Absence of a true long-range orbital order in a two-leg Kondo ladder

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(Dated: March 23, 2022)

PACS numbers: 71.10.Pm, 75.10.-b, 75.30.Mb

We investigate, through the density-matrix renormalization group and the Lanczos technique, the possibility of a two-leg Kondo ladder present an incommensurate orbital order. Our results indicate a staggered short-range orbital order at half-filling. Away from half-filling our data are consistent with an incommensurate quasi-long-range orbital order. We also observed that an interaction between the localized spins enhances the rung-rung current correlations.

I. INTRODUCTION

In 1985, it was observed that the heavy fermion superconductor $URu_2Si_2$ presents a second order phase transition at $17.5\,K$. This phase transition is characterized by sharp features in the specific heat and several others thermodynamic properties (see, e.g., Ref. 2 and References therein). The large entropy loss associated in this phase transition is equivalent to an ordered moment of about $0.5\mu_B$. However, the size of staggered moment measured by neutrons scattering measurements is $m \sim 0.03\mu_B$. The order parameter associated with this phase transition is, at the present moment, not established and it is challenging to discover the nature of the hidden order behind the transition.

Many theoretical groups have proposed several kinds of hidden order. But, until now, experiments were not able to establish which is the correct one. Certainly, also from the theoretical point of view, more studies are needed to clarify the correct order associated with this mysterious phase transition. In this front, we present here a numerical study of a microscopic model for the heavy fermion systems.

In this work we focus on the order parameter proposed a few years ago by Chandra and collaborators. They suggested the existence of a hidden incommensurate orbital order in the heavy fermion $URu_2Si_2$ below the second order phase transition. The orbital order phase is associated with currents circulating around the plaquettes, as illustrated in Fig. 1. In the case of $URu_2Si_2$, these currents produce a very week orbital moment $0.02\mu_B$ that explains the large entropy loss.

Very recently, neutron scattering measurements were unable to detect the orbital order in the heavy fermion $URu_2Si_2$. Although the orbital order was not detected, it is not possible yet to discard it as the hidden order due to the resolution limitation of the experiments performed. Note that the orbital order is expected to be 50 times smaller than the spin order.

Our goal in this work is to investigate the existence of an incommensurate orbital order in the Kondo Lattice model (KLM). This model is the simplest one believed to present the physics of heavy fermions materials (see next section). Our approach will be numerical, through the density-matrix renormalization group (DMRG) and the Lanczos technique. These techniques are non-perturbative, however limited by the system size. For this reason, we consider the two-leg Kondo ladder (2-LKL), which is the simplest geometry able to present an orbital order.

The orbital order, also called flux or orbital current phase, has already been discussed in the context of the high temperature superconductors. The standard two-leg t-J ladders model present a short-range orbital order, while an extended version has long-range orbital order for some parameters. A recent detailed discussion of the orbital order in the context of a Hubbard model can be found in Ref. 13.

We close this section mentioning that a model very similar to the KLM was used to describe the magnetism of $URu_2Si_2$. Sikkema and collaborators, through a mean field calculation, showed that the Ising-Kondo lattice model with transverse field presents a weak ordered moment, similar to the one observed in experiments. However, the Ising-KLM model was not able to reproduce the large specific heat jump.
II. MODEL

In order to investigate the heavy fermion systems, the minimum ingredients that a microscopic model must consider are two types of electrons, the conduction electrons in the s-, p-, or d-, orbital as well as the electrons in the inner f-orbitals. In the literature there are two well known standard models that consider these two kind of electrons, the periodic Anderson model (PAM) and the KLM. In an appropriate parameter regime (mainly (i) the mobility of the f electrons is very small, which is relevant for the heavy fermion system and (ii) that the Coulomb interaction of the electrons in the f orbitals is very large) Schrieffer and Wolff showed that the KLM can be derived from the PAM. We consider in this work the KLM which has less degrees of freedom per unit cell than the PAM and it is easier to explore numerically.

The KLM incorporate an interaction between the localized spins and the conduction electrons via exchange interaction $J$. To attack this model in two or three dimension by unbiased non-perturbative numerical approaches is an impossible task at the present moment. However, it is possible to consider quasi-one-dimensional systems such as the N-leg ladders model.

