Kondo Screening Cloud Around a Quantum Dot: Large-Scale Numerical Results

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Measurements of the persistent current in a ring containing a quantum dot would afford a unique opportunity to finally detect the elusive Kondo screening cloud. We present the first large-scale numerical results on this controversial subject using exact diagonalization and density matrix renormalization group (RG). These extremely challenging numerical calculations confirm RG arguments for weak to strong coupling crossover with varying ring length and give results on the universal scaling functions. We also study, analytically and numerically, the important and surprising effects of particle-hole symmetry breaking.

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The screening of an impurity spin by conduction electrons, the Kondo effect, is believed by many to be associated with the formation of a "screening cloud" around the impurity with a size $\xi_K = v_F/T_K$ where v_F is the Fermi velocity and T_K is the Kondo temperature, the characteristic energy scale associated with this screening [1]. This fundamental length scale, which has been called the "holy grail" of Kondo research [2], and which from the above estimate can be as large as 1 μm in typical situations, has never been observed experimentally and has sometimes been questioned theoretically. Although traditionally associated with dilute impurity spins in metals, the Kondo effect has been observed more recently in nanostructures [3–6]. The electron number on semiconductor quantum dots, weakly coupled to leads, can be varied in single steps with a gate voltage. When this electron number is odd, the quantum dot generally has a spin of 1/2 and can act as a Kondo impurity, screened by electrons in the leads. By attaching the dot to quantum wires of length L, the Kondo screening cloud size could be measured from the dependence of conductance properties on L [7,8]. A particularly simple case is when the dot is attached to a single quantum wire which forms a closed ring. Two simple tight-binding models have been considered corresponding to an "embedded" or "side-coupled" quantum dot (EQD or SCQD). Suppressing electron spin indices, the corresponding Hamiltonians are

$$H_{\mathrm{EQD}} = -t\sum_{i=1}^{L-2}(c_i^\dagger c_{i+1} + \mathrm{H.c.}) + H_K, \tag{1}$$

where $H_K = J_K\vec{S}\cdot(c_1^\dagger + c_{L-1}^\dagger)\frac{\vec{\sigma}}{2}(c_1 + c_{L-1})$, and

$$H_{\mathrm{SCQD}} = -t\sum_{i=0}^{L-1}(c_i^\dagger c_{i+1} + \mathrm{H.c.}) + H_K, \qquad (c_L \equiv c_0) \tag{2}$$

where $H_K = J_K\vec{S}\cdot c_0^\dagger\frac{\vec{\sigma}}{2}c_0$, and $c_{i\sigma}$ annihilates an electron at site i of spin σ; S^a are $S = 1/2$ spin operators. We generally set $t = 1$ in what follows. A magnetic flux is added to the model by adding appropriate phases to the hopping terms and the resulting persistent current, j, is measured.

The EQD must have $j = 0$ when the Kondo coupling, $J_K = 0$, since then the sites 1 and (-1) are decoupled from each other. On the other hand, the SCQD has a large j when $J_K = 0$ since the Hamiltonian then reduces to that of a free ring with periodic boundary conditions. When the Kondo coupling becomes large ($J_K \gg t$) essentially the inverse behavior occurs, due to the formation of a Kondo screening cloud. In the strong coupling limit of the EQD the screening electron goes into the symmetric orbital on sites 1 and -1. This allows resonant transmission through the antisymmetric orbital on these sites and the ideal sawtoothlike j of a free ring occurs when the system is at 1/2-filling. On the other hand, for the SCQD, the screening electron sits at site 0 and completely blocks all current flow in the strong coupling limit. The more interesting question is the behavior of j in these models for small J_K/t at large length, L. The Kondo length scale grows exponentially as $J_K/t \to 0$. The persistent current was predicted [7,8] to be given by universal scaling functions of ξ_K/L and the dimensionless magnetic flux through the ring, $\alpha \equiv e\Phi/c$:

$$jL/(ev_F) = f(\xi_K/L, \alpha), L, \xi_K \gg a, \tag{3}$$

with a the lattice constant. The crossover functions, f, are very different for the EQD and SCQD and also depend on the parity of the electron number in the ring, N. However, they are otherwise expected to be universal in the small J_K limit, not depending on details of the dispersion relation, electron density, the range of the Kondo interaction, etc. In previous work by one of us and Simon [7,8], it was argued that, in the limit $L \gg \xi_K$, strong coupling behavior occurs, since the effective Kondo coupling is expected to become large at large length scales. Thus it was predicted that $f(\xi_K/L, \alpha)$ approaches the value for an ideal ring at $\xi_K/L \to 0$ for the EQD but approaches zero for the SCQD, for either parity of N. The former prediction is in disagreement with other studies using variational [9] or cluster mean field [10] techniques where jL for the EQD was predicted to have very different L dependence, whereas the SCQD prediction is in stark contradiction with the conclusions of other studies using Bethe ansatz [11] and diagrammatic expansions [12] that predicted that j attains the value for an ideal ring at $\xi_K/L \to 0$. However, the results of Refs. [7,8] are in agreement with the slave boson mean field studies [13], interpolative perturbative approach [14], numerical renormalization group results [15] performed in zero field with open boundary conditions as well as with cluster mean field calculations [16]. Other theoretical studies include Refs. [17–20]. The behavior of the persistent current, j, in quantum dot systems is therefore the subject of considerable controversy.

In this Letter we attempt to settle this controversy using exact diagonalization (ED) and density matrix renormalization group (DMRG) techniques. These techniques are essentially exact and superior to the variational and mean field approaches used in previous studies. The calculations have been performed using fully parallelized programs on distributed SHARCNET facilities. The current $j = -edE/d\alpha$ is obtained from the ground state energy and for the DMRG we denote the number of states kept in the left and right density matrices by m_L and m_R. In the case of the EQD we find good agreement with the expected scaling picture and obtain useful results on the crossover functions, f. For the SCQD we find an extremely slow crossover with varying L or J_K but we present both numerical and analytical evidence that j scales to zero at small ξ_K/L at 1/2-filling, as predicted by the previous RG approach. We show that particle-hole (p-h) symmetry breaking leads, for small J_k/t, to small nonuniversal corrections to jL. Surprisingly, these produce a small nonzero value of j_eL, the current for even N, at $L \to \infty$ for the SCQD.

Embedded quantum dot.—In Fig. 1 we plot j vs α/π for a fixed $J_K = 1$, and various $L = N$. Here both L and N include contribution from the impurity site. Note that a crossover is seen between the weak coupling behavior at smaller lengths (small and sinusoidal) to strong coupling ideal ring behavior at the largest lengths (larger and the sawtooth). To further illustrate this crossover, we focus on one value of the flux, $\alpha/\pi = 0.05$. In Fig. 2 we plot jL/ev_F vs L for this fixed value of the flux for $L = N$ both even or odd. Small numerical errors in the DMRG calculations with ($m_L = 1024$, $m_R = 512$) are visible beyond $L = 24$ when compared to results with $m = (1024, 2048)$. As can be seen from Figs. 1 and 2 the current depends strongly on whether $L = N$ is even or odd. For $L = N$ even there is a difference between $N = 4p$ and $N = 4p + 2$, visible in Fig. 2, that can be absorbed into a redefinition [8] of the flux $\tilde{\alpha} = \alpha + \pi N/2$. From the results shown in Figs. 1 and 2 we conclude that *jL increase* with L towards the free ring limit contradicting Refs. [9,10].

Weak and strong coupling results [8] and Fig. 1 indicate that $j(\alpha)$ has period 2π for $N = L$ even but period π for $N = L$ odd. The latter result follows rigorously at 1/2-filling from p-h symmetry which takes $\alpha \to \pi - \alpha$ for $N = L$ odd together with time reversal which takes $\alpha \to -\alpha$. Away from 1/2-filling, when p-h symmetry is

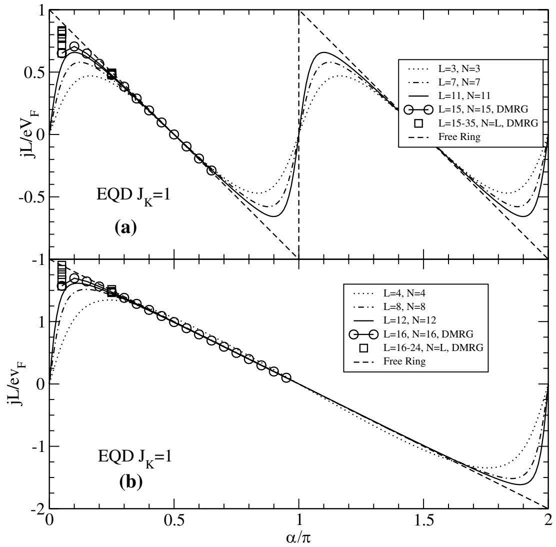

FIG. 1. The current at 1/2-filling for $N = 4p - 1$ (a) and $N = 4p$ (b) for the EQD. Results are shown for a number of system sizes with $J_K = 1$ as a function of α/π. The lines are ED, the symbols DMRG results.

