The spatial range of the Kondo effect: a numerical analysis

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The spatial length of the Kondo screening is still a controversial issue related to Kondo physics. While renormalization group and Bethe Anzats solutions have provided detailed information about the thermodynamics of magnetic impurities, they are insufficient to study the effect on the surrounding electrons, i.e., the spatial range of the correlations created by the Kondo effect between the localized magnetic moment and the conduction electrons. The objective of this work is to present a quantitative way of measuring the extension of these correlations by studying their effect directly on the local density of states (LDOS) at arbitrary distances from the impurity. The numerical techniques used, the Embedded Cluster Approximation, the Finite U Slave Bosons, and Numerical Renormalization Group, calculate the Green functions in real space. With this information, one can calculate how the local density of states away from the impurity is modified by its presence, below and above the Kondo temperature, and then estimate the range of the disturbances in the non-interacting Fermi sea due to the Kondo effect, and how it changes with the Kondo temperature $T_K$. The results obtained agree with results obtained through spin-spin correlations, showing that the LDOS captures the phenomenology of the Kondo cloud as well.

To the best of our knowledge, it is the first time that the LDOS is used to estimate the extension of the Kondo cloud.

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I. INTRODUCTION

The physics of isolated impurities inside a Fermi sea has received considerable attention since it was experimentally shown that nano-systems composed by quantum dots possess Kondo phenomena, very clearly reflected in its transport properties.¹ One signature of this effect is a narrow resonance, at the Fermi energy, in the local density of states (LDOS) of the impurity, with a width of the order of a characteristic energy, the so-called Kondo temperature, $T_K$. The transport properties of a nanoscopic structure in this regime are substantially affected by the Kondo resonance, as it creates an extra channel at the Fermi level through which the electrons can propagate. The energy $k_B T_K$ is also associated with an antiferromagnetic correlation between the impurity and the conduction electron spins in its neighborhood, favoring the emergence of a singlet ground state. These spins, localized in the impurity’s vicinity, constitute a screening cloud of the localized impurity spin, known as the Kondo cloud. While most of the physics involved in this important effect is by now well established, the nature, structure, and extension of the Kondo cloud, and even its existence, is still, to some extent, controversial.²³⁴ Theoretically, it is thought to be a crucial ingredient in helping to understand, for instance, the interaction between two nearby impurities, when one of them is sitting within the region of influence of the Kondo cloud of the other. From the experimental point of view, although it is thought that the extension of this characteristic cloud can reach very large values,² the properties of a system of impurities in metals seem to depend linear on the impurity concentration. This seems to indicate that the impurities do not see each other, although, based on the expected Kondo cloud extension, they should. Moreover, there has not been any clear experimental evidence of it existence, with the exception of the electronic conductance measurements in quantum corral models.⁵ For instance, in an ellipsoidal quantum corral, a Kondo peak produced by a magnetic atom located at one focus of the ellipse has an experimentally detectable spectral response in the other focus. This indicates a very peculiarly structured Kondo cloud, which, through the use of an Scanning Tunneling Microscope (STM), can be experimentally analyzed.

The Kondo cloud length can be estimated by considering that the mean-life of the Kondo quasi-particles are related to the time-scale $\tau_K \approx \hbar/k_B T_K$. Assuming that these quasi-particles propagate with the Fermi velocity $v_F$, then the Kondo screening length can be related to the quantity $v_F/k_B T_K$.⁶ Therefore, Eq. (1)

$$R_K \approx \frac{\hbar v_F}{k_B T_K}$$

Obviously, since all electrons whose energies fall within the Kondo peak will participate in the formation of the Kondo cloud, the quantity $v_F$ is not well defined. Moreover, one may expect that the quasi-particles do not propagate with the bulk $v_F$, but with a renormalized $v^*$, given by the presence of the impurity. From Heavy Fermion theory, we can estimate $v^* = k_F/m^*$, where $m^*$ is the effective mass of the quasi-particle.⁶ Therefore, Eq. (1) should provide inaccurate results for the screening length $R_K$. However, it should be expected to give the correct dependence with $T_K$ and some plausible order of magnitude for its length.

From the theoretical point of view, this problem has been analyzed using different approaches.⁵⁷⁸ The study of spin properties, through the local susceptibility or the spatial spin correlation function, has given significant contributions to the understanding of this phenomenon.²⁶,²⁸ More closely related to our approach, the analysis of the conductance of a quantum dot embedded in a finite wire or the persistent currents in a
finite ring using renormalization arguments or Density Matrix Renormalization Group calculations, respectively, were proposed as a way of determining the Kondo cloud, as well.

More recently, a variational approach was proposed to study the propagation, from the impurity, of the local hole-density. In this work, it was possible to show that, in two and three dimensions, the extension of the Kondo cloud is of the order of a few Fermi wave-lengths only, due to angular dispersion effects, such that $R_K$ does not play a significant role in the physics of a system of impurities in either of these dimensions. This seems to explain the situation from the experimental point of view (as mentioned above), and thus the irrelevance of the Kondo cloud in most of the real systems studied. However, for one-dimensional systems, the impurity-impurity interaction should be determined by the Kondo cloud length $R_K$. This will have important consequences to the conductance properties, and therefore will have implications to the design of quantum dot integrated nanoscopic systems.

