One-dimensional Kondo lattice model at quarter filling

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We revisit the problem of the quarter-filled one-dimensional Kondo lattice model, for which the existence of a dimerized phase and a nonzero charge gap had been reported by Xavier *et al.* [Phys. Rev. Lett. **90**, 247204 (2003)]. Recently, some objections were raised claiming that the system is neither dimerized nor has a charge gap. In the interest of clarifying this important issue, we show that these objections are based on results obtained under conditions in which the dimer order is artificially suppressed. We use the incontrovertible dimerized phase of the Majumdar-Ghosh point of the J_1-J_2 Heisenberg model as a paradigm with which to illustrate this artificial suppression. Finally, by means of extremely accurate density-matrix renormalization-group calculations, we show that the charge gap is indeed nonzero in the dimerized phase.

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I. INTRODUCTION

The Kondo lattice model plays an important role in the discussion of the physical properties of heavy fermion materials.[1] Therefore, an accurate determination of its properties and phase diagram is an important task. In this respect, even the one-dimensional case is of interest. Even though the Kondo lattice chain (KLC) has been extensively analyzed and much is known about its properties[2] (see also Ref. 3), a few controversies still remain.

A few years ago we and our collaborators presented mostly numerical evidence that the KLC has an insulating dimerized phase at quarter filling.[4,5] Our analysis was mainly based on numerical density-matrix renormalization-group (DMRG) calculations with open boundary conditions (OBC). More recently, Hotta and Shibata[6,7] (HS) raised objections to our conclusions and suggested that the KLC at quarter filling is neither dimerized nor exhibits a charge gap. They ascribed the putative errors to a lack of numerical precision and to a misinterpretation of the data. Their analysis is mainly based on modifications of the boundary conditions as compared to ours, either by using an odd number of lattice sites and/or by imposing a shift on the conduction-electron site energies at the borders or by working with periodic boundary conditions (PBC) and antiperiodic boundary conditions (APBC). Given these uncertainties and in view of the importance of this question, it is our hope to shed some light on the origin of these differences, while at the same time highlighting the intrinsic difficulties in a numerical determination of the presence of dimerization.

As we will show below, if we use an odd number of sites, a very careful interpretation of the data is necessary. We believe the discrepancy between our results and those from HS stems from this fact. In order to show this, we analyze a model with an incontrovertible dimerized phase, namely, the J_1-J_2 Heisenberg model at the Majumdar-Ghosh (MG) point and by reanalyzing the KLC at quarter filling in light of the latter results. Finally, we will also show extremely accurate DMRG data confirming the existence of a charge gap.

Before presenting our results, let us first discuss briefly the difficulties of determining numerically the presence of long-range order. Strictly speaking, a spontaneously broken symmetry can only be realized in the thermodynamic limit. Only in this limit is the order parameter nonzero. No continuous symmetry can be spontaneously broken at *finite* temperature in one and two dimensions with short-ranged interactions, as shown by the Mermin-Wagner-Hohenberg theorem.[8] At zero temperature, true long-range order is still possible for continuous symmetry in two dimensions, while in one dimension only quasi-long-range order can appear, i.e., the two point correlation function of the order parameter decays as a power law. However, a *discrete* symmetry can be broken at zero temperature even in one dimension. Such is the case of a dimerized phase, which can be characterized by a broken discrete lattice translational symmetry. Although the ordered phase is realized only in the thermodynamic limit, its signature can be observed in finite systems. One possibility is a finite-size scaling analysis of the order-parameter correlation function. For example, the Fourier transform of the spin-spin correlation function at the ordering wave vector $S(\vec{q}^*)$ can be studied as a function of system size in order to detect long-range magnetic order. If $S(\vec{q}^*)$ (appropriately normalized) tends to a constant as the system size grows, this signals the presence of long-range magnetic order. The analog in the case of dimerization would be the dimer-dimer correlation function. Another possibility is to measure the order parameter directly after the application of a small (infinitesimal) symmetry-breaking field. If the order parameter remains nonzero as the system grows, this is a sign of true long-range order.

