The fate of the Kondo cloud in a superconductor

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Magnetic impurities embedded in a metal are screened by the Kondo effect, signaled by the formation of an extended correlation cloud, the so-called Kondo or screening cloud. In a superconductor, the Kondo state turns into sub-gap Yu-Shiba-Rusinov (Shiba) states, and a quantum phase transition occurs between screened and unscreened phases once the superconducting energy gap $\Delta$ becomes sufficiently large compared to the Kondo temperature, $T_K$. Here we show that, although the Kondo state does not form in the unscreened phase, the Kondo cloud does exist in both quantum phases. However, while screening is complete in the screened phase, it is only partial in the unscreened phase. Compensation, a quantity introduced to characterize the integrity of the cloud, is universal, and shown to be related to the magnetic impurities' $g$-factor, monitored experimentally by bias spectroscopy.

Introduction. — One of the most fascinating manifestations of magnetic interactions in metals is the Kondo effect [1], where a local spin interacts with a sea of non-interacting electrons, to get there completely dissolved by quantum fluctuations below the so-called Kondo temperature, $T_K$. This magic quantum spin vanishes is accompanied by the formation of the so-called Kondo cloud, as characterized by the ground state correlation function

$$C(\mathbf{r}) \equiv \langle \hat{S}_{\text{imp}} \cdot \hat{S}(\mathbf{r}) \rangle, \quad (1)$$

with $\hat{S}(\mathbf{r})$ the electrons' spin density at position $\mathbf{r}$, and $\hat{S}_{\text{imp}}$ the spin of the magnetic impurity, which we assume to be of size $S_{\text{imp}} = 1/2$, which is typical in quantum dot devices. The antiferromagnetic correlations in Eq. (1) have been investigated theoretically [2–20] and also attempted to be measured experimentally by many [21–24]. They oscillate fast in space, and are characterized by an exponentially large length scale, the so-called Kondo scale, $\xi_K \approx v_F/T_K$, with $v_F$ the Fermi velocity [25]. In $D$ spatial dimensions, apart from logarithmic corrections [10, 11, 26], the envelope of $C(\mathbf{r})$ decays as $\sim 1/r^D$ at short distances, $r < \xi_K$, while it falls off as $\sim 1/r^{D+1}$ for $r \gg \xi_K$. Simple estimates yield the Kondo scale $\xi_K$ as large as $\sim 1\mu m$ in typical metals, a distance comparable to the physical dimensions of mesoscopic devices.

The antiferromagnetic correlations residing in this huge Kondo cloud are, however, quite small, as signaled by the sum rule [10, 27]

$$\int \langle \hat{S}_{\text{imp}} \cdot \hat{S}(\mathbf{r}) \rangle d^D\mathbf{r} = -\frac{3}{4} \kappa, \quad (2)$$

with $\langle \ldots \rangle$ referring to the ground state average, and $\kappa = 1$ a certain measure of quantum screening, introduced later. Equation (2) just expresses that, after all, there is only a single spin that is needed to forms a singlet state with the impurity, and that this compensating conduction electron spin is smeared in the Kondo volume, $\sim \xi_K^D$. Entanglement entropy [28, 29] calculations and the study of entanglement witness operators [30] also corroborate this picture, and confirm that the local spin's entanglement, i.e. the Kondo cloud resides within a distance $\xi_K$ from the impurity. Although many theoretical proposals have been put forward to measure the Kondo cloud by now [7, 11, 31], the cloud remained elusive for experimentalists for a very long time [21–24], and its large extension has only been confirmed very recently via Fabry-Pérot oscillations in a mesoscopic system [32]. In this work we investigate the fate of the Kondo compensation cloud in an s-wave superconductor. In a superconductor, the superconducting gap $\Delta$ competes with the Kondo effect, and prohibits screening of the magnetic impurity for weak interactions, $T_K \ll \Delta$. In this case, the magnetic impurity spin remains free even at very small

\[ \frac{1}{\sqrt{2}} \left\{ \begin{array}{c} \left| \cdots \right\rangle \left\langle \cdots \right| \right\} - \left| \cdots \right\rangle \left\langle \cdots \right| \left. \right\rangle \right. \]

