Numerical study of finite size effects in the one-dimensional two-impurity Anderson model

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(Received 7 May 2008; published 4 June 2008)

We study the two-impurity Anderson model on finite chains using numerical techniques. We discuss the departure of magnetic correlations as a function of the interimpurity distance from a pure $2k_F$ oscillation due to open boundary conditions. We observe qualitatively different behaviors in the interimpurity spin correlations and in transport properties at different values of the impurity couplings. We relate these different behaviors to a change in the relative dominance between the Kondo effect and the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction. We also observe that when RKKY dominates, there is a definite relation between interimpurity magnetic correlations and transport properties. In this case, there is a recovery of $2k_F$ periodicity when the on-site Coulomb repulsion on the chain is increased at quarter filling. The present results could be relevant for electronic nanodevices implementing a nonlocal control between two quantum dots that could be located at variable distance along a wire.

DOI: 10.1103/PhysRevB.77.235103 PACS number(s): 72.15.Qm, 73.23.−b, 73.63.Kv, 75.40.Mg

I. INTRODUCTION

It is well known that the main properties of the two-impurity Anderson model (TIAM) (Ref. 1) are determined by the competition between the Kondo effect[2] generated by each impurity and the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction between the impurities.[3,4] Renewed interest in this model comes from the observation of the Kondo effect in electronic devices, where a nanoscopic relatively isolated region, a quantum dot (QD), can act as a single spin-1/2.[5] In particular, it has been observed in a nanoelectronic device formed by two QDs coupled through an open conducting region[6] that transport through one of the QDs depends on the occupancy and coupling of the other QD via the RKKY interaction. The main issues involved in this and related experiments[7] are the possibility of tuning different regimes dominated by the Kondo effect or by the RKKY interaction and the dependence of transport properties on the sign of the magnetic correlation between the impurities.

Analytical studies of the TIAM are usually concerned with long-distance behaviors.[1,3] However, it should be emphasized that the properties of mesoscopic devices are determined by finite size effects rather than by bulk physics. Finite size effects have been addressed in a study of a double QD in an Aharonov-Bohm ring,[8] and it was found that RKKY dominates the transport properties. More closely related to the problems we consider in this work is a study of two impurities coupled by a finite one-dimensional (1D) wire,[9] where it was shown that the RKKY interaction is always dominant due to the strong reduction of the Kondo temperature by finite size effects. In another slave-boson study[10] it was concluded that the presence of different transport regimes depends on the sign of the RKKY interaction. In these two studies, however, the impurities are located at the edges of the chain and, hence, the effects of the outer sites in Fig. 1, or "leads," were not considered.

The main motivation for the present study is then to understand finite size effects in the 1D TIAM, which can be considered as a model of a device formed by two QDs coupled through a conducting chain and connected to 1D leads (Fig. 1). Another motivation for this work is to understand the effects of electronic correlations, which are present in materials such as carbon nanotubes[11] used in experimental realizations of quasi-1D devices.[12] Coulomb correlations in the chain affect both the Kondo temperature and RKKY interaction.[9,13]

In this work we show numerically that the spin-spin correlation between the two impurities as a function of the interimpurity distance R, $S(R)$, for a fixed length L of the whole chain, departs from the predicted $2k_F$ long-distance behavior for the TIAM.[3,4] We show how a regime where the RKKY interaction dominates over the Kondo effect appears as the impurity couplings are decreased. We also provide a measure of the conductance G, which is more relevant for applications to nanodevices. We show that this quantity, particularly in the regimes where RKKY dominates, follows an oscillatory behavior with R at a fixed L related to that of $S(R)$. We also show that an on-site Coulomb repulsion on the chain, at quarter filling, restores the $2k_F$ periodicity of $S(R)$ and $G(R)$. Finally, we provide indications that most of these finite size effects found are due to the open boundary conditions adopted for our system.

The paper is organized as follows. In Sec. II we define the Hamiltonian model, and we describe the method employed in the calculations. In Sec. III we present results for $S(R)$ and $G(R)$, first for noninteracting leads and then in the presence of correlations on the chain. We conclude in Sec. IV by providing a summary of the results and by suggesting possible connections with other theoretical approaches, as well as with experiments.