Our previous calculations followed the second route above. Since we were interested in a possible broken lattice translation symmetry, we used the open borders as small symmetry-breaking fields. However, it is essential in this case that the lattice structure itself does not suppress the possible dimer order, e.g., by working with a lattice with an odd number of unit cells, which is unable to accommodate the two-site substructure of the dimer order. Other modifications of the boundaries can also be detrimental to the observation of dimerization. As we will show, this accounts for the discrepancies between ours and the results of HS. Furthermore, even when HS followed the first route, their results

will be shown not to be incompatible with the presence of dimerization.

It should be stressed that the numerical determination of long-range order is often quite difficult as one is never sure whether a larger lattice size will eventually show that an apparent order is actually destroyed at longer length scales. However, it is very important to work in such conditions as to allow the investigated order to at least be possible. As we argue below, in the case of a dimerized phase, extra care must taken not to frustrate the order from the start by working with an odd number of sites or by artificially altering the boundary conditions.

Given these uncertainties, we chose to show results for a system in which the dimer order is well established, namely, the J_1-J_2 Heisenberg model for $J_2 \gtrsim 0.24J_1$. By showing the pitfalls of a numerical determination of dimerization in this system, we hope to both shed light on the previous works on the Kondo chain and to bring to a more general audience what should be avoided in the investigation of broken lattice translational symmetry with numerical methods.

We investigated the models above with DMRG (Refs. 9 and 10) under OBCs. For the J_1-J_2 Heisenberg model we used typically $m=400$ states per block. This number of states kept in the truncation process is enough to give very precise results, the discarded weight being typically about 10^{-10}. However, for the KLC we used a much larger number of states in order to obtain precise results (up to $m=3500$). We have done $\sim 10-26$ sweeps and the discarded weight was typically $10^{-6}-10^{-10}$ in the final sweep. The dimension of the superblock in the last sweep can reach up to 27×10^6. This large dimension is due to the fact that the center blocks in our DMRG procedure are composed of eight states. As a consequence, keeping $m=3500$ states per block in the KLC is analogous to keeping $m'=4\times 3500$ states in the J_1-J_2 Heisenberg model.

This paper is organized as follows. In Sec. II, we will use the MG point of the J_1-J_2 Heisenberg model as a paradigm of a dimerized phase and important insight will be gained as to the effect of the use of an odd number of lattice sites. In Sec. III, we will analyze the KLC for both odd and even numbers of sites and will show that indeed our numerical results point to the existence of a true long-ranged dimerized phase at quarter filling. In Sec. IV, through extremely accurate DMRG calculations we will show that the charge gap is indeed larger than zero in the dimerized phase. Finally, we will present our conclusions.

II. MAJUMDAR-GOSH POINT

One of the best established examples of a dimerized phase occurs in the Heisenberg model with nearest-(J_1) and next-nearest-neighbor (J_2) interactions,

$$H=\sum_{j=1}^{L-1}(J_1\mathbf{s}_j\cdot\mathbf{s}_{j+1}+J_2\mathbf{s}_j\cdot\mathbf{s}_{j+2}),$$

where $\mathbf{s}_j$ is a spin-1/2 operator at site j. This model is known to show dimerization for $J_2/J_1\equiv\alpha>\alpha_c\approx 0.24$.[11–14] A particularly simple point of the dimerized phase is the MG point $\alpha=0.5$. The ground state of the infinite system can be shown to be composed of independent singlets formed out of neighboring pairs of spins.[15–17] This much simpler structure, as compared to $\alpha\neq 0.5$, corresponds to a correlation length of one lattice spacing for the connected dimer-dimer correlation function. Evidently, there are two equivalent ways of realizing the broken translational-symmetry ground state by choosing the dimers to lie on pairs which are one lattice spacing apart. The exact ground-state energy follows trivially from this structure and is given by $E_0/L=-3/8J_1$.

If the model is now analyzed on a finite lattice with an *even* number of sites and OBC, *one* of the two equivalent ground states can be easily accommodated, the other becoming now an excited state. However, for an *odd* number of sites and OBC, *none* of the above ground states can be realized, as the two-site substructure cannot be accommodated in an odd-sized lattice. In other words, the additional site frustrates the dimerization. This is not specific to the MG point but applies to *any* dimerized phase. The energies at the MG point can no longer be obtained exactly when L is odd, although some variational estimates can be made.[18] Below we show some energies obtained numerically for odd L. We note that for PBC (for which there is not explicit broken translational symmetry) and finite even L, the ground state is, in general, a superposition of the two equivalent broken-symmetry states and does *not* show spontaneously broken translational invariance. This is to be expected since symmetries can only be spontaneously broken in the thermodynamic limit. Note that for OBC the average nearest-neighbor spin-spin correlation $D(j)=\langle\mathbf{s}_j\cdot\mathbf{s}_{j+1}\rangle$ is not a constant (depends on j) for a *finite system* since translational symmetry is *explicitly* broken by the chain ends, which act effectively like small symmetry-breaking fields as $L\to\infty$.

