The 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 micron 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 nano-structures [3, 4, 5, 6]. The electron number on semiconductors quantum dots, weakly coupled to leads, can sometimes be 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 anti-symmetric orbital on these sites and the ideal saw-tooth like $j$ 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 $J_K/t \rightarrow 0$. The persistent current was predicted [2] to be given by universal scaling functions of $\xi_K/L$ and the dimensionless magnetic flux through the ring, $\alpha \equiv e\Phi/c$:

$$jL/(ev_F) = f(\xi_K/L, \alpha), \quad L, \xi_K \gg a,$$

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 P. Simon [3] 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 $f(\xi_K/L, \alpha)$ ap-

\[ H_{\text{EQD}} = -t \sum_{j=1}^{L-2} \left( c_j^\dagger c_{j+1} + \text{h.c.} \right) + H_K, \quad (1) \]

where $H_K = J_K S \cdot (c_1^\dagger + c_{L-1}^\dagger) e^{i\Phi}/2 (c_1 + c_{L-1})$, and

\[ H_{\text{SCQD}} = -t \sum_{j=0}^{L-1} \left( c_j^\dagger c_{j+1} + \text{h.c.} \right) + H_K, \quad (c_L \equiv c_0) \quad (2) \]

where $H_K = J_K S \cdot c_0^\dagger c_0$ and $c_j$ annihilates an electron at site $j$ of spin $\sigma$; $S^\sigma$ 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.

$\xi_K = v_F / T_K$ 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 micron 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 nano-structures [3, 4, 5, 6].

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proaches the value for an ideal ring at $\xi_K/L \rightarrow 0$ for the EQD but approaches zero for the SCQD, for either parity of $N$. The former prediction is in disagreement with other studies [8, 11] 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 authors [11, 12] who predicted that $j$ attains the value for an ideal ring, at $\xi_K/L \rightarrow 0$. However, the results of Refs [7, 8] are in agreement with the theoretical, numerical (up to $L=8$) and mean field results of Refs. [17, 18, 19, 20]. Other theoretical studies include Refs. [13, 14, 15, 16]. 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). The calculations have been performed using fully parallelized programs on distributed SHARCNET facilities. The DMRG work turns out to be very cpu-intensive due to the necessity of using periodic boundary conditions to obtain a persistent current, the complex form of the Hamiltonian at non-integer fillings and the fact that the current is $o(1/L)$. 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 $\xi_K/L$ at 1/2-filling, as predicted by the previous RG approach. We show that particle-hole symmetry breaking leads, for small $J_k/t$, to small non-universal corrections to $jL$. Surprisingly, these produce a small non-zero value of $j_L$, the current for even $N$, at $L \rightarrow \infty$ for the SCQD.

**Embedded Quantum Dot:** In Fig. 1 we plot $j$ vs. $\alpha/\pi$ for a fixed $J_K=1$, and various $L=N$. Here both $L$ and $N$ includes 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 saw-tooth). 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 $m=(1024, 512)$ 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 re-definition of the flux $\hat{\alpha} = \alpha + \pi N/2$. From the results shown in Figs. 1 and 2 we conclude that $jL$ increase with $L$ towards the free ring limit contradicting Refs [8, 10].

**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 $\alpha/\pi$. The results for the small system sizes are obtained using exact diagonalization methods while the larger system sizes (circles) have been obtained using DMRG techniques.

**FIG. 2:** The current $jL/ev_F$ for $J_K = 1$ and $\alpha/\pi = 0.05$ as a function of $L$ for the EQD. The results for the small system sizes are obtained using exact diagonalization methods (•) while the larger system sizes have been obtained using DMRG techniques with $(m_L=1024, m_R=512)$ (○). The □ indicate DMRG results obtained using $(m_L=1024, m_R=2048)$. The dashed lines indicate the free ring result.

Weak and strong coupling results [8], and Fig. 1 indicate that $j(\alpha)$ has period $2\pi$ for $N = L$ even but period $\pi$ for $N = L$ odd. The latter result follows rigorously at 1/2-filling from particle-hole (P-H) symmetry which takes $\alpha \rightarrow \pi - \alpha$ for $N = L$ odd together with time reversal which takes $\alpha \rightarrow -\alpha$. Away from 1/2-filling, when
the continuum limit formulation with a linearized dispersion relation and a wave-vector cut-off which is symmetric around the Fermi surface, as arising from particle-hole P-H symmetry is broken, we might expect that the period of \( j/\alpha \) would be enlarged to \( 2\pi \). This can be checked at both weak and strong coupling. In the weak coupling limit, in addition to the terms calculated previously, we find an additional term, of period \( 2\pi \) in the current for odd \( N \), only present away from \( 1/2 \)-filling \( (N/L \neq 1) \):

\[
\delta j_0 \approx \frac{3J^2_K e}{\pi L} \sin \alpha \sin^2(\pi N/2L) \frac{2\pi \cos(\pi N/2L)}{4t},
\]