FIG. 1. Schematic "phase diagram" of the model at zero temperature. When $\Delta > T_K$, the ground state is a doublet with an asymptotically free spin decoupled from the superconductor, while in the opposite limit, when $\Delta < T_K$, the ground state is a many-body singlet.
temperatures, but it binds superconducting quasiparticles to itself antiferromagnetically, amounting to discrete (singlet) sub-gap electron and hole excitations [33], called the Shiba states [34–36]. Beyond a critical magnetic coupling, i.e. for $\Delta/T_K < (\Delta/T_K)_c \approx 1.1$ [37], a first order quantum phase transition occurs, and the subgap singlet excitation becomes the ground state, as illustrated in Fig. 1. A spin $S_{\text{imp}} = 1/2$ impurity embedded into a superconductor has therefore two quantum phases, a screened singlet phase for $\Delta/T_K < (\Delta/T_K)_c$, and a doublet phase for $\Delta/T_K > (\Delta/T_K)_c$.

Here we investigate the structure of the Kondo compensation cloud in these two phases. Somewhat surprisingly, we find that the superconductor does not destroy the Kondo cloud even in the unscreened doublet quantum phase, just reduces the degree of compensation, $\kappa$, from its value $\kappa = 1$ in the singlet phase to $\kappa = \kappa(\Delta/T_K) < 1$ in the doublet quantum phase. We dub the corresponding fractional compensation cloud as the Shiba cloud. The fractional compensation emerges as a result of the competition of the Kondo screening length, $\xi_K$, and the superconducting correlation length, $\xi$, and in the doublet phase the extension of the cloud is just the coherence length, $\xi$, rather than $\xi_K$. This enormous extension of the Shiba cloud is in agreement with recent experiments on side-coupled superconducting quantum dot devices, measuring the size of Shiba states [38].

**Compensation.**—We first show that Eq. (1) is satisfied with $\kappa = 1$ in the singlet phase, $\Delta/T_K < (\Delta/T_K)_c$. To prove Eq. (1), we only need to exploit SU(2) symmetry and the fact that the ground state $|G\rangle$ is a singlet, implying that $|G\rangle$ is an eigenstate of the total spin operator, $\vec{S}_T$, with zero eigenvalue,

$$\vec{S}_T|G\rangle = (\vec{S}_{\text{imp}} + \int d^3r \vec{s}(r))|G\rangle = 0.$$ 

Multiplying this equation by $\langle G| \vec{S} \ldots$ from the left and using $\vec{S}_{\text{imp}} \cdot \vec{S}_{\text{imp}} = 3/4$ yields immediately Eq. (2) with $\kappa = 1$.

We now show that a similar relation holds even in the doublet phase, but with $\kappa < 1$, defining the degree of compensation. In the doublet phase, we have two degenerate ground states, $|\uparrow\rangle$ and $|\downarrow\rangle$. These two states transform among each other upon the action of the total spin operators as

$$\vec{S}_T|\alpha\rangle = \sum_\beta \frac{1}{2} \sigma_{\beta\alpha}|\beta\rangle,$$

with $\alpha$ and $\beta$ referring to $|\uparrow\rangle$ and $|\downarrow\rangle$, and $\sigma$ the Pauli matrices. Similar to the spin $\vec{S}_T = 0$ case, we now multiply this equation by $\langle \alpha| \vec{S}_{\text{imp}} \ldots$, and average over $\alpha$. On the right hand side, however, we can now use the Wigner-Eckart theorem, according to which

$$\langle \alpha| \vec{S}_{\text{imp}}|\beta\rangle = g \frac{1}{2} \sigma_{\alpha\beta},$$

with $g$ the $g$-factor of the impurity spin. This immediately yields Eq. (2) with

$$\kappa = 1 - g.$$

For a free spin we have $g = 1$, implying no compensation, $\kappa = 0$. However, as we discuss below, for a spin embedded into a superconductor, $g$ becomes finite due to quantum fluctuations, leading to a partial compensation of the spin and a squeezed Kondo cloud.