Let us define the dimer order parameter as $|O_j|=|D(j)-D(j+1)|$. For OBC, the signature of a true long-range dimer order should be detected by plotting $|O_{L/2}|$ versus $1/L$. The dimer order exists if $\lim_{L\to\infty}|O_{L/2}|>0$ since the boundary-generated symmetry-breaking field becomes infinitesimal and the thermodynamic limit is enforced.

Let us first consider the J_1-J_2 Heisenberg model with an *even number of sites*. In Fig. 1(a), $D(j)$ is shown for the J_1-J_2 Heisenberg model with OBC for some values of α and $L=180$ [note that there are $L-1$ data points for $D(j)$ in an L-site lattice]. As we mentioned before, with OBC $D(j)$ oscillates. In particular, for the MG point ($\alpha=0.5$) $D(j)$ is 0 for even j and $-3/4$ for odd j, as expected. The fact that $D(j)$ exhibits a robust oscillation in the middle of the system suggests that a dimer order may exist. In order to establish the dimer phase, we now have to plot $|O_{L/2}|$ as a function of $1/L$. This is shown in Fig. 1(b), where we clearly see that the order parameter tends to a nonzero value only for $\alpha>0.2$. Though not intended to determine the critical value $\alpha_c\sim 0.24$, this plot shows that it is possible to numerically determine *the presence or the absence* of long-ranged dimer order using the second route mentioned before.

Now, let us investigate the same model with an *odd number of sites*. In Fig. 2(a), we present the average nearest-neighbor spin-spin correlation $D(j)$ at the MG point ($\alpha=0.5$) and at $\alpha=0.4$ as a function of j for odd system sizes with OBC. As expected, $D(j)$ oscillates. However, we clearly

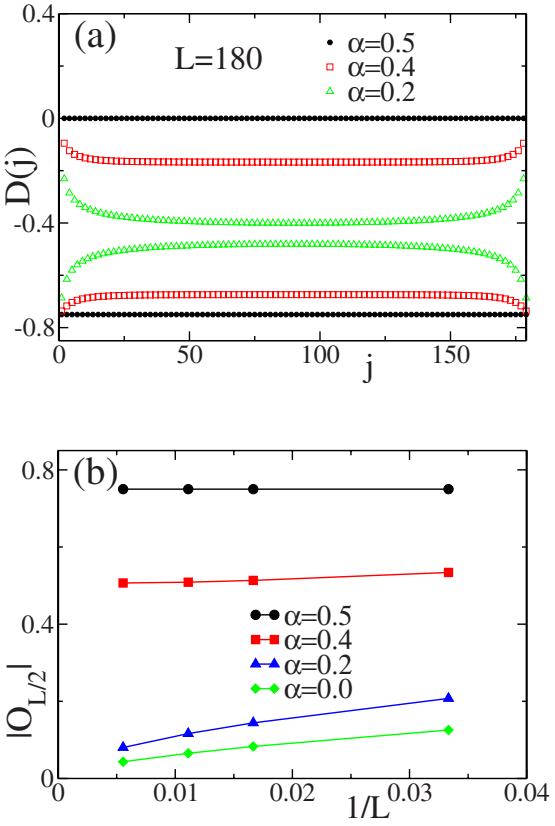

FIG. 1. (Color online) (a) The nearest-neighbor spin-spin correlation $D(j)$ versus distance from the lattice boundary for the J_1-J_2 Heisenberg model with $L=180$ and some values of α. (b) The dimer order parameter at the chain center $|O_{L/2}|$ as a function of $1/L$ for lattices with even numbers of sites for the same model.