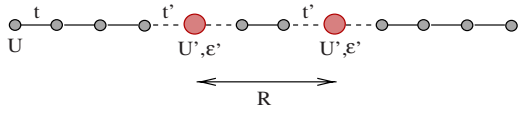

FIG. 1. (Color online) Picture of model (1), $L=12$, $R=3$.

II. MODEL AND METHODS

The 1D two-impurity Anderson model with Hubbard repulsion on the chain is defined by the Hamiltonian

$$\mathcal{H}_0 = -t_0 \sum_{i,i+1\in\Lambda,\sigma} (c^\dagger_{i+1\sigma} c_{i\sigma} + \text{H.c.}) + U \sum_{i\in\Lambda} n_{i\uparrow} n_{i\downarrow}$$
$$- t' \sum_{\mu=\pm 1,\sigma} (c^\dagger_{r_1+\mu\sigma} c_{r_1\sigma} + c^\dagger_{r_2+\mu\sigma} c_{r_2\sigma} + \text{H.c.})$$
$$+ U' \sum_{i=r_1,r_2} n_{i\uparrow} n_{i\downarrow} + \epsilon' \sum_{i=r_1,r_2} (n_{i\uparrow} + n_{i\downarrow}), \quad (1)$$

where the notation is standard. The Anderson impurities or QDs, with parameters U', ϵ', are symmetrically located with respect to the center of the chain, i.e., at sites $r_{1,2}=(L\pm R+1)/2$, with R odd (see Fig. 1). The QDs are connected to the rest of the system Λ with a hopping t'. The subsystem Λ comprises the leads ($i<r_1$, $i>r_2$) and the region between both impurities ($r_1<i<r_2$), and it is described by a Hubbard Hamiltonian with couplings t_0 and U. $t_0=1$ is adopted as the unit of energy.

Model (1) will be studied on finite clusters using density matrix-renormalization group (DMRG) (Ref. 14). Open boundary conditions (OBC) were adopted throughout. We would like to emphasize that OBC are the realistic boundary conditions for the devices that motivate the present work. There has been a previous study of a related model using DMRG, but the two impurities were fixed at the chain edges[15], that is, leads were not included in that model.

We provide a measure of the response of the system to the application of a small bias voltage $\Delta V=V_R-V_L$ ($V_R=-V_L$), where V_L (V_R) are on-site potentials applied to the ten sites at the edge of the left (right) lead. Although these 1D leads have to be connected to massive two- or three-dimensional metallic or semiconducting contacts, we believe that as a first step it is necessary to consider the system formed only by the two QDs connected to the 1D leads. The current $J_L(t)$ [$J_R(t)$] on the bond connecting the left (right) QD to the left (right) lead is computed with the time-dependent DMRG.[16] In the case of a single QD and noninteracting leads, this numerical setup has been shown[17–20] to reproduce the results for equivalent systems, which were treated analytically.[21] In the following, we employed the "static" algorithm,[17] which although less precise than the "adaptive" algorithm[18] still gives qualitatively correct results, as we have explicitly checked in some cases,[22,23] but is much faster than the adaptive scheme, thus, allowing to explore different couplings and densities, and a wide range of R and L. All of the results reported below correspond to $\Delta V=0.01$. We compute $J(t)=[J_L(t)+J_R(t)]/2$, which follows with time very approximately a sinusoidal function, and we adopt as a measure of the response or "conductance," G, the average of the sinusoidal fitting to $J(t)/\Delta V$ over a half period. This qualitative behavior is mostly independent of various criteria that have been proposed to quantify G.[19] We want to emphasize that our main purpose in this study is to obtain *relative* values of G as a function of the interimpurity distance R. In this sense, the application of the bias potential on only ten sites at the edges of the system instead of applying to the whole leads is then a necessary condition to treat all distances R on an equal foot.

