Finite-size-scaling study of the gap formation in the "Kondo-necklace" model

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The "Kondo-necklace" model is studied by exact numerical diagonalization on finite chains up to $N = 12$ sites. The gap extrapolated to infinite systems can be well fitted by a Kosterlitz-Thouless-like form with a critical coupling $(J/W)_c = 0.24$. Although this value is appreciably smaller than the best estimate from real-space renormalization, our results indicate strongly a finite critical coupling in contrast to the one-dimensional Kondo lattice.

I. INTRODUCTION

Since the discovery of heavy fermion systems the periodic Anderson model (Anderson lattice) has been the subject of numerous studies using a variety of different approaches. This model is expected to describe the properties of such seemingly very different systems as mixed-valence compounds, heavy fermion systems, magnetically ordered materials or even superconductors. As general reviews see Refs. 1–3.

In this model at every site there are two kinds of electronic states, corresponding to d and f orbitals. The d electrons can propagate by hopping to neighboring sites, and they are hybridized to the f electrons on the same site. The f electrons, on the other hand, feel a strong on-site Coulomb repulsion U if there is another f electron of opposite spin on that site.

While in mixed-valence compounds the valence can fluctuate since the average number of f electrons on any site is not close to an integer due to the hybridization, in other cases, at least for high temperatures, a well-developed magnetic moment may exist. This could be the case in the limit when the energy ϵ_f of the f level lies deep in the Fermi sea so that the level is occupied, and at the same time U is large enough to prevent the occupancy of the site by another f electron that could compensate the spin of the first one. This is the Kondo lattice limit of the Anderson lattice.

In this model localized spins exist at every site and they are coupled to the band electrons. This system can be described by the Hamiltonian

$$H_{\mathrm{KL}} = -W\sum_{n,\alpha}(d^{\dagger}_{n,\alpha}d_{n+1,\alpha} + d^{\dagger}_{n+1,\alpha}d_{n,\alpha}) + J\sum_{n}[(d^{\dagger}_{n,\uparrow}d_{n,\uparrow} - d^{\dagger}_{n,\downarrow}d_{n,\downarrow})S^{z}_{n} + d^{\dagger}_{n,\uparrow}d_{n,\downarrow}S^{-}_{n} + d^{\dagger}_{n,\downarrow}d_{n,\uparrow}S^{+}_{n}], \quad (1.1)$$

where $d^{\dagger}_{n,\alpha}$ ($d_{n,\alpha}$) is the creation (annihilation) operator of a d electron at site n with spin α. The states of f electrons at site n are represented by the spin operator $\mathbf{S}_n$.

Although at every site there is a well-developed localized magnetic moment, the overall behavior of the system may be that of a magnetically ordered antiferromagnet or that of heavy fermions. For strong Kondo coupling J the local moments will form singlets with the conduction electrons. Any excitation that breaks these singlets will cost a finite energy and therefore there should be a finite gap in the excitation spectrum when the number of conduction electrons is equal to the number of localized spins (half-filled band). For general band filling or weaker coupling the f electrons (localized spins) screen each other producing a global Kondo singlet ground state. One of the most interesting problems in the study of the Kondo lattice is how this singlet state is formed in the weak coupling case and how the gap opens as J increases.

Analytic calculations for the Kondo lattice use quite often a $1/N$ expansion and the slave boson technique[4–6] or a variational approach with the Gutzwiller ansatz and Gutzwiller approximation.[7–9] Although these calculations give an overall picture, it is useful to have results by other methods. In the one-dimensional case numerical calculations are also possible, solving exactly the spectrum of a finite system and then trying to extrapolate to infinitely long chains. In the Anderson lattice both the d and f electrons can be in four different states at every site, making the Hilbert space very large even for a short chain. In the Kondo lattice, where the empty and doubly occupied f states are excluded, the Hilbert space is somewhat smaller, allowing us to study somewhat longer chains. The longest chains that have been studied by exact numerical diagonalization have $N = 6$ sites for the Anderson lattice,[10] and $N = 7$ sites for the Kondo lattice.[11] Monte Carlo simulations, either in the quantum projector version[12] or at finite temperatures[13,14] allow the study of longer chains.

A simplified version of the Kondo lattice, called "Kondo necklace," was proposed by Doniach,[15] where the number of states per site is reduced further, and therefore it is more amenable to numerical studies.