see that this oscillation seems to vanish in the middle of the lattice. At first sight, this seems to suggest that in the thermodynamic limit $D(j)$ does not oscillate, indicating the absence of a dimerized phase in both cases. In order to check this, we present in Fig. 2(b) $|O_{(L-1)/2}|$ versus $1/L$ for odd L (only for the MG point). As can be seen, $|O_j|$ indeed tends to zero in the thermodynamic limit, indicating, at first thought, the absence of a dimerized phase. This result is in contradiction with the well-known dimerized phase of this model both at the MG point and at $\alpha=0.4$. How is it possible? The explanation lies in the frustration of translational-symmetry breaking induced by the last site of an odd-sized lattice, as explained above. In fact, the ground state at the MG point (and at $\alpha=0.4$) with an odd number of sites has a solitonic spin-1/2 excitation, which is delocalized and acts to suppress the dimer order.[18,19] An estimate of the ground-state energy at the MG point can be obtained assuming that the wave function for odd L is given by a free solitonic excitation.[18] In fact, numerical data support this picture.[19]

In Fig. 2(c), the ground-state energy per site, for odd and even L, is presented as a function of $1/L$ (only at the MG point). Clearly, the energy per site for odd L is larger than that for even L. This is due to the fact that there is a gap for the creation of the solitonic excitation. In Fig. 2(d), we show $\langle S_z(i)\rangle$ at the MG point and at $\alpha=0.4$ for a system size of $L=181$ (similar results were obtained in Ref. 19 for $L=101$).

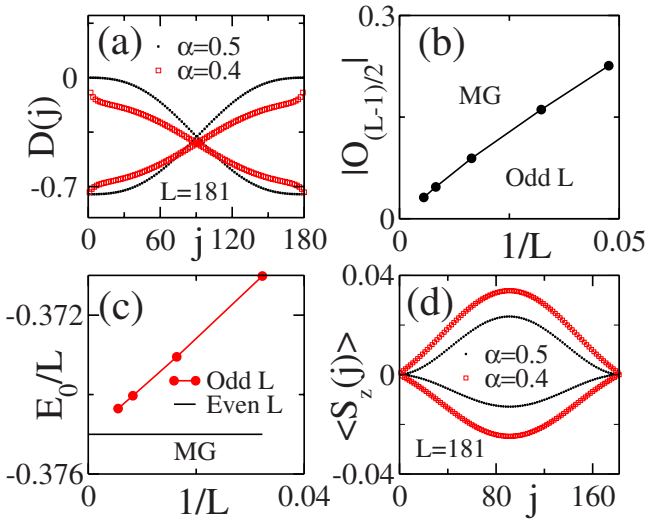

FIG. 2. (Color online) Some expectation values and energies for the J_1-J_2 Heisenberg model ($J_2/J_1\equiv\alpha$). (a) $D(j)$ vs distance from the lattice boundary for $L=181$ at the Majumdar-Ghosh point ($\alpha=0.5$) and at $\alpha=0.4$; (b) $|O_{(L-1)/2}|$ as a function of $1/L$ for lattices with odd numbers of sites at the MG point; and (c) the ground-state energy per site E_0/L vs $1/L$ for even and odd L at the MG point. (d) $\langle S_z(j)\rangle$ vs lattice site for $L=181$, showing the solitonic excitation, at the MG point and at $\alpha=0.4$.

The delocalization of the soliton is clear in both cases and its envelope can be modeled as a free quantum particle in a box of size L.[19] The soliton has a finite extent for $\alpha\neq 0.5$, due to the larger dimer correlation length, and this picture becomes less accurate.[19] As we argue in Sec. III, the frustration of the dimer order in an odd-sized lattice is the origin of the discrepancy between ours and HS's work.

III. DIMERIZATION IN THE QUARTER-FILLED KONDO LATTICE CHAIN

Having obtained some insight into the ground-state wave function at the MG point with an odd number of sites, we consider now the KLC with OBC given by

$$H=-\sum_{i=1,\sigma}^{L-1}(c_{i,\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})+J\sum_{j=1}^{L}\mathbf{S}_j\cdot\mathbf{s}_j,$$

where $c_{j\sigma}$ annihilates a conduction electron in site j with spin projection σ, $\mathbf{S}_j$ is a localized spin-1/2 operator, $\mathbf{s}_j=\frac{1}{2}\Sigma_{\alpha\beta}c_{j,\alpha}^{\dagger}\boldsymbol{\sigma}_{\alpha\beta}c_{j,\beta}$ is the conduction electron-spin-density operator, and $\boldsymbol{\sigma}_{\alpha\beta}$ are Pauli matrices. Here, $J>0$ is the Kondo coupling constant between the conduction electrons and the local moments and the hopping amplitude was set to unity to fix the energy scale.