**Perturbation theory.**—In the limit $\Delta \gg T_K$ perturbation theory and a renormalization group approach can be used to assess the origin of $g$. We consider for that the Kondo model

$$H = J \vec{s}_{\text{imp}} \cdot \vec{s}(0) + H_{\text{host}},$$

with $J$ the local Kondo coupling, and $\vec{s}(0) = \frac{1}{2} \psi(0)\sigma \psi(0)$ the spin density at the origin, expressed now in terms of the conduction electrons’ field operator, $\psi_\sigma(r) = \sum_k e^{ikr} / \sqrt{\xi} c^{\dagger}_{k\sigma}$. The term $H_{\text{host}}$ describes the non-interacting superconducting host,

$$H_{\text{host}} = \sum_{k,\sigma} c_k^{\dagger} c_k c_{k\sigma} + \sum_{k,\sigma} (\Delta c^k_{\uparrow} c^\dagger_{k\downarrow} + h.c.) .$$

To determine $\kappa$, we simply compute $\langle \uparrow | \vec{S}_{\text{imp}} | \uparrow \rangle = g/2$ perturbatively in $J$. A straightforward calculation yields [39]

$$\kappa = 1 - g = a \frac{\ln \frac{\Lambda_0}{\Delta}}{\ln \frac{\Lambda_0}{\Delta}} + O(j_0^2),$$

with $\Lambda_0$ a bandwidth cutoff of the order of the Fermi energy, and $j_0 = J\theta_0$ the usual dimensionless Kondo coupling, defined by means of the local density of states at the Fermi energy, $\theta_0$. Clearly, the compensation contains a logarithmic singularity, which must be handled by resumming the perturbation series up to infinite order. We have performed this resummation in subleading (so-called leading logarithmic) order by using the multiplicative renormalization group (RG) [39], and exploiting the invariance of the impurity contribution to the free energy under the RG. This calculation yields the expression

$$\kappa = 1 - \exp \left( - \frac{1}{2} j_0 - \frac{1}{2} j(\Delta/T_K) \right),$$

with $j(\Delta/T_K)$ the renormalized exchange coupling,

$$j(\Delta/T_K) \approx \frac{1}{\ln \frac{\Delta}{\Delta_K}} - \frac{1}{\ln \left( \frac{\Delta}{\Delta_K} \right)} .$$

Here $T_K = A_0 \sqrt{\theta_0} e^{-1/j_0}$ denotes the Kondo temperature in the next to leading logarithmic approximation, with $\bar{F} \approx 2.5$ determined numerically to fit the Kondo temperature, defined as the half-width of the Kondo resonance [40]. Obviously, in the limit $j_0 \to 0$, Eq. (6) becomes a universal function, $\kappa = \kappa(\Delta/T_K)$. 


FIG. 2. Compensation \( \kappa \) across the quantum phase transition as a function of \( \Delta/T_K \), for \( j_0 = 0.05 \). In the fully screened regime, \( \Delta/T_K \ll 1.1 \), \( \kappa \) remains 1, and it displays a universal jump of size \( \Delta \kappa \approx 0.719 \) at the quantum phase transition, followed by a monotonic decrease in the partially screened regime. Blue and yellow squares represent DMRG and NRG results, while the solid line presents the theoretical result, Eq. (6).

"Numerics." To verify the above scenario and to determine the compensation \( \kappa(\Delta/T_K) \) accurately, we carried out detailed numerical simulations using numerical renormalization group (NRG) [41] as well as density matrix renormalization group (DMRG) [42, 43] methods. In both approaches, we can compute the ground state expectation value of the local spin, extract the \( g \)-factor from that, and express the compensation \( \kappa \) as

\[
\kappa = 1 - 2 \langle \uparrow \mid S^c_{\text{imp}} \mid \uparrow \rangle
\]

in the unscreened phase. The results are presented in Fig. 2. They show perfect agreement with each other, and also with the analytical expressions, Eqs. (6) and (7). The compensation right at the quantum phase transition is around \( \kappa_c \approx 0.28 \), thus quantum fluctuations screen around 1/3rd of the total spin, even in the doublet phase.