A. Holzner et al., using DMRG, have calculated the spin-spin correlations involved in the formation of the Kondo cloud in a one-dimensional system and found the dependence of the range of the Kondo cloud with the Kondo temperature to agree with Eq. [1][2]

Motivated by this situation, we study the Kondo cloud in a one-dimensional system, focusing our attention on its electronic properties. The study of the propagation of the Kondo resonance, located at the vicinity of the Fermi energy, will shine light, for instance, into the transport properties of a quantum dot connected to leads where the distance from the dot to an STM tip is changed in a controlled and continuous way. This will be experimentally similar to the transport properties studies of a system formed by a magnetic atom located in one focus of an elliptical quantum corral, as mentioned above, and can be experimentally implemented for a quantum dot connected into an infinite wire.

In the present work, we discuss the spatial behavior of the Kondo cloud by alternative means in an infinite one-dimensional system. Indeed, to estimate the cloud range, three different numerical techniques are used to track the effects of the impurity over the LDOS far away from the impurity. These effects are calculated above and below the Kondo temperature $T_K$, and their difference is used as a fingerprint of the extension of the Kondo cloud. The calculations are carried out using the Embedded Cluster Approximation (ECA)[13] and the Finite-U Slave Bosons Mean-Field approximation (FUSBMF)[14] and the Numerical Renormalization Group (NRG) method [15].

The paper is organized as follows: In the next section (Sec. [II]), we present the model used and the methods to solve it. In Sec. [III] we briefly describe the behavior of the LDOS, in real space, within the metal lead and define the function used to estimate $R_K$. In Sec. [IV] the numerical results calculated using ECA, FUSBMF and NRG are discussed and compared. Finally, in the last Section, we present our conclusions.

![FIG. 1: (Color online) Schematics of the system used to determine the spatial extension of the Kondo cloud. The exactly diagonalized (ED) cluster (with a variable number of sites $L+1$, where the QD is numbered as site zero) is indicated by the dashed box. Note that the (integer) index $0 \leq N < \infty$ runs over all sites inside and outside the cluster. By applying the numerical methods employed in this work, the dressed (interacting) Green function for all sites in the cluster is obtained (note that for FUSBMF and NRG, the cluster can be considered as just the impurity – see end of Sec. [III]B for details). A simple Equation of Motion procedure allows the calculation of the GF in any site of the semi-chain outside the cluster. With that, the effect of the Kondo screening effect over the non-interacting Fermi sea, the so-called Kondo cloud, can be probed at an arbitrary distance from the impurity.](image)
is the number operator at the impurity. The first two terms of $H_T$ represent the Hamiltonian of the impurity and the non-interacting band, respectively, and the last term is the hybridization between them. An important quantity for this system is the broadening of the impurity level $\Gamma = 2\pi t^2 \rho_{\text{lead}}(E_F)$, where $\rho_{\text{lead}}(E_F)$ is the LDOS of the first site in the semi-chain at the Fermi energy $E_F$. Note

In this paper, we will concentrate our attention on the electron-hole symmetric point ($V_g = -U/2$), although the results can be generalized to an arbitrary value of gate potential. As mentioned in the introduction, we want to estimate the NRG methods, which are briefly described next.

At the end of this section we will describe how the LDOS in a site $N$ far away from the impurity is calculated using the Equation of Motion (EOM) method. Note that the EOM method described in Sec. II B does not depend on the method used to calculate $G_{dd}$; any of the three methods described below provide essentially the same kind of input for the EOM procedure.

### A. Numerical methods

#### 1. Embedded Cluster Approximation method

The ECA method has been developed to treat localized impurity systems consisting of a many-body interacting region weakly coupled to non-interacting conduction bands. The approach is based on the idea that the many-body effects of the impurity are local in character (the Kondo cloud, for instance). With this in mind, we proceed in three steps: first, out of the complete system (the impurity plus a non-interacting band, described by a tight-binding Hamiltonian), one isolates a cluster consisting of the impurity plus their $L$ nearest neighboring sites in the tight-binding semi-chain. This cluster, with a variable size $L + 1$, as it includes the impurity, is shown in Fig. I by dashed lines. The first site outside the cluster is labeled $N = L + 1$ (remember that $N$ is an index, as opposed to a number of sites). Most of the many-body effects are expected to be confined to this cluster.

The second step of the method consists in exactly diagonalizing the cluster, using, for example, the Lanczos method, and calculate all the GFs. Finally, in the third step, the cluster is embedded into the rest of the tight-binding semi-chain using a Dyson equation. Being $g_{i,j}$ a cluster-GF that propagates an electron from site $i$ to $j$ and $g_{L+1,i}$ the GF of the first site out of the cluster ($N = L + 1$), the Dyson equation to calculate a dressed (by the presence of the semi-chain), GF for sites inside the cluster can be written as,

$$ G_{i,i} = g_{i,i} + g_{i,L} \, t \, G_{L+1,i} \, , $$

$$ G_{L+1,i} = g_{L+1,i} \, t \, G_{i,i} \, . $$

Note that the hopping parameter $t$ in Eq. 6 corresponds to the broken link shown by a dashed line in Fig. I. This matrix element has the same value as all the other hopping parameters within the chain. Properties like conductance through the impurity and its LDOS, for example, can be obtained solving this set of equations (for more details, see Ref. [14]).

#### 2. Finite-U slave bosons mean-field approximation

The slave boson mean field is a method proposed originally to treat the problem when the Coulomb repulsion $U$ is the larger quantity. The double occupancy is excluded from the Hilbert space with the help of projectors-bosons operators. After taking a mean field in the boson operators, the many-body Hamiltonian is mapped into an effective one-body Hamiltonian that can be solved exactly.