broken, we might expect that the period of $j(\alpha)$ would be enlarged to 2π. This can be checked at both weak and strong coupling. In the weak coupling limit, in addition to the terms calculated previously [8], we find an additional term, of period 2π in the current for N odd, only present away from 1/2-filling ($N/L \neq 1$):

$$\delta j_o \approx \frac{3J_K^2 e}{\pi L} \sin\tilde{\alpha} \sin^2(\pi N/2L) \frac{2\pi \cos(\frac{\pi N}{2L})}{4t}, \qquad (4)$$

where $\tilde{\alpha} = \alpha + \pi(N-1)/2$. In the weak coupling limit, the period 2π term in j for odd N can be understood, in the continuum limit formulation with a linearized dispersion relation and a wave-vector cutoff which is symmetric around the Fermi surface, as arising from particle-hole symmetry breaking potential scattering terms in the effective Hamiltonian, of $O(J_K^2)$. These terms are strictly mar-

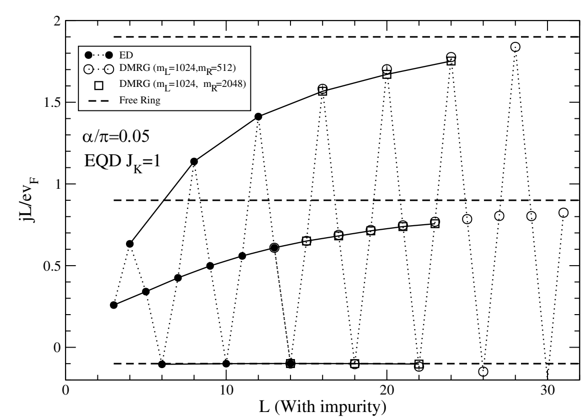

FIG. 2. The current jL/ev_F for $J_K = 1$ and $\alpha/\pi = 0.05$ vs L for the EQD. Shown are ED results (•), DMRG results with ($m_L = 1024$, $m_R = 512$) (∘) and ($m_L = 1024$, $m_R = 2048$) (□). The dashed lines indicate the free ring result.

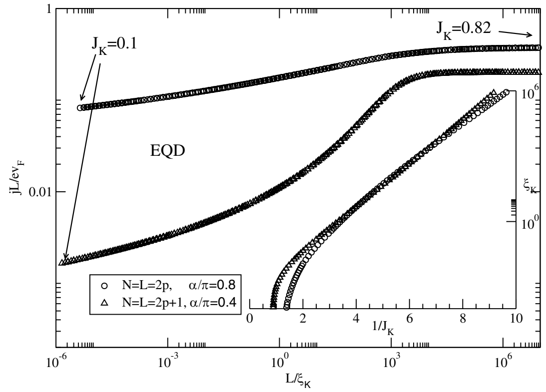

FIG. 3. The current at $1/2$-filling jL/ev_F, at $\alpha/\pi = 0.4$ ($N = 4p$ $\circ$) and at $\alpha/\pi = 0.8$ (N odd $\triangle$), plotted vs L/ξ_K obtained by combining our results for various values of J_K for the EQD. We fix $\xi_K(J_K = 0.3) \equiv 1$ and obtain the remaining ξ_K relatively to $\xi_K(J_K = 0.3)$ by rescaling. The inset shows the obtained $\xi_K(J_K)$ as a function of $1/J_K$ for even ($\circ$) and odd ($\triangle$) N.

