Finite-Size Effects in Conductance Measurements on Quantum Dots

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The observation of the Kondo effect in quantum dots has provided new opportunites to finally observe the controversial Kondo screening cloud. Here we study the conductance of a quantum dot embedded in a finite length quantum wire, predicting a change in behavior when the length of the wire is comparable to the size of the screening cloud.

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One of the most remarkable triumphs of recent progress in nanoelectronics has been the observation of the Kondo effect in a single semiconductor quantum dot [1–3] and carbon nanotubes [4]. The quantum dot is formed in a semiconductor heterolayer by applying voltages which confine electrons to an island of size a fraction of a micron. When the tunneling amplitude to the dot from the external leads is sufficiently small, the number of electrons on the dot becomes quite well defined, leading to the Coulomb blockade effect on the conductance. When the number of electrons on the dot is odd, it can behave as an $S = 1/2$ magnetic impurity and the transmission and backscattering of electrons is described by a magnetic exchange interaction between this impurity and the conduction electrons. The Kondo effect is a renormalization of this exchange interaction to large values at low temperature, $T < T_K$, where T_K is the Kondo temperature, leading ultimately to ideal $2e^2/h$ conductance [5]. In a simple-minded picture, this Kondo effect results from the formation of a spin singlet between the impurity spin and a conduction electron in a very extended wave function, known as the screening cloud. The size of this screening cloud is of the order of $\xi_K \approx v_F/T_K$, where v_F is the Fermi velocity and is of the order of 1 μm.

Some of these semiconductor devices have the quantum dot embedded in a quantum wire of width comparable to the dot dimension and length of the order of 1 μm. The ends of the wire must be connected, ultimately, to three-dimensional leads in order to perform conductance measurements. In this situation, the Kondo screening cloud may fill the entire quantum wire and even extend beyond it into the macroscopic leads. One might expect some modification, perhaps suppression, of the Kondo effect to occur if the quantum wire is shorter than the screening cloud. If so, this could provide an ultimate limitation on miniaturization of some nanoelectronic devices.

We have recently investigated this effect in a somewhat different situation where the quantum wire containing the quantum dot is made into a closed ring. Unfortunately, it is then impossible to perform a standard conductance measurement. However, the persistent current induced by a magnetic flux is also sensitive to screening cloud effects and is drastically reduced when the circumference of the ring becomes smaller than ξ_K or equivalently, the energy level spacing of the ring Δ becomes larger than T_K [6]. However, such a persistent current measurement would be a difficult experiment. Thus we turn our attention here to an experimentally easier but theoretically more challenging device: a quantum dot embedded in a quantum wire which is in turn connected to external leads by weak tunnel junctions. We assume that a gate voltage can be applied to the dot and also to the quantum wires. We note that a related device has been proposed recently by Thimm *et al.* [7] where a Kondo impurity was equally coupled to all energy levels of a finite size box. The energy level spacing was assumed constant and of $O(1/V)$, where V is the volume of the (three dimensional) box. These two aspects differ considerably from the geometry studied here. A simplified one-dimensional tight-binding model which describes our device is indicated in Fig. 1 and has the Hamiltonian

$$H = H_L + H_W + H_D + H_{LW} + H_{WD}, \qquad (1)$$

where L, W, and D stand for leads, wires, and dot, respectively. Here

$$\begin{aligned} H_L &= -t\left[\sum_{j=-\infty}^{-L-2} + \sum_{j=L+1}^{\infty}\right](c_j^\dagger c_{j+1} + \text{h.c.}), \\ H_W &= -t\left[\sum_{j=-L}^{-2} + \sum_{j=1}^{L-1}\right](c_j^\dagger c_{j+1} + \text{h.c.}) \\ &\quad + \epsilon_W\left[\sum_{-L}^{-1} + \sum_{1}^{L}\right]n_j, \qquad (2) \\ H_D &= \epsilon_D n_0 + U n_{0\uparrow} n_{0\downarrow}, \\ H_{LW} &= -t_{LW}(c_{-L-1}^\dagger c_{-L} + c_L^\dagger c_{L+1} + \text{h.c.}), \\ H_{WD} &= -t_{WD}(c_{-1}^\dagger c_0 + c_0^\dagger c_1 + \text{h.c.}). \end{aligned}$$

Here $n_{j\sigma} \equiv c_{j\sigma}^\dagger c_{j\sigma}$ and $n_j \equiv n_{j\uparrow} + n_{j\downarrow}$.