We consider the 2-LKL with $2 \times L$ sites defined by

$$H_{KM} = - \sum_{<i,j>,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + H.c.) + J \sum_j S_j \cdot s_j + J_{AH} \sum_{<i,j>} S_i \cdot S_j,$$

(1)

where $c_{j,\sigma}$ annihilates a conduction electron in site $j$ with spin projection $\sigma$, $S_j$ is a localized spin $1/2$ operator, $s_j = \frac{1}{2} \sum_{\alpha,\beta} c_{j,\alpha}^\dagger \sigma_{\alpha,\beta} c_{j,\beta}$ is the conduction electron spin density operator and $\sigma_{\alpha,\beta}$ are Pauli matrices. Here $<ij>$ denote nearest-neighbor sites, $J > 0$ (when the KLM is deduced from the PAM obtain $J > 0$) 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.

We also consider an interaction between the localized spins $J_{AH}$, we choose $J_{AH} > 0$ since antiferromagnetism had been observed in $URu_2Si_2$. The same model above also represents the manganites when $J < 0$. In this latter case, the interaction between the localized spins seems to be important to stabilize some phases. This is the motivation to also consider this interaction. Note that several others terms in the Hamiltonian could also be included, like the Coulomb interaction of the electrons in the conduction band, extra electrons hopping, etc. However, at the present moment, there are no evidences indicating that such extra terms are relevant to the low energy physics of the heavy fermion systems. Up to now, it is well established that $J$ is essential to describe the magnetism observed in the heavy fermion systems. At small values of $J$, an antiferromagnetic long-range order (LRO) is expected due the Ruderman-Kittel-Kasuya-Yosida interaction, whereas for large $J$ a paramagnetic phase emerges. Doniach was the first to point out the existence of a quantum critical point (QCP) due the competition between these two phases.

Unlike other models, such as the $t-J$ model, much less is known about the Kondo lattice model. Even in the one dimension version, where the ground state of the Kondo chain is quite well known (see also Ref. 22). New phases have been reported recently, such as a new ferromagnetic phase inserted into the paramagnetic phase as well as a dimerized phase at quarter-filling. The latter has been questioned recently by Hotta and Shibata. Those authors claim that the dimerized phase is an artifact of the open boundary conditions. Indeed, the boundary condition is very important, as well as the number of sites considered. In Ref. 23 the authors observed, mainly, that with an odd number the sites the dimer state does not exist. The parity of the number of sites is thus very relevant and an odd number destroys the dimerization.

In quasi-one-dimensional systems, such as the N-leg ladders, very few non-perturbative studies have been reported. Recently, quantum Monte Carlo (QMC) and DMRG calculations of the half-filled Kondo lattice model in small clusters found the existence of a quantum critical point (QCP) at $J \sim 1.45$, in agreement with previous approximated approaches (see also Ref. 31). Note that the QMC calculations were feasible only at half-filling, where the famous sign problem is absent. Moreover, the DMRG results of the N-LKL at half-filling show that the spin and charge gaps are nonzero for any number of legs and Kondo coupling $J$. These results are quite different from the well known N-leg Heisenberg ladders were the spin gap is zero for an even number of legs.

The phase diagram of the 2-LKL has also been explored numerically. In this case, a ferromagnetic phase was observed only for small densities, very distinctively from the phase diagram of the 1D Kondo lattice chain, where the ferromagnetism is present at all electronic densities for large values of $J$. However, it is similar to the mean field phase diagram of the 3D Kondo lattice model. In this sense, the 2-LKL presents a better signature of the phases appearing in real systems than its one-dimensional version. Interesting that it was also observed dimerization in the 2-LKL at conduction electron densities $n = 1/4$ and $n = 1/2$. As in the one-dimension version, the RKKY interaction explains these unusual spin structures. In fact, in some real heavy fermion systems some unusual spin order structures have indeed been observed.

Here, we consider electronic densities $n$ larger than 0.4, where a paramagnetic phase have been observed. In particular, we focus on the electronic densities $n = 1$ and $n = 0.8$. We choose these densities since the magnitude of the rung-rung current correlation is bigger for larger electronic densities. We investigate the model with the DMRG technique under open boundary conditions and
use the finite-size algorithm for sizes up to $2 \times L = 120$, keeping up to $m = 1600$ states per block in the final sweep. The discarded weight was typically about $10^{-5} - 10^{-7}$ in the final sweep. We also cross-checked our results with Lanczos technique for small systems.

