Gap formation and phase transition of the anisotropic Kondo necklace model: Density matrix renormalization group analysis

J. J. Mendoza-Arenas, R. Franco, and J. Silva-Valencia*
Departamento de Física, Universidad Nacional de Colombia, Bogotá, Colombia
(Received 28 May 2009; revised manuscript received 21 October 2009; published 8 January 2010)

We analyze the one-dimensional Kondo necklace model, at zero temperature, with an anisotropy parameter η in the interaction of the conduction chain, by means of the density matrix renormalization group. We calculate the energy gap and estimate the quantum critical points that separate a Kondo singlet state from an antiferromagnetic state, assuming a Kosterlitz-Thouless tendency. We also observe the correlation functions and the structure factors that support our critical points. The resulting phase diagram is presented and compared to that reported previously using Lanczos calculations. It is shown that the quantum critical points vary very slowly with η, but when η approaches zero, they drop abruptly.

DOI: 10.1103/PhysRevB.81.035103 PACS number(s): 71.27.+a, 75.10.Pq, 75.30.Mb

I. INTRODUCTION

The magnetic properties of heavy fermion materials, such as their quantum phase transition between an antiferromagnetic ordered state and a nonmagnetic spin liquid (Kondo singlet) state, have been analyzed theoretically and experimentally using many methods.[1–3] These systems (intermetallic compounds containing rare-earth or actinide elements, such as Ce, Yb, and U) possess two types of electrons: the conduction electrons (in s, p, and d orbitals), which propagate through the lattice of the system, and the localized ones, which stay in the f orbitals for low energies. The coupling between these electrons generates two distinct effects: the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. The first consists of a screening of the localized magnetic moments by the conduction electrons, due to the formation of singlets, and favors the spin liquid phase. The second, which is an indirect exchange between the localized spins mediated by the conduction electrons, tends to establish the antiferromagnetic order. The interplay between these mechanisms determines the magnetic phase of the system.

In order to investigate heavy fermions and the properties described above, some theoretical models, like Anderson's and the Kondo lattice, have been exhaustively studied. These models contain charge and spin degrees of freedom, so their treatment is rather complicated. But it has been determined that the magnetic behavior mentioned above is driven by the spin degrees of freedom, not by the charge ones. In order to focus on the magnetic properties of the system, Doniach[4] introduced a simpler model that ignores charge fluctuations, and that maintains the interplay between the RKKY interaction and the Kondo effect. This model is called the Kondo necklace, and is characterized by the following Hamiltonian:

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

where $\vec{s}_i$ and $\vec{S}_i$ represent the spins of the conduction and localized electrons at site i, respectively, t is the hopping parameter, and J is the Kondo exchange coupling. The first term (XY interaction in the conduction chain) attempts to emulate the hopping of conduction electrons to their nearest neighbors, and the second term is the interaction between localized and conduction spins. The behavior of the system is determined by the ratio of both coupling parameters, J/t. The quantum critical point $(J/t)_c$ separates an antiferromagnetic phase [for $J/t < (J/t)_c$] from the spin liquid phase [for $J/t > (J/t)_c$]. Materials such as $CeRh_2Si_{2-x}Ge_x$,[5] $CeIn(Ag_{1-x}Cu_x)_2$,[6] and $Ce_{1-x}La_xAl_3$ (Ref. 7) seem to behave according to this model, modifying the value of J either by varying x or by applying external pressure.

