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The Kondo necklace model with planar anisotropy

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ABSTRACT

We study the one-dimensional anisotropic Kondo necklace model at zero temperature through White's density matrix renormalization group technique. The ground state energy and the spin gap were calculated as a function of the exchange parameter for two anisotropy values. We found a finite critical point separating a Kondo singlet from an antiferromagnetic phase. The transition is highly congruent with a Kosterlitz–Thouless form. We observed that the critical point increases with the anisotropy.

1. Introduction

Strongly correlated electron systems are some of the most studied systems in condensed matter physics. Important examples are the heavy fermions, which in the last years have been the object of intense theoretical and experimental investigation. In these kinds of materials (like intermetallic compounds containing rare earths and actinides such as Ce, Yb and U), there are two different types of electronic states: the s, p and d orbitals, which correspond to conduction electrons that move through the lattice, and the inner f orbitals, in which electrons stay at low energies. The interaction between these electrons leads to two different effects, which compete between them to determine the magnetic behavior of the system. The first, known as the Kondo effect, is the screening of the localized magnetic moments (of f electrons) due to the conduction electrons, and generates a non-magnetic state by creating singlets along the system. The second, called the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction, is an indirect exchange between the spins of the localized electrons, mediated by the conduction electrons, and tends to establish an antiferromagnetic order.

One of the most important Hamiltonians that incorporate the competition mentioned above is given by the Kondo lattice model:

$$H_{KL} = -t\sum_{i,\sigma}(c^{+}_{i,\sigma}c_{i+1,\sigma} + \text{H.c.}) + J\sum_{i}\boldsymbol{S}_i\cdot\boldsymbol{s}_i, \tag{1}$$

where $c^{+}_{i,\sigma}$ ($c_{i,\sigma}$) is the creation (annihilation) operator of a conduction electron in site i, t is the hopping between nearest neighbors and J is the antiferromagnetic coupling between the localized spins ($\boldsymbol{S}_i$) and the spins of the conduction electrons ($\boldsymbol{s}_i$). In order to simplify the study of the magnetic behavior and keep only the spin degrees of freedom, neglecting the charge fluctuations, Doniach [1] proposed a different Hamlitonian, known as the Kondo necklace model:

$$H_{KN} = t\sum_{i}(s^{x}_{i}s^{x}_{i+1} + s^{y}_{i}s^{y}_{i+1}) + J\sum_{i}\boldsymbol{S}_i\cdot\boldsymbol{s}_i. \tag{2}$$

In this Hamiltonian, a nearest-neighbor XY interaction between $\frac{1}{2}$ spins tends to emulate the propagation of the conduction electrons. The coupling of conduction spins to localized ones is maintained, so it is expected that the competition between the Kondo effect and the RKKY interactions is still present. Materials such as $CeRh_2Si_{2-x}Ge_x$ [2] and $Ce_{1-x}La_xAl_3$ [3] can be understood on the basis of this model.

Many analyses have been made of the one-dimensional Kondo necklace model at zero temperature. Some of them found that a phase transition from the Kondo singlet state to the (quasi-long-range ordered) antiferromagnetic one takes place at a finite value of J (J_c), such as the study by Doniach [1] on the basis of mean field theory ($J_c = 1$), or the finite size scaling [4] by Santini and Sólyom ($J_c = 0.24$), consistent with a Kosterlitz–Thouless-like transition. Nevertheless, most approaches support the idea that any phase transition at finite couplings occurs (that is, the system is always in the singlet phase), as quantum Monte Carlo simulations [5], bosonization [6,7], density matrix renormalization group (DMRG) [6,8] and the bond operator method within mean field theory [9]. A Kosterlitz–Thouless tendency has also been suggested with this result [6,8].

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An anisotropy parameter in the *XY* interaction of (2) was first added by Saguia et al. [10] by means of the following Hamiltonian:

$$H_{AKN} = t\sum_i (s_i^x s_{i+1}^x + (1-\eta) s_i^y s_{i+1}^y) + J\sum_i (\boldsymbol{S}_i \cdot \boldsymbol{s}_i). \quad (3)$$

This model is important because real heavy fermion materials present anisotropic features; for example, the $\eta = 1$ case is useful to describe systems with a strong Ising character. Also, it is interesting to study its critical behavior, because there is no consensus among the results obtained for different approaches: using real-space renormalization group it was determined that, for $\eta > 0.58$, there was a phase transition at a finite J, and that for $\eta < 0.58$ the system was in the Kondo singlet phase for all non-zero values of J [10,11]. But recent studies have obtained different results. Using spin wave theory and a numerical Lanczos method, it was seen that there was always a phase transition for $\eta > 0$ [12], and applying the bond-operator method for one dimension, there was no evidence of transition at finite J for any anisotropy [13].

In the present paper, we try to clarify some aspects of the critical behavior of the anisotropic Kondo necklace model (3), calculating the spin gap for two η values as a function of J ($t = 1$ for simplicity) using the density matrix renormalization group [14–16]. We implemented a finite system algorithm for lattices of up to 100 sites, and kept up to 100 states. Our highest errors were on the order of 10^{-9}. In order to have a high degree of precision in the gap calculation, we used as target states the ground and first excited state of the superblock.

