Is there an exponentially large Kondo screening cloud?

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Abstract

We make a precise scaling conjecture, based on renormalization group ideas, regarding the screening cloud around an impurity spin in the Kondo effect and test it numerically using the Density Matrix Renormalization Group method.

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The renormalization group (RG) theory of the Kondo effect \[1\] suggests the existence of an exponentially large length scale, \(\xi_K \equiv v_F/T_K \approx a e^{1/\rho J}\) where \(v_F\) is the Fermi velocity, \(T_K\) the Kondo temperature, \(a\) the unit cell dimension, \(J\) the Kondo coupling and \(\rho\) the density of states (per spin). One imagines a cloud of electrons of this size, typically microns, which screens the impurity spin. The meaning, or even the existence of this screening cloud has been a subject of some controversy \[2–4\] with no clear consensus emerging either experimentally or theoretically. In particular, the experiments of Boyce and Slichter \[2\] were interpreted as indicating that the screening cloud had a size of order a lattice spacing, about a hundred times smaller than predicted by the renormalization group theory. In this letter we make a more precise statement of what the existence of this screening cloud really means, based on renormalization group scaling ideas, and test it against results from perturbation theory, local Fermi liquid theory and numerical simulations. A detailed account of our results will be presented elsewhere \[5\]. Related theoretical work includes perturbative calculations \[6,4\], RG approaches \[7,4\] and numerical work on the Anderson model \[8\]. For a general review of the Kondo effect see Ref. \[9\] and references therein.

We consider the standard Kondo model:

\[
H = \sum_k \epsilon_k \psi_k^\dagger \psi_k + JS_{\text{imp}} \cdot \sum_{k,k'} \psi_k^\dagger \frac{\sigma^\beta}{2} \psi_{k'},
\]

with \(S_{\text{imp}} = 1/2\). We are interested in the Knight shift, proportional to the local susceptibility:

\[
\chi(r,T) \equiv (1/T) \langle \psi^\dagger(r) \frac{\sigma^z}{2} \psi(r) S_{\text{tot}}^z \rangle.
\]

Here \(S_{\text{tot}}\) is the total spin operator, including both impurity and conduction electron spins; we set the two g-factors equal. In the scaling limit, \(rk_F \gg 1\), \(T \ll E_F\), we conjecture the scaling form:

\[
\chi(r,T,J) - \frac{\rho}{2} = \frac{1}{v_F r^2} \left\{ f \left( \frac{rT}{v_F}, \frac{T}{T_K} \right) \cos \left[ 2k_F r + \delta \left( \frac{rT}{v_F}, \frac{T}{T_K} \right) \right] + g \left( \frac{rT}{v_F}, \frac{T}{T_K} \right) \right\},
\]

where \(f\), \(g\) and \(\delta\) are universal functions of two scaling variables, and the bulk Pauli susceptibility has been subtracted. The prefactor of \(1/r^2\) arises from reducing the 3 dimensional...
problem to an effective one-dimensional problem, [10] which is assumed to obey scaling. Instead of the second scaling variable, \( T/T_K \), we may equivalently use the renormalized Kondo coupling at scale \( T, \lambda_{\text{eff}}(T) \), where \( \lambda \) is the dimensionless Kondo coupling, \( \lambda \equiv \rho J \). For weak bare coupling and high temperatures, \( T/T_K \approx \exp[1/\lambda_{\text{eff}}(T)] \). Eq. (3) follows naturally from the expected asymptotic limits of \( \chi \) and standard scaling hypotheses. This scaling form is probably the best definition of what it means to have a screening cloud since it implies that for \( T \leq T_K, \chi(r) \) varies over at least a distance of \( \xi_K \).