The one-dimensional Kondo necklace model at zero temperature has been studied using several methods. First, Doniach[4] obtained $(J/t)_c = 1$ using mean field theory. Later, Santini and Sólyom[8] used finite size scaling and obtained $(J/t)_c = 0.24$. They also proposed that the phase transition was of Kosterlitz-Thouless type. Nevertheless, most approaches, such as quantum Monte Carlo simulations,[9] bosonization,[10,11] density matrix renormalization group,[10,12,13] bond-operator mean field theory,[14,15] and flow equation method[16] support the idea that no phase transition at finite couplings occurs [that is, the system is always in the spin liquid phase, $(J/t)_c = 0$]. A Kosterlitz-Thouless tendency has also been suggested for this case.[10,13]

According to the latter results, the physical behavior of the system is as follows: for $J/t \gg 1$, the coupling between neighboring sites is very small, and the ground state is made up of nearly independent spin singlets in each site. As J/t diminishes, the nearest neighbor interaction gets stronger and the Kondo effect loses importance. For $J/t \ll 1$, the RKKY exchange becomes the dominant interaction in the system, and the antiferromagnetic phase tends to be established, without success for finite coupling parameters, with a Kosterlitz-Thouless tendency.

In order to study the effect of anisotropy, Saguia *et al.*[17] introduced an anisotropic Kondo necklace model, which will be considered using the following Hamiltonian:

$$H_{AKN} = t\sum_{i=1}^{N} (s_i^z s_{i+1}^z + (1-\eta) s_i^y s_{i+1}^y) + J\sum_{i=1}^{N} (\vec{S}_i \cdot \vec{s}_i). \qquad (2)$$

This model takes into account an Ising-like anisotropy parameter η in the interaction of conduction spins. This pa-

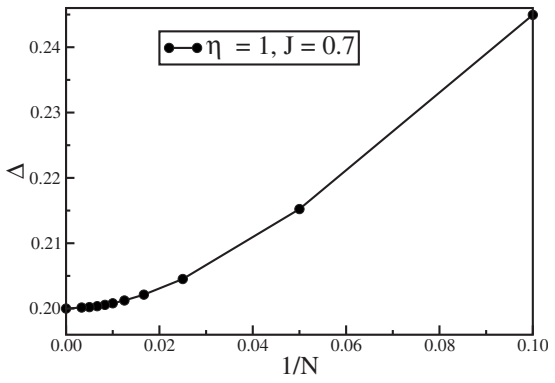

FIG. 1. Energy gap Δ for $J=0.7$, $\eta=1.0$, and different sizes of the chain. The solid line is a guide for the eye.

rameter takes values from $\eta=0$ (original Kondo necklace) to $\eta=1$ (full anisotropic case). Different results for the quantum critical behavior of this model (in one dimension, at zero temperature) have been obtained: using a real-space renormalization group[17] it was determined that for $\eta>0.58$, there was a phase transition at a finite J/t, and that for $\eta<0.58$, the system was in the Kondo singlet phase for all nonzero values of J/t. Using spin wave theory and a numerical Lanczos method for systems up to 24 sites,[18] it was seen that there was always a phase transition for $\eta>0$, and with the bond-operator method,[19] no transition at finite J/t for any anisotropy was found.

In this paper, we study the one-dimensional anisotropic Kondo necklace model (2) at zero temperature, using White's density matrix renormalization group (DMRG) method.[20–22] In Sec. II, we calculate the energy gap for several η values, and estimate the critical points J_c considering a Kosterlitz-Thouless tendency, and $t=1$ for simplicity. In Sec. III, we support our results with the correlation functions and structure factors. In Sec. IV we show the resulting phase diagram, and compare it to that of Mahmoudian and Langari.[18] The conclusions are presented in Sec. V.

