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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 subgap Yu-Shiba-Rusinov states, and a quantum phase transition occurs between screened and unscreened phases once the superconducting energy gap Δ exceeds sufficiently 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.

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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 noninteracting electrons, to get there completely dissolved by quantum fluctuations below the so-called Kondo temperature, T_K. This magic quantum spin vanish is accompanied by the formation of the so-called *Kondo cloud*, as characterized by the ground state correlation function

$$C(\mathbf{r}) \equiv \langle \vec{S}_{\text{imp}} \cdot \vec{s}(\mathbf{r}) \rangle, \tag{1}$$

with $\vec{s}(\mathbf{r})$ the electrons' spin density at position $\mathbf{r}$, and $\vec{S}_{\text{imp}}$ the spin of the magnetic impurity, which we assume to be of size $S_{\text{imp}} = 1/2$, typical in quantum dot devices. The antiferromagnetic correlations in Eq. (1) have been investigated theoretically [2–19] and also attempted to be measured experimentally by many [20–23]. 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 [24]. In D spatial dimensions, apart from logarithmic corrections [8,9], the envelope of $C(r)$ 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 a Kondo scale ξ_K as large as $\sim 1\ \mu$m in typical metals, a distance comparable with 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 [8,25]

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

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 form a singlet state with the impurity, and that this conduction electron spin is smeared within the Kondo volume, $\sim \xi_K^D$. Entanglement entropy [26] calculations and the study of entanglement witness operators [27] also corroborate this picture, and confirm that the local spin's entanglement, i.e., the Kondo cloud resides within a distance ξ_K from the impurity. Although many theoretical proposals have been put forward to measure the Kondo cloud by now [5,9,28], the cloud remained elusive for experimentalists for a very long time [20–23], and its large extension has only been confirmed very recently via Fabry-Pérot oscillations in a mesoscopic system [29].

In this work, we investigate the fate of the Kondo compensation cloud in an s-wave superconductor. In a superconductor, the superconducting gap Δ 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 temperatures, but it binds superconducting quasiparticles to itself antiferromagnetically, amounting to discrete (singlet) subgap electron and hole excitations [30], called the Yu-Shiba-Rusinov (YSR) states [31–33]. Beyond a critical magnetic coupling, i.e., for $\Delta/T_K < (\Delta/T_K)_c \approx 1.1$ [34], a

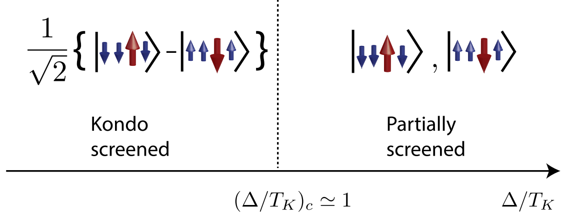

FIG. 1. Schematic "phase diagram" of the model at zero temperature. When $\Delta > T_K$, the ground state is a doublet with an asymptotically free spin decoupled from the superconductor, while in the opposite limit, when $\Delta < T_K$, the ground state is a many-body singlet.

first order quantum phase transition occurs [36], and the subgap singlet excitation becomes the ground state, as illustrated in Fig. 1. A spin $S_{\rm imp} = 1/2$ 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 $\Delta/T_K > (\Delta/T_K)_c$ [37–39].

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, but it reduces the degree of compensation κ 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 YSR *cloud*. The fractional compensation emerges as a result of the competition of the Kondo screening length ξ_K and the superconducting correlation length ξ and in the doublet phase the extension of the cloud is the coherence length, ξ, rather than ξ_K. This enormous extension of the YSR cloud is in agreement with recent experiments on side-coupled superconducting quantum dot devices, measuring the size of YSR states [40].

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,

$$\vec{S}_T|G\rangle = \left(\vec{S}_{\rm imp} + \int \mathrm{d}^D\,\mathbf{r}\,\vec{s}(\mathbf{r})\right)|G\rangle = 0. \qquad (3)$$

Multiplying this equation by $\langle G|\vec{S}_{\rm imp}\ldots$ from the left and using $\vec{S}_{\rm imp}\cdot\vec{S}_{\rm imp} = 3/4$ 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

$$\vec{S}_T|\alpha\rangle = \sum_\beta \frac{1}{2}\vec{\sigma}_{\beta\alpha}|\beta\rangle, \qquad (4)$$

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

$$\langle\alpha|\vec{S}_{\rm imp}|\beta\rangle = g\frac{1}{2}\vec{\sigma}_{\alpha\beta}, \qquad (5)$$

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

$$\kappa = 1 - g. \qquad (6)$$

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 combined with a renormalization group approach can be used to assess the origin of g. We consider for that the Kondo model

$$H = J\vec{S}_{\rm imp}\cdot\vec{s}(0) + H_{\rm host}, \qquad (7)$$

with J the local Kondo coupling, and $\vec{s}(0) = \frac{1}{2}\psi^\dagger(0)\boldsymbol{\sigma}\psi(0)$ the spin density at the origin, expressed now in terms of the conduction electrons' field operator, $\psi_\sigma(\mathbf{r}) = \sum_{\mathbf{k}} e^{i\mathbf{kr}}/\sqrt{V}\,c_{\mathbf{k}\sigma}$. The term $H_{\rm host}$ describes the superconducting host in terms of the mean field BCS Hamiltonian,

$$H_{\rm host} = \sum_{\mathbf{k},\sigma}\epsilon_{\mathbf{k}}\,c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma}(\Delta c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} + \mathrm{H.c.}). \qquad (8)$$

We consider a homogeneous superconducting gap, and neglect any spatial dependence of Δ, generated by the presence of the magnetic impurity [41].