In our previous work,[4] we showed that the KLC at quarter filling is dimerized from $\lim_{L\to\infty}|D(L/2)|>0$ for even L. Note that for the KLC, $D(j)$ oscillates in sign and, for this reason, we can use $D(j)$ as the dimer order parameter. In analogy to the MG point, we can destroy the dimerization by breaking the two-site substructure of the dimers. For example, we can add or remove just one site. In this case,

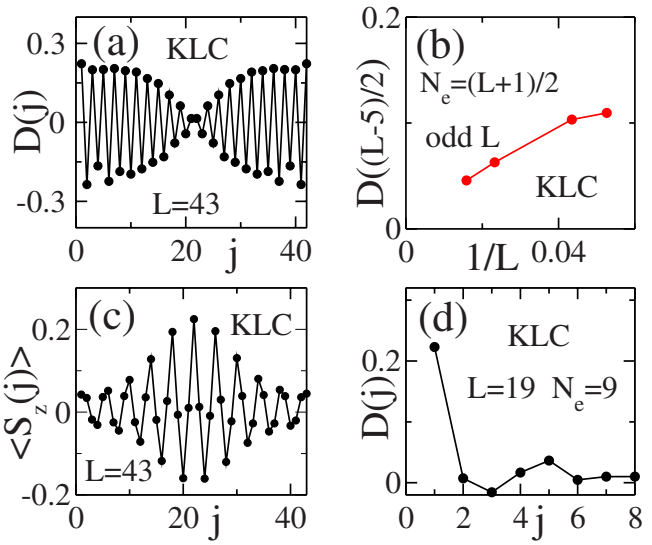

FIG. 3. (Color online) (a) The dimer order parameter $D(j)$ vs distance to the boundary for the KLC, $J=0.5$, $N_e=22$, and $L=43$ (only half the sites are shown). (b) The dimer order parameter at the chain center $\{D[(L-5)/2]\}$ as a function $1/L$ for odd L and the same parameters as in (a); (c) $\langle S_z(j)\rangle$ vs j for the KLC and the same parameters as in (a); and (d) same as (a) but for $L=19$ and $N_e=9$.

keeping the electronic density as close as possible to quarter filling, the electronic densities are $n=\frac{1}{2}\pm\frac{1}{2L}$. For odd L the ground-state total spin is not zero. If the number of conduction electrons N_e is even, it is 1/2. On the other hand, for odd N_e the total spin of the ground state is 1(2) if $L=2N_e-1$ ($L=2N_e+1$). It is interesting that if we keep the lattice size even and add or remove just one electron in the conduction band, we may also destroy the dimerization, as will be discussed below.

In Fig. 3(a), the order parameter $D(j)$ is shown as a function of the distance to the boundary for the KLC with $J=0.5$ and $N_e=\frac{L+1}{2}$. As in the case of the MG point, the order parameter seems to decrease away from the boundary. This result suggests that the dimerization does not exist in the thermodynamic limit for the KLC with odd L. Indeed, as shown in Fig. 3(b), the dimer order parameter measured at the center of the lattice tends to zero as we increase the system size. We also show in Fig. 3(c) $\langle S_z(j)\rangle$ as a function of the lattice site. Note the similarity with the MG point [Fig. 2(d)]. These results suggest that the ground state of KLC with odd L also possesses a solitonic excitation, as at the MG point with odd L. If L is odd and $N_e=\frac{L-1}{2}$ the dimer order parameter decays much faster away from the edges, as can be seen in Fig. 3(d) for a representative set of data. Although the energy converges quite rapidly in this case, the convergence of the correlations is slower, and for this reason we restrict our results to "small" lattice sizes.

For even L and odd N_e the total spin of the ground state is 3/2. For even L and $N_e=\frac{L}{2}+1$, the dimerization also seems to decay away from the boundary, although it does so in an oscillatory fashion, as seen in Fig. 4(a). One would perhaps naively think that also for $N_e=\frac{L}{2}-1$ and even L the dimerization might not exist. However, as shown in Fig. 4(b), the order is robust in this case. It is likely that the solitons are localized at the boundaries in the case of $N_e=\frac{L}{2}-1$.