II. ENERGY GAP STUDY

In order to analyze the anisotropic Kondo necklace Hamiltonian (2), we have implemented a finite system DMRG with open boundary conditions. Since, in general, the Hamiltonian (2) does not commute with the total spin in z direction, the algorithm was constructed without symmetries. In this case, we took the gap Δ as the energy difference between the ground state and the first excited state. To improve our calculation, both states were taken as targets. For a specific case, namely, $\eta=1.0$ and $J=0.7$, we have calculated the gap for different sizes of the chain N, from $N=10$ to $N=300$. These results are shown in Fig. 1. We also used the extrapolation method of Vanden Broeck-Schwartz[23] to estimate the value of the gap at the thermodynamic limit ($N\to\infty$), obtaining $\Delta=0.20000152$. We observe that for $N>100$, the gap varies very slowly, and that its corresponding value in the thermodynamic limit is close to that of 100 sites (difference of 0.4%), so to obtain values of the gap close to those of very large chains without a huge computational effort, we took $N=100$; because of the latter, we do not obtain the critical points with absolute certainty, but a close estimate to those when $N\to\infty$ is showed. As the anisotropy parameter η and the Kondo coupling J diminish, that is, as we get closer to the original Kondo necklace model and the RKKY interactions become stronger, more states are needed to preserve the order of the error; so in our code, we maintained $m=20$ states for high values of J and η, and $m=115$ for low values. Our highest errors were on the order of 10^{-7}.

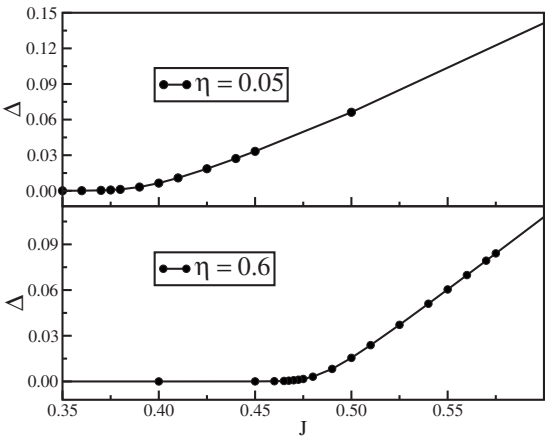

FIG. 2. Energy gap Δ as a function of J. For $\eta=0.05$. and $\eta=0.6$. The solid lines are guides for the eye.

In Fig. 2, the gaps for $\eta=0.6$ and $\eta=0.05$ as functions of J are presented; the solid lines are guides for the eye. They clearly fall to zero at finite values of J, which correspond to the quantum critical points J_c.

In order to estimate J_c for the different anisotropies η, we fitted the gap to the following exponential form, which corresponds to a Kosterlitz-Thouless transition:[24]

$$\Delta = A\ \exp[-b/(J-J_c)^{0.5}]. \tag{3}$$

We could consider the exponent s of $(J-J_c)$ as a variable, but it turned out to be very close to $\frac{1}{2}$, which is the expected case for a Kosterlitz-Thouless transition (for example, $s=0.46$ for $\eta=1.0$ and $s=0.50$ for $\eta=0.2$). In Fig. 3, we show the logarithmic tendency of the gap at $\eta=0.6$ near $J_c=0.4564(7)$, which is linear with $1/\sqrt{J-J_c}$ for points with small errors.

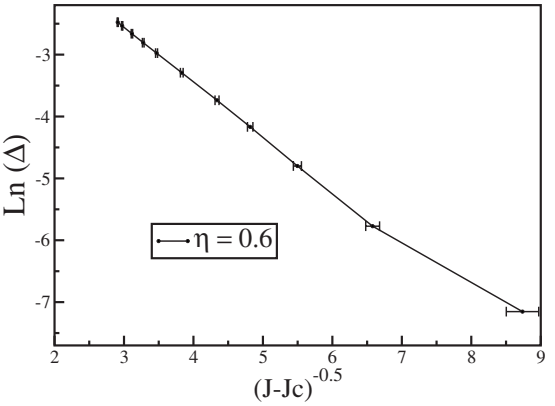

FIG. 3. Logarithmic tendency of the gap near J_c for $\eta=0.6$.

TABLE I. Critical points J_c obtained with a Kostelitz-Thouless decay for the gap.

η	1.0	0.8	0.6	0.4	0.2	0.1	0.05	0.01
J_c	0.4691(7)	0.4668(7)	0.4564(7)	0.439(1)	0.407(1)	0.381(1)	0.3544(9)	0.293(2)

This indicates that a Kosterlitz-Thouless decay corresponds well to the closing of the gap.