The Hamiltonian of the "Kondo necklace" is

$$H_{\mathrm{KN}} = W\sum_{n}(\tau^{x}_{n}\tau^{x}_{n+1} + \tau^{y}_{n}\tau^{y}_{n+1}) + J\sum_{n}\boldsymbol{\sigma}_{n}\boldsymbol{\tau}_{n}, \quad (1.2)$$

where both τ_n and σ_n are Pauli operators. The term with W should imitate the propagating d electrons, since it is equivalent after a Jordan-Wigner transformation to

a band of spinless fermions. These fermions interact with the localized spins $\boldsymbol{\sigma}_n$ via an antiferromagnetic spin-spin coupling. The main difference compared to the original Kondo lattice model is the absence of charge fluctuations. Since the essential feature of the Kondo lattice is the antiferromagnetic coupling of localized spins to itinerant electrons, it is expected that the main physical properties of the Kondo lattice are maintained in this model as well.

Doniach[15] himself solved the model in a simple mean-field approximation. He found two different regimes, depending on whether $J/W > 1$ or $J/W < 1$. In the first case the ground state is a singlet. In a mean-field approach this means that a singlet is formed at every site. A finite excitation energy is needed to break them. In the weak-coupling region, on the other hand, an antiferromagnetic long-range order has been found.

Soon afterwards the model has been investigated by real-space renormalization-group calculations.[16–18] It turned out that there is no long-range order in the weak-coupling case, only long-range correlations. The best estimate for the critical coupling is $(J/W)_c = 0.375$ from calculations with two-site clusters and $(J/W)_c = 0.382$ when using three sites. On the other hand, the same kind of calculation gives $J_c = 0$ for the Kondo lattice,[19] i.e., any positive Kondo coupling will always generate a finite gap.

Recently Scalettar, Scalapino, and Sugar[20] have studied the Kondo necklace by Monte Carlo simulations. They used chains up to $N = 16$ sites. Since this finite-temperature procedure is not very convenient to calculate the energy gap directly, they determined the spectrum indirectly from the correlation functions. They concluded that a gap seems to be present for any J, as in the Kondo lattice.

In this paper we present results obtained for the correlation functions and for the energy gap on finite chains using exact diagonalization. With the help of finite-size scaling and by analyzing the results obtained after extrapolating to infinite systems we will attempt to determine where and how the gap opens.

II. CORRELATION FUNCTIONS

We performed numerical diagonalizations of the Kondo necklace Hamiltonian for $N = 4, 6, 8, 10$, and 12 sites. The full Hilbert space for the Kondo necklace has dimension $D = 4^N$. However, the computational effort can be much diminished by exploiting all the constants of motion of H_{KN}. Obviously H_{KN} conserves the z component of the total spin $S^z_{\mathrm{tot}} = \sum_n (\tau^z_n + \sigma^z_n)/2$, and H_{KN} can be diagonalized separately within each S^z_{tot} subspace. The largest such subspace is the one corresponding to $S^z_{\mathrm{tot}} = 0$, which has dimension $(2N!)/(N!)^2$. Since H_{KN} is invariant under translations, a further reduction to block-diagonal form can be achieved by forming Bloch states with a given value of the total wave vector $K \in \{0, 2\pi/N, \ldots, 2\pi(N-1)/N\}$. In this way, the size of the greatest block to be diagonalized reduces roughly to $(2N!)/N(N!)^2$, which is about 225 000 for $N = 12$. Moreover, the matrices are highly sparse, and only a relatively small number of nonzero elements have to be kept in the computer memory. The diagonalization technique we used was the simultaneous (subspace) iteration method,[21] which permits us to find the ground state and a few excited states, and is particularly suited for sparse matrices. The accuracy of the procedure was checked by comparing with a standard diagonalization routine for N=6.

The ground state is found to have quantum numbers $S^z_{\mathrm{tot}} = 0$, $K = 0$, while the first excited state is in the subspace $S^z_{\mathrm{tot}} = \pm 1$, $K = \pi$ for all N and J/W. Owing to the lack of rotational invariance in the model, this excited state has no counterpart in the $S^z_{\mathrm{tot}} = 0$ subspace. This anisotropy clearly shows up in the correlation functions.

