The Kondo screening cloud: what can we learn from perturbation theory?

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We analyse the role which the distance scale \( \xi_K = v_F/T_K \) plays in the single-impurity Kondo problem using renormalization group improved perturbation theory. We derive the scaling functions for the local spin susceptibility in various limiting cases. In particular, we demonstrate exactly that the non-oscillating part of it should be short-range, i.e., vanish for distances \( r \gg 1/k_F \) and show explicitly that the interior of the screening cloud does not exhibit weak coupling behavior.

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Although the Kondo effect has been very thoroughly studied for over thirty years [1], comparatively little theoretical work concentrated on the role of spatial correlations. Part of the problem is that it is inaccessible to the Bethe ansatz and difficult to analyse using Wilson’s renormalization group. No theoretical and experimental consensus has emerged on the question of the length scale at which screening of the impurity takes place. On one hand, in the scaling language [3, 4], the low energy scale \( T_K \propto e^{-1/\rho J} \) implies the presence of the exponentially large length scale \( \xi_K = v_F/T_K \); here \( v_F \) is the Fermi velocity, \( T_K \) is the Kondo temperature, \( J \) is the Kondo coupling, and \( \rho \) is the density of states (per spin). On the other hand, in the Knight shift experiments of Boyce and Slichter [5] no such scale was observed. It also appears experimentally [6] that alloys with impurity concentration \( n \gg (1/\xi_K)^3 \), i.e., where the inter-impurity distances are much less than \( \xi_K \), display single-impurity behavior. In this letter we attempt to clarify these questions using renormalization group improved perturbation theory. We derive the scaling functions explicitly that the interior of the screening cloud exhibit weak coupling behavior.

\[
H = \sum_k \epsilon_k \psi_k^\dagger \psi_k + JS_{\text{imp}} \cdot \sum_{k,k'} \psi_{k'}^\dagger \frac{\sigma^z}{2} \psi_k \cdot \sigma^z. \tag{1}
\]

The quantity measured in the Knight shift experiments is the local spin susceptibility,

\[
\chi(r,T) \equiv \langle (1/T) \psi^\dagger(r) \frac{\sigma^z}{2} \psi(r) S^z_{\text{tot}} \rangle > -\chi_0, \tag{2}
\]

where \( S^z_{\text{tot}} = S^z_{\text{imp}} + (1/2) \int dr \psi^\dagger(r) \sigma^z \psi(r) \) is the total spin operator of the impurity and conduction electrons. The bulk Pauli contribution, \( \chi_0 \equiv \rho J/2 \) has been subtracted. Recently a scaling conjecture was made [8], supported by numerical results, that in the scaling limit, \( r_k \gg 1, T \ll E_F \), the spin susceptibility has the following form:

\[
\chi = \frac{\chi_{2k_F} \left( \frac{T}{v_F}, \frac{T}{K} \right)}{4 \pi^2 r^2 v_F} \cos(2k_Fr) + \frac{\chi_{\text{un}} \left( \frac{T}{v_F}, \frac{T}{K} \right)}{8 \pi^2 r^2 v_F}, \tag{3}
\]

where \( \chi_{2k_F} \) and \( \chi_{\text{un}} \) are universal functions of two scaling variables [10]. This form follows from the relativistic one-dimensional formulation of the Kondo problem [11]. The one-dimensional Hamiltonian in terms of the left-moving fields is:

\[
H = v_F \left[ v_F \int_{-\infty}^\infty \left( d\psi_L^\dagger(r) (id/dr) \psi_L(r) + v_F \lambda \psi_L^\dagger(0) \frac{\sigma}{2} \psi_L(0) \right) \right] \cdot S_{\text{imp}}. \tag{4}
\]

The local spin susceptibility \( \chi(r,T) \) in this formalism is a sum of uniform and \( 2k_F \) parts.

\[
\chi_{\text{un}}(r,T) \equiv \langle v_F/T \rangle \left( \psi_L^\dagger(r) \frac{\sigma^z}{2} \psi_L(r) + \psi_L^\dagger(-r) \frac{\sigma^z}{2} \psi_L(-r) \right) S^z_{\text{tot}} >, \tag{5}
\]

and \( \chi_{2k_F} \) is given by the same expression with \( r \) replaced by \( -r \) in the argument of \( \psi_L \). Here \( S_{\text{tot}} \) is the total spin in the one-dimensional theory:

\[
S_{\text{tot}} = S_{\text{imp}} + S_{\text{el}} \tag{6}
\]

\[
S_{\text{el}} = \frac{1}{2\pi} \int_{-\infty}^\infty dr \psi_L^\dagger(r) \frac{\sigma}{2} \psi_L(r).
\]