In Table I, we show the resultant critical values J_c for each η considered. We obtained very good fits (that is, we obtained regression correlation factors larger than 0.99994). We also were able to calculate J_c introducing some changes in the function (3). For example, we add prefactors to the exponential such as J^d, with d a constant, and fix b to some value [we take $b=1$, since the obtained b values in the fittings with Eq. (3) are close to 1]. In this case, the regression correlation factors are of the same order and, for $\eta>0.1$, the critical points don't change significantly. But for very small anisotropies, they are considerably larger: for example, for $\eta=0.01$, the critical point would be $J_c'=0.318$. This shows the difficulty of accurately establishing the critical points, but in any case, as we shall see in Sec. IV, the phase diagram keeps its main features if we choose the latter critical points instead of those reported in Table I.

Implementing a DMRG algorithm with symmetries for $\eta=1.0$ (full anisotropic model) and $\eta=0$ (original Kondo necklace), we found that for the former case, the gap Δ defined above is not a spin gap, whereas for the latter case it is, between sectors of total spin 0 and 1.

III. CORRELATION FUNCTIONS AND STRUCTURE FACTORS

We will now report our results for the correlation functions $\langle s_0^z s_i^z\rangle$, $\langle s_0^+ s_i^-\rangle$, $\langle S_0^z S_i^z\rangle$, and $\langle S_0^+ S_i^-\rangle$, with respect to the ground state of the superblock. Here, $s_0(S_0)$ denotes a conduction (localized) spin in the middle of the chain, and $s_i(S_i)$ another conduction (localized) one separated from the former i sites. We have calculated the correlation functions for $\eta=1.0$ and $\eta=0.2$ in systems of 60 sites, taking values of J around the critical points we obtained before. We also calculated the local correlation functions $\langle \vec{S}\cdot\vec{s}\rangle$ for each site, which on average tend to $-\frac{3}{4}$ at large J values (as well as for $\eta=0$).[13] For example, we obtained $\langle \vec{S}\cdot\vec{s}\rangle=-0.7487$ for $J=5.0$ and $\eta=1.0$. This was expected, since for large J the anisotropy η loses importance, the Kondo effect dominates the system and nearly independent singlets are established in each site.

In Fig. 4, we present our results for the z correlation functions of conduction spins $\langle s_0^z s_i^z\rangle$ for $\eta=1.0$, and in Fig. 5, we show their absolute values. For $J=0.6$ and $J=0.5(J>J_c)$, we found RKKY antiferromagnetic oscillations that decay rapidly as the separation i between spins increases. As J takes larger values, the oscillations decrease faster. This is expected, since the Kondo effect becomes stronger as J increases. This behavior is similar to that of the in-plane correlation functions found by Moukouri *et al.* for the original Kondo necklace model.[13] Also, for both J values, without taking into account the sites near the end of the chain, the decrease in the functions in Fig. 5 fits very well with an exponential decay. Otherwise, for $J=0.2$ and $J=0.4$, we don't perceive a decrease in the correlation functions at a glance (except for the last sites, which could be caused by finite size effects). But looking carefully at the obtained values, we can see that, in fact, the functions are always decreasing, although very slowly and not exponentially. This indicates a quasi-long-range antiferromagnetic order (in agreement with the Mermin-Wagner theorem). So, the conduction z-correlation functions are consistent with the reported critical point. This is also true for localized correlation functions $\langle S_0^z S_i^z\rangle$, which are equal to the conduction ones for every J that we considered. The planar correlation functions $\langle s_0^+ s_i^-\rangle$ and $\langle S_0^+ S_i^-\rangle$ are zero, even for nearest neighbors, indicating no correlations in x and y directions.

