are characterized as metallic hosts in which magnetic impurities with a partially filled f shell are immersed. The unstable f shell leads to some attractive properties for quantum computation [4], since it is shielded from the environment by the outer electrons.

The one-dimensional KN model is defined by the Hamiltonian

$$H = W\sum_{i=1}^{N}(\tau_i^x\tau_{i+1}^x + \tau_i^y\tau_{i+1}^y) + J\sum_{i=1}^{N}\vec{S}_i.\vec{\tau}_i, \tag{1}$$

where τ_i^α and S_i^α are independent spin-1/2 operators acting on a site i, which are given by $\sigma^\alpha/2$, with σ^α ($\alpha = x, y, z$) denoting the Pauli matrices. A schematic arrangement of the system is displayed in Fig. 1. The spin operators τ_i^α and S_i^α are associated with the conduction electrons[1] and the innercore spins hanging from the τ-spin chain, respectively. The Hamiltonian Eq. (1) describes an one-dimensional KN lattice with N sites, where periodic boundary conditions are adopted, *i.e.*, $\tau_{N+1}^x = \tau_1^x$ and $\tau_{N+1}^y = \tau_1^y$. The positive parameter W represents the hopping energy and J is the Kondo exchange coupling, which can be either ferromagnetic ($J < 0$) or antiferromagnetic ($J > 0$). Note that, since the KN model is defined with two spins on each site, the smallest representative cell of the system is described by four spins, each spin being taken as a quantum bit (qubit).

Before describing our results we present the definition of concurrence, which is the measure of entanglement used throughout this paper. The concurrence C_{12} for a pair of qubits labelled as 1 and 2 is defined [5] by $C_{12} = \max(\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0)$, where the λ_i are the square roots, in decreasing order, of the eigenvalues of the operator $R \equiv \rho_{12}(\sigma_y \otimes \sigma_y)\rho_{12}^*(\sigma_y \otimes \sigma_y)$. In the definition of R, ρ_{12} denotes the density matrix, which can be either pure or mixed, for the pair of qubits 1 and 2, and ρ_{12}^* its complex conjugate in the the standard basis $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$. In a system with more than two qubits, ρ_{12} is obtained by tracing the density operator over the other qubits. The concurrence ranges from 0, implying an unentangled state, to 1, in which the two qubits are maximally entangled.

In pure states of N qubits, it has been conjectured [6] that entanglement is distributed following the inequality for the squared concurrence

$$C_{12}^2 + C_{13}^2 + ... + C_{1N}^2 \leq C_{1(23..N)}^2, \tag{2}$$

[1] In the KN model, the conduction electrons are represented by a set of pseudo-spins on a linear lattice, the charge degrees of freedom being frozen out.

where $C_{1(23..N)}$ is the single-qubit concurrence, defined as the concurrence between the qubit 1 and the rest of lattice $(23...N)$. This quantity represents collective contributions of the entanglement between the qubit 1 and all the other qubits of the system and can be obtained from $C_{1(23..N)} = 2\sqrt{\det \rho_1}$, where ρ_1 is the density matrix for the qubit 1. A relevant aspect of the single-qubit concurrence is that, as it has been suggested in ref. [2], it may be a useful tool to identify a quantum critical point in a lattice system.

We begin by considering the entanglement for the pairs of qubits of the two-site KN model, whose spins are labelled with τ_1, τ_2, S_1, and S_2, as represented in Fig. 1. For simplicity, we will refer to τ_1, τ_2, S_1, and S_2, as qubits A, B, C, and D, respectively. The qubits A and B form a ring coupled via antiferromagnetic XY interaction ($W > 0$), while A and C, as well as B and D, are coupled via Heisenberg interaction, which can be either ferromagnetic or antiferromagnetic. The symmetry of the lattice ensures that the entanglement is the same for the following pairs: AC and BD, AD and BC, and AB and CD. Therefore we will only refer to the pairs AB, AC, and AD along the paper.