Renormalizability implies that the functions \( \chi_A (A = 2k_F, \text{un}) \) obey equations of the form:

\[
\left[ D \frac{\partial}{\partial D} + \beta(\lambda) \frac{\partial}{\partial \lambda} + \gamma_A(\lambda) \right] \chi_A(T, \lambda, D, rT/v_F) = 0, \tag{7}
\]

where \( D \) is the ultra-violet cut-off (the bandwidth), \( \lambda \equiv \rho J/2 \) is the dimensionless coupling constant, \( \beta(\lambda) \) is the \( \beta-
function and \( \gamma_A(\lambda) \) is the anomalous dimension, which is a sum of contributions from the local fermion bilinears and from \( S^2_{\text{tot}} \). In this case, both contributions to \( \gamma_A \) vanish. \( S^2_{\text{tot}} \) has zero anomalous dimension because it is a conserved operator. The fermion bilinear at \( r \neq 0 \) has vanishing anomalous dimension because the interactions occur only at the origin; only “boundary operators” receive anomalous dimensions in such theories [11]. The most general solution of this equation is a general function of the effective coupling constant at scale \( T, \lambda_T \) and of the parameter \( rT/v_F \). Swapping the dependence on \( \lambda_T \) for dependence on \( T/T_K \) and using the fact that \( \chi_{2k_F} \) is real we obtain Eq. (3).

\[
\chi_{2k_F}(x = rT/v_F, \lambda_T) = \frac{(\lambda_E + (3\pi/2)\lambda_E^2 + \text{const}\lambda_E^3)(1 - \lambda_T)}{(4/\pi^2)\sin(2\pi x)},
\]

where \( \lambda_T \) is given by:

\[
\lambda_T = \lambda + \lambda^2 \ln(D/T) + \lambda^3[\ln^2(D/T) - (1/2)\ln(D/T) + \text{constant}].
\]

\( \lambda_E \) is also given by Eq. (10), with \( T \) replaced by another effective scale, \( E(x) = T/[1 - \exp(-4\pi x)] \). Eq. (10) is universal up to a rescaling of the cut-off, \( D \) and a change in the constant term. We use this freedom to redefine \( D \) to simplify our expressions. It is important to note that the infrared divergences of perturbation theory are not cut off at low \( T \) by going to small \( r \), as was first noticed by Gan [11]. It is also necessary to have a high \( T \) so that \( \lambda_T \) is small. In the third order, these divergences are associated with the graph shown in Fig.2. Due to the non-conservation of momentum by the Kondo interaction, the bubble on the right gives a logarithmic \( T \)-dependent factor which is independent of \( r \). Thus, at low \( T \), the interior of the screening cloud does not exhibit weak coupling behavior. \( \chi(r, T) \) decreases exponentially, \( \propto e^{-2\pi x} \), for \( r \gg v_F/T \). In the opposite limit, \( r \ll v_F/T \), \( \chi_{2k_F} \) can be expressed as a polynomial in \( \lambda_T \) and \( \ln x \), or equivalently \( \lambda_T \) and \( \lambda_r \), the effective coupling at scale \( r \). (Note that \( \lambda_r \equiv \lambda_E \) for \( r \ll v_F/T \)). To third order, the local spin susceptibility has the following form:

\[
\chi_{2k_F}(\lambda_T, \lambda_r) = \frac{(\lambda_r + c\lambda^3_r)(1 - \lambda_T)}{(r/\pi v_F)^2} \quad (x \ll 1),
\]

where \( c \) is a constant. The \( T \)-dependent factor is, to the order we work, precisely the total impurity susceptibility, \( \chi_{\text{tot}}(T) \). This is the total susceptibility less the bulk
Pauli term and its value has been determined accurately \[1\]. At low \(T\) it approaches \(1/T_K\). \(\lambda r \ll 1\) provided that \(r \ll \xi K\), even if \(T \ll T_K\).

\[\text{FIG. 2. Singular third-order graph for } \chi(r,T).\]