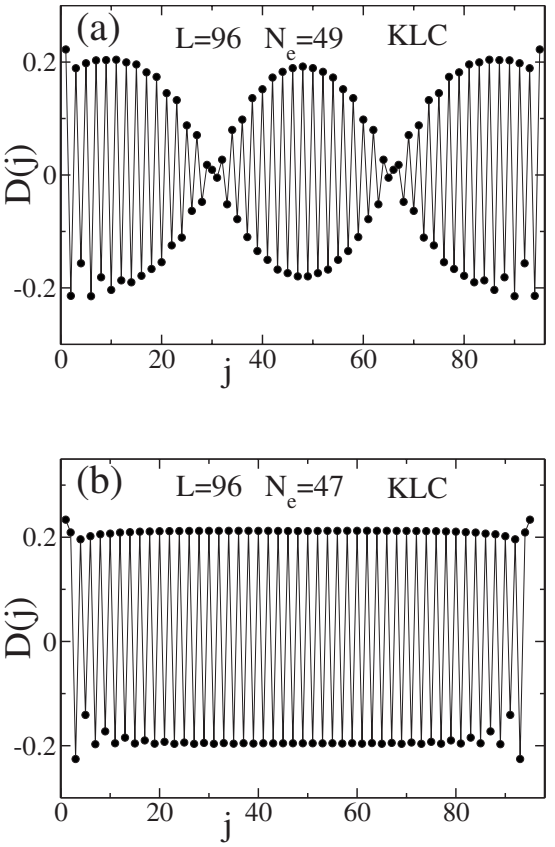

FIG. 4. The dimer order parameter $D(j)$ vs distance to the boundary for the KLC and $J=0.5$: (a) $L=96$ and $N_e=49$ and (b) $L=96$ and $N_e=47$.

IV. CHARGE GAP IN THE KONDO LATTICE CHAIN

Finally, we investigate the charge gap of the KLC at quarter filling. We define the charge gap as $\Delta=E(N+2)+E(N-2)-2E(N)$, where $E(M)$ is the ground-state energy for M conduction electrons. In our previous work[4] we presented numerical results with DMRG keeping $m=800$ indicating that there exists a finite charge gap at quarter filling in the thermodynamic limit. We also used bosonization arguments to show that if the KLC has a dimerized ground state at quarter filling, then a charge gap could exist. However, Hotta and Shibata[7] raised objections to our previous results arguing for a lack of precision in our numerical data for the coupling value $J=0.5$. It should be stressed that these authors only showed results for $J=1$ (and $m=1100$). Here, we present new DMRG results, keeping up to $m=3500$ states, showing that their objections are unfounded.

In Fig. 5(a), the charge gaps for coupling constants $J=0.6$ and $J=0.5$ are shown as functions of $1/L$ for two different values of m. As can be observed, there is very little difference between the charge gaps $\Delta_L(m=3500)$ and $\Delta_L(m=2000)$. We also show a fit of our data with $m=3500$ with the function $\Delta_L=\Delta_\infty+a_0/L+a_1/L^2$. The charge gaps clearly tend to a nonzero value. Our fit gives $\Delta_\infty=0.070$ and $\Delta_\infty=0.072$ for $J=0.6$ and $J=0.5$, respectively. However, HS did