The Hamiltonian for the two-site model is obtained from Eq. (1) by setting $N = 2$. The ground state of the system with either $J < 0$ or $J > 0$ is nondegenerate and can be written as the following pure state of $ABCD$:

$$|0\rangle_{xy} = N_{xy}\Big(|++--\rangle + \alpha_1(|+--+\rangle + |-++-\rangle) + \alpha_2(|+-+-\rangle + |-+-+\rangle) + |--++\rangle \Big), \tag{3}$$

where the positions in the kets denote the qubits A, B, C, and D in this order. The normalization constant N_{xy} and the functions α_1 and α_2, which depend on the parameters J and W, are found to be

$$\alpha_1 = \frac{J + 2\lambda_{xy}}{2J} \;\;,\;\; \alpha_2 = \frac{\lambda_{xy}^2 + \lambda_{xy}J - 3J^2/4}{WJ} \;\;,\;\; N_{xy} = \frac{1}{\sqrt{2(1+\alpha_1^2+\alpha_2^2)}}, \tag{4}$$

with λ_{xy} being the ground state energy

$$\lambda_{xy} = -\frac{J}{6} - 2\sqrt{Q}\,\cos\frac{\theta}{3} \;\;,\;\; \theta = \arccos\left(\frac{-J(9W^2 - 16J^2)}{54\sqrt{Q^3}}\right) \;\;,\;\; Q = \frac{4J^2 + 3W^2}{9}. \tag{5}$$

At temperature T=0, only the ground state is populated. If the XY coupling is taken as zero ($W = 0$), the system becomes two decoupled Heisenberg dimers, namely, AC and BD. In this regime, all the pairs of qubits are completely unentangled for $J < 0$. In fact, the absence of entanglement between qubits coupled by ferromagnetic Heisenberg interaction is a general property already pointed out in ref. [1]. On the other hand, if $J > 0$ then the qubits in the dimers are maximally entangled for any value of the parameter J, with the concurrence vanishing for all the other pairs.

Consider now the parameter $W > 0$. We obtain, in the limit $J = 0$, the two-qubit antiferromagnetic XY ring in the presence of two other non-interacting spins (C and D). In this case, the pair of qubits AB is maximally entangled for any W and the concurrences for the other pairs are zero. For the Heisenberg coupling $J > 0$, the pair AD is always unentangled and there is a competition, governed by the values of J and W, between the entanglement of the pairs AB and AC coupled by Heisenberg and XY interactions, respectively. Actually, the concurrences AB and AC are complementary, *i.e.*, if the qubit A is partially entangled with B, then A can have only a limited quantity of entanglement with C. These results completely satisfy the inequality (2), with the upper bound limit for the entanglement being obtained from the single-qubit concurrence between A and BCD, given by $C_{A(BCD)} = 1$ independently of the values of J and W. For the case $J < 0$, the entanglement is distributed between the pairs AB and AD. However, although there is no concurrence between qubits coupled with Heisenberg interaction, an increase of the value of J decreases the entanglement of the pair AB and increases the concurrence for AD. In fact, it can be observed from Eqs. (3-5), that a variation in J affects C_{AB} and C_{AD}, since the functions α_1 and α_2 depend on this parameter. As in the case $J > 0$, the inequality (2) is satisfied with $C_{A(BCD)} = 1$.

In order to take into account the effect of the temperature on the entanglement in the KN model, we consider the density matrix for the system at thermal equilibrium as given by $\rho(T) = exp(-H/kT)/Z$, where Z is the partition function and k the Boltzmann's constant. Starting from $T = 0$ and a fixed W, if we slowly increase the temperature, then the entanglement for the pair AB also increases, for all values of J, before beginning to decrease. This is explained by observing that, for $J = 0$, the ground state

is degenerate, being a statistical mixture of four states with energy eigenvalue $-W$. In this case, the entanglement AB assumes the maximum value 1 at $T = 0$, independently of the parameter W. When J is "turned on", the degeneracy splits up and the ground state turns out to be given by Eq. (3). However, for a nonvanishing value of the coupling J, there are some excited states contributing with a greater portion of entaglement AB than the ground state. Thus, since the effect of the temperature is to populate the excited states, entanglement AB turns out to increase before being completely destroyed. In contrast, the entanglement for the pair AC always decreases with temperature. We can understand this behavior by noting that, for $W = 0$, the ground state of the system is nondegenerate and the pair AC is maximally entangled for any value of J at $T = 0$. For nonvanishing W, the ground state of the system remains nondegenerate and there are no excited states contributing with a quantity of entanglement greater than the ground state. Therefore, the mixing of Eq. (3) with higher energy levels, in this case, can only destroy the entanglement. Similar results hold true for the case of ferromagnetic Heisenberg interaction, where it is possible to have thermal entanglement for the pairs AB and AD .

We also investigate how an external magnetic field applied in the KN model along the z direction can modify the entanglement of the system. The Hamiltonian for this case is given by

$$H_B = H + B \sum_{i=1}^{N} (s_i^z + \tau_i^z), \tag{6}$$

where H is the Hamiltonian previously defined in Eq. (1) and B is a constant magnetic field. As in the above discussion, we shall deal with the case of a chain with two sites. Furthermore, only the case $J > 0$ will be considered, since similar results are found in the case of ferromagnetic Heisenberg interactions.

