Kondo Screening Cloud and Charge Quantization in Mesoscopic Devices

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We propose that the finite size of the Kondo screening cloud, \(\xi_K\), can be probed by measuring the charge quantization in a one-dimensional system coupled to a small quantum dot. When the chemical potential in the system is varied at zero temperature, one should observe charge steps that are controlled by the Kondo effect when the system size \(L\) is comparable to \(\xi_K\). We show that, if the standard Kondo model is used, the ratio between the widths of the Coulomb blockade valleys with odd or even number of electrons is a universal scaling function of \(\xi_K/L\).

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The Kondo effect can be described as the strong renormalization of the exchange coupling between an electron gas and a localized spin at low energies [1]. Below some characteristic energy scale, known as the Kondo temperature \(T_K\), a non-trivial many-body state arises in which the localized spin forms a singlet with one conduction electron. In the recent realizations of the Kondo effect [2], a semiconductor quantum dot in the Coulomb blockade regime plays the role of a spin \(S = 1/2\) impurity when the number of electrons in the dot is odd. The Kondo temperature in these systems is a function of the coupling between the dot and the leads and can be conveniently controlled by gate voltages. As a clear signature of the Kondo effect, one observes that the conductance through a quantum dot with Kondo effect, one observes that the conductance through a Kondo impurity was treated in [3]. On the other hand, we expect that in a finite system the infrared singularities that give rise to the Kondo effect are cut off not by temperature, but by the level spacing \(\Delta\) if \(\Delta \gg T\). For a one-dimensional (1D) system with length \(L\) and characteristic velocity \(v\), the relevant dimensionless parameter is \(\Delta/T_K \sim \xi_K/L\), where \(\xi_K \equiv v/T_K\) is identified with the size of the Kondo screening cloud, the mesoscopic sized wave function of the electron that surrounds and screens the localized spin. This long length scale (\(\xi_K \sim 0.1–1 \mu\text{m}\)) is comparable with the size of currently studied mesoscopic devices, which has motivated several proposals that the Kondo cloud should manifest itself through finite size effects in such systems [4, 5, 6].

One familiar property of small metallic islands in the Coulomb blockade regime is the quantization of charge. Since each electron added to the system costs a finite energy, the number of electrons changes by steps as one varies the chemical potential and sharp conductance peaks are observed at the charge degeneracy points [2]. In AlGaAs-GaAs heterostructures, the level spacing of a 1D system with size \(L \sim 1 \mu\text{m}\) is of order \(\Delta \sim 100 \mu\text{eV}\), large enough to be resolved experimentally. Clearly, the energy levels should be affected by the Kondo interaction with an adjacent dot. Therefore, the addition spectrum should exhibit signatures of the finite size of the Kondo cloud.

We consider the geometry shown in Fig. 1. One of the ends of a wire of length \(L\) with a large number of electrons (such that \(\Delta \ll \epsilon_F\), where \(\epsilon_F\) is the Fermi energy) is weakly coupled to a small quantum dot via a gate voltage \(V_{dw}\). Both the dot and the wire (which can be thought of as a very long and thin dot) are in the Coulomb blockade regime. The dot has a very large charging energy and a ground state with \(S = 1/2\). We assume that the wire is very weakly connected to a reservoir and that transfer of a single electron between wire and reservoir could be measured by some Coulomb blockade technique. This coupling is assumed weak enough so as not to affect the energy levels of the wire-dot system. Experiments with small dots and large dots have been performed, for example, in [7] and considered theoretically in [8].

Here we investigate this effect using the basic Kondo model, ignoring charge fluctuations on the dot, assuming the wire contains a single channel and ignoring all electron-electron interactions in the wire. Within the constant interaction approximation [2] these interactions are represented by a simple charging energy whose effects on the charge steps are easily subtracted off. We postpone a more complete treatment of these complications, to a later work. (The effect of short range interactions on the conductance through a Kondo impurity was treated in the Luttinger liquid framework in [7].)