Boyce and Slichter \[3\] have measured the Knight shift from Cu nuclei near the doped Fe impurities, at distances up to 5-th nearest neighbor. At these very small distances of order of a few lattice spacings, they have found empirically that the Knight shift obeyed a factorized form, \(\chi(r,T) \approx f(r)/(T + T_K)\), with rapidly oscillating function \(f(r)\) for a wide range of \(T\) extending from well above to well below the Kondo temperature. This is essentially the same form as Eq. (11) at \(T \gg T_K\) and low \(r\). We observe from Eq. (11) that the factorization breaks down for \(r > v_F/T\). Our perturbative approach isn’t valid unless \(T \gg T_K\), so we can’t check factorization at low \(T\). This question can certainly be addressed for the overscreened large-\(k\) Kondo problem, where it is possible to obtain reliable low-temperature results from the weak-coupling perturbative expansion \[12\]. The factorized behavior of the local spin susceptibility was also obtained in Ref. \[13\].

\[
4T \chi_j(T, \lambda, \Lambda) = \exp \left[ \int_{\lambda}^{\Lambda} \frac{\gamma_j(\lambda')}{\beta(\lambda')} d\lambda' \right] \Pi_j(\lambda_T) = \Phi_j(\lambda_T) \exp \left[ -\int_{\lambda}^{\Lambda} \frac{\gamma_j(\lambda')}{\beta(\lambda')} d\lambda' \right].
\]

Here \(\Phi_j(\lambda_T), \Pi_j(\lambda_T)\) are some scaling functions. From our third-order perturbative analysis using Wilson’s result \[3\] for \(\chi_{tt}(T)\) we have obtained that the functions \(\Phi_j(\lambda_T)\) coincide for all three susceptibilities up to and including terms of order \(\lambda^2\). When \(\lambda\) is small, the scale factor in Eq. (14) can be easily calculated from perturbative expansion of \(\beta\) and \(\gamma_{\text{imp}}:\)

\[
\exp \left[ -\int_{0}^{\lambda} \frac{\gamma_{\text{imp}}(\lambda')}{\beta(\lambda')} d\lambda' \right] \approx 1 + \frac{\lambda}{2}.
\]

Thus, at least at high temperatures, where our perturbative calculation of the scaling functions is valid, the integrated electronic susceptibility obeys:

\[
\int \chi(r,T) dr \approx -\frac{\lambda}{2} \chi_{tt}(T).
\]

This result is mostly given by the electron-impurity correlator, while the electron-electron piece,

\[
\chi_{ee} \equiv \int_{0}^{\beta} d\tau \langle S_{\gamma,\lambda}(\tau)S_{\gamma,\lambda}(0) \rangle = \frac{\lambda^2}{4} \chi_{tt}(T),
\]

is further suppressed by a power of \(\lambda\). In the scaling limit of small bare coupling, \(\lambda \to 0\), the total polarization of the conduction electrons vanishes, at least at high temperature. The oscillating function \(\chi(r)\) integrates to 0, and \(\chi_{tt}\) comes entirely from the impurity-impurity part. It should be emphasized, however, that the result is non-zero at finite bare coupling \(\lambda\). (A typical experimental value of \(\lambda\) might be \(1/\ln(E_F/T_K) \approx .15\).) We conjecture that the equality of the scaling functions, \(\Phi_j(\lambda_T)\) defined in Eq. (14) holds at all \(T\), so that Eq. (14) is true at all \(T\) and small bare coupling. In particular, the integrated electronic susceptibility then vanishes in the scaling limit of zero bare coupling at all \(T\). Precisely this result was found at \(T = 0\) from the Bethe ansatz \[14\]. However, this conjecture is not completely consistent with recent work of Lesage et al. \[15\] which extrapolates to the isotropic Kondo Hamiltonian from an anisotropic model. While this may well indicate that our conjecture is wrong, it is
also possible that there is a problem with the extrapolation since we find the susceptibilities to be very singular in the isotropic limit.