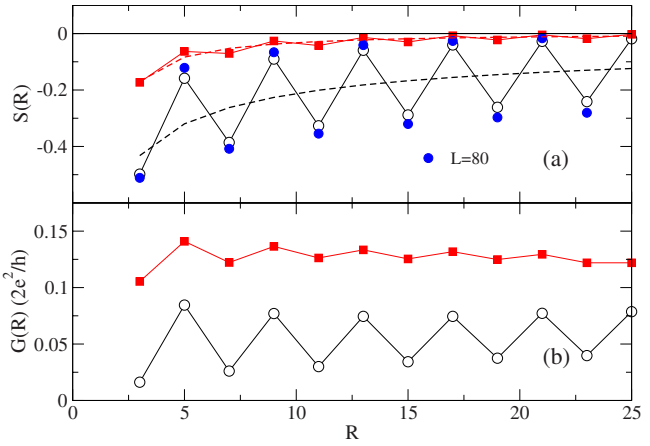

FIG. 2. (Color online) (a) Spin-spin correlations between the impurities and (b) conductance as a function of the interimpurity distance R at $n=1$ for $t'=\sqrt{2}/2$ (circles) and $t'=1$ (squares), on the $L=120$ chain except otherwise stated. In (a), dashed lines show fits to $2k_F$ oscillations.

We adopted $U'=8$ and $\epsilon'=-4$ (symmetric point) in order to ensure a strong magnetic character of the impurities, which we checked in all cases. In the following we will consider two values of t', $\sqrt{2}/2$ and 1. The Kondo effect for the single impurity Anderson model for $t'=1$ was studied using the same method as in the present work in Ref. 22. Most of our calculations reported below were obtained for $L=120$. The truncation error in DMRG calculations for this cluster was kept below 10^{-6}. In all cases we worked in the subspace of total $S^z=0$. Thus, taking into account the isotropy of the Hamiltonian (1), we computed the spin-spin correlations between sites $i\neq j$ as $S_{ij}=3\langle S^z_i S^z_j\rangle$. In particular, the spin-spin correlation between impurities is $S(R)=3\langle S^z_{r_1+R} S^z_{r_1}\rangle$.

III. RESULTS AND DISCUSSION

Let us start by discussing results at half filling, $n=1$. In Fig. 2(a), it can be seen that for $t'=\sqrt{2}/2$ and $t'=1$, $S(R)$ presents a four-site period, which corresponds to a k_F oscillation. To be more precise there is a k_F modulation on top of the antiferromagnetic (AF) $2k_F$ oscillation. This $2k_F$ component can be fitted for R odd by the law $-1.102/x^{0.59}$ ($t'=\sqrt{2}/2$) and $-1.021/x^{1.38}$ ($t'=1$). The k_F component decays much slower, as $x^{-0.22}$ ($t'=\sqrt{2}/2$) and $x^{-0.68}$ ($t'=1$). At this point we could advance the hypothesis that the departure of the present results from the pure $2k_F$ oscillation is due to the OBC used in DMRG calculations. That is, $2k_F$ oscillations starting from the chain edges would modulate the magnetic correlations from each of the impurities, and hence, as a function of R, this would enhance the k_F component of $S(R)$. The large intensity of $S(R)$ and its survival at long distances for $t'=\sqrt{2}/2$ suggest that we are in the regime where the RKKY interaction dominates over the Kondo effect. On the other hand, the smaller amplitude and rapid suppression of $S(R)$ with R for $t'=1$ indicate the presence of a