Effects being left out of our simple model include other impurities and electron-electron interactions in the wires and leads; we only keep them on the dot. We also ignore the effect of multiple channels. (The quantum wires studied in [3] apparently contained about ten channels, whereas a metallic carbon nanotube contains 2 channels.)

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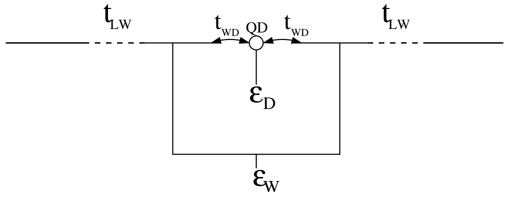

FIG. 1. Schematic representation of the device under consideration. ϵ_D and ϵ_W control, respectively, the dot and wire gate voltage.

In the single channel case $\xi_K/L \approx T_K/\Delta$ so the effects that we study could be regarded as depending either on this ratio of length scales or of energy scales. It is thus important to consider more realistic multichannel models, where these ratios are different, to obtain a better understanding of what effects are dependent on which ratio.

We will assume that the system is in the strong Coulomb blockade regime, so that $t_{WD} \ll -\epsilon_D$, $U + \epsilon_D$, where $\epsilon_D < 0$. Then we may eliminate the empty and doubly occupied states of the dot, so that $H_D + H_{WD}$ gets replaced by a Kondo interaction plus a potential scattering term

$$H_{WD} + H_D \rightarrow H_K = J(c_{-1}^\dagger + c_1^\dagger)\frac{\vec{\sigma}}{2}(c_{-1} + c_1) \cdot \vec{S} + V(c_{-1}^\dagger + c_1^\dagger)(c_{-1} + c_1), \qquad (3)$$

with $J = 2t_{WD}^2[\frac{1}{-\epsilon_D} + \frac{1}{U+\epsilon_D}]$, $V = \frac{t_{WD}^2}{2}[\frac{1}{-\epsilon_D} - \frac{1}{U+\epsilon_D}]$. Here $\vec{S}$ is the spin operator for the quantum dot. We assume that the Kondo interaction and the lead-wire tunneling are weak, $J, t_{LW} \ll t$.

In the case of a closed ring, we showed earlier that the renormalization of the Kondo coupling is cut off, even at low temperatures, by the ring circumference [6]. In the present situation, this renormalization would be cut off by the finite length L of the quantum wires, if $t_{LW} = 0$. Essentially, if the Kondo cloud does not have sufficient room to form, then the growth of the Kondo coupling constant is cut off. The effective Kondo coupling at the length scale L becomes of $O(1)$ when $L \approx \xi_K$.

What is less obvious, is what happens for small but finite t_{LW}. Then, even if $L \ll \xi_K$, the Kondo cloud can still form by leaking into the leads. The growth of the Kondo coupling is not cut off by the finite size of the wire. Nonetheless, we might expect some noticeable effects to occur when L is reduced to a value of $O(\xi_K)$, associated with the screening cloud beginning to leak into the leads. It is these effects which we wish to study in the present paper.