\[ \chi_{2k_F}(r,T) \] is a sum of impurity and electron parts, \( \chi_{2k_F,\text{imp}} \) and \( \chi_{2k_F,\text{el}} \). While the former obeys the RG equation Eq. (1) with \( \gamma_A = \gamma_{\text{imp}} \), the latter obeys a more complicated RG equation due to operator mixing of \( S_{\text{el}} \) and \( S_{\text{imp}} \). \( \chi_{2k_F,\text{imp}} \) has the same \( \lambda \)-dependent factor as in Eq. (1), multiplied by a scaling function:

\[ \chi_{2k_F,\text{imp}} \approx \left( 1 + \frac{\lambda}{2} \right) \chi_{2k_F}^{(1)}(\lambda T, x), \]  

where the scaling function

\[ \chi_{2k_F}^{(1)}(\lambda T, x) = \frac{(\lambda F + const\lambda F^2)(1-\lambda T)}{(4/\pi^2)\sinh(2\pi x)} \]

is not the same as in Eq. (3). Thus, we obtain for all \( r \) at weak bare coupling:

\[ \chi_{2k_F,\text{el}} \approx \frac{\lambda}{2} \chi_{2k_F}^{(1)}(\lambda T, x) + \frac{(3\pi/2)\lambda F^x(1-\lambda T)}{(4/\pi^2)\sinh(2\pi x)}. \]  

Hence two different scaling functions are present in the experimentally measured Knight shift, and their share depends upon the gyromagnetic ratios for the impurity and conduction electrons. Unlike for the total spin susceptibility, \( \chi_{2k_F,\text{el}} \) doesn’t vanish in the scaling limit of zero bare coupling. However, it is small compared to \( \chi_{2k_F,\text{imp}} \) when the bare coupling and \( x \) are both small.

We may summarize the response of the weak-coupling Kondo model to a small magnetic field as follows. The impurity spin is much more strongly affected by a weak Kondo coupling than is the electron gas. This is connected with the fact that the free impurity susceptibility blows up as \( T \to 0 \), whereas the free conduction electron susceptibility does not. Thus even a weak Kondo coupling drastically affects \( \chi_{\text{el}} \) at low \( T \), causing the diverging Curie susceptibility to level off at \( 1/T_K \). On the other hand the affect on the electron gas can only become appreciable in a long distance, infrared limit. The effect of this, however, is not very dramatic, because of the factor of \( 1/r^2 \), which arises for purely dimensional reasons.

At short distances, of \( O(1/k_F) \), the excess polarization of the electron gas produced by the Kondo interaction is small. This together with the oscillating nature of the long-distance polarization gives rise to a small integrated excess polarization of the electron gas of \( O(\lambda/T_K) \).

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[1] A. C. Hewson, *The Kondo Problem to Heavy Fermions*, Cambridge University Press, Cambridge 1993.
[2] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
[3] (a) Ph. Nozières, J. Low Temp. Phys. 17, 31 (1974); Ph. Nozières, J. de Phys. 39, 1117 (1978); (b) For a review see Ph. Nozières, in *Proc. 14th Int. Conf. on Low Temperature Physics*, eds. M. Krusius and M. Vuorio, Vol. 5, (North Holland, Amsterdam 1975).
[4] J. P. Boyce and C. P. Slichter, Phys. Rev. Lett. 32, 61 (1974); Phys. Rev. B 13, 379 (1976).
[5] J. Kondo, Solid State Physics 23, 183 (1969).
[6] K. Chen, C. Jayaprakash and, H. R. Krishnamurthy, Phys. Rev. B 45, 5368 (1992).
[7] J. Gan, J. Phys.:Cond. Mat. 6, 4547 (1994).
[8] E. S. Sørensen and I. Affleck, preprint (1995), to appear in Phys. Rev. B, cond-mat 9508030.
[9] O. Újsághy, A. Zawadowski, and B. Gyorffy, preprint 1995.
[10] Definitions of \( \chi_{2k_F} \) and \( \chi_{2u} \) differ by a factor of \( v_F \) from those used in Ref. [5].
[11] See, for example, I. Affleck and A. W. W. Ludwig, Nucl. Phys. B 360, 641 (1991).
[12] V. Barzykin, I. Affleck, in progress
[13] E.Kim, M.S.Makivik, D.L.Cox, Phys. Rev. Lett. 75, 2015 (1995).
[14] A. A. Abrikosov and A. A. Migdal, J. Low. Temp. Phys. 3, 519 (1970); M. Fowler and A. Zawadowski, Sol. State Comm. 9, 471 (1971).
[15] J. H. Lowenstein, Phys. Rev. B 29, 4120.
[16] F. Lesage, H. Saleur and S. Skorik, cond-mat/9603043.