2. Results

In Fig. 1 the ground state energies per number of sites for $\eta = 0.2$ and 1.0 are shown (for a lattice of length $N = 60$). They decrease monotonically as J increases, and for large values of J they are very similar, tending to the isotropic Kondo necklace values, for example, at $J = 4.0$, E_0/N is -3.015, -3.013 and -3.008 for $\eta = 0$, 0.2 and 1.0, respectively. At smaller J values, where the gap has linear behavior (see below), the energies are quite different, so the result of including the anisotropy is appreciable even when the Kondo effect is more dominant in the system than the RKKY interactions.

We now study the spin gap Δ. This analysis is important since a finite value of the gap, which is defined as the energy difference between the states of total spin 0 (ground state) and total spin 1 (first excited state), is characteristic of the Kondo singlet phase and represents the needed energy to break a singlet and produce a triplet. The quantum critical point is that at which the gap becomes zero.

In Fig. 2 the gap is shown as a function of J for $\eta = 1.0$ in a 60 site lattice. In this case, for $J > 0.5125$ (approximately), the gap is linear. This indicates that for this range of J, the Kondo effect is more dominant in the system than the RKKY interactions. That is because when the singlets are independent, the energy needed to break one of them and create a triplet is just J, but if the singlets are nearly independent, we obtain that the spin gap is $\Delta \propto J$, with the proportionality constant close to 1. In fact, we found this constant to be 0.987. At $J \approx 0.5125$, the linear behavior of the gap is lost, so the RKKY interactions begin to dominate the system. So we can think of $J = 0.5125$ as the point at which a smooth crossover from Kondo to the RKKY regime begins.

As mentioned before, the RKKY interactions are not strong enough to generate the phase transition to the antiferromagnetic state in the one-dimensional Kondo necklace model (2). In the anisotropic model (3), this is not the case. For very small J, the gap oscillates with values smaller than 10^{-12} (which can be considered as 0). In order to give an estimate of the point at which

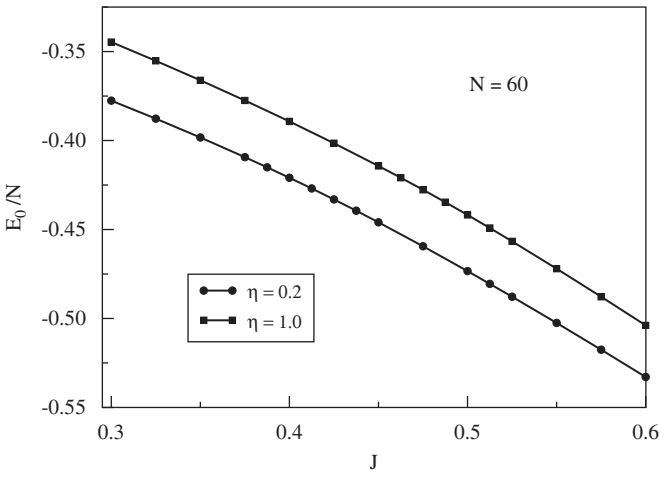

Fig. 1. Ground state energy per number of sites for $\eta = 0.2$ and 1.0. Here the lattice size is $N = 60$.

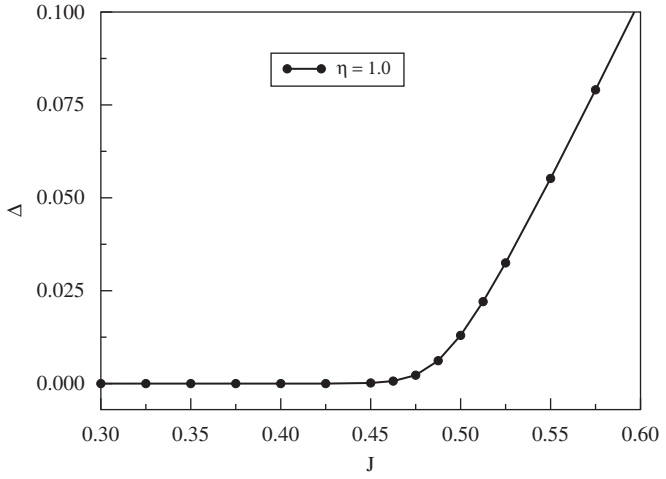

Fig. 2. The spin gap Δ as a function of J for $\eta = 1.0$. Here the lattice size is $N = 60$.

the gap becomes 0 (the critical point J_c), we assume a Kosterlitz–Thouless type transition, as was proposed in earlier works for the isotropic model. In such a case, the gap takes the following exponential form:

$$\Delta = A\ \exp[-b/(J - J_c)^s]. \quad (4)$$

In a Kosterlitz–Thouless transition, s is expected to be $\frac{1}{2}$. The best fit to the gap values of Fig. 2 was obtained with $J_c = 0.448$ and $s = -0.46$ (very close to $\frac{1}{2}$). Fixing s to this value we found, with almost the same correlation coefficient and smaller errors than before, $J_c = 0.445$, which is very close to the first value. We also got a better fit and smaller errors fixing b (for example, to 1) and including a prefactor to the exponential of the form J^d, obtaining a critical point close to the one already mentioned ($J_c = 0.4518$, $d = 0.50$). So the latter kind of behavior could be considered to describe the gap's approach to zero.

Following the gap tendency found by Reyes et al. [13] for two and three dimensions, we also fitted our gap values to a power law of the form

$$\Delta = a|J - J_c|^b, \quad (5)$$

with this behavior, and giving a determined value of the quantum critical points is a complicated task, since it is difficult to choose the best fit. The correlation coefficients were worse than the ones in the Kosterlitz–Thouless decay, and the errors were bigger.