III. RESULTS

Before presenting our results, we briefly discuss the order parameter associated with a circulating current phase. Such a phase breaks rotational, translational as well as time reversal symmetries. The appropriated order parameter to detect this phase is the current between two nearest-neighbour sites, i.e., $\langle \hat{J}_{i,j} \rangle$ where the current operator between two nearest-neighbours $i$ and $j$ is given by

$$\hat{J}_{i,j} = i \sum_{\sigma} (c_{i,\sigma}^{\dagger} c_{j,\sigma} - c_{j,\sigma}^{\dagger} c_{i,\sigma}).$$

Strictly speaking, a spontaneous symmetry breaking only appears in the thermodynamic limit. Only in this limit $\langle \hat{J}_{i,j} \rangle \neq 0$ in the ordered phase. The signature of a spontaneous symmetry breaking appears in the two point correlation function of the operator that measures the symmetry. We utilize this fact to infer about the orbital order. If a continuous symmetry is broken, no long-range order exist at finite temperature in one and two dimensions, as stated by the Mermin-Wagner-Hohenberg theorem. At zero temperature a true long-range order may exist (a famous example is the dimerized phase of magnetic systems). If a continuous symmetry is broken in the orbital phase, a true long-range order may occurs in the ground state of the 2-LKL. Our results indicate strongly that the rung-rung current correlation has an exponential decay at half-filling. Close to half-filling our results indicate an incommensurate quasi-long range orbital order.

A. Half-filling

We start presenting some results for the conduction density $n = 1$. We observed, in this case, that the averaged rung-rung current correlation behaves as

$$C(l) = a_0 (-1)^l \exp(-l/\xi),$$

for all values of $J$ and $J_{\text{AH}}$ explored in this work. In Fig. 2(a), we present a typical example of the magnitude of $C(l)$ at half-filling for a system size $L = 30$. As we see, our results indicate strongly that $C(l)$ has an exponential decay due to the linear decay in the linear-log plot. The inset in Fig. 2(a) also shows that $C(l)$ is staggered. The solid line in Fig. 2(a) correspond to a fit of Eq. 2 with $a_0 = 0.16$ and a decay length $\xi = 1.43$. We performed a least-squares fitting, resulting in a root mean square (RMS) of 0.0018 and a correlation coefficient of 0.996. We found that $C(l)$ has a very small dependence on the number $m$ of states retained in the truncation process for $J > 0.8$, as can be observed in Fig. 2(a). For $J < 0.8$ is
Figure 2: (Color online) (a) The linear-log plot of $|C(i)|$ for two distinct value of $m$ with $L = 30$ at half-filling. The solid line in Fig. 2(a) correspond to a fit of Eq. 2 with $\xi = 1.43$ and $a_0 = 0.06$, the RMS per cent error is 0.18. Inset: $C(l)$ vs distance with $m = 1000$. Only few sites are presented. The couplings are $J = 0.8$ and $J_{AH} = 0$. (b) The cosine transform $N(q)$ of $C(l)$ presented in Fig. 1(a) with $m = 1000$. (c) The linear-log plot of $|C(l)|$ for two distinct size, both with $m = 1000$. The couplings are $J = 0.35$ and $J_{AH} = 0$.

The signature of the sign alternation is observed through the cosine transform of $C(l)$. In Fig. 2(b), we show the cosine transform of $C(l)$ present in Fig. 2(a) with $m = 1000$. Clearly, we observed a peak at $q = \pi$ due the sign alternation of $C(l)$. Note that the finite-size effects are small, as can be seen in Fig. 2(c). For this reason, we restrict most of our calculus to system size $2x30$ in order to save computational time.

very hard to get accurate results, however even for small $J$ we believe to have captured the correct qualitative behaviour. Nevertheless, we present most of our results for $J > 0.8$, where the results are more accurate.
Our results indicate that for small $J$, where the RKKY is expected to be dominant, the rung-rung current correlations has a bigger correlation length as we see in Fig. 3(a). On the other hand, for large $J$, which favors formation of singles, the correlation length is smaller. This result is expected, since for $J \to \infty$ the rung-rung current correlations must go to zero.

The Hamiltonian Eq. (1) with $J_{AH} = 0$ does not lead to a long-range orbital order at half-filling, as we have observed. Since $J_{AH}$ seems to be important to stabilise some phases for $J < 0$, it may be possible that it also stabilises the orbital phase for $J > 0$. For these reason, we also investigate the effect of $J_{AH}$ in the ground state of the 2-LKL. As we see in Fig. 3(b), for small values of $J$, $J_{AH}$ does not affect significantly $C(l)$. On the other hand, for larger $J$ as shown in Fig. 3(c), $J_{AH}$ clearly enhances the length correlation. Although $J_{AH}$ enhanced $C(l)$, at half-filling only short-range orbital order is observed for several parameters investigated.