It is instructive to begin with a calculation of the conductance that treats t_{LW} exactly but treats J in lowest nonvanishing order of perturbation theory. We expect this to be valid at sufficiently high T when the renormalized coupling is sufficiently small. To do this calculation, we first diagonalize the Hamiltonian at $J = 0$, i.e., we diagonalize $H_0 \equiv H_L + H_W + H_{LW}$. For nonzero t_{LW}, the spectrum of H_0 is continuous. In order to study the Kondo interaction in perturbation theory, it is useful to express $c_1 + c_{-1}$ in terms of the even eigenstates, c_ϵ of $H_0 - \mu N_e$: $\frac{(c_1 + c_{-1})}{\sqrt{2}} = \int_{-2t-\mu}^{2t-\mu} d\epsilon f(\epsilon) c_\epsilon$. We normalize c_ϵ so that $\{c_\epsilon, c_{\epsilon'}^\dagger\} = \delta(\epsilon - \epsilon')$. Then $f(\epsilon)$ obeys the normalization condition $\int_{-2t-\mu}^{2t-\mu} d\epsilon |f(\epsilon)|^2 = 1$. For small t_{LW}, this "local density of states," $\rho(\epsilon) \equiv |f(\epsilon)|^2$, has sharp peaks at the energies $\epsilon_n = \epsilon_W - \mu - 2t\cos[k_n]$, where the momenta $k_n \approx \pi n/L + O(t_{WL}^2/Lt^2)$. The separation between these peaks near zero energy is $\Delta_n \approx \pi v_F/L$. The width of these peaks is approximately $\delta_n = (2t_{LW}^2 \sin^3(k_n)\eta_{n,W}/tL$, with $\eta_{n,W} = \sqrt{1 + \epsilon_W \cos k_n/(t\sin^2 k_n) - \epsilon_W^2/(4t^2\sin^2 k_n)}$.

We see that the ratio of width to separation is of the order of $\delta_n/\Delta_n \approx \frac{t_{LW}^2}{t^2}\frac{\sin^2 k_n}{\pi}\eta_{n,W}$. We will assume that this quantity is $\ll 1$. The full Hamiltonian may be written in this basis as

$$H - \mu N_e = \int_{-2t-\mu}^{2t-\mu} d\epsilon \epsilon c_\epsilon^\dagger c_\epsilon + \int d\epsilon d\epsilon' f^*(\epsilon) f(\epsilon') \times \left(2Jc_\epsilon^\dagger \frac{\vec{\sigma}}{2} c_{\epsilon'} \cdot \vec{S} + 2Vc_\epsilon^\dagger c_{\epsilon'}\right). \qquad (4)$$

Following [8] the linear conductance (for $t_{LW} \neq 0$) at cubic order in J, V is given by

$$G(T) = \frac{e^2}{\pi\hbar}\pi^2 \int d\epsilon \rho(\epsilon)^2[-dn_F/d\epsilon]\frac{3}{4}J^2[1 + 2JI_1(\epsilon)] + \frac{e^2}{\pi\hbar}4\pi^2V^2 \int d\epsilon \rho(\epsilon)^2[-dn_F/d\epsilon], \qquad (5)$$

with $I_1(\epsilon) = \int d\epsilon' \frac{\rho(\epsilon')}{(\epsilon' - \epsilon)}[1 - 2n_F(\epsilon')]$. $n_F(\epsilon)$ is the Fermi distribution function at temperature T. Notice that the potential scattering term does not renormalize at this order in agreement with [8]. The integral $I_1(\epsilon)$ depends on the local density of states $\rho(\epsilon)$.

Let us focus on the second order terms in J and V, and ignore, for the moment, the corrections of higher order. We must distinguish three regimes of temperature resulting simply from the fact that the width of $(-dn_F/d\epsilon)$ is $O(T)$. If $T \gg \Delta_n$, then the integral in Eq. (5) averages over many peaks of $\rho(\epsilon)$ so that G is approximately independent of ϵ_W:

$$G \approx \frac{e^2}{\pi\hbar}(\pi\rho_0)^2[3J^2/4 + 4V^2], \qquad (6)$$

where $\rho_0 = \sin k_F/\pi t$ is the average local density of states. When $\delta_n \ll T \ll \Delta_n$, the conductance depends strongly on ϵ_W. If ϵ_W is tuned to a resonance peak, $\epsilon_W = \mu + 2t\cos[k_n]$, then the integral in Eq. (5) is dominated by the peak at k_n and we find

$$G(T) \approx \frac{e^2}{\pi\hbar}\frac{(3J^2/4 + 4V^2)}{4TLt_{LW}^2\eta_{n,W}}\pi t \sin k_n. \qquad (7)$$