Eq. (3) is consistent with perturbation theory at \( T \gg T_K \), where \( \lambda_{\text{eff}}(T) \) is small. The first order result is:

\[
\chi(r, T) - \frac{\rho}{2} = \frac{\lambda}{16r^2v_F \sinh \frac{2\pi r}{v_F}} \cos 2k_Fr,
\]

consistent with Eq. (3). Including the next order term, [6,4] and assuming also, \( rT/v_F \ll 1 \) we find:

\[
\chi(r) - \frac{\rho}{2} = -\frac{\cos 2k_Fr}{32\pi r^3T} \{\lambda + \lambda^2[\ln(k_Fr) + \text{constant}]\}.
\]

(5)

In low order perturbation theory, the effective coupling at temperature \( T \) is given by [11]

\[
\lambda_{\text{eff}}(T) = \lambda + \lambda^2 \ln(v_Fk_F/T) + O(\lambda^3).
\]

(6)

Thus, to \( O(\lambda^2) \), the quantity in brackets in Eq. (3) may be written, as

\[
\{\lambda_{\text{eff}}(T) + \lambda_{\text{eff}}(T)^2[\ln(rT/v_F) + \text{constant}]\},
\]

consistent with Eq. (3).

Conversely, at \( T \ll T_K \) and \( r \gg \xi_K \), we expect local Fermi liquid theory [11] to apply. \( \chi \) then reduces to the magnetic susceptibility of a non-magnetic impurity with a \( \pi/2 \) phase shift. This can be obtained by differentiating the Friedel oscillation formula for the local charge density:

\[
n(r) = n_0 - \frac{1}{2\pi^2r^3} \cos[2k_Fr + \pi/2],
\]

(8)
with respect to the chemical potential yielding:

\[
\chi(r,T) = \frac{1}{4v_F}\frac{dn}{dk_F} = \frac{\rho}{2} + \frac{1}{4\pi^2v_F r^2}\cos(2k_Fr),
\]  

(9)

again consistent with Eq. (3). Note that \(\chi(r,T)\) is longer-range at low T after the screening cloud has formed, \(\chi \propto 1/r^2\), than at higher T before it has formed, \(\chi \propto 1/r^3\), (Eq. (5)).

Integrating Eq. (3) over \(d^3r\), to obtain the long-range contribution to the total susceptibility, only \(g\) contributes, giving (after a change of variables):

\[
\chi_{\text{long range}} = \frac{4\pi}{T}\int_0^\infty dxg(x,T/T_K).
\]  

(10)

This is consistent with the low temperature Fermi liquid prediction \[\chi \approx 1/T_K\] provided that \(\int_0^\infty dxg(x,y) \propto y\) (for \(y \ll 1\)).

The functions \(f(x,y), g(x,y), \) and \(\delta(x,y),\) in the regime \(y \leq 1, \ x/y = r/\xi_K \leq 1\) are of special interest. They describe the interior of the screening cloud at low T. One might naively suppose that a small \(r \ll \xi_K\) would also cut off the renormalization of the effective coupling so that deep inside the screening cloud we recover weak-coupling behavior (for weak bare coupling) even at low T. However, explicit RG calculations by Gan \[4\] show this not to be the case. He showed that a small \(r\) does not cut off the infrared divergence of the Kondo coupling in perturbation theory. Thus the scaling functions are expected to be non-trivial in this region.

Now let us consider the experiments of Boyce and Slichter \[2\] on Fe doped Cu. They measured the Knight shift from different shells of Cu atoms within a few lattice spacings from the impurities from \(T=300K\) down to well below the Kondo temperature of 29K. They found the factorized form: \(\chi(r,T) = f(r)/(T + T_K),\) with some rapidly varying function \(f(r)\) (which, in fact, changes sign over the small range of \(r\) considered). Note that all measurements are taken in the regime \(rT/v_F \ll 1, rT_K/v_F \ll 1.\) In fact the values of \(r\) are so small that it is unclear whether the scaling form of Eq. (3) holds at all. Assuming it does, we may essentially consider \(x \to 0\) in the scaling functions. Assuming that, in this limit, \(f\) dominates over \(g,\) and that \(\delta\) is essentially constant, we can obtain the above result if \(f(x,y)\)
exhibits an approximately factorized form for $x/y \ll 1$ and all $y$: $f(x, y) \approx f(x/y)/(y + 1)$. Note that such factorization could not also occur at large $r$, $r \gg \xi_K$ if our assumed scaling and asymptotic behaviors are correct. In this region, the $1/r^3$ behavior of the $2k_F$ part at $T \gg T_K$ crosses over to $1/r^2$ at $T \ll T_K$. Thus, a conclusive test of the existence of the screening cloud would probably require experiments which probe length scales of $O(\xi_K)$.

