Correlation exponent K_ρ of the one-dimensional Kondo lattice model

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We present results for the correlation exponent K_ρ of the Tomonaga-Luttinger liquid description of the one-dimensional Kondo lattice as a function of conduction-electron density and coupling constant. K_ρ is obtained from the first derivative of the Fourier transform of the charge-charge correlation function. We also show that the spin correlation function can only be described in this picture if we include logarithmic corrections, a feature that had been previously overlooked. A consistent description of both charge and spin sectors is then obtained. Finally, we show evidence that the spin sector of the dimerized phase at quarter-filling is gapless.

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The Kondo lattice model is the simplest model believed to describe the low energy physics of heavy fermion materials.[1] Its one-dimensional version has been thoroughly studied in the last 10 years and a great deal of understanding has been gained. However, some outstanding issues remain, some of which may have implications in the higher dimensional cases. For example, the question of whether the localized spins should be counted in a Luttinger's theorem determination of the size of the Fermi momentum is still controversial.[2–6] Furthermore, even the phase diagram still presents some surprising phases: at quarter conduction electron filling the spins are dimerized and the charge sector is gapped.[7] The latter phase may be at the origin of the spin-Peierls phase observed in the quasi-one-dimensional organic compounds $(\mathrm{Per})_2M(\mathrm{mnt})_2$ ($M=\mathrm{Pt},\mathrm{Pd}$).[8] At a *generic incommensurate filling*, however, the system is gapless in both the spin and charge sectors and it is reasonable to assume[9] that it is a Tomonaga-Luttinger liquid (TLL).[10] In this paper, we will assume that this is the case. In an attempt to systematically characterize this behavior, we have determined the nonuniversal TLL exponent K_ρ as a function of coupling constant and conduction electron density. We found that a consistent picture of charge and spin sectors can be obtained, only if logarithmic corrections are included in the spin correlations. Moreover, we also show that the spin excitation spectrum of the quarter-filled case is gapless. We give arguments showing that the presence of dimerization and the absence of a spin gap are not mutually exclusive.

We considered the one-dimensional spin-$\frac{1}{2}$ Kondo lattice Hamiltonian with L sites

$$H = -\sum_{\substack{j=1 \\ \sigma=\pm1}}^{L-1} c^\dagger_{j,\sigma}c_{j+1,\sigma} + \mathrm{h.c.} + J\sum_{j=1}^{L} \mathbf{S}_j \cdot \mathbf{s}_j,$$

where $c_{j\sigma}$ annihilates a conduction electron in site j with spin projection $\sigma/2$, $\mathbf{S}_j$ is a localized spin-$\frac{1}{2}$ operator and $\mathbf{s}_j = \frac{1}{2}\Sigma_{\alpha\beta}\, c^\dagger_{j,\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{j,\beta}$ is the conduction electron spin density operator. $J>0$ is the Kondo coupling constant between the conduction electrons and the local moments and the hopping amplitude has been set to unity to fix the energy scale. We studied the model with the density matrix renormalization group (DMRG) technique[11] with open boundary conditions. We used the finite-size algorithm for sizes up to $L=120$ keeping up to $m=600$ states per block. The discarded weight was typically about $10^{-5}-10^{-8}$ in the final sweep.

TLLs with periodic boundary conditions and SU(2) symmetry have charge and spin correlation functions given asymptotically by[10]

$$\langle \delta n(0)\,\delta n(x)\rangle = \frac{K_\rho}{(\pi x)^2} + A_1\frac{\cos(2k_F x)}{x^{K_\rho+1}} + A_2\frac{\cos(4k_F x)}{x^{4K_\rho}}, \quad (1)$$

$$\langle \mathbf{S}^T(0)\cdot\mathbf{S}^T(x)\rangle = \frac{1}{(\pi x)^2} + B_1\frac{\cos(2k_F x)}{x^{K_\rho+1}}, \quad (2)$$

where $\delta n(x)=n(x)-\langle n(x)\rangle$, $\mathbf{S}^T(j)=\mathbf{S}_j+\mathbf{s}_j$, K_ρ is the nonuniversal charge correlation exponent and k_F is the Fermi momentum. Local charge perturbations, such as introduced by impurities or boundaries, induce density oscillations, called Friedel oscillations. In the case of a TLL, they take the form [3,4,12]

$$\langle \delta n(x)\rangle = C_1\frac{\cos(2k_F x)}{x^{(K_\rho+1)/2}} + C_2\frac{\cos(4k_F x)}{x^{2K_\rho}}. \quad (3)$$