On the other hand, if ϵ_W is far from a resonance peak (compared to T) then

$$G(T) \approx \frac{e^2}{\pi\hbar}(3J^2/4 + 4V^2)\frac{t_{LW}^4 \sin^6 k_n \eta_{n,W}^2}{t^6}. \qquad (8)$$

Finally, in the ultralow temperature regime, $T \ll \delta_n$, and ϵ_W on resonance, we can evaluate

$$G(T) \approx \frac{e^2}{\pi\hbar}\frac{(\frac{3J^2}{4} + 4V^2)t^2}{t_{LW}^4 \eta_{n,W}^2 \sin^2 k_n}. \qquad (9)$$

The conductance is still given by Eq. (8) when ϵ_W is tuned off resonance for $T < \delta_n$. These approximate formulas certainly break down when they do not give $G\pi\hbar/e^2 \ll 1$, due to higher order corrections in J and V. So our approximate formulas will certainly break down before T is lowered to δ unless $J \ll t_{LW}^2/t$, a condition which might typically not be satisfied. When these formulas apply, we clearly see that the conductance is much larger when ϵ_W is tuned on resonance.

However, there is another, more interesting reason why these formulas can break down at low T, namely, Kondo physics. The cubic correction in Eq. (5) contains a $\ln T$ term which essentially replaces J by its renormalized value at temperature T, $J_{\rm eff}(T)$. We expect that this will remain true at higher orders. At sufficiently high T we can calculate this quantity to lowest order in perturbation theory, using the Hamiltonian in the form of Eq. (4). If the bandwidth is lowered from $\pm D_0$ [where D_0 is $O(t)$] to $\pm D$, then

$$J \to J + J^2\left[\int_{-D_0}^{-D} + \int_{D}^{D_0}\right]\frac{d\epsilon\rho(\epsilon)}{|\epsilon|}. \qquad (10)$$

The renormalization of J is quite different depending on how far we lower the cutoff D. If $D \gg \Delta_n$, the integral in Eq. (10) averages over many peaks in the density of states so its detailed structure becomes unimportant and we obtain the result for the usual Kondo model, unaffected by the weak tunnel junctions $J \to J[1 + 2J\rho_0 \ln(D_0/D)]$.

On the other hand, for smaller D, $D \ll \Delta_n$, the renormalization of J in Eq. (10) becomes strongly dependent on ϵ_W. Let us first assume that ϵ_W is tuned to a resonance of the density of states of width δ_n. Then the integral in Eq. (10) gives a very small contribution as D is lowered from Δ_n down to δ_n so $J_{\rm eff}(D)$ practically stops renormalizing over this energy range. Finally, when $D < \delta_n$, the density of states grows rapidly. By approximating the local density of states by a Lorentzian of width δ_n, we can express the result in terms of the change in $J_{\rm eff}(D)$ as D is lowered from Δ_n

$$J_{\rm eff}(D) \approx J_{\rm eff}(\Delta)\left[1 + J_{\rm eff}(\Delta)\frac{4\sin^2 k_n}{\pi L\delta_n}\ln\left(\frac{\delta_n}{D}\right)\right]. \qquad (11)$$

The density of states appearing in this renormalization is enhanced by a factor of $(2t\sin k_n/[L\delta_n]) \approx t^2/[t_{LW}^2\eta_{n,W}^2 \sin^2 k_n]$. This leads to a rapid growth of $J_{\rm eff}(T)$. On the other hand, if ϵ_W is off resonance then the density of states is small, of order $(\delta_n/\Delta_n^2 L)$ so the growth of the Kondo coupling is very slow at all energies $D < \Delta_n$. Related observations about the renormalization of J, based on numerical results, were made in [9].