The FUSBMF approach is an extension of the usual slave boson mean field in order to treat problems with finite $U$. The first step is to enlarge the Hilbert space, by introducing a set of slave boson operators $\hat{e}$, $\hat{p}_\sigma$ and $\hat{d}$, and replacing the creation ($d_\sigma^\dagger$) and annihilation ($d_\sigma$) operators in the Hamiltonian by $d_\sigma^z \equiv d_\sigma^+ \hat{d}$ and $\hat{z}_\sigma$, respectively. Following Kotliar and Ruckenstein, the operator $\hat{z}$ takes the form

$$ \hat{z}_\sigma = \frac{1}{2} \hat{d} \hat{d}^\dagger - \frac{1}{2} \hat{d}^\dagger \hat{d} + \frac{1}{2} \hat{d}^\dagger \hat{d}^\dagger \, . $$

Notice that the bosonic operators $\hat{d}$ and $\hat{d}^\dagger$ do not carry an spin index. The enlarged Hilbert space is then restricted to the physically meaningful subspace by imposing the constraints

$$ \hat{P} = \hat{d} \hat{d}^\dagger + \sum_\sigma p_\sigma^z \hat{p}_\sigma + \hat{d}^\dagger \hat{d}\, = \, 1 \, = \, 0 $$

and

$$ \hat{Q}_\sigma = n_d \hat{d}^\dagger \hat{d} - \hat{p}_\sigma^z \hat{p}_\sigma - \hat{d} \hat{d}^\dagger \, = \, 0 \, . $$

Both constraints are included into the Hamiltonian through Lagrange multipliers $\lambda^{(1)}$ and $\lambda^{(2)}$. The constraint described by Eq. 5 force the dots to have empty, single, or double occupancy only, while the constraint of Eq. 10 relates the boson with the fermion occupancies. In the mean-field approximation, we replace the boson operators $\hat{e}$, $\hat{p}_\sigma$ and $\hat{d}$ (and their Hermitian conjugates) by their thermodynamical expectation values $\langle \hat{e} \rangle = \langle \hat{p}_\sigma \rangle$, $\langle \hat{d} \rangle = \langle \hat{d}^\dagger \rangle$ and $\langle \hat{d}^\dagger \hat{d} \rangle = \langle \hat{d} \hat{d}^\dagger \rangle$. These expectation values, plus the Lagrange multipliers, constitute a set of parameters to be determined by minimizing the total energy $\langle \hat{H} \rangle$. In principle, it is necessary a set of seven self-consistent parameters. Once again, as in the infinite $U$ case, the problem was reduced to a one-body Hamiltonian whose energy can be minimized easily. The quantity we need to calculate is the Green function at the impurity, around the Fermi level. Thus,

$$ G_{dd} = \langle \hat{z}_\sigma \hat{d}_\sigma^z ; \hat{d} \hat{d}^\dagger \rangle \, , $$

which is the propagator that carries the correct weight of the Kondo resonance.

In Sec. II B it will be shown how to calculate the GF in the lead’s sites using $G_{dd}$ as an input.
3. Numerical renormalization group approach

The NRG method was originally proposed by K. G. Wilson to study magnetic impurity problems. Initially, it was applied to the Kondo Hamiltonian, and later extended to the Anderson model. It can be shown that for these two models, at low temperatures, the states close to the Fermi level (i.e. with the lowest energy contribution) are the most relevant. Therefore, perturbation theories are not the most adequate approach to these problems. As a brief description of the method (a full detailed description can be found in Refs. [17][19], we present the two main steps in the implementation of the method.

The first one consists in sampling the energy interval of the conduction band by a set of logarithmically decreasing energy intervals \([x_N, x_{N-1}],\) defined by \(x_N = \pm D \Lambda^{-N},\) where \(\Lambda\) is the discretization parameter and \(D\) is the half-width of the conduction band. Then, from each interval, only one representative energy value is kept (chosen according to a well defined criterion, see Bulla in Ref. [19] for details). The total number of representative energies, one from each interval, result in the set of discrete energies that couples to the impurity. After these two basic steps, the total Hamiltonian is mapped into a semi-infinite chain, commonly known as Wilson-chain, where each site of the chain corresponds to an energy scale in the logarithmically discretized conduction band, with the impurity sitting at its first site. It is important to notice that the \(t_n\) couplings, between adjacent sites \(n\) and \(n + 1,\) decrease, away from the impurity, as \(\Lambda^{-n/2}.\) The final form for the Hamiltonian in the NRG framework is

\[
H = \lim_{N \to \infty} \Lambda^{-(N-1)/2} H_N
\]

where,

\[
H_N = \Lambda^{(N-1)/2} \left[ \sum_{\sigma} c_{0\sigma}^\dagger c_{0\sigma} + \text{h.c.} \right] + \sum_{n=0}^{N} \epsilon_n c_{n\sigma}^\dagger c_{n\sigma} + \sum_{n=0}^{N-1} t_n \left( c_{n\sigma}^\dagger c_{n+1\sigma} + \text{h.c.} \right)
\]

with \(d_{\sigma}\) annihilates an electron with spin \(\sigma\) at the impurity, and \(c_{n\sigma}\) annihilates one at site \(n\) in the semi-infinite chain (indexed from \(n = 0\) to \(N\)).