The main goal of this work is to present K_ρ as a function of the conduction electron density and the Kondo coupling J for the one-dimensional Kondo lattice model. A previous work[4] determined K_ρ, but only for the density $n=\frac{2}{3}$. Besides, in that work, the authors argued that the system has a "large" Fermi surface, with $2k_F^L=\pi(n+1)\ (\mathrm{mod}\ 2\pi)$, not a "small" one with $2k_F^S=\pi n\ (\mathrm{mod}\ 2\pi)$. Indeed, under some assumptions, the presence of low-lying excitations with momentum $2k_F^L$ can be proved.[2] Assuming a "large" Fermi surface, the numerical results show that the dominant term in the charge Friedel oscillations is the second one in Eq. (3). From the decay of the envelope function of this term, K_ρ was determined at $n=\frac{2}{3}$.[4] However, more recent work has called into question the presence of a "large" Fermi surface, particularly for small J.[5] If the Fermi surface is small, both terms in Eq. (3) oscillate with the same period at $n=\frac{2}{3}$ and the envelope function method cannot be unambiguously applied. In order to avoid this ambiguity, we determined K_ρ from the first term in Eq.

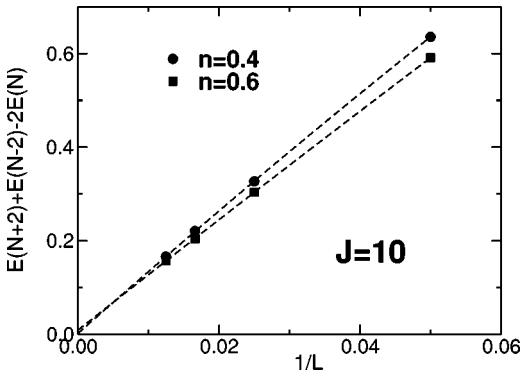

FIG. 1. Charge gap versus $1/L$ for $J=10$ and densities $n=0.4$ and $n=0.6$. Here, $E(N)$ is the ground state energy of the sector with N electrons. The dashed lines are fits to $\Delta_\infty + c_1/L + c_2/L^2$.

(1), or, equivalently, from the derivative of the Fourier transform of the charge-charge correlation function at $q=0$,

$$K_\rho = \pi \left. \frac{\partial C(q)}{\partial q} \right|_{q=0}, \tag{4}$$

where

$$C(q) = \frac{1}{L} \sum_{j,k} e^{iq(j-k)} \langle \delta n(j)\, \delta n(k) \rangle .$$

This method has been shown to give very accurate results by Daul and Noack.[13] These authors determined the exponent K_ρ (by the DMRG technique) for the one-dimensional Hubbard model and found good agreement with the exact results. For this reason, in the present work we will use this procedure to estimate the exponent K_ρ.

Haldane has conjectured that the TLL is the generic universality class of one-dimensional gapless systems.[14] Although a rigorous proof usually relies on the integrability of the model, renormalization group arguments confirm this conjecture in paramagnetic phases.[10] Much less is known about the case of systems with ferromagnetic ground states.[15] However, even in this case, the spin sector usually decouples from the charge sector and it is possible for the latter to remain a TLL. The one-dimensional Kondo lattice model is ferromagnetic for sufficiently large J.[16] In Fig. 1 we show its charge gap as a function of system size for $J=10$ (inside the ferromagnetic phase) and the densities $n=0.4$ and $n=0.6$. The extrapolated values suggest that the ferromagnetic phase, like the paramagnetic one, has no charge gap. Thus, it is quite natural to expect that, inside the ferromagnetic phase, the charge sector may also be described as a TLL and we will assume this to be the case. In fact, as we will see below, our results are consistent with this assumption. Note that this appears to happen also in the case of the Hubbard model with next-nearest neighbor hopping.[13]