FIG. 1: Possible experimental setup. \(V_{dw}\) controls the tunneling \(t'\) between the small dot (on the left) and the wire and \(V_g\) varies the chemical potential in the wire.
Weak coupling. – The tunneling between the wire and the dot is well described by the Anderson model \cite{Anderson1958}. For zero tunneling amplitude the system reduces to an open chain and a free spin. In the continuum limit, we introduce the fermionic field \( \Psi(x) \) for the electrons in the wire, as well as its right- and left-moving components

\[ \Psi(x) = e^{ikFx} \psi_R(x) + e^{-ikFx} \psi_L(x). \]

The open boundary conditions \( \Psi(0) = \Psi(L) = 0 \) imply that \( \psi_{L,R} \) are not independent. Instead, \( \psi_{L,R} \) can be regarded as the extension of \( \psi_R \) on the negative-x axis: \( \psi_R(-x) = -\psi_L(x) \). We can then work with right movers only and write down an effective Kondo model (we drop the index \( R \) hereafter)

\[ H = -iv_F \int_{-L}^L dx \psi^\dagger \partial_x \psi + 2\pi v_F \lambda \psi^\dagger(0) \frac{\delta}{2} \psi(0) \cdot \mathbf{\hat{S}}, \]

where \( \lambda \) is the dimensionless Kondo coupling. We assume that \( \lambda \) is independent of \( V_0 \), which may require that \( t' \) and the energy of the localized state in the dot be tuned accordingly. For \( \lambda \ll 1 \), the size of the Kondo screening cloud (defined in the thermodynamic limit) is exponentially large: \( \xi_K \sim (v_F/D) e^{1/\lambda} \), where \( D \ll \epsilon_F \) is a high-energy cutoff. The boundary condition in the weak coupling fixed point \( (L/\xi_K \to 0) \) reads \( \psi(-L) = e^{i\delta \lambda} \psi(L) \), where \( \delta = 2k_F L \mod \pi \). Using the mode expansion \( \psi(x) = -(i/\sqrt{2D}) \sum_k e^{iks} c_k \), we obtain the momentum eigenvalues \( \xi_n = (n\pi - \delta)/L, n \in \mathbb{Z} \).

We denote by \( N(\mu) \) the total number of electrons in the system, including the one in the quantum dot. We are interested in the elementary steps of \( N \) around some initial value \( N_0 \equiv N(\mu_0) \). At \( T = 0 \), we calculate \( N(\mu) \) as the integer value of \( N \) that minimizes the thermodynamic potential \( \Omega(N) = E(N) - \mu N \), where \( E(N) \) is the ground state energy. Defining \( \mu_{\ell+\frac{1}{2}} \) as the value of \( \mu \) where \( N \) changes from \( N_0 + \ell \) to \( N_0 + \ell + 1 \), we obtain from the charge degeneracy condition \( \Omega(N_0 + \ell + 1) = \Omega(N_0 + \ell) \) that \( \mu_{\ell+\frac{1}{2}} = E(N_0 + \ell + 1) - E(N_0 + \ell) \). For \( \lambda = 0 \), we set \( \mu_0 \) halfway between the highest occupied and the lowest unoccupied energy level of the open chain. In this case, \( N_0 = \text{odd} \): the ground state is doubly degenerate (total spin \( S_{\text{tot}} = 1/2 \)) and consists of one electron in the dot and pairs of conduction electrons in the Fermi sea. The energy levels measured from \( \mu_0 \) are \( \epsilon_n = (n - 1/2) \Delta \), where \( \Delta = \pi v_F/L \). It is easy to see that, as we raise \( \mu > \mu_0 \), \( N \) jumps whenever \( \mu \) crosses an energy level. Moreover, there are only two steps due to the spin degeneracy of the single-particle states \( (\mu_{2m+\frac{1}{2}} = \mu_{2m+\frac{3}{2}}) \). As a result, \( N(\mu) - N_0 \) takes on only even values and \( N \) is always odd (see dashed line in Fig. 2).