In Fig. 6, the z structure factor is presented, which, for a wave vector q, is given by

$$s^z(q)=\frac{1}{N}\sum_{j,l=1}^{N}\langle s_j^z s_l^z\rangle e^{iq(j-l)}, \tag{4}$$

with $N=60$ (the size if the chain) and

$$q=\frac{2\pi}{N}m, \quad m=0,\ldots,\frac{N}{2}. \tag{5}$$

For an antiferromagnetic order, it is expected that $s^z(q)$ diverges at $q=\pi$ when $N\to\infty$, so looking at the structure factor, we can obtain information about where this phase is present. The pronounced peak of $s^z(\pi)$ for $J=0.4$ and $J=0.2$ clearly indicates the existence of an antiferromagnetic phase there, while for the other J values, this can not be established. This is consistent with the critical point J_c found with the gap.

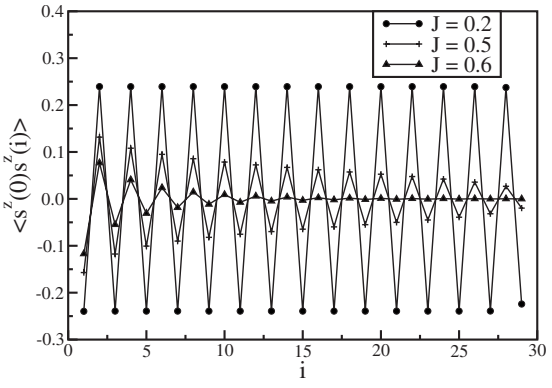

FIG. 4. z correlation functions of conduction spins $\langle s_0^z s_i^z\rangle$ for $\eta=1.0$; s_0^z corresponds to a conduction spin in the middle of the chain.

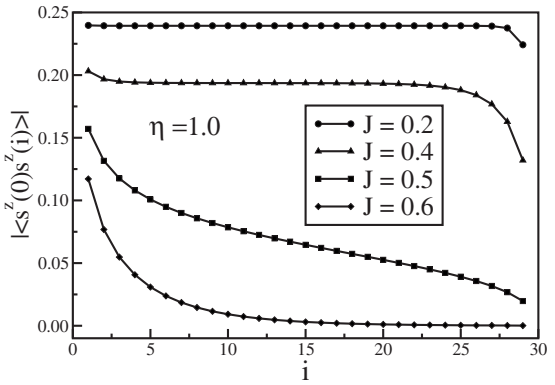

FIG. 5. $|\langle s_0^z s_i^z \rangle|$ for $\eta=1.0$.

In Fig. 7, the expected values for both spins ($\langle s^z \rangle$ and $\langle S^z \rangle$) are shown for $\eta=1.0$ and $J=0.2<J_c$, so we can see the antiferromagnetic configuration explicitly. As for the correlation functions, the absolute values for both types of spins are equal in magnitude.

For $\eta=0.2$, the z correlation functions and the corresponding structure factors show a behavior similar to those in the case for $\eta=1.0$, so they are not shown. These results are also in agreement with the critical point obtained with the gap: the z correlation function for $J=0.5$ decreases exponentially, and for $J=0.3$, decreases very slowly up to the sites near the end of the chain. Also, the structure factor $s^z(q)$ presents a pronounced peak at $q=\pi$ for $J=0.3$ indicating antiferromagnetism, while for $J=0.5$ this does not happen. So J_c seems to be between those values of J, as we found earlier. This time, the correlation functions are appreciably different for both types of spins, the magnitude for the conduction spins being smaller than the magnitude for the localized ones (Fig. 8 for $J=0.3$). Nevertheless, they have the same form, and give the same information about where the critical point could be. The expected values for conduction spins are also smaller than the ones for localized spins, but have the same configuration that is shown in Fig. 7. As J takes larger values, the difference between both types of spins diminishes, since the interaction in the conduction chain becomes less important. It is worthwhile to mention that neither for localized nor for conduction spins are the planar correlation functions different from zero for $\eta=0.2$, as can be seen in Fig. 9. Nevertheless, they do not give us any