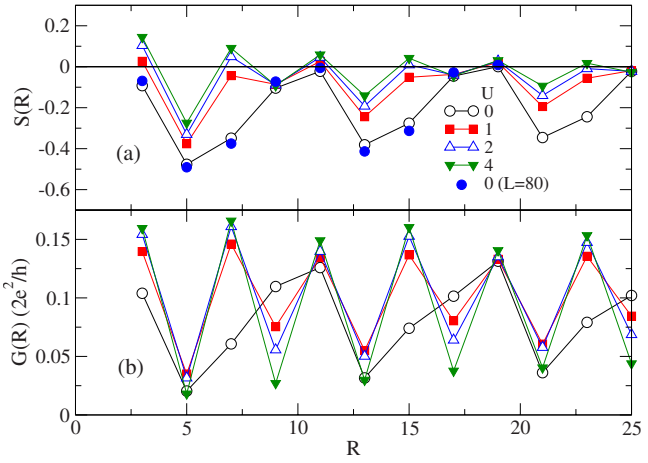

FIG. 3. (Color online) (a) Spin-spin correlations between the impurities and (b) conductance as a function of the interimpurity distance R for $t'=\sqrt{2}/2$ at $n=0.5$, parametrized with U, on the $L=120$ chain except otherwise stated.

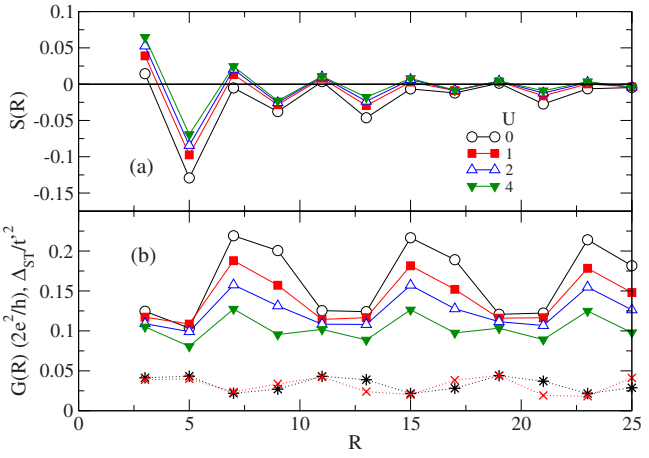

FIG. 4. (Color online) (a) Spin-spin correlations between the impurities and (b) conductance as a function of the interimpurity distance R for $t'=1$ at $n=0.5$, parametrized with U, on the $L=120$ chain. In (b) the singlet-triplet energy Δ_{ST}/t'^2 is shown for $t'=1$ (stars) and $t'=\sqrt{2}/2$ (crosses).

strong screening of the magnetic moment of the impurities implying a dominance of the Kondo effect.

The conductance [Fig. 2(b)] presents an oscillation with R that follows that of $S(R)$. There is a set of minimum values of $G(R)$ for $R=4m+3$ (m integer) that corresponds to the stronger AF spin-spin correlations between impurities and a set of maximum values of $G(R)$, which occur at $R=4m+1$, corresponding to the weaker AF $S(R)$. The expected difference in amplitude of $G(R)$ between both values of t' considered, since the current is proportional to t', can also be observed. The most important feature in these results is that, for the case of $t'=\sqrt{2}/2$, there is a factor of 2 or larger between the conductances for $R=4m+1$ with respect to the one for $R=4m+3$. We believe that this large difference can be detected experimentally in appropriate devices. In our calculation, the maximum of $G(R)$ could not possibly reach the expected unitary limit as a consequence of applying the bias potential to only few sites on the leads as discussed in Sec. II.

Although half filling is perhaps more realistic for actual devices, it is interesting to study also the case of quarter filling, $n=0.5$. In this case it is possible to study transport properties in the presence of electron correlations on Λ. In Fig. 3(a), for $t'=\sqrt{2}/2$, it can be seen that for the noninteracting chain ($U=0$) $S(R)$ presents an oscillation with period 8, which again corresponds to an overall k_F oscillation. As in Fig. 2(a), results for $L=80$ show an oscillation in $S(R)$ slightly larger in amplitude to that for $L=120$. A systematic study of the effect of L is presented at the end of this work. Similarly to what happened at $n=1$, the conductance, shown in Fig. 3(b), has the same dependence on R as the spin-spin correlations. At $n=0.5$, the minimum (maximum) of G occurs at $R=8m+5$ ($R=8m+3$), which coincides with the values of R at which $S(R)$ has the strongest (weakest) AF values.