Note that an explicit analytical expression for \(t_n\) in Eq. [13] cannot be obtained for a band of arbitrary shape. For the present problem, where a semi-elliptical band is used, we are forced to calculate the \(t_n\) numerically. The hoppings \(t_n\) that define the Wilson-chain must not be confused with the matrix elements \(t\) of the real space chain, shown in Fig I. The elements \(t_n\) correspond to the band obtained after the logarithmic discretization of the real space chain. It can be shown that when \(\Lambda \to 1,\) the hoppings \(t_n \to t^\text{Diag.}\)

The second important step consists in solving numerically the resulting Hamiltonian given by Eq. [12]. To this end, we start with a system consisting of the isolated impurity, described by the Hamiltonian \(H_{\text{imp}}.\) Then, the subsequent sites are added one by one. This procedure generates a sequence of Hamiltonians \(H_N,\) which are solved as follows: at a given iteration \(N\) the Hamiltonian \(H_N\) is diagonalized numerically. The eigenvectors and the corresponding eigenvalues are obtained. Next, a new site \(N + 1\) is added. This is done by enlarging the current Hilbert space (associated to iteration \(N\)) through a tensorial product of its elements with the states of the site being added in the next iteration. This process results in an exponential growth of the dimension of the Hilbert space of successive iterations. Due to computational constraints, it is necessary to truncate the Hilbert space at each iteration, after it reaches a certain size. The NRG truncation criterion is to keep only the \(M\) lowest energy states of \(H_N\) (typically, \(M = 1000\)), and neglect the higher energy spectrum.

The process of adding a single site to \(H_N\) is repeated until the system reaches the strong coupling fixed point. When this fixed point is reached, \(H_N\) and \(H_{N+2}\) have the same eigenvalues.

The sequence of iterations described above can be thought of as a renormalization group (RG) process. Adding one site to the chain, and obtaining the new low-energy spectra, can be understood as an RG transformation \(R\) that maps the Hamiltonian \(H_N\) into a new Hamiltonian \(H_{N+1} = R(H_N),\) which has the same form as \(H_N.\) Once the fixed points are obtained, the static and dynamic properties, as well as temperature effects, can be calculated. In particular we are interested in the local GF at the impurity.

At this point it is worth to remind the reader that the information about the high energy dynamics is not accurately taken into account, since the high-energy spectra is partially neglected after the truncation.

All the NRG data presented in this work was calculated with \(\Lambda = 2.5\) and keeping the \(M = 1000\) lower energy states in each iteration. To calculate the LDOS at the impurity, the delta functions were broadened using Logarithmic-Gaussians with a \(b = 0.6\) factor (see Ref. [19]).

Finally, we want to stress, once again, the difference between the real space semi-infinite chain and the Wilson-chain. The first one, shown in Fig I, has all the hopping terms equal to \(t.\) The Wilson-chain is just used to calculate the GF at the impurity, and it is obtained after the discretization of the real space chain. With the impurity propagator, obtained from NRG, the LDOS at any site of the real space chain can be calculated, as explained below.

B. LDOS away from the impurity: Equation of Motion

In this section, we will explain how to calculate the LDOS at any site of the semi-chain, which models the electron reservoir. Note that, for all numerical methods used in this work, once the dressed GF is known at the impurity (and, in the case of ECA, for all the other sites of the cluster), a procedure based on the construction of a Dyson equation, through the use of a sequence of Equation of Motion, can yield the dressed GF for any site in the tight-binding semi-chain, no matter how far away from the impurity. This can be most easily understood in the case of ECA, as this idea is built into the very core of the method. Indeed, ECA allows us to calculate not just the LDOS in all the sites of the cluster, but also in
all the sites in the rest of the semi-infinite tight-binding chain used to represent the lead. An important fact that we want to remark regarding ECA is that the embedding procedure results in a feedback of the leads into the central region, but also reciprocally. The physics under study does not need to be restricted to entirely occurring within the exactly solved region. I.e., many-body effects taken into account exactly inside the ED cluster are propagated, by the Dyson equation, into the electron reservoir (the semi-chain), which now does not have anymore the LDOS of a non-interacting system. It is important to remark, as will be clearly explained shortly, that the change of the LDOS in the semi-chain from tight-binding to many-body lies at the core of the method used in this work to estimate the range of the Kondo cloud. One added benefit of the procedure to be described below is that the physics of the Kondo effect at the impurity (the Kondo resonance) does not need to be calculated with ECA for the EOM procedure to work. In the present work, it is also calculated with FUSBMF and NRG.

To calculate the dressed propagators at any site of the semi-chain, we write down the EOM of the local propagators at a site \( M \). In the case of ECA, the site \( M \) must be outside the cluster, i.e., \( M \geq L + 1 \) (see Fig. 1). This restriction does not apply to FUSBMF or NRG, where the equivalent to the ECA cluster can be considered to be just the impurity. A brief description of the EOM method can be found in Ref. 22. To simplify the notation, in what follows we will ignore the spin index \( \sigma \). The set of equations to solve, in order to calculate \( G_{M,M} \), is given by

\[
\begin{align*}
G_{M,M} &= g_0 + g_0 t G_{M-1,M} + g_0 \tilde{G}_{M+1,M}, \\
G_{M+1,M} &= \tilde{g}_{sc} t G_{M,M}, \\
G_{M-1,M} &= G_{M-1,M-1}, \\
G_{M+1,M-1} &= \tilde{g}_{sc} t G_{M+1,M-1},
\end{align*}
\]

where \( g_0 = 1/\omega \) is the atomic GF at site \( M \) and \( \tilde{g}_{sc} \) is the bare propagator for the rest of the semi-chain starting at the site \( M + 1 \) and is given by,

\[
\tilde{g}_{sc} = \frac{\omega \pm \sqrt{\omega^2 - 4t^2}}{2t^2}.
\]

In Eq. 16, we used explicitly the equivalence between \( G_{M-1,M} \) and \( G_{M,M-1} \). This is only valid if the hopping parameters \( t \) are real (e.g., no magnetic field inside the chain, although a more general EOM, involving a magnetic field, can also be found.