where \( \alpha = \alpha + \pi(N - 1)/2 \). In the weak coupling limit, the period \( 2\pi \) term in \( j_0 \) for odd \( N \) can be understood, in the continuum limit formulation with a linearized dispersion relation and a wave-vector cut-off which is symmetric around the Fermi surface, as arising from particle-hole P-H symmetry breaking potential scattering terms in the effective Hamiltonian, of \( O(J^2_K) \). These terms are strictly marginal under renormalization group transformations and hence their effects do not grow larger with growing \( L/\xi_K \), but remain of \( O(J^2_K) \), where \( J_K \) is the bare coupling, at all length scales. Thus the period \( 2\pi \) term in \( j_0 \) 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 \( j_L/evF \) is plotted vs. \( L/\xi_K \) for a fixed \( \alpha/\pi = 0.40(0.80) \) for \( L = N \) odd(even). If \( \xi(J^0_K) \) is fixed at a given \( J^0_K \), \( \xi(J^1_K) \) can be estimated by rescaling \( L/\xi_K \) until \( j_L/evF \), calculated with \( J^1_K \) superposes \( j_L/evF \) calculated with \( J^0_K \) and so forth. The results of Fig. 3 nicely confirms the scaling picture and shows that \( f \) is an increasing function of \( L/\xi_K \).

**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 \( L/\xi_K \) 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 \( L/\xi_K \) 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 couple the two sides of the quantum dot and thus allow for a small non-zero current. By doing perturbation theory to 3rd order in \( 1/J_K \), we obtain an effective Hamiltonian valid at \( J_K \gg
1:

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

where the tunneling terms are:

\[ H_T = \frac{4}{9J_K} e^{-\alpha}(c_{1}^\dagger c_{L-2} + c_{L-1}^\dagger c_{1}) + h.c. \]
\[ - \frac{32}{3J_K} e^{-2\alpha} c_{1}^\dagger c_{1}^\dagger c_{L-1} c_{L-1} + h.c. \]
\[ + \frac{4}{3J_K}(n_1 + n_{L-1} - 2)e^{-\alpha} c_{1}^\dagger c_{L-1} + h.c. \tag{6} \]

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 \( O(1/J_K^2) \), by calculating the \( \alpha \)-dependence of the groundstate energy in first order perturbation theory in \( H_T \). Considering 1/2-filling, this gives, for odd or even \( N \),

\[ j_o L/e \approx \frac{32}{9J_K} \left[ \tan(\pi/2L) + \tan(3\pi/2L) + 18 \right] \frac{\sin(\hat{\alpha})}{3J_K L^2} \]
\[ j_e L/e \approx \frac{32}{9J_K} \left[ 1 + \cos(\pi/L) \right]^2 \sin(2\hat{\alpha}). \tag{7} \]

The absence of period 2\( \pi \) 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 \( j_o \) 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 cross over from weak to strong coupling behavior as \( L/\xi_K \) is varied.

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

\[ j_o L/e \approx \frac{32}{9J_K} \sin(\hat{\alpha}) \]
\[ \times \left[ \frac{\sin(\frac{\pi(N-1)}{2L})}{\cos(\frac{\pi}{2L})} + \frac{\cos(\frac{\pi(N-1)}{2L})}{\sin(\frac{\pi}{2L})} \right] \]
\[ j_e L/e \approx \frac{32}{9J_K} \sin(\hat{\alpha}) \left[ \frac{\cos(\frac{\pi(N-1)}{2L})}{\cos(\frac{\pi}{2L})} + \frac{\sin(\frac{3\pi(N-1)}{2L})}{\sin(\frac{3\pi}{2L})} \right]. \tag{8} \]

Note that \( j_o L/e \) is \( O(1/L) \) and actually gets smaller as we move away from 1/2-filling. We see that \( j_o L \) approaches zero as \( L \to \infty \). Surprisingly, we see that \( j_e L \) attains a non-zero limit as \( L \to \infty \), away from 1/2-filling, in stark contrast to \( j_o L \) and the behavior of both \( j_o L \) and \( j_e L \) at 1/2-filling. We have numerically verified Eqs. \( 3 \) in detail finding excellent agreement for \( J_K > 100 \). For an intermediate coupling of \( J_K = 4 \) we show ED results for \( j_o L/e \) in Fig. \( 3 \), at a flux \( \hat{\alpha}/\pi = 0.75 \) and 1/4-filling, clearly approaching a non-zero limit for \( N \) even with opposite sign and a much smaller amplitude than that of the ideal ring. For odd \( N \), \( j_o L/e \to \text{const}/L \) in accordance with Eq. \( 8 \). This \( O(1/L) \) behavior of \( j_o \) away from 1/2-filling results from non-universal 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 \( j_o \) at \( L \gg \xi_K \), which has the form:

\[ j_o = (ev_F/L)\left[ (A\xi_K/L) \sin 2\alpha + B(J_K/D)^2 \sin \hat{\alpha} \right] \]

where \( A \) is a universal constant and \( B \) is a non-universal 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. \[3\]. 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. \[14\].

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 \( (\psi_+^\dagger \sigma^x \psi_-)^2 \), \( \psi_+^\dagger \sigma^y \psi_- \cdot (\psi_+^\dagger \sigma^x \psi_-) \), 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 \( \xi_K \), 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 \( ev_F^2/T_K L^2 \) at 1/2-filling, or for even \( N \) at arbitrary filling, as well as making various other predictions that could be compared with numerical simulations and experiments.\[21\]

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. This research is supported by NSERC of Canada, CFI, SHARCNET and CIAR. 1A acknowledges interesting conversations with P. Simon.
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