We first focus on the general q-dependence of $C(q)$. In Fig. 2 we present the Fourier transform of the charge-charge correlation function for $n=0.8$, $L=40$, and several values of J. We have checked that the *qualitative* behavior of $C(q)$ presents no finite size effects, and also observed that the simple sum rule $C(0)=0$ is satisfied (within the accuracy of

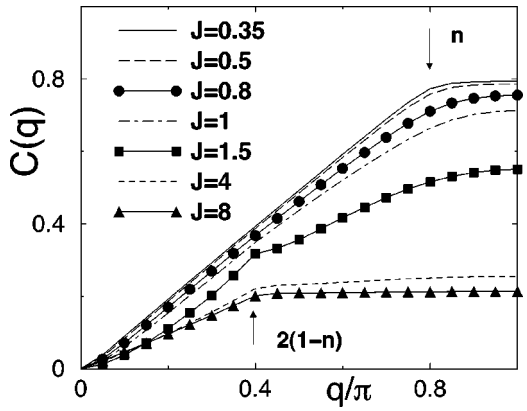

FIG. 2. Fourier transform $C(q)$ versus momentum for several values of J, $L=40$, and density $n=0.8$. The arrows indicate the position of the cusp.

the DMRG) for all values of density and Kondo coupling J shown. For small values of J and all densities, $C(q)$ increases linearly with q up to $q=\pi n$, and then saturates at $C(q)=n$ for $n<q/\pi<1$. On the other hand, for large Kondo coupling $C(q)$ increases linearly with q up to $q=2\pi n \pmod{2\pi} < \pi$ and then saturates at $C(q)=n\ (1-n)$ for $n<\frac{1}{2}$ $(n>\frac{1}{2})$ and $2\pi n \pmod{2\pi} < q < \pi$.

In order to get some insight into the behavior of $C(q)$ we consider free fermions with spin-S in a one-dimensional nearest-neighbor tight-binding lattice. In this case, the Fourier transform of the charge-charge correlation function $C_0^S(q)$ is

$$\frac{C_0^S(q)}{(2S+1)} = \begin{cases} q/2\pi, & 0 \leqslant q/\pi \leqslant 2m, \\ m, & 2m \leqslant q/\pi \leqslant 1, \end{cases} \tag{5}$$

where $m=\min[n/(2S+1), 1-n/(2S+1)]$. We will need two particular cases, with the restriction $n<1$. For spin-$\frac{1}{2}$ fermions

$$C_0^{1/2}(q) = \begin{cases} q/\pi, & 0 \leqslant q/\pi \leqslant n, \\ n, & n \leqslant q/\pi \leqslant 1, \end{cases} \tag{6}$$

while for spinless fermions, if $n<\frac{1}{2}$,

$$C_0^0(q) = \begin{cases} q/2\pi, & 0 \leqslant q/\pi \leqslant 2n, \\ n, & 2n \leqslant q/\pi \leqslant 1, \end{cases} \tag{7}$$

and if $n>\frac{1}{2}$,

$$C_0^0(q) = \begin{cases} q/2\pi, & 0 \leqslant q/\pi \leqslant 2(1-n), \\ 1-n, & 2(1-n) \leqslant q/\pi \leqslant 1. \end{cases} \tag{8}$$

Our results for $C(q)$ in the one-dimensional Kondo lattice model all tend to the free spin-$\frac{1}{2}$ case when $J \to 0$ (see Fig. 2), as expected. Besides, for $J \gg 0$, $C(q)$ tends to the $S=0$ case, $C_0^0(q)$. This is also to be expected, since in this case the conduction electrons form unbreakable mobile singlets with the localized spins, effectively behaving like spinless fermions.[16]

The cusp of $C(q)$ at $q=2k_F^S=n\pi$, for small values of J, is the signature that the charge density oscillations [Eq. (1)] are

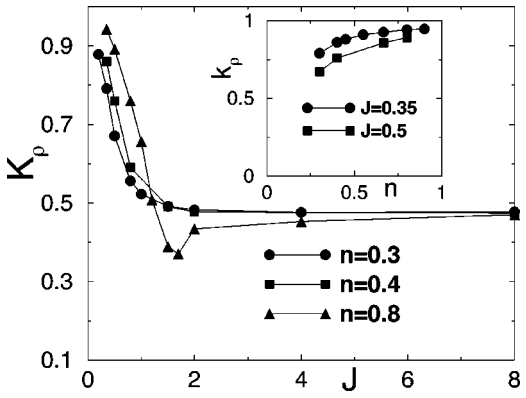

FIG. 3. The exponent K_ρ obtained with Eq. (4) as a function of J with $L=40$. The densities are indicated. Inset: K_ρ vs density for $J=0.35$ and $J=0.5$.