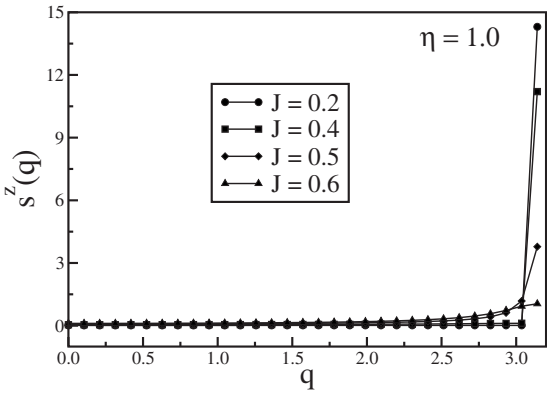

FIG. 6. z structure factor of conduction spins for $\eta=1.0$.

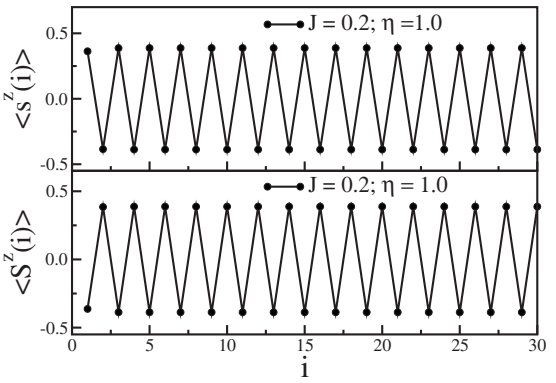

FIG. 7. Comparison between z expected values of conduction and localized spins, for $J=0.2$ and $\eta=1.0$.

information about the quantum phase transition, since they are very similar for $J=0.3$ and $J=0.5$. They tend very quickly to zero, and we can't even distinguish if the decay is exponential or a power law (both behaviors fit very well). The planar structure factors, defined by

$$s^{+-}(q) = \frac{1}{N}\sum_{j,l=1}^{N} \frac{1}{2}(\langle s_j^+ s_l^- \rangle + \langle s_l^+ s_j^- \rangle) e^{iq(j-l)} \tag{6}$$

and shown in Fig. 10, do not provide information about the transition either. They are very similar for both J values and do not present a sharp maximum at $q=\pi$. So, according to our results, the planar correlations do not allow us to identify a range in which the quantum phase transition could take place.

It is known that for systems undergoing a Kosterlitz-Thouless transition, besides the gap tendency of the form (3), the correlation functions $g(r)$ decay exponentially with the distance r above the critical point, and when the phase transition takes place, the decay changes to a power law of the form

$$g(r) \sim r^{-\delta}, \tag{7}$$

where $\delta=0.25$ at the critical point.[24] As already stated, the z correlation functions obtained fit very well with an exponential decay above J_c. For $\eta=1.0$, we have tried to establish if

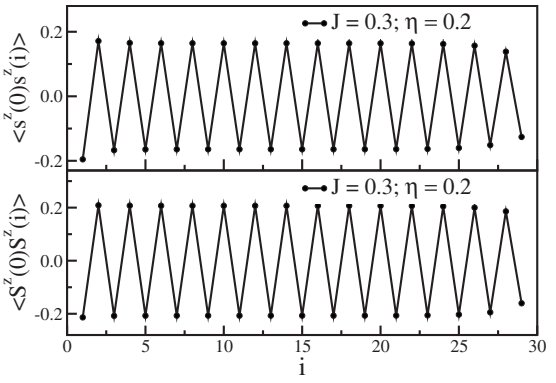

FIG. 8. Comparison between z correlation functions of conduction and localized spins, for $J=0.3$ and $\eta=0.2$.