Now consider the implications of this renormalization for the value of T_K, defined as the temperature where $J_{\rm eff}(T)$ becomes of $O(1)$. When $J_{\rm eff}(T)$ becomes large at $T \gg \Delta_n$ then T_K is related to the bare Kondo coupling and bandwidth as in the usual case (with no weak links): $T_K \approx T_K^0 \equiv D_0 e^{-1/2J\rho_0}$. Furthermore, in this case, T_K does not depend strongly on ϵ_W. We may characterize this case by $T_K^0 \gg \Delta_n$ or equivalently $\xi_K \ll L$. The screening cloud fits inside the quantum wires and the weak links do not modify the Kondo effect significantly.

On the other hand, suppose that $T_K^0 \ll \Delta_n$ implying that $J_{\rm eff}(\Delta_n) \ll 1$. In this case T_K depends strongly on ϵ_W. If the system is tuned to a resonance then T_K will be slightly less than δ_n:

$$T_K^R \approx \delta_n\left(\frac{T_K^0}{D_0}\right)^{t_{LW}^2\eta_{n,W}^2 \sin^2 k_n/t^2} = O(\delta_n). \qquad (12)$$

On the other hand, if the system is off resonance then $T_K \ll \delta_n$:

$$T_K^{OR} \approx \Delta_n\left(\frac{T_K^0}{D_0}\right)^{t^2/(t_{LW}^2 \sin^2 k_n)}, \qquad (13)$$

effectively zero for most purposes. This behavior of T_K vs T_K^0 is plotted in the inset of Fig. 2 for both ϵ_W on resonance and off resonance. The curves coincide for $T_K^0 \gg \Delta_n$ and differ strongly for $T_K^0 \ll \Delta_n$. The off-resonance Kondo temperature T_K^{OR} drops sharply at $T_K^0 < \Delta_n$ to very small values ($\ll \delta_n$). On the other hand, T_K^R also has a sharp drop at $T_K^0 < \Delta_n$ but then becomes almost flat and of the order of δ_n. Note that the crossover may occur at a smaller value of T_K^0 in the N-channel case (which may depend on some details about the other channels).

Now consider the behavior of the conductance as a function of T and ϵ_W in the two cases. In the case $\xi_K \ll L$, we may calculate the conductance perturbatively in $J_{\rm eff}(T)$ at $T \gg T_K^0$ and using local Fermi liquid theory for $T \ll T_K^0$ [5]. For $T \gg T_K^0$, we obtain Eq. (6), essentially independent of ϵ_W. On the other hand, for $T \ll T_K^0$, the conductance reduces to that of an ideal wire containing no quantum dot, i.e., our original model with $U = 0$, $\epsilon_d = 0$, $t_{WD} = t$, and some effective length $\tilde{L} \sim L$. ($\tilde{L}$ can be somewhat reduced from L by an amount of order ξ_K). As T is lowered below Δ_n this conductance develops peaks with spacing of the order of $\Delta_n/2$. This is the spacing of peaks in the density of states of a wire of length $2L$, containing no quantum dot. It is half the spacing in the density of states of the model with $J = 0$, discussed above. Initially, as T is lowered below Δ_n, the peak width is $O(T)$ and the peak height is $O(2e^2\Delta_n t_{WL}^2/hTt^2)$. As T is lowered below δ_n the peak width becomes $O(\delta_n)$ and the peak height becomes $O(2e^2/h)$.

On the other hand, when $\xi_K \gg L$, the dependence of conductance on T and ϵ_W is very different. As T is