Solving this set of equations, we obtain,

\[
G_{M,M} = \frac{g_0 + g_0 t g_0}{1 - g_0^2 \tilde{g}_{sc}} G_{M-1,M-1}.
\]

Note that the GF at the site \( M \) can be calculated after the GF at \( M - 1 \). Note that the equation above clearly indicates that, to calculate the dressed GF at site \( M \), the only many-body information needed is the dressed GF at site \( M - 1 \). This fact automatically defines a procedure to find the propagator at any site in the semi-chain. Note that Eq. 19 is defined for a site, within the semi-chain (i.e. \( M \geq 2 \)), that is connected to both adjacent sites by a matrix element \( t \). Thus, this still leaves us with the task of calculating \( G_{1,1} \). To calculate the correct propagator at site 1, we have to rewrite Eqs. 14 to 17 in order to obtain \( G_{1,1} \) as a function of \( G_{0,0} \), without overlooking that the hopping between sites 0 and 1 is \( t' \), not \( t \).

For FUSBMF and NRG, we start with the GF calculated at the impurity, i.e., \( G_{0,0} \). Using the EOM method, we calculate the propagator at the first site of the chain, \( G_{1,1} \). Then, using Eq. 19 the propagator \( G_{M,M} \) can be calculated at any site. The procedure for the ECA method is slightly different, as in ECA all the dressed propagators inside the ED cluster are calculated already within the method. Therefore, in ECA, the EOM procedure starts at site \( L + 1 \) (see Fig. 1), using Eq. 19 where \( G_{L,L} \) is an input from the ECA calculations. In that case, there is no special procedure to calculate \( G_{1,1} \).

Once \( G_{M,M} \) is calculated for the desired site \( M \), the LDOS can be calculated as,

\[
\hat{\rho}_M(\omega) = \frac{-1}{\pi} \text{Im}[G_{M,M}].
\]

As we are using the same procedure to find the LDOS away from the impurity for three very diverse numerical methods (ECA, FUSBMF, and NRG), some explanation about the adopted terminology is necessary, so that the same term, with slightly different meanings, can be unambiguously used throughout the manuscript. As explained in Fig. 1 in ECA, cluster means a variable size finite group of sites (including the impurity), which is exactly diagonalized and embedded (as explained above). In this manuscript, the ECA cluster contains up to \( L + 1 = 10 \) sites (i.e., the impurity plus up to \( L = 9 \) tight-binding sites). For sites \( N \geq L + 1 \), the LDOS will be found through the EOM method, as described above. On the other hand, an FUSBMF or an NRG cluster, given the very nature of both methods, contains just the impurity itself (therefore, \( L = 0 \), see Fig. 1). Because of that, there is a slight difference to the application of the EOM method to these last two methods, viz., \( G_{1,1} \) has to be calculated first, and then all the other \( G_{i,j} \) are calculated by using Eq. 19 in sequence, as explained above.

### III. LOCAL DENSITY OF STATES WITHIN THE METAL HOST

Using the FUSBMF approximation, we can obtain analytically self-consistent expressions for the GF, and then the LDOS. The local GF is also obtainable within NRG, i.e., the LDOS at the impurity can be found with very good accuracy, and, as explained in Sec. 18 the GF (and therefore the LDOS) can be calculated within the semi-chain that models the non-interacting band. The same is valid for ECA, despite the distinctions drawn above between ECA, in the one hand, and FUSBMF and NRG, in the other hand.

In Fig. 2 we show the LDOS for several different sites within the non-interacting semi-chain (\( N > 0 \)), calculated by ECA. The parameters used are \( U = t \) and \( \Gamma = 0.1t \), and
FIG. 2: (Color online) (a-f) The LDOS for sites (note that the impurity is located at and 100 (see Fig. 1), calculated by ECA for a cluster with while dashed (red) curves show results for values for show the LDOS at panels, which were calculated using the EOM method described in the text. The LDOS for the first three sites (were calculated using ED, in contrast to the ones for the last three sites. which were calculated using the EOM method described in the text. The LDOS for the first three sites ( were also calculated with EOM and, as expected, there was a very good agreement between the results obtained with the two different methods.

FIG. 3: (Color online) (a) LDOS for site \( N = 0 \), where the impurity is located (see Fig. 1), calculated by ECA. Solid line shows LDOS for \( V_g = -U/2, U = t, \) and \( t' = 0.3t \), while in dashed lines, results are shown for \( T > T_K \) and the same parameter values for \( V_g, U \) and \( t' \). An imaginary part \( \nu = 0.001 \) was used to regularize the LDOS. The dashed (black) curve displays an example of the normalized Lorentzian used to convolute the data in Eq. 22. (b) LDOS for the first and third sites of a non-interacting semi-chain with bandwidth \( D = 4t \). (c) Same as (b), but now for the second and fourth sites.