In the strong-coupling limit $J/W \gg 1$ a perturbational calculation can be performed by splitting the Hamiltonian as $H_{\mathrm{KN}} = H_0 + H_1$, where H_0 is the on-site coupling between the spins $\boldsymbol{\tau}_n$ and $\boldsymbol{\sigma}_n$ with strength J, and H_1 contains the hopping term with overlap W. Since the perturbational calculation goes in powers of W/J, the correlations between first, second, etc., neighbors build up successively. Up to second order this calculation gives the following nonzero transverse and longitudinal correlations:

$$\langle \sigma^+_n \sigma^-_{n+1} \rangle = -\frac{1}{2}\left(\frac{W}{J}\right) + \cdots, \tag{2.1}$$

$$\langle \sigma^+_n \sigma^-_{n+2} \rangle = +\frac{3}{16}\left(\frac{W}{J}\right)^2 + \cdots, \tag{2.2}$$

$$\langle \sigma^z_n \sigma^z_{n+1} \rangle = -\frac{3}{32}\left(\frac{W}{J}\right)^2 + \cdots. \tag{2.3}$$

We checked that in the large-J/W limit our numerical results agree with the predictions of perturbation theory.

In Figs. 1 and 2 we show the correlation between the transverse components of the localized spins σ at sites n and $n + i$ for the longest available chain with $N = 12$ sites. Using a periodic boundary condition the distance between the two spins can at most be six lattice spacings. As mentioned before and seen from the perturbational calculation, due to the anisotropy of the model the longitudinal correlations are much weaker than the

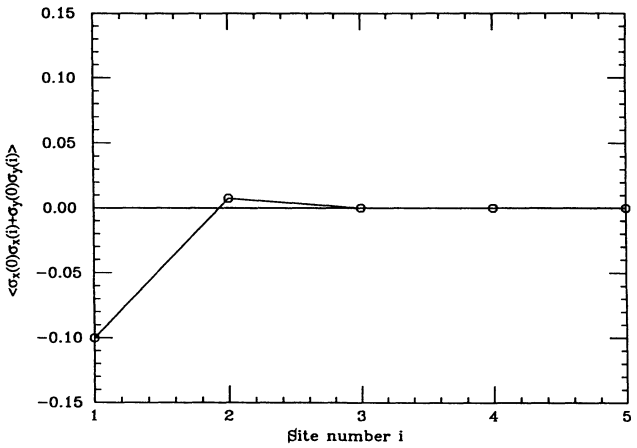

FIG. 1. Transverse correlation function between the localized spins σ_n and σ_{n+i} in a chain with 12 sites at $J/W = 5$.

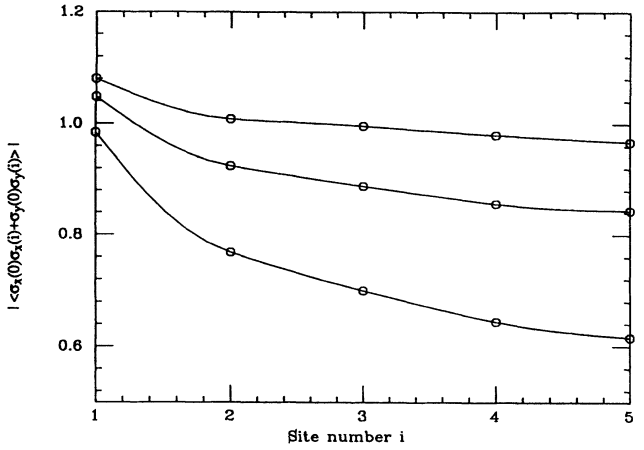

FIG. 2. The envelope of the transverse correlation function between the localized spins σ_n and σ_{n+i} in a chain with 12 sites for $J/W = 0.2$ (upper curve), $J/W = 0.3$ (center curve), and J/W=0.4 (lower curve). The lines connecting the values at integer i are only drawn as a guide to the eye.

transverse ones. The alternation in the sign of the correlation shows up in the transverse correlations only, therefore the longitudinal correlations are not given here. For large J/W, where the correlations are of short range, the envelope has a clear exponential fall-off with distance, signaling the presence of the singlet-triplet gap. These rapidly vanishing oscillating correlations are shown in Fig. 1 for $J/W = 5$. For decreasing J/W the correlations become of longer and longer range. We show in Fig. 2 the envelope of the transverse correlation function in that range of J/W, where the transition is expected to occur. When J and W become of the same order, on the length scale of our finite chain it is impossible to distinguish between an exponential and an algebraic decay of the correlations, since the correlation length gets larger than the chain size. Therefore, from the study of the correlation functions we cannot determine whether there is a critical $(J/W)_c$ where the exponential decay of correlations would change to power-law behavior due to the closing of the gap, even less whether this transition is of Kosterlitz-Thouless type. For this reason, rather than trying to determine the gap from the correlation functions, we calculated it directly from the excitation spectrum.