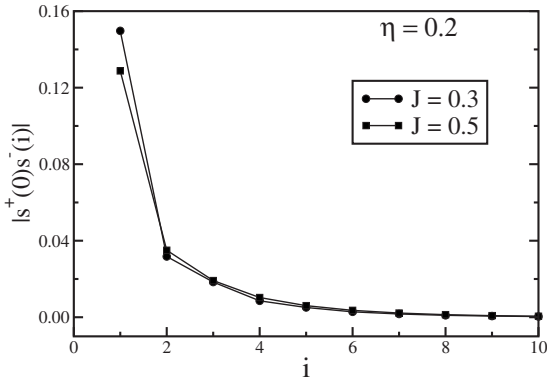

FIG. 9. $|\langle s_0^+ s_i^- \rangle|$ for η=0.2.

a behavior of the form (7) corresponds to the z correlation functions near the critical point found with the gap (excluding sites near the end of the chain). We obtained a value of δ=0.224 at J=0.49, somewhat close to the critical point. The finite size of the lattice considerably affects the behavior of the correlation functions (see Fig. 5), and also could be important for the gap values. So, in order to determine beyond doubt if the correlation function decays with δ=0.25 at the critical point and if the transition corresponds to a Kosterlitz-Thouless one, finite size effects should be reduced even more.

IV. PHASE DIAGRAM

In Fig. 11, we show the resulting phase diagram, which we constructed using the values in Table I. Below the line, the system is in the antiferromagnetic state, and above it, it is in the spin liquid phase. Qualitatively, this diagram is similar to that of Mahmoudian and Langari,[18] since we found a phase transition even for very small anisotropies [for example, J_c=0.293(2) for η=0.01], but their critical points are rather different from ours.

First, our J_c are larger for all anisotropies. Furthermore, for high η values, the critical line in Fig. 11 increases with η a little more slowly than the one obtained by Mahmoudian and Langari. For $0.01<\eta<0.1$, the increase we obtained is less abrupt than theirs, and for $\eta<0.01$ the rise is extremely

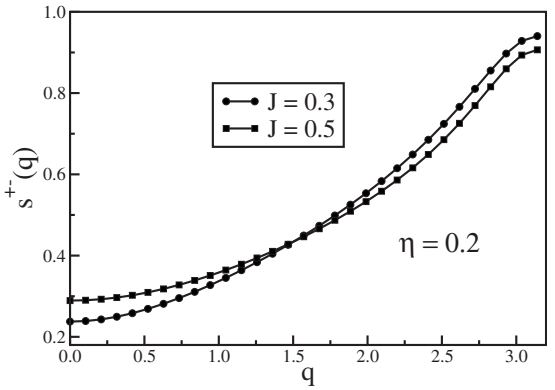

FIG. 10. Planar structure factor of conduction spins for η=0.2

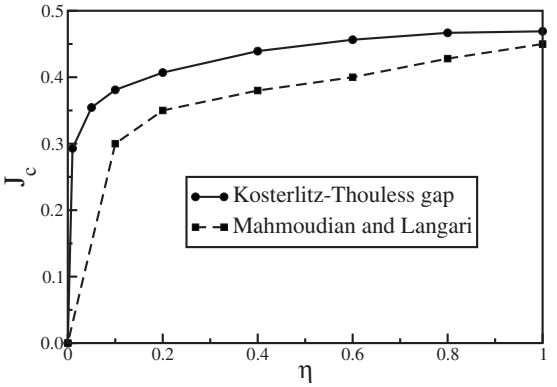

FIG. 11. Phase diagram for the anisotropic Kondo necklace model at T=0, compared to that of Mahmoudian and Langari.

sharp, since J_c=0 at η=0. Anyway, our results suggest that a quantum phase transition between antiferromagnetic and spin liquid states takes place at a finite critical point J_c for any $\eta>0$. As we said before, if we consider the prefactor J^d in the gap decay (3), the critical points change significantly for very small anisotropies, making the rise for lower η even sharper than before (since these values of J_c are larger than those of Table I). Nevertheless, the phase diagram still indicates that for any $\eta>0$ a phase transition occurs at finite coupling parameters, and that the increase in the critical line for $\eta>0.01$ is slower than the one Mahmoudian and Langari obtained.