To test our scaling hypothesis using the density matrix renormalization group (DMRG) method [1] we consider a tight-binding model with open boundary conditions:

$$H = -t \sum_{i=1}^{L-1} \left( \psi_i^{\dagger} \right) \left( \sigma^\alpha \right)_{i+1} \psi_{i+1,\alpha} + J S_{\text{imp}} \cdot \psi_i^{\dagger} \frac{\sigma^\beta}{2} \psi_i^\beta, \quad (11)$$

with the total number of sites, $L$, even. We shall always take the hopping strength, $t$, to be unity, and we only consider ground-state properties at half-filling. We keep $m = 128$ states and for optimal precision we apply the finite lattice DMRG [1] to each step in the infinite lattice DMGR method. In the ground-state the total magnetization, $S^z_{\text{tot}} = 1/2$, is a constant and we therefore consider the local magnetization, $<S^z_j>$, instead of $\Delta \chi \equiv \chi(r, T, J) - \rho/2$.

Here $S^z_j$ is the $z$-component of the electron spin at site $j$. With the DMRG method we can obtain results for finite systems, $L \leq 40 - 50$, at $T = 0$. Hence we need a finite-size form of Eq. (3). This can be obtained by noting that since $k_F = \pi/2$ at half-filling, $\delta$ can be eliminated from Eq. (3). Substituting $rT/v_F \rightarrow r/L$ and $T/T_K \rightarrow \xi_K / L$ we get:

$$<S^z_j> = \frac{1}{L} \left\{ \tilde{f} \left( j \frac{L}{\xi_K} \right) \langle -1 \rangle^j + \tilde{g} \left( j \frac{L}{\xi_K} \right) \right\}. \quad (12)$$

In writing this equation we have included a factor of $T/r^2$ in going from 3D to 1D and converting to the local magnetization.

We briefly mention a few useful results regarding the weak and strong coupling behavior of Eq. (11). In the weak coupling limit, $J \ll t$, using perturbation theory, we find for large $L$:

$$<S^z_j> \rightarrow \frac{(J/t)}{4\pi j} (-1)^j. \quad (13)$$

In the strong coupling limit, $J \gg t$, it can be shown that the on-site magnetization behaves in the following way:
\[ < S_j^z > = \frac{1}{L} \sin^2 \frac{\pi j}{2}, \quad j > 2. \]  

These results are consistent with the scaling form Eq. (12) if we note that in the weak coupling limit we can substitute \( J/t \) with the effective coupling \( 1/\ln(\xi_K/L) \).

We start by considering \( < S_{L/2}^z > \). Restricting our analysis to even values of \( L/2 \) Eq. (12) takes the simpler form \( L < S_{L/2}^z > = h(L/\xi_K) \). If this scaling form is obeyed it should be possible to collapse data for different \( L \) and \( J \) onto a single scaling curve. In Fig. 1 we show our results for a large range of Kondo couplings \( J \) with \( \xi_K(J = 2.5) \) fixed to 1. Choosing appropriate values of \( \xi_K \) all the data can clearly be brought onto the predicted scaling form. A very dramatic crossover from weak to strong coupling behavior is evident. Note that for strong coupling \( L < S_{L/2}^z \) approaches 1 consistent with the result Eq. (14). The weak coupling result Eq. (13) predicts a roughly constant value of \( < S_{L/2}^z > \) for fixed \( J \) consistent with the behavior in Fig. 1. The fact that \( < S_j^z > \rightarrow \text{constant}/L \) for \( j \gg \xi_K \) is analogous to the prediction that local susceptibility, \( \chi(r, T) \), should be longer range when the screening cloud has formed than when it has not, as discussed above.