Let us turn on the interaction on Λ. It can be seen in Fig. 3(a) that there is a rapid suppression of the k_F modulation in $S(R)$ with increasing U, leaving behind a well-defined $2k_F$ oscillation, which is already apparent at $U=2$. For $U\geq 2$ the spin-spin correlations at $R=4m+3$ become slightly positive, that is, they become ferromagnetic (FM). Consequently, as it can be observed in Fig. 3(b), there is a similar change in the dependence of the conductance on R, with the minima (maxima) of G located at the same values as the AF (FM) correlations in Fig. 3(a). Notice that for $U\geq 2$ the ratio between the maximum and the minimum values of G becomes equal to 8 or larger. Again this very large ratio should be detectable experimentally if a device with the geometry of Fig. 1 and working at quarter filling could be fabricated.

In Fig. 4(a), we show the spin-spin correlations between impurities at $n=0.5$ for $t'=1$. At this filling, there is an additional important difference with the corresponding results for $t'=\sqrt{2}/2$ depicted in Fig. 3(a), which is that the $2k_F$ periodicity is now clearly dominant. This behavior of $S(R)$ supports the idea that these two values of t' belong to different regimes. On the other hand, the behavior of the conductance with R shown in Fig. 4(b), in the noninteracting case $U=0$, is similar to the one for $t'=\sqrt{2}/2$, shown in Fig. 3(b), with a large k_F component. However, in the presence of interactions on the chain, the amplitude of $G(R)$ is *suppressed* by increasing $U>0$ for $t'=1$, while it seems *enhanced* by U for $t'=\sqrt{2}/2$. This suppression of $G(R)$ would be expected in a Luttinger liquid, since it is proportional to K_ρ, which decreases with increasing U.[24,22] For $t'=1$, it can be also observed in Fig. 4(b) that only for the largest value of the interaction considered, $U=4$, a $2k_F$ periodicity becomes dominant. Finally, the relation between the location of the maximum and minimum values of $G(R)$ with the ones of $S(R)$ observed in Fig. 3(b) is absent for small U, but it is recovered for $U=4$.

These clearly different behaviors of $S(R)$ and $G(R)$ for the two types of impurities considered have to be traced to the essential competition between the Kondo effect and RKKY interactions. For the noninteracting case, the Kondo temperature may be estimated as[2] $T_K=t'\sqrt{U'/(2t_0)}\times\exp[-\pi t_0 U'/(8t'^2)]$ (in units of $k_B=1$), which gives $T_K=0.0026$ for $t'=\sqrt{2}/2$ and $T_K=0.086$ for $t'=1$. That is, if for the case of $t'=\sqrt{2}/2$ it is reasonable to assume that RKKY

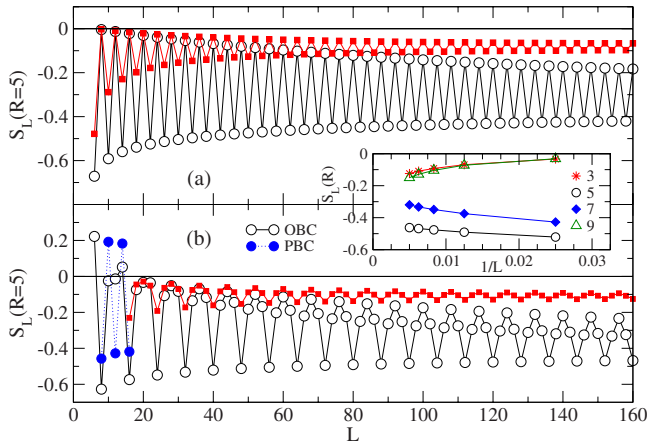

FIG. 5. (Color online) Spin-spin correlations between the impurities at $R=5$ as a function of the total length L for $t'=\sqrt{2}/2$ (circles), $t'=1$ (squares), and (a) $n=1$, (b) $n=0.5$. The inset shows the scaling of $S_L(R)$ with L for $t'=\sqrt{2}/2$, $n=0.5$, and for various values of R as indicated.