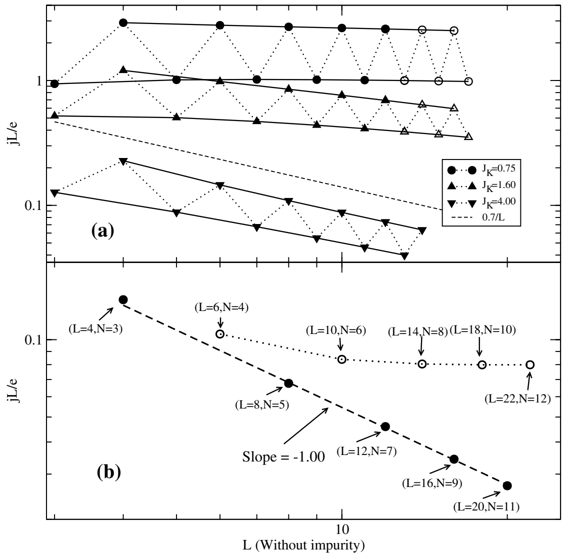

FIG. 4. (a) The current jL/e at $1/2$-filling for the SCQD for $\tilde{\alpha}/\pi = 0.15$ and $J_K = 0.75$, 1.60, 4.00 vs L. Solid (open) symbols are ED (DMRG with $m_L = 1024$, $m_R = 2048$) results. A function with pure $1/L$ behavior is shown. (b) The current jL/e at $1/4$-filling for the SCQD for $\tilde{\alpha}/\pi = 0.75$ and $J_K = 4$ vs L. ED results are shown for even N ($\circ$) and odd N ($\bullet$). The dashed line is a power-law fit to the points with $N = 5 - 11$, of slope $= -1$. The symmetry reduced Hilbert space at $N = 12 (L = 22)$ is 3, 929, 717, 484.

ginal under renormalization group transformations and hence their effects do not grow larger with growing L/ξ_K, but remain of $O(J_K^2)$, where J_K is the *bare* coupling, at all length scales. Thus the period 2π term in j becomes negligible at all length scales, when $L \gg \xi_K$, in the limit of small bare coupling and hence do not appear in the universal scaling functions, $f(\xi_K/L, \alpha)$.

We have also attempted to numerically calculate an approximation to the scaling function f by rescaling ED results out to $L = 13$ for a range of J_K. Our results are shown in Fig. 3 where jL/ev_F is plotted vs L/ξ_K for a fixed $\alpha/\pi = 0.40(0.80)$ for $L = N$ odd (even). If $\xi_K(J_K^0)$ is fixed at a given J_K^0 to set the scale of the x axis, all the data can be rescaled to follow a single curve as shown. (See Ref. [21] for details.) Even though the results in Fig. 3 are only an approximation to the scaling function, they nicely confirm the scaling picture and show that f is an *increasing* function of L/ξ_K.

Side-Coupled Quantum Dot.—[Now L does *not* include the impurity site while N *does* include the impurity electron. For N odd $\tilde{\alpha} = \alpha + \pi(N-1)/2$ and for N even $\tilde{\alpha} = \alpha + \pi N/2$.] In Fig. 4(a) we show exact diagonalization and DMRG results for the SCQD at $\tilde{\alpha} = 0.15\pi$ analogous to Fig. 2. These results are consistent with jL going to zero at $L \gg \xi_K$; however, it appears necessary to go to extremely large L/ξ_K to see this behavior. A calculation of the scaling function, f, equivalent to Fig. 3, shows that f for the SCQD is a *decreasing* function of L/ξ_K in contradiction to the results of Refs. [11,12].

In order to test our conjectured scaling behavior, we have studied both analytically and numerically the strong coupling limit, $J_K \gg 1$, in greater detail. In this limit one electron sits at site 0 and forms a singlet with the impurity spin, effectively cutting the ring at the origin. Perturbation theory in $1/J_K$ generates terms in a low energy effective Hamiltonian which couples the two sides of the quantum dot and thus allows for a small nonzero current. By doing perturbation theory to third order in $1/J_K$, we obtain an effective Hamiltonian valid at $J_K \gg 1$:

$$H_{\text{eff}} = -\sum_{j=1}^{L-2} (c_j^\dagger c_{j+1} + \text{H.c.}) + H_T, \tag{5}$$

where the tunneling terms are:

$$H_T = \frac{4}{9J_K^2} e^{-i\alpha}(c_1^\dagger c_{L-2} + c_2^\dagger c_{L-1}) + \text{H.c.} \quad - \frac{32}{J_K^3} e^{-2i\alpha} c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{L-1\uparrow} c_{L-1\downarrow} + \text{H.c.} \quad + \frac{4}{3J_K^3}(n_1 + n_{L-1} - 2) e^{-i\alpha} c_1^\dagger c_{L-1} + \text{H.c.} \tag{6}$$

Here n_i is the electron number on site i. We have ignored additional terms in the effective Hamiltonian which do not contribute to the current at low orders in $1/J_K$. We may now evaluate the current, up to $O(1/J_K^3)$, by calculating the α dependence of the ground state energy in first order perturbation theory in H_T. Considering $1/2$-filling, this gives, for odd or even N,

$$j_o L/e \approx \frac{32}{9J_K^2}\left[\tan\left(\frac{\pi}{2L}\right) + \tan\left(\frac{3\pi}{2L}\right)\right]\sin\tilde{\alpha} + \frac{128}{3J_K^3 L}[2\sin\tilde{\alpha} - \sin(2\tilde{\alpha})] \qquad j_e L/e \approx \frac{32}{3J_K^3 L}[1 + 1/\cos(\pi/L)]^2 \sin 2\tilde{\alpha}. \tag{7}$$