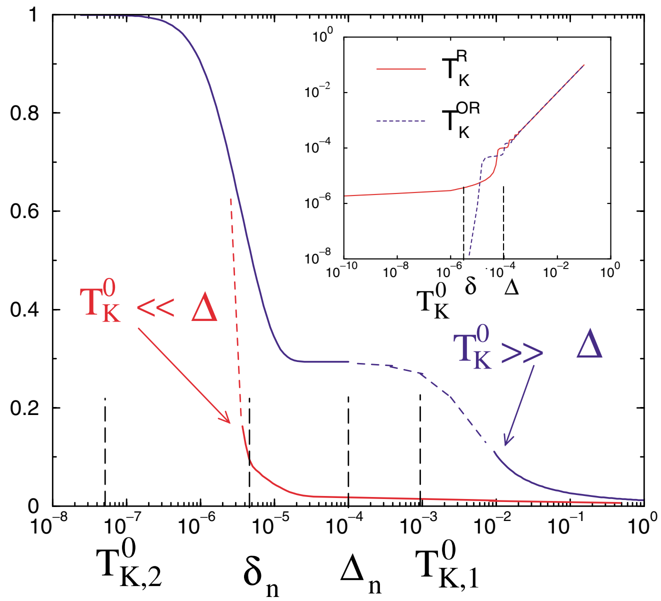

FIG. 2 (color online). On-resonance conductance as a function of temperature (assuming ϵ_W is on resonance) for both cases $\Delta_n \ll T^0_{K,1}$ (right blue curve) and $\Delta_n \gg \delta_n \gg T^0_{K,2}$ (left red curve). The curves in plain style correspond to the perturbative calculations plus the Fermi liquid result for the first case only. We have schematically extrapolated these curves (dotted lines) where neither the perturbative nor the Fermi liquid theory applies. The inset represents $T_K = f(T_K^0)$ in a log-log scale for ϵ_W on resonance (plain curve which becomes almost flat at low $T_K^0 \ll \delta_n$), and ϵ_W off-resonance (dashed curve which drops sharply at low T_K^0). Both curves coincide at $T_K^0 > \Delta_n$.

lowered below Δ_n the *on-resonance* conductance starts to grow both because of the single electron effects reflected in Eqs. (7) and (9) and, eventually, when $T \leq \delta_n$ because of the growth of $J_{\rm eff}(T)$. In this regime it is more difficult to calculate the on-resonance conductance both because of the breakdown of the perturbative results and because it appears considerably more difficult to extract unambiguous predictions from local Fermi liquid theory. Nonetheless, it seems very reasonable to expect a conductance of $O(1)$ on resonance at $T \leq \delta_n$, where $J_{\rm eff}(T)$ is $O(1)$ on resonance. However, we can show quite rigorously that the *off-resonance* conductance remains very small, given by the perturbative formula Eq. (8), at least down to $T \ll \delta_n$ of $O(T_K^{OR})$ given by Eq. (13). Note, in particular, that the values of ϵ_W where T_K is large have spacing Δ_n, not $\Delta_n/2$. *Thus the halving of the period, which we argued above to occur in the other case, $\xi_K \ll L$, does not occur in this case at least down to extremely low T of $O(T_K^{OR})$.* (The behavior of the conductance at very low $T \leq T_K^{OR}$ in the case $\xi_K \gg L$ appears more difficult to determine. However, this is such an unphysically low T that it is not an important limitation of the methods that we are using here.)

In Fig. 2, we have drawn schematically the conductance on resonance as a function of temperature for two different bare Kondo temperatures $T^0_{K,1} \gg \Delta_n$ and $T^0_{K,2} \ll \delta_n \ll \Delta_n$, using the perturbative formula given by Eq. (5) and the Fermi liquid picture valid for the first case only. For the first case, the conductance has a plateau which corresponds to the quantum dot being screened and the ϵ integral in Eq. (5) averaging over many peaks. The conductance reaches $2e^2/h$ only when $T \ll \delta_n$. (This second increase is essentially just a single electron effect.) Conversely, in the second case, the conductance remains small until $T \approx \delta$, where the Kondo coupling becomes strongly renormalized [see Eq. (11)]. We may expect a very abrupt increase of the conductance in this regime as schematically depicted in Fig. 2. Notice that for this choice of $T^0_{K,2}$, the renormalized Kondo temperature $T^R_{K,2}$ is actually enhanced and of the order of δ_n. These different behaviors lead to different shapes of the curves.

One can easily extend this analysis to the nonparity symmetric case by considering two local densities of states ρ^L and ρ^R. To have both local density of states on resonance, it would in general be necessary to introduce two independent gate voltages ϵ^L_W and ϵ^R_W controlling the left and right wire.

In conclusion, we have studied how the finite temperature conductance and effective Kondo temperature of a quantum dot embedded in a wire depend strongly on the ratio between the size of the wire and the size of the Kondo screening cloud.

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