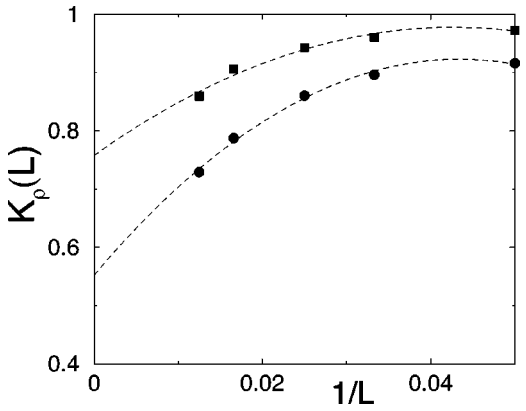

FIG. 4. The exponent K_ρ vs $1/L$ for $J=0.35$, $n=0.4$ (circles) and $n=0.8$ (squares). The dashed lines are fits according to Eq. (9), with $K_\rho=0.55$ (0.76), $a=17.0$ (10.3), and $b=-196.1$ (-120.5) for $n=0.4$ (0.8).

dominated by the $2k_F^S$ term. As we increase J the cusp moves to $q=2\pi n \pmod{2\pi}$. At first sight, this might seem like an indication that the system crosses over from a $2k_F^S$-dominated region to a $4k_F^S$-dominated one as J increases. Indeed, this is what happens in the Hubbard model when we increase the on-site repulsion U.[17] However, since $4k_F^S=2\pi n=4k_F^L \pmod{2\pi}$, the change might be due to a phase transition from a small Fermi surface to a large one.[6] Indeed, there have been indications of an intervening ferromagnetic phase at intermediate values of J,[18] which could give rise to this change. Unfortunately, the study of other (spin-spin) correlation functions has not shed any light on the issue:[5] the size of the Fermi surface for intermediate values of J remains an open question.

In Fig. 3 we show the exponent K_ρ calculated through Eq. (4) for several values of n and Kondo coupling J. For all densities we see that K_ρ tends to unity when $J\to 0$, in agreement with our expectation that the system tends to a noninteracting spin-$\frac{1}{2}$ electron gas with $K_\rho^0=1$. On the other hand, in the strong coupling limit $K_\rho\sim 0.5$, as expected for free spinless fermions [cf. Eqs. (4) and (7)]. We have observed that for densities $n>\frac{1}{2}$ and $J\sim 1.5$, K_ρ attains its smallest values. This is a region where charge oscillations are enhanced (see, e.g., Fig. 1 of Ref. 3). Actually, for some values of J and $n>\frac{1}{2}$ we were unable to determine K_ρ, as for example at $J=1.7$ and $n=0.9$. At these points, our data did not satisfy the simple sum rule $C(0)=0$, even increasing the truncation m up to $m=600$. The exponent K_ρ also did not converge as a function of m. A truncation of $m=600$ is more than enough to get precise values in other parameter regions. Typically, for small values of J and $L=40$, K_ρ obtained with truncations $m=400$ and $m=600$ differ by less than 5×10^{-2} and $C(0)\sim 10^{-4}$ with $m=400$. It is interesting to note that this region where the charge oscillations are strongest corresponds to the ferromagnetic phase at intermediate J.[18] For completeness, we also show in the inset of Fig. 3 the dependence of K_ρ on the density for $J=0.35$ and $J=0.5$ with $L=40$. As we can see, K_ρ decreases with increasing J.