Let us first analyse the magnetic entanglement in the KN model at zero temperature. For $B = 0$, the ground state is given by Eq. (3) and the single-qubit concurrence is always 1, independently of the values of the parameters J and W. After the external magnetic field B is "turned on", the ground state suddenly changes, as B crosses a specific value, from Eq. (3) to

$$|0\rangle_{xy}^B = N_{xy}^B \left(\gamma_1(|---+\rangle - |--+-\rangle) - \gamma_2(|-+--\rangle + |+---\rangle) \right), \tag{7}$$

where N_{xy}^B is the normalization constant and the γ_i are functions of the parameters J and W. In this state, the single-qubit concurrence has a little decrease from 1 to a value which depends on J and W. For example, when $J = W = 1$, the value of the single-qubit concurrence is 0.989. By increasing the magnetic field to a critical value $B_c = B_c(J, W)$ the single-qubit concurrence vanishes, since the ground state becomes the fully unentangled state $|----\rangle$. Hence, for any fixed value of the parameter W, we obtain a critical line $B_c = B_c(J)$. Taking $J = W$, we can numerically interporlate the straight line $B_c \approx 1.707\, J$. We remark that the effect of the external magnetic field is the gradual alignement of all the spins in the chain, leading the ground state always to an unentangled state for a high value of B.

We now consider the thermal entanglement in the model by taking into account the presence of the magnetic field B. As discussed before, the increase of the temperature can rise the concurrence of AB due to the mixing of the ground state with some higher entangled excited states. In contrast, the concurrence for the pair AC is always decreased as the temperature is "turned on". However, when a magnetic field B greater than the critical value B_c is applied in the system, entanglement for the pair AC can considerably be generated as the temperature rises (for $J > 0$), as exhibited in Fig. 2. This is because, as B crosses B_c, the ground state of the two-site model suddenly changes from a highly entangled to an unentangled state. Hence, an increase in temperature can here produce entanglement also for the pair AC due to the mixing of the unentangled ground state with some entangled excited states. For $B > B_c$, as B approaches the critical field B_c, the content of entanglement which can be yielded with the increase of temperature becomes higher. Moreover numerical simulations point to the existence of a temperature for which entanglement is always destroyed indenpendently of the magnetic field applied. For $J = W = 1$, this temperature is given by $kT_c \approx 0.79$ (see Fig. 2) when we compute the concurrence for a Heseinberg coupled pair.

In conclusion, we have discussed the thermal and magnetic entanglement in the two-site KN Hamiltonian, which is a simple model for describing heavy fermion systems. Concerning the natural entanglement present in the model, we have studied how the concurrence for a pair of qubits is distributed according to the fundamental couplings of the theory. The effect of temperature and the presence of an external magnetic field applied in the z direction have also been analysed. These variables have been

shown to be adjustable to control the entanglement available in the system. In particular, it has been found a critical magnetic field $B_c(J,W)$ which separates phases exhibiting a completely different pattern of entanglement. Concerning the features of the model when a larger number of sites is taken into account, the results for the entanglement are qualitatively close to that obtained here for two-site KN ring [8]. In fact, this behavior seems to rest on the competition between the two couplings of the theory, which will take place independently of the number of sites considered.

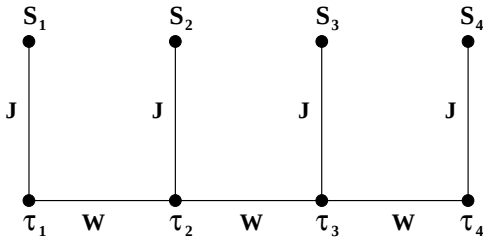


Figure 1: Schematic arrangement of the KN chain with four sites, with τ_i and S_i spin-1/2 operators.

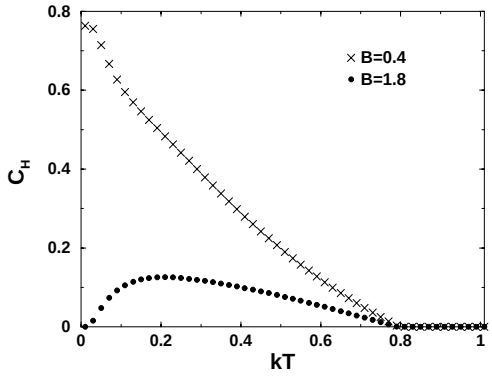


Figure 2: Thermal concurrence for the pairs of qubits coupled by antiferromagnetic Heisenberg interaction in the two-site KN model. The parameters J and W are set to 1.

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