dominates over the Kondo effect, since T_K for $t'=1$ is ≈ 33 times larger, while the effective RKKY interaction[4] $\mathcal{K}\sim t'^2$ would be only a factor of 2 larger, then it is plausible that the case of $t'=1$ belongs to the regime where the Kondo effect dominates over the RKKY interaction. Particularly for the case of $t'=\sqrt{2}/2$, where RKKY can be assumed as dominant, it is instructive to estimate $\mathcal{K}$ as the difference in ground state energy between the singlet and triplet states. For this case one gets that Δ_{ST} oscillates with R with maximum values of $\mathcal{K}\sim\Delta_{ST}\approx 0.04$ $(n=1)$. This value is larger than the above estimated T_K for this impurity. At $n=0.5$ the oscillation of Δ_{ST} with R has period 8 as it can be observed in Fig. 4(b). Although these estimates are instructive and consistent with our numerical results, one should bear in mind that the above expression for T_K is valid in the bulk limit, while the results for Δ_{ST} were obtained for the $L=120$ chain. The strong suppression of T_K due to the finite size of the system found in Ref. 9 may not appear in our system due to the presence of the leads, which may provide room for the Kondo cloud to develop. We would also like to notice that in all cases we examined, the ground state is a singlet, which is consistent with the result that $S(R)$ is always AF or at most weakly FM.

Finally in Fig. 5 we show the dependence of $S(R)$ at a fixed interimpurity distance $R=5$ on the length L. The period of $S_L(R=5)$ is 4 $(n=1)$ and 8 $(n=0.5)$ for the two types of impurities considered, which correspond to the wave vector k_F. It is interesting to examine here the dependence of these results on the boundary conditions (BC) of the system. Periodic boundary conditions (PBC) and antiperiodic boundary conditions (APBC) have, separately, a period of 8 as with OBC. However, if for each L we adopt the BC with minimum energy, then a doubling of the wave vector of the oscillation is obtained. By using exact diagonalization we obtained that the energy is minimum for PBC for $L=4m$ (m integer) and for APBC when $L=4m+2$. The minimum of energy for $L=4m+1$ and $L=4m+3$ falls alternatively on PBC or APBC depending on R. The resulting $S_L(R=5)$ is shown in Fig. 5(b). This result is then another example of the effects caused by OBC.[25] The inset of Fig. 5 shows a slow dependence of $S_L(R)$ on L for various R. Since, particularly for $t'=\sqrt{2}/2$, $G(R)$ follows the oscillation of $S(R)$, it is quite likely then that an oscillation of the conductance could be experimentally observed in a real device for a fixed interdot distance as the length of the 1D leads is varied.

IV. CONCLUSION

In conclusion, we have shown for the two-impurity Anderson model on finite chains the presence of different behaviors of the interimpurity magnetic correlations $S(R)$ for the two values of the coupling between the impurities and the chain, t'. We suggested that these different behaviors indicate that the relative dominance between the Kondo effect and the RKKY interaction can be tuned by the single parameter t'. In the case when RKKY dominates, we found important oscillations in the conductance with interimpurity distance, $G(R)$, following that of the spin-spin correlations. It would be tempting to relate these different behaviors of $S(R)$ and $G(R)$ to the presence of an unstable fixed point suggested by numerical renormalization group calculations.[3] Although certainly such a fixed point could not strictly appear in a finite-size calculation, some traces of its presence, for example, an admixture of the singlet and triplet states, could be detected. However, we found that the ground state of our model is always a singlet consistently with dominating AF interimpurity correlations. It would be interesting to explore other parameters of our model to find such a critical point.[26]

Finally, we have observed that the k_F modulation of the $2k_F$ oscillation of $S(R)$ and $G(R)$ observed for noninteracting leads is suppressed by an on-site electron repulsion on the chain. We hope that some of the present results could be found in a 1D realization of the device developed in Ref. 6, which we believe could be built on a carbon nanotube with the QDs defined with an appropriate array of gates.[12]

ACKNOWLEDGMENT

One of us (S.C.) wishes to acknowledge partial financial support from the Josefina Prats Foundation.

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