III. OPENING OF THE GAP

As mentioned before, a straightforward perturbational calculation can be performed on the model in powers of W/J. Since H_0 is the sum of independent on-site terms, singlets will be formed in the ground state on all sites. Their energy per site is $\epsilon_s = -3J$. The perturbation will mix this state to configurations where some of the sites are in the triplet state with energy $\epsilon_t = -J$. Up to second order in W/J the ground-state energy is

$$E_0/N = -3J\left[1 + \frac{1}{12}\left(\frac{W}{J}\right)^2 + \cdots\right]. \tag{3.1}$$

The first excited state of the unperturbed system will have one triplet site, while all other sites remain in the singlet state. Denoting by Ψ_n the state, where the triplet is on site n, a triplet wave can be formed by assuming the wave function of this state in the form

$$\Psi_k = \frac{1}{\sqrt{N}}\sum_n \Psi_n e^{ikR_n}. \tag{3.2}$$

Starting from this unperturbed state, the wave functions Ψ_k with different k will not mix and the energy of this state can be determined in nondegenerate perturbation theory. After subtracting the ground-state energy we obtain

$$E_k = 4J + 2W\cos(ka) - \frac{1}{4}\frac{W^2}{J}\cos(2ka). \tag{3.3}$$

The lowest-energy excitations are at the zone boundary and the gap is

$$\Delta = 4J\left[1 - \frac{1}{2}\frac{W}{J} - \frac{1}{16}\left(\frac{W}{J}\right)^2 + \cdots\right]. \tag{3.4}$$

Higher-order corrections could in principle be calculated similarly, but they will not help much to locate the point where Δ vanishes.

We have therefore calculated the gap Δ_N numerically exactly for finite systems with N sites. The results are shown in Fig. 3. In order to extrapolate to $N \to \infty$, we assumed first that the finite-size corrections can be described with three parameters in the following form:

$$\Delta_N = \Delta + \frac{A}{N} + \frac{B}{N^2}. \tag{3.5}$$

The extrapolated gap Δ was determined from the best fit to the calculated values.

Due to marginal operators the next-to-leading corrections may be logarithmic, instead of higher powers of N.[22] In the spin-$\frac{1}{2}$ Heisenberg model, near its Kosterlitz-Thouless-like transition the finite-size corrections are known to have terms of the form $1/N \ln N$.[23]

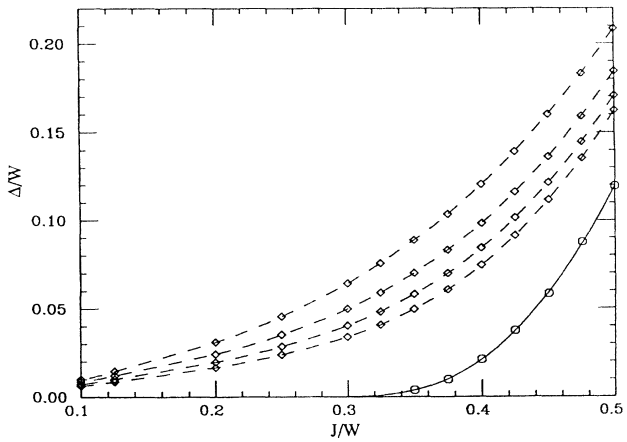

FIG. 3. Numerical values of the gap Δ_N for chains with $N = 6, 8, 10, 12$ sites are marked by squares. The gap decreases with increasing chain length. The extrapolated values for $N \to \infty$ are shown by circles.

We have therefore made another extrapolation by a four-parameter law

$$\Delta_N = \Delta + \frac{A}{N} + \frac{B}{N \ln N} + \frac{C}{N^2}. \tag{3.6}$$

The two procedures gave very similar values for Δ. They are also shown in Fig. 3.

Since the real-space renormalization-group calculations predict the transition to the gapless phase at around $J/W = 0.4$, in our study we concentrated on the region $0.2 < J/W < 0.5$. The calculated gap shows a rapid decrease from about 0.12 (in units of W) at $J/W = 0.5$ to 4×10^{-3} at $J/W = 0.325$ and a value of order 10^{-4} at $J/W = 0.3$. For $J/W < 0.3$ it oscillates around zero with very small values, which we interpret as the gap being smaller than the accuracy (around 10^{-5}) to which the eigenvalues were calculated.