The build-up of finite compensation is accompanied by the evolution of the screening cloud. We can directly monitor this latter in one dimension with DMRG computations. In the absence of superconductivity, \( \kappa \) apart from an oscillating part \( \sim \cos(2k_Fx) \), spin-spin correlations decays as \( |C(x)| \sim \xi_K/x \) at short distances, \( x \ll \xi_K \), while they fall off quadratically for \( x \gg \xi_K \), where \( |C(x)| \sim (\xi_K/x)^2 \) [6, 11, 27, 44]. The power law decay originates in both regimes from electron-hole excitations. In a superconductor, however, electron-hole excitations of energy \( \delta E < 2\Delta \) are forbidden. Correspondingly, the power law behavior is suppressed beyond the associated superconducting correlation length, \( \xi = \Delta/v_F \), beyond which correlations show an exponential decay, as also demonstrated by perturbation theory (see Ref. [39]). The Shiba phase transition occurs right when the Kondo and coherence lengths become approximately equal, \( \xi \approx \xi_K \): the spin becomes fully screened under the condition that the Kondo compensation cloud fits into the coherence volume \( \sim \xi^D \).

This behavior is clearly observed in our DMRG simulations performed on a one-dimensional superconducting lattice, with a Kondo impurity placed at its end (see Fig. 3). In our simulations, we focused on the case of half filling, and extracted the envelope function of \( C(x) \) from the value of \( C(x) \equiv \langle \hat{S}_{\text{imp}} \cdot \hat{\vec{s}}(x) \rangle \) at the even sites [45]. For \( \Delta = 0 \), the envelope function shows the expected universal scaling in the near and far regions. For \( \Delta \neq 0 \), the algebraic behavior turns into an exponential decay, \( C(x) \propto \exp(-x/\xi) \), with \( \xi = v_F/\Delta \) the coherence length.

Connection to experiments – These predictions can be tested experimentally. The degree of compensation, in particular, can be measured by investigating the magnetic splitting of an artificial atom (quantum dot), attached to a superconductor, and placed in a local field, as realized in the setup presented in Fig. 4. The local exchange field is induced by attaching a ferromagnetic electrode to the quantum dot, and the strength of this field can be tuned efficiently by shifting the quantum dot’s level [46–49]. A tunnel coupling to the superconductor establishes the exchange coupling, \( J \), and gives rise to Kondo screening [48, 50–52]. Finally the third,
normal electrode is used to perform co-tunneling spectroscopy [38] and thus measure the exchange field induced splitting [47–49]. All elements of this circuit have been demonstrated experimentally.

Conclusions.— We have investigated the fate of the Kondo cloud of a magnetic impurity embedded in a superconducting host, and have shown that the impurity’s spin remains partially compensated by quantum fluctuations even in the superconducting phase. The extension of the fractional compensation cloud is just the superconducting correlation length, ξ. The degree of compensation displays a universal jump at the parity changing transition point, and is a universal function of Δ/TK, which we determined analytically and numerically, and which can be accessed experimentally by a proposed experimental set-up.

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SUPPLEMENTAL INFORMATION

Here we present certain details of the perturbative and renormalization group calculations outlined in the main paper, and give some further details on the numerical renormalization group computations.

Perturbation theory

We consider an $S_{\text{imp}} = \frac{1}{2}$ impurity spin embedded in an $s$-wave BCS superconductor, with the impurity coupled to the spin density at position $r = 0$. The Hamiltonian, as already given in the main text, is the sum of the Kondo interaction,

$$ H_K = J \tilde{S}_{\text{imp}} \cdot \mathbf{s}(0), \quad (9) $$

and the BCS Hamiltonian

$$ H_{\text{host}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} (\Delta c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{-k}\bar{\sigma}} + \text{h.c.}). \quad (10) $$

The spin density at $r = 0$ is given by $s(0) = \frac{1}{2} \sum \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\bar{\sigma}}$, where $c_{\mathbf{k}\sigma}$ denotes the creation operator of electrons with momentum $\mathbf{k}$ and spin $\sigma$. The energy $\epsilon_{\mathbf{k}}$ is measured with respect to the Fermi energy $E_F$, and we assume half filling. We perform a perturbative calculation in $J$ in the free spin regime, $T_K \ll \Delta$, and compute the expectation value $\langle \tilde{S}_{\text{imp}}^z \rangle$. In the non-interacting limit, $J = 0$, the unperturbed ground state is a direct product of the BCS ground state and the impurity spin, $|\phi_0\rangle = |\text{BCS}\rangle \otimes |\uparrow\rangle$. Here, we assume the presence of a small external magnetic field, which lifts the spin degeneracy and selects the spin up state. First order of perturbation yields a state $|\phi\rangle = |\phi_0\rangle + |\delta\phi\rangle$, with