At half-filling, for all parameters studied, $N(q)$ always presents a peak at $q = \pi$. In Fig. 4, we present this peak intensity for $J = 0.8$ and $J = 1.8$ as function of $J_{AH}$. As we see, the peak intensity increases with $J_{AH}$ and saturates for large $J_{AH}$ around ~0.45.

Our main conclusion, for the half-filling case, is absence of long-range orbital order. Note that it may be possible that the inclusion of the Coulomb interaction between the electrons in the conduction band leads the system into a phase with long-range orbital order, as occurs in an extend $t - J$ model. This is under investigation in the present moment by one of the authors.

B. Close to half-filling

Away from half-filling the DMRG calculation of $C(l)$ is less stable, for this reason we consider system sizes smaller than 2x40 and keeping up to $m = 1600$ states in the truncation process. Although we obtained results for a few densities away from half-filling, we focus on density $n = 0.8$ where the magnitude of $C(l)$ is larger. For small densities is very hard to get accurate results since the current intensity is very small. In Fig. 5(a), we present the log-log plot of $|C(l)|$ at conduction density $n = 0.8$ for a system size $2 \times 30$ with $J = 0.8$ and $J_{AH} = 1.0$ for two different values of $m$. Since in the log-log plot we obtain a linear decay (see the solid line in this figure) $C(l)$ must have a power law decay. If we use a linear-log plot our data does not have a linear decay. As can be seen from that Figure, it is very hard to get good accuracy even working with $m = 1600$ states. Although we were not able to obtain the current-current correlations at large
distances with a high accuracy, we believe to have captured the correct behavior, i.e., a power law decay. The large oscillations appearing in those Figures are due to fact that some values of \( C(l) \) are very close to zero.

Since our data of \( C(l) \) in the log-log plot strongly suggest a power law decay close to half-filling (note that for the half-filling case the decay is exponential) we tried to fit \( C(l) \) with the function

\[
C_{\text{fit}}(l) = a_0 \frac{\cos(n\pi l)}{l^{\alpha_1}} + a_1 \frac{\cos(2n\pi l)}{l^{\alpha_2}},
\]

where \( n = 0.8 \) is the density. The dashed curve in Fig. 5(a) corresponds to a fitting of our data with \( m = 1600 \). We were not able to reproduce precisely \( C(l) \), however the general behavior is quite well described.

Note also that finite-size effect are larger away from half-filling, as we can see by comparing the Figs. 5(b) and 2(c). It is important to mention that we observed, away from half-filling and in very few distances \( l \), that the sign of the averaged correlation \( C(l=j-k) \) does not have the same sign of \( C(j,k) \) for some pairs of \( (j,k) \) satisfying \( l=\lvert j-k \rvert \). This does not seem to be due to the number of states kept in the truncation process since we also obtained the same effect for small clusters with exact diagonalization.

In Fig. 6 we present \( N(q) \) for a representative set of parameters at conduction density \( n = 0.8 \). As shown in that Figure, there is no peak at \( q = \pi \), signaling an absence of staggered rung-rung current correlations. For the conduction density \( n = 0.8 \) we observed a cusp at \( q = n\pi \). These results indicate that close to half-filling the 2-LKL presents an *incommensurate* quasi-long-range orbital order.

**IV. CONCLUSION**

In this paper, we have investigated the possibility of a two-leg Kondo ladder present an orbital order. In particular, we focus on the densities \( n = 1 \) and \( n = 0.8 \). For the several couplings investigated we did not find any trace of a true long-range orbital order, which would be relevant to explain the large entropy loss observed in the second order phase transition of \( URu_2Si_2 \). Our data indicate that the half-filling case presents a staggered short-range orbital order, while close to half-filling our results are consistent with an incommensurate quasi-long-range orbital order. Although we did not find evidence of a long-range orbital order in the ground state of the two-leg Kondo ladder, we can not yet completely discard this possibility. It may occur that an extended version of the Kondo lattice model presents the long-range orbital order. So, we may conclude that either the orbital phase does not exist and is not the origin of the mysterious phase transition observed in the the heavy fermion \( URu_2Si_2 \) or the standard Kondo lattice Model is not able to reproduce the correct order observed in the experiments.

**Acknowledgments**

The authors thank E. Miranda for useful discussions. This work was supported by Brazilian agencies FAPESP and CNPq.

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