The LDOS of the first four edge sites of an isolated non-interacting semi-chain. The results shown in Fig. 2 panels (a) to (d) display essentially the hybridization between the LDOS of the impurity (panel (a) in Fig. 3) and the LDOS of the sites in the semi-chain (panels (b) and (c) in Fig. 3), once the impurity is coupled to the semi-chain. The solid (black) curve shows the LDOS for \( T = 0 \), while the dashed (red) curve shows the LDOS for \( T > T_K \), at the first four sites in the semi-chain, after it couples to the impurity. This hybridization can be described in a simple way: a peak in the LDOS of the impurity [Fig. 3(a)], centered at \( \omega_p \), will generate either a resonance or an anti-resonance (at \( \omega_p \)) in the LDOS of a semi-chain site when the impurity couples (hybridizes) to the semi-chain. On the one hand, a resonance (a peak) will result if the semi-chain’s LDOS, in one specific site, vanishes at \( \omega_p \). On the other hand, an anti-resonance (a dip) results when the site’s LDOS at \( \omega_p \) is finite. This resonance/anti-resonance site to site oscillation effect in the LDOS will have important consequences in the next section. Our interest is to be able to distinguish the effect caused over the semi-chain’s LDOS, far away from the impurity, by the presence \( (T < T_K) \) or absence \( (T > T_K) \) of a resonance at the Fermi energy (the Kondo peak) in the LDOS at the impurity [compare the solid and dotted curves in Fig. 3(a)]. The extent to which this hybridization effect can spread away from the impurity will be used as a measure of the extent of the Kondo cloud.

Figure 2 clearly displays this kind of hybridization effect, as described above. Indeed, if one concentrates the attention on the features close to the Fermi energy (\( \omega = 0 \)) in the differ-
FIG. 4: (Color online) (a) Main panel: Absolute value of the cloud extension function, $|F(N)|$, calculated by ECA as a function of the semi-chain site $N$ for several different cluster sizes ($L = 1$ to $9$, in steps of $2$ – see legend). The parameter values are $U = t$ and $\Gamma = 0.1t$. Note that $L$ is the number of nearest neighboring sites to the impurity within the cluster solved exactly in ECA. The curves shown are the data obtained through Eq. 22. Fits to these data (not shown), for each value of $L$, using Eq. 23, result in exactly the same curves as the ones shown. It is clear that the data for each different cluster size decays exponentially with $N$ (notice the logarithmic scale in the vertical axis). (b) ECA extrapolation to the thermodynamical limit for each $\Gamma$ value and (b) FUSBMF results. Note that, as $\Gamma$ increases, the reach of the distortion in the LDOS of a given site $N$ ($R_{K}$), produced by the impurity, is reduced, reflecting the shorter range of the Kondo effect. Note also that the dependence of $|F(N)|$ with $N$ for all $\Gamma$ values shown is perfectly linear.

FIG. 5: (Color online) Cloud extension function $F(N)$ as a function of the site in the semi-chain, for several values of $\Gamma$. (a) Extrapolation to the thermodynamical limit for each $\Gamma$ value and (b) FUSBMF results. Note that, as $\Gamma$ increases, the reach of the distortion in the LDOS of a given site $N$ ($R_{K}$), produced by the impurity, is reduced, reflecting the shorter range of the Kondo effect. Note also that the dependence of $|F(N)|$ with $N$ for all $\Gamma$ values shown is perfectly linear.

IV. NUMERICAL RESULTS

As mentioned in Sec. I, considering that the width of the Kondo resonance in the LDOS at the impurity, $\Delta$, is proportional to $T_{K}$, we expect that,

$$R_{K} \approx \frac{1}{\Delta},$$

(21)
In this section, we will estimate the screening length $R_K$ by evaluating the distortion in the LDOS, produced by the Kondo resonance at the impurity, in sites N arbitrarily far away from the impurity. The distortion produce in site N will be quantified by the absolute value of the function $F(N)$, as defined by

$$F(N) = \int_{-\infty}^{\infty} \left( \rho^K_N(\omega) - \rho^{NK}_N(\omega) \right) L(\omega) \, d\omega,$$  \quad (22)$$

where $\rho^K_N$ ($\rho^{NK}_N$) is the local density of states at the site N in the Kondo regime (out of Kondo), and $L$ is the Lorentzian distribution of width $\Delta$ [dashed curve in Fig. 3(a)]. Note that the distance to the impurity is given by $r = Na$, where a is the lattice parameter. It is important at this point to remind the reader that all the calculations here were done at $V_h = 0$ (i.e., at the particle-hole symmetric point). To evaluate $\rho^K_N$, we applied the EOM procedure to the impurity’s GF (where the dotted line in Fig. 5(a) shows the negative of its imaginary part).

Note that, for a site far away from the impurity, where the many-body effects are not important, $\rho^K_N$ must be equal to $\rho^{NK}_N$, thus $F(N) \approx 0$. This can be seen in the last panel of Fig. 3. $F(N)$ will be used to find a length scale beyond which the presence of the impurity is not relevant any more. We will call $F(N)$ the cloud extension function.

As already mentioned, to calculate $\rho^K_N$, we will use ECA, FUSBMF, and NRG.

In Fig. 4(a), it is shown the absolute value of the cloud extension function, $|F(N)|$, calculated with ECA, as a function of $N$, for $U = t$, $\Gamma = 0.1t$, and for several values of $L$ (note that the vertical axis has a logarithmic scale). The scatter plots show the data obtained from Eq. 22 for some selected values of $N$, for different cluster sizes $L$ (see legend). We find that the behavior of $|F(N)|$, for all values of $L$ used, is a decaying exponential (the correlation factor, when fitting the curves with an exponential, was exactly 1 for all values of $L$):

$$|F(N)| = A_0 \exp(-N/R_K).$$  \quad (23)$

where $R_K$ marks the distance from the impurity where the value of $|F(N)|$ has fallen by $1/e$, in comparison to its value at the impurity ($N = 0$). The solid lines in panel (a) show the result of fitting each set of data with Eq. 23. In the inset of Fig. 3(a), it can be observed that $F(N)$ oscillates between positive and negative values for successive N. This is a direct consequence of the resonance/anti-resonance oscillation in the LDOS discussed in the previous section. The extrapolation of $R_K$ to an ‘infinite’ ECA cluster ($1/L \to 0$) is explained in detail next.