$$ |\delta\phi\rangle = -\frac{J}{2} \sum_{\sigma\sigma'} \sum_{\mathbf{k},\mathbf{k'}} \frac{\tilde{S}_{\text{imp}}}{E_{\mathbf{k}} + E_{\mathbf{k'}}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{\sigma'}\bar{\sigma}} c_{\mathbf{\sigma'}\bar{\sigma}} |\text{BCS}\rangle \otimes |\uparrow\rangle, $$

with $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$ the quasiparticles’ excitation energy. Second order corrections to the wave function can be shown to cancel and, to order $O(J^2)$, the expectation value of the impurity spin $\langle \tilde{S}_{\text{imp}}^z \rangle$ is given by

$$ \langle \tilde{S}_{\text{imp}}^z \rangle = \frac{\langle \phi | S_{\text{imp}}^z | \phi \rangle}{\langle \phi | \phi \rangle} \approx \frac{1}{2} \left( 1 - \frac{1}{4} J^2 \sum_{\mathbf{k},\mathbf{k'}} \frac{1}{(E_{\mathbf{k}} + E_{\mathbf{k'}})^2} \right). $$

Replacing the momentum sums by integrals $\rho_0 \int_{-A_0}^{A_0} d\epsilon$, we obtain with logarithmic precision

$$ \langle \tilde{S}_{\text{imp}}^z \rangle = \frac{1}{2} \left( 1 - \frac{1}{4} J_0^2 \ln(A_0/\Delta) + O(j_0^2) \right), \quad (11) $$

where $j_0 = \theta_0 J$ is the dimensionless exchange coupling. This is just Eq. (5) of the main text.

We can also use the same approach to compute the correlation $\langle \tilde{S}_{\text{imp}}^z \cdot \mathbf{s}(x) \rangle$ in a one dimensional version of the model, where we replace $H_{\text{host}}$ by

$$ H_{\text{chain}} = -t \sum_{x=1}^{L-1} \sum_{\sigma} (c_{x\sigma}^\dagger c_{x+1\sigma} + \text{h.c.}) \quad (12) $$

and couple the impurity spin to the spin density at the first site, $\mathbf{s} = \frac{1}{2} c_{1\bar{\sigma}}^\dagger c_{1\langle\sigma}$. Hamiltonian (12) can be solved directly in real space by using the density matrix renormalization group (DMRG) approach. Figure 5 compares the results of a complete DMRG computation and those of second order perturbation theory, which are demonstrated to provide good approximation for $\langle \tilde{S}_{\text{imp}}^z \cdot \mathbf{s}(x) \rangle$, away from the quantum phase transition.

Multiplicative renormalization group approach

In this section we show, how one can derive Eqs. (6) and (7) by means of the multiplicative renormalization group approach. The multiplicative renormalization group for the Kondo problem is best formulated in terms of pseudofermions, $\tilde{f}_s$, used to express the spin operator as $\tilde{S}_{\text{imp}} = \sum_{s,s'} \tilde{f}_{s} \tilde{S}_{ss'}^s f_{s'}$ with the additional constraint, $\sum_s \tilde{f}_s f_s \equiv 1$. In this language, the impurity part of the Hamiltonian is

$$ H_{\text{imp}} = \frac{J}{\sum_{s,s',\sigma,\sigma'} f_s^\dagger \tilde{S}_{ss'}^s f_{s'} \cdot \psi_{\sigma}^\dagger \sigma \psi_{\sigma'} - h \sum_s s f_s^\dagger f_s, \quad (13) $$