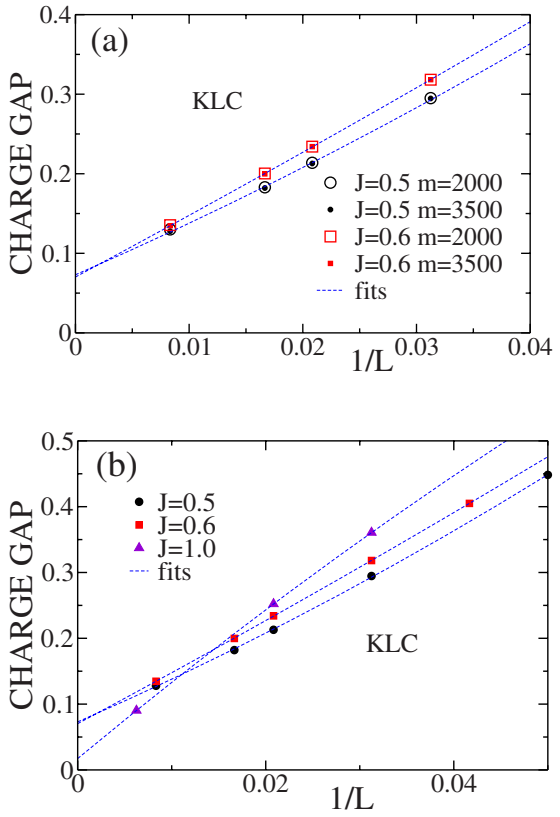

FIG. 5. (Color online) Charge gaps Δ for the KLC at quarter filling. (a) Δ vs $1/L$ for $J=0.5$ and $J=0.6$ and two values of the DMRG truncation m. The dotted lines are fits (see text for details). (b) Δ vs $1/L$ for $J=0.5$, 0.6, and 1.

not present results for $J=0.5$ or $J=0.6$ where the charge gaps are expected to be larger than for $J=1$ since the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction which we argued induces the dimerization[4] is expected to dominate the "Kondo effect" for small J. Indeed, this is what we obtain [see Fig. 5(b)]. The results of Hotta and Shibata[7] are confined to $J=1$, where the charge gap is quite small as we see in Fig. 5(b). Finally, the extrapolations for densities away from half-filling presented in our previous papers give $\Delta_\infty < 0.002$, which are much smaller than the charge gaps found for quarter filling and beyond our precision.

V. CONCLUSIONS

In the above, we have shown how an uncritical finite-size analysis can lead to wrong conclusions in the incontrovertibly dimerized phase of the MG point. A very similar situation was found in the case of the quarter-filled KLC, where very different results are obtained for even and odd numbers of lattice sites. This shows how care must be taken in a numerical determination of dimerization, especially with the number of sites and the boundary conditions.

In their work, HS used different boundary conditions (OBC and APBC), odd and even numbers of sites, and even modified the site energies at the edges of the chain.[6,7] As argued above, any of these *ad hoc* changes can severely affect the dimer order and in many cases suppress it to zero. The use of OBC with an even number of sites, thus commensurate with a possible dimerized substructure, is an unbiased way of probing the long-range nature of the broken lattice translational symmetry in the thermodynamic limit.

Another unbiased strategy is the investigation of the long-distance behavior of the dimer-dimer correlation function $C(i-j) \equiv \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_j \cdot \mathbf{S}_{j+1}) \rangle$ with PBC and even L. This procedure is much less convenient in a DMRG calculation since the DMRG is much less efficient under PBC or APBC and one is thus confined to small system sizes. HS showed also results under APBC. Although we are not certain whether the additional phase introduced under APBC suppresses dimerization or not, it is clear that their results are fully compatible with a dimerized ground state. Indeed, for $J=1$ and $L=120$ our calculations give a dimer order parameter $|\langle d(j) \rangle| = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle| \approx 0.128$. This corresponds to $|\langle o_j \rangle| \equiv |\langle d(j) - d(j+1) \rangle| \approx 0.256$ and to $\lim_{|i-j| \to \infty} |\langle o_i o_j \rangle| = |\langle o_i \rangle|^2 \approx 0.066$. It can be seen from the data reported by HS (Refs. 6 and 7) that the asymptotic behavior of their dimer-dimer correlation function seems to be just converging to about this value for $L=32$ and APBC. Thus, although it is hard to say whether they have reached the asymptotic bulk value, their results for APBC are certainly not incompatible with true long-ranged dimer order. It would be interesting to investigate this question under PBC and larger system sizes in order to have a complete picture. Unfortunately, with the DMRG this may well turn out to be impossible with currently available computer power.

Finally, we have also shown that even the most accurate DMRG calculations ($m=3500$) point to the existence of a nonzero charge gap at quarter filling. HS confined their results to the $J=1$ case (and $m=1100$), where this gap is very tiny (also from the $m=3500$ results), which makes the analysis more difficult. By working at smaller coupling-constant values, we were able to accurately extrapolate to the thermodynamic limit and found that the charge gap indeed tends to a nonzero value.

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