As mentioned already, each curve in Fig. 4(a) (from $L = 1$ to $L = 9$) is fitted using Eq. 23. Therefore, a value for $R_K(L)$ is found for each cluster size used in ECA ($1 \leq L \leq 9$). Figure 4(b) shows the values obtained this way for $R_K(L)$ as a function of $1/L$ (solid (black) dots), for the different values of $L$ used in panel (a). A fitting of these results by a quadratic polynomial is also shown (dashed (red) curve). The intercept of the dashed (red) curve with the vertical axis provides an extrapolation of $R_K$ to the thermodynamical limit.

FIG. 6: (Color online) Range ($R_K$) of the Kondo cloud as a function of $\Delta$. The open dots show the results obtained for $R_K$ through the fitting of curves like the ones in Fig. 5 for various values of $\Gamma$ (therefore, different $\Delta$, i.e., the width of the resonance at the Fermi level $\Delta$). (a) ECA, (b) FUSBMF, and (c) NRG results. A fixed parameter $U = t$ was used for the three methods, and the parameter $\Gamma$ was changed in order to obtain different $\Delta$ values. The solid (red) line in each panel shows the interpolation of an $1/\Delta$ function, as expected for $R_K$ vs $\Gamma$ (which is proportional to $\Delta$). The value of the proportionality factor for each method is shown in the respective label.

FIG. 7: (Color online) ECA results for the size of the Kondo cloud vs. $1/\Delta$ for $U = 0.5t$, $U = t$ and $U = 1.5t$. Note that, for the interval of values of $U$ and $\Gamma$ shown, $R_K$ is exactly a linear function of $1/\Delta$, and does not depend on the values of $U$ and $\Gamma$ used.
$R_{K}(L \rightarrow \infty)$. This extrapolated value of $R_{K}$ can then be used in Eq. 23 to obtain the thermodynamical limit for the $|F(N)|$ curve, which, for $\Gamma/t = 0.1$, is the open (red) triangles in Fig. 4(a). 23

Obviously, Eq. 23 has two free parameters, viz., $A_{0}$ and $R_{K}$. Although the vertical axis in Fig. 4(a) is logarithmic, making it difficult to judge the convergence of $A_{0}$, it is true that $A_{0}$ converges with $L$ faster than $R_{K}$ (note that, in accordance with Eq. 23, $A_{0}$ is the y-intercept and $R_{K}$ is the negative of the inverse of the slope of the curves for different cluster sizes). The values of $A_{0}$ for different values of $L$ as obtained from the fitting, of each data set in Fig. 4(a), done with Eq. 23. The dependence of $A_{0}$ on the model parameters will be discussed below. 23

At this point, it is important to note that, as the cluster used in the FUSBMF and NRG calculations has a fixed size ($L = 0$), there is no extrapolation to be done to find $|F(N)|$ for both methods. There is only a fitting to Eq. 23 to find $R_{K}$ and $A_{0}$.

Now that we have clarified how the thermodynamical limit value for $R_{K}$ is found for each method, we want to show how it varies with the model parameters. Figure 5(a) shows the extrapolated (ECA) $|F(N)|$ curves, for $U = 1.0$ and different values of $\Gamma$ (from 0.0625 (solid black curve) to 0.4 (dashed magenta curve). From the data, it is clear that $R_{K}$ (the negative of the inverse of the slope) increases with increasing values of $\Gamma$. In panel (b), the corresponding $|F(N)|$ curves obtained with FUSBMF are shown, for comparison. The overall agreement between both methods is quite good. As expected, we observe that the size of the Kondo cloud (measured through the cloud extension function) increases with $U/T$. We can understand this behavior by noting that, as $\Gamma$ increases (with a fixed $U$), $T_{K}$ also increases, and $R_{K}$, as predicted by Eq. 1, decays.

Figure 6 shows the results obtained [open dots in panels (a), (b) and (c)] by extrapolating $R_{K}$ from $|F(N)|$ for different values of $\Gamma$ (at $V_{g} = -U/2$), using ECA (a), FUSBMF (b), and NRG (c). These results are plotted as a function of $\Delta$ (which is taken as the full-width at half-height of the Kondo peak for each different value of $\Gamma$). We observe that the dependence of the Kondo length $R_{K}$ with $\Delta$ satisfies the relationship given by Eq. 21 (as $\Delta$, the width of the Kondo peak, is proportional to $T_{K}$). To emphasize that, each set of data (obtained by the three different methods) was fitted by a function $\propto 1/\Delta$ (see the solid (red) line in each panel). It is important to stress that the proportionality coefficient between $R_{K}$ and $1/\Delta$ obtained by all the three different methods is very similar, i.e., $R_{K} \sim 2.0/\Delta$. The proportionality factor in Eq. 21 are 1.874 for ECA, 1.964 for FUSBMF, and 2.102 for NRG. While this factor is similar for ECA and FUSBMF, there is a 10% difference between ECA and NRG. We believe that this difference comes from the parameter $b$ used in NRG to broaden the logarithmic-Gaussian functions in the LDOS, as the value of $\Delta$ obtained by NRG is very sensitive to the choice of this arbitrary parameter.