Given this qualitative behavior of K_ρ as a function of J, we now set out to determine some quantitative values of the exponent. For this, we must be careful to take into account finite-size effects. In Fig. 4 we show K_ρ for the densities $n=0.4$ (circles) and $n=0.8$ (squares) as a function of $1/L$ at $J=0.35$. In order to incorporate the finite-size dependence, we determined the extrapolated exponent assuming that $K_\rho(L)$ behaves like

$$K_\rho(L)=K_\rho+a/L+b/L^2. \tag{9}$$

In Fig. 4 the dashed lines are fits to our data using Eq. (9). The exponents K_ρ obtained through the fits are 0.55 and 0.76 for $n=0.4$ and $n=0.8$, respectively. The values of K_ρ shown in the inset of Fig. 3 for small values of J and $L=40$ should be seen as upper limits. From the uncertainty of about 0.05 in the values of K_ρ for fixed L, we estimate the error in the extrapolated values to be $\lesssim 0.1$.

Now that we have accurately determined the exponent K_ρ we should be able to describe all correlation functions, since the only parameters needed are K_ρ and the Fermi momentum k_F [$K_\sigma=1$ because of SU(2) symmetry]. In particular, we can cross-check our results with the spin-spin correlation function [Eq. (2)]. Previous work showed that for small values of the Kondo coupling J the size of the Fermi surface is small,[5] so that k_F is fixed (see also Ref. 18). To eliminate the effect of the open boundaries on the spin-spin correlation function, we considered a large system and averaged the correlations over pairs of sites separated by a given distance j to get $\langle \mathbf{S}^T(0)\cdot\mathbf{S}^T(l)\rangle$, as discussed by other authors.[5,13,19] In Fig. 5, the circles correspond to this averaged spin-spin correlation function $P(l)=\langle \mathbf{S}^T(0)\cdot\mathbf{S}^T(l)\rangle_{aveg}$ for $n=0.4$ and $n=0.8$ at $J=0.35$ and $L=120$. We restricted the values to the interval $30\leqslant l\leqslant 90$, because the TLL description only makes sense asymptotically and large values of l may be compromised by the open boundaries. *A direct attempt at fitting the data of Fig. 5 with Eq. (2) yields $K_\rho<0$, which is clearly incorrect.* We believe the discrepancy is due to logarithmic corrections, which are well established in other models with SU(2) symmetry, e.g., the Heisenberg model.[20,21] Thus, assuming a generic form

$$\langle \mathbf{S}^T(0)\cdot\mathbf{S}^T(x)\rangle=\frac{1}{(\pi x)^2}+B_1\frac{\cos(2k_Fx)\ln^\alpha x}{x^{K_\rho+1}}, \tag{10}$$

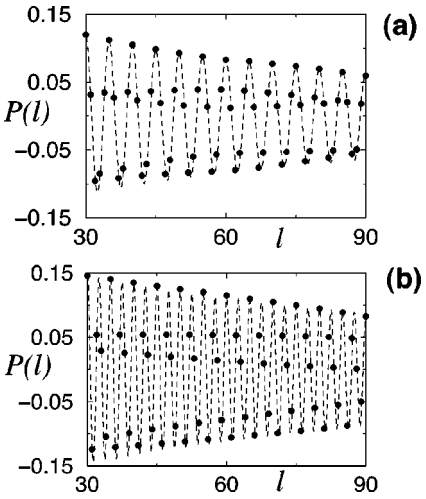

FIG. 5. The spin-spin correlation function for densities $n=0.4$ (a) and $n=0.8$ (b) ($J=0.35$ and $L=120$). The dashed line is a fit of Eq. (10) with $\alpha=4.0$ and $K_\rho=0.55$ for $n=0.4$, and $\alpha=5.1$ and $K_\rho=0.76$ for $n=0.8$.

we can produce an excellent fit to the numerical results *using the exponents K_ρ independently obtained before* and only two fitting parameters: $\alpha=4.0$ ($\alpha=5.1$) and $B_1=0.17$ ($B_1=0.11$) for $n=0.4$ ($n=0.8$). This is seen as the dashed line in Fig. 5. Logarithmic corrections thus appear to be crucial for a complete description of the spin correlations of the one-dimensional Kondo lattice model. As far as we know, this point has not been stressed before. We note that the above values of α differ from the expected values of $\frac{1}{2}$.[22] A more accurate determination of the exponent of the log correction may require much larger system sizes.