We obtain the charge steps in the weak coupling limit by calculating the correction to the ground state energy using perturbation theory in \( \lambda \) \cite{Fradkin1991}. In the limit \( \lambda \to 0 \), the ground state for \( N \) odd is still doubly degenerate and we write \( |GS(N = \text{odd})\rangle = \prod_{n \leq 0} c_{n+\frac{1}{2}}^\dagger c_{n+\frac{1}{2}} |0\rangle \otimes |\gamma\rangle \), where \( |\gamma\rangle = |\uparrow\rangle, |\downarrow\rangle \) is the spin state of the dot. However, for \( N \) even, there is one single electron occupying the state at the Fermi surface (with momentum \( k_F \)). To lowest order in degenerate perturbation theory, the ground state for \( \lambda \to 0 \) is \( |GS(N = \text{even})\rangle = \prod_{n \leq 0} c_{n+\frac{1}{2}}^\dagger c_{n+\frac{1}{2}} |0\rangle \otimes |0\rangle \), where \( |0\rangle \equiv |\uparrow\rangle \otimes |\uparrow\rangle - |\downarrow\rangle \otimes |\downarrow\rangle |2/\sqrt{2} \) is the singlet state between the spin of the dot and the electron at \( k_F \). This state has \( S_{\text{tot}} = 0 \) and \( \langle \hat{S} \cdot \hat{S}_{cl} \rangle = -3/4 \), where \( \hat{S}_{cl} = \sum c_{\ell+\frac{1}{2}}^\dagger \sigma^x c_{\ell+\frac{1}{2}} \) is the total spin of the conduction electrons. The singlet formation lowers \( E(N) \) for \( N = \text{even} \) relatively to \( N = \text{odd} \). As a result, the Kondo interaction splits the double steps and gives rise to small plateaus with \( N \) even (Fig. 2). To \( O(\lambda^2) \), we find

\[ \frac{\mu_{\ell+\frac{1}{2}} - \mu_0^*}{\Delta} = \frac{[\ell]}{2} - \frac{3}{4} (-1)^\ell \left( \lambda + 2\lambda^2 \ln \frac{DL}{v_F} + \ldots \right), \]

where \( [\ell] \equiv \ell + 1 \) for even and \( [\ell] \equiv \ell \) for odd. Note the logarithmic divergence at \( O(\lambda^2) \) as \( L \to \infty \), characteristic of the Kondo effect. We recognize the expansion of the effective coupling \( \lambda_{\text{eff}}(L) \sim \ln \left( \xi_K/L \right)^{-1} \) in powers of the bare \( \lambda \), as expected from scaling arguments. We have verified that the scaling holds up to \( O(\lambda^3) \), i.e., \( \mu_{\ell+\frac{1}{2}} \) has no dependence on the cutoff \( D \) but the implicit one in the expansion of \( \lambda_{\text{eff}}(L) \). This is remarkable given that \( E(N) \) itself is cutoff dependent. Based on this, we conjecture that the relative width of the plateaus with \( N \) odd/even is a universal scaling function of \( \xi_K/L \). We define the ratio (see Fig. 2)

\[ R \equiv \frac{\delta \mu^*}{\delta \mu} = \frac{E(N_0 + 3) - 2E(N_0 + 2) + E(N_0 + 1)}{E(N_0 + 2) - 2E(N_0 + 1) + E(N_0)}. \]

From Eq. 3, we have that in the weak coupling limit

\[ R \left( \frac{\xi_K}{L} \gg 1 \right) \approx \frac{2}{3} \ln \left( \frac{\xi_K}{L} \right) - \frac{1}{3} \ln \ln \left( \frac{\xi_K}{L} \right) + \text{const}. \]
Strong coupling. – When $\lambda_{eff} \to \infty$, the spin of the dot forms a singlet with one conduction electron and decouples from the other electrons in the chain. In this limit the Kondo cloud is small ($\xi_K / L \to 0$). The strong coupling boundary conditions reflect the $\pi / 2$ phase shift for the particle-hole symmetric case: $\psi(-L) = -\psi(L) [8]$. This implies that the $k$ eigenvalues are shifted with respect to weak coupling: $k_n = (n\pi + \pi / 2 - \delta) / L$. At this fixed point we recover the spin degeneracy of the single-$k$ original plus pairs of electrons in the wire, thus from which we obtain $c_n = n\Delta$ as measured from the original $\mu_0^*$. The ground state consists now of a singlet for the particle-hole symmetric case: $\chi_{imp} = 1/(4T_K)$. This interaction lowers the ground state energy when there is an odd number of remaining conduction electrons ($S_{cl} = 1/2$), thus splitting the charge steps in the strong coupling limit. To lowest order in $1/T_K$, we find