Figure 7 shows ECA results of $R_{K}$ v.s. $1/\Delta$ for three different values of $U$ (0.5, 1.0, and 1.5). As shown in the figure, the functional form $R_{K} \propto 1/\Delta$ is valid for the intervals of $U$ and $\Delta$ (and therefore $\Gamma$) inside which the calculations were done. More importantly, as all the curves collapse to a single line, the proportionality coefficient is also independent of these intervals. This indicate that the ‘propagation’ of the Kondo effect into the leads (which is essentially measured by $R_{K}$) depends only on the width of the Kondo resonance at the Fermi level (measured by $\Delta$).

Figure 9 shows, for ECA and FUSBMF, the parameter $A_{0}$ as a function of $\Delta$. We can see that, the ECA and FUSBMF curves agree quite well, for the same value $U = 1.0$. Additional calculations, with different $U$ values ($U = 0.5$ and $U = 1.5$), were done just with ECA. For these additional results, one sees that the curves start to diverge from each other for large $\Delta$, but agree for small values ($\Delta < 0.04$). The agreement for small $\Delta$ can be easily understood if one takes in account the universal behavior of the Kondo effect, in the sense that it is determined by a single energy scale, the Kondo temperature $T_{K}$. Therefore, $A_{0}$ (as $R_{K}$) does not depend on either $U$ or $\Gamma$ independently, but on their ratio ($U/\Gamma$), at least until the system enters the mixed valence regime, at higher $\Delta$ (equivalent to $\Gamma$). Notice that the curve for lower $U$ ($U = 0.5$) starts to diverge from the other two at a lower value of $\Delta$ (proportional to $\Gamma$), while the opposite occurs for the larger-$U$ curve. 23

V. CONCLUSIONS

Using, for the first time, the LDOS within the metal lead, we have estimated the effective length, in real space, of the effect of the many-body correlations originating at the impurity site. For the Kondo effect, we defined a cloud extension function $F(N)$ in order to estimate when an electron located at a site $N$, away from the impurity, is not affected anymore by its presence.
Indeed, we have used the electronic properties reflected in the LDOS function (charge spectra) of the one-dimensional metallic lead, to study the spatial propagation of the Kondo effect away from the magnetic impurity. The length of the Kondo cloud, $R_K$, has been defined in the literature to be the extension of the spin-screening-cloud, formed by the conduction electrons, in the vicinity of the impurity. From this point of view, it is essentially the spatial size of a magnetic property, as it is associated to the spin-spin correlations between the local impurity and the conduction electron spins. However, here we claim that, as far as the Kondo cloud is concerned, the charge spectra counterpart of the Kondo physics (defined as the effect of the impurity’s Kondo peak over the LDOS of the leads) is equivalent to its magnetic expression, as they are both manifestations of the same physical phenomenon. Moreover, we claim that $|F(N)|$, being dependent just on the LDOS, is easier to calculate and measure than spin-correlation-based functions.

As far as transport properties are concerned, if the Kondo effect is thought to be the way in which two or more QDs can interfere, the relevant way of studying the Kondo cloud is by analyzing the effect of the impurity over the LDOS of the rest of the system.

In order to study the Kondo effect spatial propagation, we define what we call a cloud extension function, denoted $F(N)$ (see Eq. 27). It measures, in an interval of width $T_K$ around the Fermi energy, the distortion of the LDOS, at site N, created by a Kondo impurity sitting at the origin. We evaluated this function using three totally different formalisms, ECA, FUSBMF, and NRG, and obtained almost identical results for the variation of $R_K$ with the parameters of the system. The fact that three different formalisms provide the same physical description makes this study quite robust and reliable. We demonstrate, as well, that the length of the Kondo cloud is controlled by the unique, scaling invariant, relevant parameter of the Kondo effect, the Kondo temperature $T_K$. These results permit a very accurate determination of the functional form of $R_K(T_K)$, in agreement with intuitive ideas, summarized in Eq. [1].

Finally, it is important to emphasize that the measurement of spin-spin correlations between different sites, in a real STM experiment, is difficult to perform, as the use of two different STM tips, at the same time, is required. On the other hand, the mapping of the Kondo cloud through the difference in the conductance, measured by an STM tip, at different points in a 1D system, looks more feasible, as it has already been performed in metallic surfaces.

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ity for a non-Kondo solution consists in decoupling the impurity from the semi-chain (by making $t' = 0$). Our calculations were done both ways, i.e., Hubbard-I and $t' = 0$, and we found agreement between the two results for the extension of the Kondo cloud $R_K$.

Note that, in ECA, $\Delta$ was calculated as the thermodynamical limit $-1/L \to 0$ of the width of the Kondo resonance at the impurity’s LDOS.

A second extrapolation method can also be used (although not as accurate as the one described in Sec.IV): one can extrapolate the value of $|F(N)|$ to the thermodynamical limit $(1/L \to 0)$ for each value of $N$, and then obtain $R_K$ by fitting the extrapolated $|F(N)|$ to Eq. 23. Although there is good qualitative agreement on the values obtained for $R_K$ between the two extrapolation methods, we favor the first one, as it involves much less computational effort and is therefore more accurate.

The limit in which $|F(N)| \to 0$ determines the order of magnitude of the Kondo cloud. However, the actual values and functional variation of both $A_0$ and $R_K$ in Eq. 23 clearly indicate that $R_K$ has a leading contribution in determining the size of the Kondo cloud, given the small variation of $A_0$ in the region of parameter space associated to the Kondo effect (compare the scales of the vertical axis in Figs. 6 and 8).

Note that $A_0$ was not calculated as $|F(0)|$, but through the fittings discussed in Figs. 4 and 5. Therefore, its value, and its dependence with $\Delta$, as seen in Fig. 8, do not represent the value or the variation of the area of the Kondo peak.

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