Finally, we would like to address the quarter-filled case, $n=\frac{1}{2}$, which has been shown to exhibit spin dimerization.[7] At this filling, the system has a charge gap and the charge sector cannot be described as a TLL.[7] Furthermore, since the spins are dimerized, we would naively expect a finite spin gap, as in the frustrated J_1-J_2 Heisenberg model.[23] We would now like to show that in fact the spin sector is gapless. In Fig. 6 we show the spin gap as a function of the lattice size L for $J=1.2$ and densities $n=0.5$, $n=0.8$, and $n=1.0$. We chose to work with a large J value in order to produce large spin gaps, since the spin gap generally increases with J. At half-filling, where the system is known to be fully gapped,[16] the data clearly tend to saturate at a nonzero value in the thermodynamic limit. By contrast, at $n=0.5$ and $n=0.8$ the data strongly indicate that the spin sector is gapless. Thus, the dimerized phase discovered in Ref. 7 has a charge gap but no spin gap. In that reference, the effect of dimerization in the localized spin subsystem on the conduction electrons was discussed. If we integrate out the local moments, an effective exchange interaction among the conduction electrons is generated. This is in a sense the "complement" of the RKKY interaction, which induces an effective exchange interaction between local moments once the conduction electrons are integrated out. This effective exchange interaction is proportional to the static spin susceptibility of the dimerized localized spins

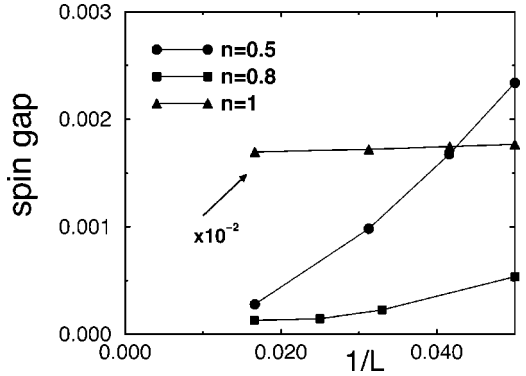

FIG. 6. Spin gap as function of $1/L$ for the densities $n=0.5$, $n=0.8$ and $n=1$ ($J=1.2$). The data for $n=1$ have been multiplied by 10^{-2} for comparison.

$$H_{eff} \sim J^2 \sum_{jk} \chi^l(j-k)\mathbf{s}_j \cdot \mathbf{s}_k. \tag{11}$$

If only nearest neighbor terms are retained, $\chi^l(j-k)=\delta_{j,k+1}D(j)$, where $D(j)\sim(-1)^j D_0$ is the dimer order parameter. This leads to a *staggered exchange interaction* between conduction electron spin densities

$$H_{eff} \sim \sum_j (-1)^j \mathbf{s}_j \cdot \mathbf{s}_{j+1}. \tag{12}$$

This kind of interaction can be analyzed through bosonization.[10] Among the many terms that are generated, those which involve combinations like $e^{-i4k_F x}\psi_R^\dagger(x)\psi_L(x)\times\psi_R^\dagger(x+1)\psi_L(x+1)$ will have just the right oscillating factor to cancel the $(-1)^j$ in Eq. (12), *since $4k_F=\pi$ at quarter filling*. One of the terms is $\sim\sin(2\sqrt{2}\phi_\rho)$ (in the notation of Ref. 10), which is relevant and opens a charge gap if $K_\rho<1$.[10] The DMRG results show that this condition is fulfilled throughout the phase diagram. Thus, the above analysis seems to be consistent with the presence of a charge gap. A term of the form $\sim\sin(2\sqrt{2}\phi_\sigma)$ is also generated. However, it is *marginal* if $K_\sigma=1$ and only generates a spin gap if the coefficient has the right sign. We conclude that the presence of a charge gap and the absence of a spin gap we find are consistent with the bosonization analysis.

In conclusion, we have presented a systematic study of the nonuniversal exponent K_ρ in the Kondo lattice model, as a function of the conduction electron density and the Kondo coupling. The qualitative behavior of the charge structure factor $C(q)$ in the weak and strong coupling limits could be ascribed to free spin-$\frac{1}{2}$ and spinless fermions, respectively. We also showed that the spin correlation function can be described within a Tomonaga-Luttinger liquid scheme only if logarithmic corrections are included. Finally, we have demonstrated that, although the charge sector has a gap at quarter filling, there are gapless spin excitations.

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