The absence of period 2π terms for N even can be understood from the p-h symmetry of the unperturbed Hamiltonian in Eq. (5) which is broken, for N even, by H_T. Note that these formulas predict that j goes to zero as $1/L^2$ at large L. In the strong coupling limit, this amounts to an analytic proof that the current is not the same as for the ideal ring, in contradiction with the claims of Ref. [11]. We have verified that Eqs. (7) are in excellent agreement with our numerical results for large J_K. However, we find that surprisingly large values of J_K, of about 100, are necessary before these formulas become accurate. This is consistent with the results of our study of length dependence of j which suggests a very slow crossover from weak to strong coupling behavior as L/ξ_K is varied.

From Eqs. (7) it is also possible to calculate the current away from 1/2-filling; at large J_K we find:

$$j_oL/e \approx \frac{32}{9J_K^2}\sin(\tilde{\alpha}) \times \left[\sin\frac{\pi(N-1)}{2L}\tan\frac{\pi}{2L} - \sin\frac{3\pi(N-1)}{2L}\tan\frac{3\pi}{2L}\right] \quad (8)$$

$$j_eL/e \approx \frac{32}{9J_K^2}\sin(\tilde{\alpha})\left[\frac{\cos(\frac{\pi(N-1)}{2L})}{\cos(\frac{\pi}{2L})} - \frac{\cos(\frac{3\pi(N-1)}{2L})}{\cos(\frac{3\pi}{2L})}\right].$$

Note that j_oL/e is $O(1/L)$ and actually gets smaller as we move away from 1/2-filling. We see that j_oL *approaches zero* as $L \to \infty$. Surprisingly, we see that j_eL attains a nonzero limit as $L \to \infty$, away from 1/2-filling, in stark contrast to j_oL and the behavior of both j_oL and j_eL at 1/2-filling. We have numerically verified Eqs. (8) in detail finding excellent agreement for $J_K > 100$. For an intermediate coupling of $J_K = 4$ we show ED results for jL/e in Fig. 4(b), at a flux $\tilde{\alpha}/\pi = 0.75$ and 1/4-filling, clearly approaching a nonzero limit for N even with opposite sign and a much smaller amplitude than that of the ideal ring. For odd N, $jL/e \sim \text{const}/L$ in accordance with Eq. (8). This $O(1/L)$ behavior of j_e away from 1/2-filling results from nonuniversal particle-hole symmetry breaking terms in the low energy effective Hamiltonian. For small J_K/D (where $D \approx t$ is the bandwidth) these terms are small, and remain so under renormalization. They contribute to j_e at $L \gg \xi_K$, which has the form: $j_e = (ev_F/L)[(A\xi_K/L) \times \sin 2\alpha + B(J_K/D)^2 \sin\tilde{\alpha}]$ where A is a universal constant and B is a nonuniversal constant, both of $O(1)$. Thus the universal $(1/L^2)$ behavior is destroyed at large length scales, $\approx \xi_K(D/J_K)^2 \gg \xi_K$, away from 1/2-filling, in contrast to the claim in Ref. [8]. Note, however, that the current at these large length scales is smaller by a factor of $(J_K/D)^2$ than that of an ideal ring, in contrast to the claim in Ref. [11].

Following Nozières [1] we have developed a local Fermi liquid theory description of the low temperature fixed point of the SCQD. This fixed point corresponds to the impurity forming a singlet with one conduction electron and the remaining low energy electrons being repelled from the origin, corresponding to a broken ring with zero persistent current. In the 1/2-filled case, the leading irrelevant operators at this fixed point, which control the persistent current at large L, are $(\psi_+^\dagger \vec{\sigma}\psi_-)^2$, $\psi_+^\dagger \vec{\sigma}\psi_- \cdot (\psi_+^\dagger \vec{\sigma}\psi_+ + \psi_-^\dagger \vec{\sigma}\psi_-)$, and their complex conjugates. Here $+$ and $-$ label the electron operators on the right- and left-hand side of the impurity. In the limit of weak bare Kondo coupling, or large ξ_K, the coupling constants in front of these terms can all be fixed uniquely up to one overall factor with dimensions of inverse energy, proportional to the inverse of the Kondo temperature. This theory predicts that the persistent current scales to zero as ev_F^2/T_KL^2 at 1/2-filling, or for odd N at arbitrary filling, as well as making various other predictions that could be compared with numerical simulations and experiments [22]. In conclusion, we have given strong numerical evidence and analytical results in support of the scaling picture of the persistent current in quantum dot systems resolving a number of outstanding controversies.

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