$$H_{FL} = -\frac{2\pi^2}{3} \frac{\psi^*}{T_K} \left[ \psi(0) \frac{\delta}{2} \psi(0) \right]^2,$$

where the prefactor is fixed such that the impurity susceptibility is $\chi_{imp} = 1/(4T_K)$. This interaction lowers the ground state energy when there is an odd number of remaining conduction electrons ($S_{cl} = 1/2$), thus splitting the charge steps in the strong coupling limit. To lowest order in $1/T_K$, we find

$$\frac{\mu_{\ell + \frac{1}{2}} - \mu_{0}^*}{\Delta} = \frac{[\ell - 1] + 1}{2} \Delta + (-1)^\ell \frac{\pi}{8} \frac{\xi_K}{L},$$

from which we obtain

$$R\left(\frac{\xi_K}{L} \ll 1\right) \approx \frac{\pi}{4} \frac{\xi_K}{L}.$$ (6)

Bethe Ansatz results. – In order to check the scaling property of $R = \delta\mu^{\text{odd}} / \delta\mu^{\text{even}}$ for any $L/\xi_K$ we use the Bethe Ansatz (BA) solution of the one-channel Kondo problem [10]. We start with a half-filled band of $N_0 - 1$ conduction electrons ($N_0$ odd) coupled to a localized impurity spin, corresponding to a system size $L = (N_0 - 1) / 2$ in units where the Bethe ansatz cutoff parameter $D$ [10], related to the band-width, is set equal to one. Since the BA solution can be obtained for any filling factor, we can add particles one by one in the system ($N = N_0, N_0 + 1, N_0 + 2, \ldots$) and compute the corresponding energies. This has been done by solving numerically the coupled BA equations [10], using a standard Newton-Raphson method. In Fig. 3 we present results obtained for the ratio $R = \delta\mu^{\text{odd}} / \delta\mu^{\text{even}}$ with $N_0 = 51, 101, 201, 301, 1001, 2001$ and 13 different values of the Kondo coupling in the range $0.06 \leq J \leq 0.8$.

The universal scaling curve has been obtained by rescaling the x-axis $L \to L / \xi_K(J)$ in order to get the best collapse of the data. The entire crossover curve is obtained, ranging from the strong coupling $L \gg \xi_K$ to the weak coupling regime $L \ll \xi_K$. Both strong coupling [Eq. (7)] and weak coupling [Eq. (4)] results are perfectly reproduced. As displayed in the inset (a) of Fig. 3, BA results agree with Eq. (4) using only one fitting parameter: constant $\approx 0.33$. The Kondo length scale, extracted from the universal data collapse of the main panel (black squares), is described by the exponential fit Eq. (5) with $\xi_0 \approx 0.31$ (dashed green line).

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\begin{figure}[ht]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{(Color online) Universal ratio $R = \delta\mu^{\text{odd}} / \delta\mu^{\text{even}}$ as a scaling function of $\xi_K / L$. Bethe ansatz results obtained for various systems sizes ($N_0 = 51, 101, 201, 301, 1001, 2001$) and 13 different values of the Kondo exchange $J$, indicated by different symbols. For each value of $J$, the system lengths $L$ have been rescaled $L \to L / \xi_K(J)$ in order to obtain the best collapse of the data using the strong coupling curve Eq. (7) (dashed red line) as a support for the rest of the collapse. The weak coupling regime for $L \ll \xi_K$, enlarged in the inset (a), is described by the weak coupling expansion Eq. (4) with constant $\approx 0.33$ (continuous blue curve). Inset (b): The Kondo length scale, extracted from the universal data collapse of the main panel (black squares), is described by the exponential fit Eq. (5) with $\xi_0 \approx 0.31$ (dashed green line).}
\end{figure}

\begin{equation}
\xi_K(J) = \xi_0 e^{c/J},
\end{equation}

with $c = 2J(1 - 3/4J^2)$. Fitting $\xi_K$ to this expression gives $\xi_0 \approx 0.31$ (see inset (b) of Fig. 3) which is in very good agreement with the expected value of $\xi_0 = 1/\pi$, resulting from the impurity susceptibility normalized to $1/(4T_K)$.