We proceed to analyze the on-site magnetization for fixed \( L/\xi_K \) as a function of \( j \). Our results are shown in Fig. 2 where we display results for \( J = 1.5 \) and \( J = 1.8 \) with \( \xi_K(J = 1.5) \approx 4.85 \) and \( \xi_K(J = 1.8) \approx 2.7 \), and we use \( L = 36, 20 \) for \( J = 1.5, 1.8 \) respectively. Thus, \( L/\xi_K \approx 7.4 \) is kept fixed. An almost complete data collapse is clearly visible. This is a highly non-trivial test of the scaling relation Eq. (12) and hence also of Eq. (3). Analogous scaling plots can be performed for the other couplings studied.

Having extracted \( \xi_K \) from the scaling of \( L < S_{L/2}^z > \), we can study \( \xi_K \) as a function of \( J \). As mentioned in the introduction, usual renormalization group arguments predicts to lowest order an exponential form for \( \xi_K \). Including one more term in the renormalization group equation for the effective coupling we have [12],

\[ - \frac{d\lambda}{d\ln \Lambda} = \lambda^2 - \lambda^3/2. \]  

Here \( \Lambda \) is the momentum space cut-off. We can integrate this equation to get an improved expression for \( \xi_K \). This gives
Here $c$ is positive and $O(1)$. The inverse of the bare cut-off, $\xi_0$, should satisfy $1 \ll \xi_0 \ll \xi_K$ and $\lambda_0$, the bare coupling, is given by $\lambda_0 = J\rho + (J\rho)^2 \ln[\tan(2\xi_0/a)]$ with the density of states for the tight-binding model, $\rho = 1/2\pi t$. This form is valid for small $\lambda_0$. The corrections arising from the constant $c$ is presumably only one of several equally important terms; we have included it here to improve the agreement with the numerical results. In the limit $\lambda_0 \to 0$ Eq. (16) reduces to: $\xi_K \propto e^{1/\lambda_0}/\sqrt{\lambda_0}$, in agreement with previous results [13]. The form, Eq. (16), is obtained using weak coupling RG and should therefore only be valid for the range of $J$ where $1 \ll \xi_K \ll L$. In this region we can now try to fit our previously obtained results for $\xi_K$ to the form Eq. (16). This is shown in Fig. 3 where the DMRG results are shown as circles and the solid line indicates a least square fit to Eq. (16) with the parameters $\xi_0 = 1.76$, $c = 0.21$. For these intermediate couplings the RG form works surprisingly well, and the data seems clearly consistent with the expected form. However, one should bear in mind that for weaker couplings $\xi_K$ has sizable error bars that we cannot estimate; secondly, the extracted $\xi_K$ is only determined up to a multiplicative constant.

In conclusion we have presented several non-trivial tests showing that the scaling form Eq. (3) clearly is obeyed in its finite-size form. Finite-size effects may be important in recent experiments using samples with lengths of order $\xi_K$ or smaller [3]. The associated Kondo length scale, $\xi_K$, which roughly determines the size of the screening cloud diverges at weaker couplings with a behavior consistent with higher order renormalization group calculations, Eq. (16). The Knight shift associated with the local susceptibility is longer range at low temperatures where the screening cloud has formed than at higher temperatures where it has not. Inside this screening cloud, as shown by Gan [4], one does not expect weak coupling behavior to be recovered.

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FIG. 1. $L < S_{L/2}^z >$ as a function of $L/\xi_K$ for a range of different coupling constants. The initial point corresponds in all cases to $L = 4$, subsequent points have $L$ increased by 4.
FIG. 2. $L$ times the expectation value of the z-component of the electron spin, $< S^z_j >$, as a function of $j/\xi_K(J)$. Two systems are shown: $J = 1.8$, $\xi_K = 2.7$, $L = 20$ and $J = 1.5$, $\xi_K = 4.85$, $L = 36$. Thus in both cases we have $L/\xi_K \approx 7.4$. 
FIG. 3. The Kondo length, $\xi_K$, as a function of Kondo coupling, $J$. The circles denote the numerical DMRG results. The solid line indicates a least square fit of $\xi_K(J)$ for $J = 1 - 4$ to the form Eq. (16). The fitted parameters are $\xi_0 = 1.76$, $c = 0.21$. 