That this effect is an artifact of the numerical calculations is clearly seen if we consider negative J/W values. In this region the model is expected to be in a gapless phase. In fact for $J/W = 0$ it reduces to the XY model, which is gapless. Negative J favors a triplet state formed by the spins τ_n and σ_n. In the limit $J/W \to -\infty$ these triplet spins can be rotated easily, so there will be no gap in the spectrum of spin excitations. For large negative J/W perturbation theory in W/J predicts a gapless excitation spectrum. Assuming that there is no phase transition for negative J/W, a gapless spectrum is expected for any intermediate negative J/W. Applying the numerical extrapolation procedure described above to the gap for $J/W < 0$, again actually very small oscillations around zero are found, showing that this is in fact a finite-size effect.

In order to try to establish the law that governs the opening of the gap, we considered only the values obtained in the region $0.35 \leq J/W \leq 0.5$. In this region the gap is much larger than the error in the numerical diagonalization, and, on the other hand, we should be near the critical point. Assuming that the transition is of Kosterlitz-Thouless type, the critical behavior of the gap is described by the usual exponential law with four parameters,

$$\Delta = A \exp[-b/(J - J_c)^s]. \tag{3.7}$$

This form was fitted to the extrapolated values of the gap. The best fit was obtained with $(J/W)_c = 0.24$ and $s = 0.63$. This value for the exponent s is very close to the expected value $s = \frac{1}{2}$. However, fits with error of the same order of magnitude may be obtained with $(J/W)_c$ in the range 0.21–0.28 and s between 0.4 and 0.7.

A somewhat worse fit could be obtained by assuming a simple power-law behavior for the gap, but in this fit, too, we had to allow for a finite value of the critical coupling. These fits give a $(J/W)_c$ of the same order as the earlier fit.

In finite-size scaling the critical coupling is usually located as the point where the scaled mass-gap ratio

$$R_{N,N+2} = \frac{(N+2)\Delta_{N+2}}{N\Delta_N} \tag{3.8}$$

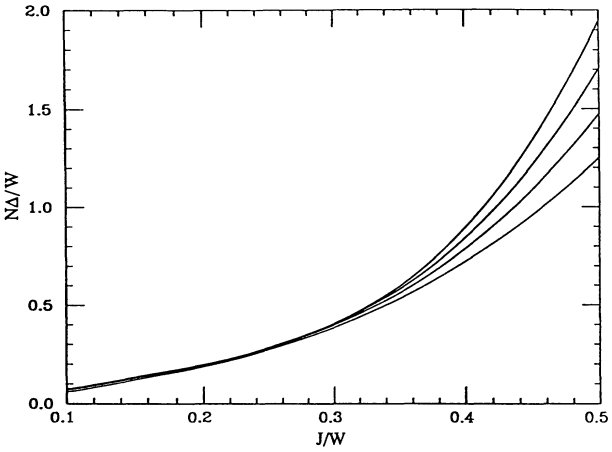

FIG. 4. The scaled gap $N\Delta_N$ for $N = 6, 8, 10, 12$. The scaled gap increases with the chain length.

is equal to unity. In our case this never happens. However, as seen in Fig. 4 the scaled gap $N\Delta_N$ shows a typical Kosterlitz-Thouless-like behavior. The scaled mass-gap ratio is very close to unity over a wide range of couplings, and starts to increase at a finite J/W. From this we cannot give a precise value for the critical point, but we can say with certainty that the transition takes place at a finite value of $(J/W)_c$.

IV. CONCLUSIONS

In this paper we have presented calculations for the opening of the gap in the Kondo necklace. Determining numerically the energy of the ground state and of the first excitation on finite systems, the results were extrapolated to infinitely long chains and then fitted to a Kosterlitz-Thouless-like behavior. Although there is some uncertainty in the value of the critical coupling, all our attempts indicate strongly that the critical value $(J/W)_c$ where the gap opens is finite. It is somewhat smaller than the value obtained in the real-space renormalization-group calculations, and is about a quarter of the value in mean-field theory.

In the Kondo lattice model the critical coupling is $J_c = 0$. The finiteness of the critical coupling in the Kondo necklace indicates that the charge fluctuations that are neglected in the Kondo necklace may play an important role to give the full behavior of the Kondo lattice. Therefore, the two models may not belong to the same universality class.

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