Flux dependence in quantum rings. – The effect we have described is not unique to the wire geometry. One interesting alternative is to suppose that the quantum dot is embedded in a ring with circumference $L$ (inset of Fig. 3). This geometry offers the possibility of looking at the dependence of the charge steps on the magnetic flux.
For $\lambda$ where $\alpha$ crossings at $\ell$ are flux dependent and exhibit zigzag lines with level can be labeled as right or left movers. The energy level is equivalent to an ideal 1D ring, whose eigenstates satisfies the boundary conditions in such a way that the transmission $\ell$ is open chain by their symmetry under the parity transformation $x \to L - x$. We define the even and odd fields $\psi_{e,o}(x) = [\psi_{R}(x) \pm e^{-ik_{F}L}\psi_{L}(L-x)]/\sqrt{2}$, in terms of which the Kondo interaction takes the form\cite{4}

$$H_{K} = 4\pi v_{F}\lambda \left[ \cos \frac{\alpha}{2}\psi^{\dag}_{e}(0) - i \sin \frac{\alpha}{2}\psi^{\dag}_{o}(0) \right] \times \frac{\delta}{2} \left[ \cos \frac{\alpha}{2}\psi_{e}(0) + i \sin \frac{\alpha}{2}\psi_{o}(0) \right] \cdot \vec{S},$$ \hspace{1cm} (9)

where $\alpha \equiv 2\pi\Phi/\Phi_{0}$ and $\Phi_{0} = hc/e$ is the flux quantum. For $N_{0} = 4p + 1$ ($p$ integer), the lowest unoccupied state of the open chain ($\lambda = 0$) is even under parity. Defining $\delta\mu_{n} \equiv \mu_{2n+\frac{1}{2}} - \mu_{2n-\frac{1}{2}}$ as the splitting of the charge steps in the weak coupling limit, we find

$$\frac{\delta\mu_{n}}{2\Delta} = \frac{3}{4} [1 + (-1)^{n}\cos \alpha] \lambda_{\ell}(L) + O\left(\lambda_{\ell}^{2}\right).$$ \hspace{1cm} (10)

Notice that for $\alpha = 2m\pi$ only the even channel couples to the impurity and the steps in the odd channel (corresponding to odd values of $n$) do not split. The opposite happens when $\alpha = (2m+1)\pi$ (see Fig. 4). In the strong coupling limit, the $\pi/2$ phase shift modifies the boundary conditions in such a way that the transmission across the dot becomes perfect\cite{3,5}. The system is then equivalent to an ideal 1D ring, whose eigenstates can be labeled as right or left movers. The energy levels are flux dependent and exhibit zigzag lines with level crossings at $\alpha = m\pi$\cite{12}. The major effect of a Fermi liquid interaction analogous to Eq. (5) is to lift the degeneracy between right and left movers at $\alpha = m\pi$ and to split two out of the four values of $\mu_{\ell}\pm\frac{1}{2}$\cite{9}. We calculate the splitting $\delta\mu_{n} \approx 2\mu_{2n+\frac{1}{2}} - \mu_{2n-\frac{1}{2}}$ using degenerate perturbation theory to $O(1/K)$ and find ($\xi_{K} \ll L$)

$$\frac{\delta\mu_{n}}{2\Delta} \approx \frac{\pi}{8}\xi_{K}^{2} \left[ \frac{1}{L} + \frac{C_{L}}{L} \right],$$ \hspace{1cm} (11)

for $\alpha \approx m\pi, m = n, n \pm 2, \ldots$ (Fig. 4). This striking difference in the flux dependence of the charge steps is consistent with the results in\cite{3}.

Finally, we would like to point out that the constant interaction model assumed here neglects the exchange interaction between electrons in the wire. However, such interaction could be cast into one empirical parameter that gives a constant contribution to the even-odd splitting, even in the weak and strong coupling limits\cite{2}.

In conclusion, we have shown that the width of the charge steps in a mesoscopic device depends on the finite size of the Kondo cloud. The signature of this effect would be the broadening of the Coulomb blockade valleys with total $N$ even as we increase $T_{K}$ (decrease $\xi_{K}$). The crossover between weak ($\xi_{K} \gg L$) and strong ($\xi_{K} \ll L$) coupling could be used to extract the characteristic length scale of the Kondo problem.

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