with $\psi = \psi(0)$ the electrons’ field operator at the impurity site, and the second term a Zeeman field, $h$, acting on the impurity spin.
Thermodynamics as well as dynamical correlations can then be formulated in terms of the pseudofermions’ unperturbed Green’s function, \( G_{σσ'}^{0}(τ) \equiv −i⟨T_{τ} f_{σ}(τ) f^{†}_{σ'}(0)⟩_{0} \), the conduction electrons’ unperturbed local Green’s function, \( G_{σσ'}^{0}(τ) \equiv −i⟨T_{τ} ψ_{σ}(τ) ψ^{†}_{σ'}(0)⟩_{0} \), and the vertex, \( f_{σσ'}^{(0)}(τ) = \frac{τ}{2} \overline{S}_{σσ'} \cdot \overline{σ}_{σσ'} \). Similar to quantum electrodynamics, multiplicative renormalization is a transformation

\[ \Lambda \rightarrow \Lambda', \ J \rightarrow J', \ h \rightarrow h', \quad (14) \]

which transforms the electron-impurity vertex function, \( Γ \), and the impurity’s dressed Green’s function \( G \) multiplicatively,

\[ G \rightarrow Z G, \quad Γ \rightarrow Z^{-1} Γ, \]

while it leaves the impurity contribution to the free energy, \( F_{\text{imp}} \) unchanged. This transformation can be formulated in terms of simple scaling equations \([53, 54]\)

\[ \frac{dj}{dl} = j^2 - \frac{1}{2} j^3 + \ldots, \quad (15) \]

\[ \frac{d \ln h}{dl} = -\frac{1}{2} j^2 + \ldots = -\frac{1}{2} \frac{dj}{dl} + \ldots, \quad (16) \]

where \( l = \ln(A_{0}/A') \) denotes the scaling variable, \( j = J_{0} \) is the dimensionless coupling and we have displayed terms appearing only in the next to leading logarithmic order. These equations are valid for \( \omega, A' \gg Δ \), where the gap has only little effect and can therefore be disregarded, and must be solved with the initial condition, \( j(A' \rightarrow A_{0}) = j_{0} \).

To compute the expectation value of the spin in the presence of a finite gap, \( Δ \), we first notice that the size of the spin can be obtained as

\[ ⟨\uparrow | S_{\text{imp}}^{z} | \uparrow⟩ = \lim_{h \rightarrow 0^+} -\frac{1}{k_{B} T} \frac{∂}{∂h} F_{\text{imp}}(j,h,A_{0}). \quad (17) \]

However, the impurity’s free energy is invariant under the renormalization group, implying that

\[ \frac{∂}{∂h} F_{\text{imp}}(j,h,A_{0}) = \frac{∂h'}{∂h} \frac{∂}{∂h'} F_{\text{imp}}(j',h',A'), \quad (18) \]

and therefore

\[ ⟨\uparrow | S_{\text{imp}}^{z} | \uparrow⟩_{j,A_{0}} = \left( \frac{∂h'}{∂h} \right) ⟨\uparrow | S_{\text{imp}}^{z} | \uparrow⟩_{j',A'}. \quad (19) \]

If we now set the renormalized bandwidth equal to the superconducting gap, \( A' \rightarrow Δ \), then we have no more conduction electrons, and the impurity remains unscrambled: \( ⟨\uparrow | S_{\text{imp}}^{z} | \uparrow⟩ = \frac{1}{2} \). The prefactor in Eq. (19) is thus just the \( g \)-factor, which we can determine by simply integrating Eq. (16) to yield

\[ g = \frac{∂h'}{∂h} = \exp \left\{ -\frac{1}{2} (j_{Δ} - j_{0}) \right\}, \quad (20) \]

with \( j_{Δ} = j'(A'\rightarrow Δ) \). This amounts to \( κ = 1 - g \), given by Eq. (6).

To derive Eq. (7), we integrate (15) to obtain

\[ \ln \frac{A_{0}}{A'} = f(j') - f(j_{0}) \quad (21) \]

with the function \( f(j) \) given as

\[ f(j) = -\frac{1}{j} + \frac{1}{2} \ln j - \frac{1}{2} \ln (1 - \frac{j}{2}). \quad (22) \]

The Kondo temperature is determined by the condition that the effective coupling be of a value \( j' ≡ j^{*} \sim 1 \),

\[ \ln \frac{A_{0}}{T_{K}} = f(j^{*}) - f(j_{0}). \quad (23) \]

Combining this with Eq. (21), we arrive at the equation,

\[ \ln \frac{A'}{T_{K}} = f(j^{*}) - f(j'). \quad (24) \]