V. CONCLUSIONS

Using the DMRG method, we have studied the one-dimensional anisotropic Kondo necklace model at T=0 for a long chain. Calculating the energy gap Δ as function of the Kondo coupling J for different anisotropies η, we have estimated the critical points J_c in which a quantum phase transition between quasi-long-range antiferromagnetic and spin liquid phases takes place. To do that, we assumed a Kostelitz-Thouless tendency for the vanishing of the gap. The results of the z correlation functions and the structure factors are consistent with the determined critical points. The gap and the correlation functions present features similar to what is expected in a Kosterlitz-Thouless transition. Our phase diagram is quantitatively different from that obtained by Mahmoudian and Langari for smaller systems,[18] the former showing a more abrupt tendency for small anisotropies and a slower variation for larger ones. Nevertheless, our diagram supports the idea that there is a quantum phase transition at a finite J for any $\eta>0$.

ACKNOWLEDGMENTS

The authors wish to thank the Bogotá Research Division (DIB) of the National University of Colombia. This work was also supported by the Projects No. DIB-8003295, No. DIB-8003255, and No. DIB-8003357. J.J.M.-A. wishes to thank the Mazda Foundation for Arts and Science for their economic support.

*jsilvav@unal.edu.co

[1] P. Gegenwart, Q. Si, and F. Steglich, Nat. Phys. **4**, 186 (2008).
[2] H. Tsunetsugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. **69**, 809 (1997).
[3] A. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, England, 1997).
[4] S. Doniach, Physica B&C **91**, 231 (1977).
[5] G. Godart, L. C. Gupta, C. V. Tomy, J. D. Thompson, and R. Vijayaraghavan, EPL **8**, 375 (1989).
[6] T. Hiraoka, T. Nobata, R. Hara, G. Nakamoto, and M. Kurisu, J. Magn. Magn. Mater. **177-181**, 383 (1998).
[7] R. Pietri and B. Andraka, Phys. Rev. B **66**, 224421 (2002).
[8] P. Santini and J. Sólyom, Phys. Rev. B **46**, 7422 (1992).
[9] R. T. Scalettar, D. J. Scalapino, and R. L. Sugar, Phys. Rev. B **31**, 7316 (1985).
[10] H. Otsuka and T. Nishino, Phys. Rev. B **52**, 15066 (1995).
[11] Y. Chen, Q. Yuan, H. Chen, and Y. Zhang, Phys. Lett. A **245**, 167 (1998).
[12] J. J. Mendoza-Arenas, R. Franco, and J. Silva-Valencia, Physica B **404**, 2868 (2009).
[13] S. Moukouri, L. G. Caron, C. Bourbonnais, and L. Hubert, Phys. Rev. B **51**, 15920 (1995).
[14] G.-M. Zhang, Q. Gu, and L. Yu, Phys. Rev. B **62**, 69 (2000).
[15] A. Langari and P. Thalmeier, Phys. Rev. B **74**, 024431 (2006).
[16] F. H. L. Essler, T. Kuzmenko, and I. A. Zaliznyak, Phys. Rev. B **76**, 115108 (2007).
[17] A. Saguia, T. G. Rapoport, B. Boechat, and M. A. Continentino, Physica A **344**, 644 (2004).
[18] S. Mahmoudian and A. Langari, Phys. Rev. B **77**, 024420 (2008).
[19] D. Reyes, M. A. Continentino, and H.-T. Wang, J. Magn. Magn. Mater. **321**, 348 (2009).
[20] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[21] S. R. White, Phys. Rev. B **48**, 10345 (1993).
[22] K. Hallberg, Adv. Phys. **55**, 477 (2006).
[23] J. M. V. Broeck and L. W. Schwartz, SIAM J. Math. Anal. **10**, 658 (1979).
[24] A. M. Tsvelik, *Quantum Field Theory in Condensed Matter Physics* (Cambridge University Press, Cambridge, England, 1998), Chap. 23.