Setting now \( A' \rightarrow Δ \) we thus obtain the implicit equation

\[ \frac{1}{j_{Δ}} = \ln \frac{Δ}{T_{K}} - C + \frac{1}{2} \ln j_{Δ} + \frac{j_{Δ}}{4} + \ldots, \quad (25) \]

where \( C = f(j^{*}) \). An iterative solution of this equation gives

\[ j_{Δ} ≈ \frac{1}{\ln \left( \frac{Δ}{T_{K}} \right) - \frac{1}{2} \ln \left( \ln \left( \frac{Δ}{T_{K}} \right) \right) + \frac{1}{4 \ln \left( \frac{Δ}{T_{K}} \right)}} \quad (26) \]

with \( F = e^{-C} \). Dropping the last, negligible term yields the expression in the main text. The value of \( j^{*} \) and thus that of \( F \) is somewhat arbitrary. We set it such that the resulting Kondo scale, \( T_{K} = F \cdot A_{0} \cdot \sqrt{j_{0}} \exp(-1/j_{0}) \) be identical to the Kondo scale extracted from the NRG calculations, defined there as the half-width of the so-called composite fermion’s resonance (see next subsection). This yields the value, \( F \approx 2.5 \), which allows us to compare the perturbative and numerical calculations without any other adjustable parameter.

**Details of NRG calculations**

In the strongly correlated regime, where the Kondo correlations are dominant, the numerical renormalization group (NRG) method provides accurate predictions \([41, 55]\). Contrary to DMRG, NRG works in the energy space, where it uses a logarithmic discretization, allowing one to reach very small energy scales. The NRG Hamiltonian defined on the Wilson chain for our problem has the form

\[ H_{\text{NRG}} = J \cdot \hat{S}_{\text{imp}} \cdot \hat{s}_{0} + \sum_{i=0}^{N} ξ_{i} (f_{i,i+1σ}^{†} f_{i,i+1σ} + h.c.) + Δ \sum_{i=0}^{N} (f_{i,i}^{†} f_{i,i}^{†} + h.c.), \quad (27) \]
where the impurity spin is coupled by the Kondo exchange to the local spin at site 0. In Eq. (27), \( N \) is the length of the chain, and \( \xi_i \) denotes hopping amplitudes, exponentially decreasing along the chain. The operator \( f_i^{\dagger} \) denotes the creation operator at site \( i \) for a fermion with spin \( \sigma \), and \( \bar{s}_0 = \frac{1}{2} \sum_{\sigma \sigma'} f_0^{\dagger} \bar{\sigma}_{\sigma} f_0^{\dagger} \) is the spin density at site \( i = 0 \).

We solve the Hamiltonian (27) iteratively, by keeping at least 1024 lowest-energy eigenstates at each step of the iteration, and by exploiting the U(1) symmetry associated with the conservation of the total \( S_z \) spin component. For these computations, we have used our open access flexible DM-NRG code [56–59].

The Kondo temperature is determined as the half width at half maximum of the spectral function of the composite fermion, \( F^{\dagger} = \bar{S}_{\text{imp}} \cdot \bar{\sigma} f_0^{\dagger} \). Typical results for the composite fermion spectral function are displayed in Fig. 6, together with the corresponding values of dimensionless couplings, \( j_0 \), and Kondo temperatures, \( T_K \). This comparison allows us to extract the prefactor \( \mathcal{F} \approx 2.5 \) in Eq. (7).

Details of DMRG calculations

For the DMRG calculation we used the two-site approach introduced by White [42] within the matrix product state formalism [43]. The chain Hamiltonian is given by Eq. (12), and the impurity spin is coupled to the first site. To determine the ground state and compute the spin-spin correlator we used the \( U(1) \) symmetry for the \( z \) component of the total spin \( S_T \). The chain length used in the calculations was in general fixed to \( L = 200 \), but larger chain lengths, up to \( L = 400 \) were also tested. The bond dimension \( M \) was fixed in between 400 to 1000.

For each set of parameters the ground state was computed in the \( S_T = 0 \) and \( S_T = 1/2 \) sectors, which allowed us to capture the parity changing transition. Our findings for the phase diagram using DMRG match those obtained by using the NRG approach.