To determine κ, we compute $\langle\Uparrow|S^z_{\rm imp}|\Uparrow\rangle = g/2$ perturbatively in J. A straightforward calculation yields [42]

$$\kappa = 1 - g = \frac{j_0^2}{4}\ln\left(\frac{\Lambda_0}{\Delta}\right) + \mathcal{O}(j_0^3), \qquad (9)$$

with Λ_0 a bandwidth cutoff of the order of the Fermi energy, and $j_0 = J\varrho_0$ the usual dimensionless Kondo coupling, defined by means of the local density of states at the Fermi energy, ϱ_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 next to leading logarithmic) order by using the multiplicative renormalization group (RG) [42], and exploiting the invariance of the impurity contribution to the free energy under the RG. This calculation yields the expression

$$\kappa = 1 - \exp\left[\frac{1}{2}j_0 - \frac{1}{2}j(\Delta/T_K)\right], \qquad (10)$$

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

$$j_\Delta \approx \frac{1}{\ln(\frac{\mathcal{F}\Delta}{T_K}) - \frac{1}{2}\ln\left[\ln(\frac{\mathcal{F}\Delta}{T_K})\right] + \frac{1}{4\ln(\frac{\mathcal{F}\Delta}{T_K})}}. \qquad (11)$$

Here $T_K = \Lambda_0 \mathcal{F}\sqrt{j_0}e^{-1/j_0}$ denotes the Kondo temperature in the next to leading logarithmic approximation, with $\mathcal{F} \approx 2.5$ determined numerically to fit the Kondo temperature, defined as the half width of the Kondo resonance [35]. In the so-called universal limit $j_0 \to 0$, $\Lambda_0 \to \infty$, and $T_K =$ finite, Eq. (10) becomes a universal function, $\kappa = \kappa(\Delta/T_K)$.

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) [43,52] as well as density matrix renormalization group (DMRG) [44,45] 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 κ as

$$\kappa = 1 - 2\langle \Uparrow | S^z_{\mathrm{imp}} | \Uparrow \rangle, \qquad (12)$$

in the unscreened phase. The results are presented in Fig. 2. They show perfect agreement with each other [53], and also with the analytical expressions, Eqs. (10) and (11). The compensation right at the quantum phase transition is around $\kappa_c \approx 0.28$, thus quantum fluctuations screen approximately one-third of the total spin, even in the doublet phase. Notice that the RG expression for the compensation in Eq. (10) and, correspondingly, the jump in the compensation, remain the same in any spatial dimension D, as also confirmed by our one-dimensional DMRG and dimension independent NRG calculations.

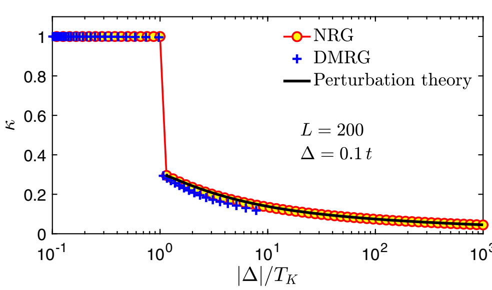

FIG. 2. Compensation κ across the quantum phase transition as a function of Δ/T_K, for $j_0 = 0.05$. In the fully screened regime, $\Delta/T_K \lesssim 1.1$, κ remains 1, and it displays a universal jump of size $\Delta\kappa \simeq 0.719$ at the quantum phase transition, followed by a monotonous decrease in the partially screened regime. Blue and yellow squares represent DMRG and NRG results, while the solid line presents the theoretical result, Eqs. (10) and (11).

The buildup 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, apart from an oscillating factor $\sim \cos(2k_F x)$, spin-spin correlations decay 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 $|C(x)| \sim (\xi_K/x)^2$ [4,9,25,54]. 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, $\xi = v_F/\Delta$, where correlations show an exponential decay, as also demonstrated by perturbation theory (see Ref. [42]). The YSR phase transition occurs right when the Kondo and coherence lengths become approximately equal, $\xi \approx \xi_K$. Thus 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 $C(x) \equiv \langle \vec{S}_{\mathrm{imp}} \cdot \vec{s}(x) \rangle$ at the even sites [55]. For $\Delta = 0$, the envelope function shows the expected behavior of $C(x) \sim 1/x$ and $C(x) \sim 1/x^2$ for small and large distances, respectively. The presence of the superconducting gap alters this behavior fundamentally, and induces an exponential decay of the form, $C(x) \propto \exp(-2x/\xi)$, once x gets larger than ξ.

These results can be generalized to any dimension. As discussed in Ref. [56], one can reduce the Kondo problem to a one-dimensional chiral Fermion problem in any

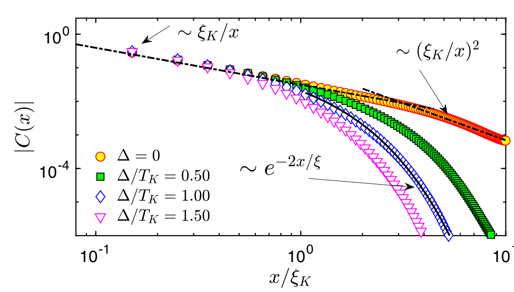

FIG. 3. Envelope for the equal-time spin-spin correlation function $C(x)$ defined in Eq. (1) as a function of the distance from the impurity spin in a one-dimensional chain, as computed by DMRG. For $\Delta = 0$, the envelope function shows the expected universal scaling in the near and far regions. For $\Delta \neq 0$, the algebraic behavior turns into an exponential decay, $C(x) \propto \exp(-2x/\xi)$, with $\xi = v_F/\Delta$ the coherence length. We used a chain length $L = 200$, the Kondo temperature was fixed to $T_K = 0.1t$, with t the hopping along the chain, which corresponds to a dimensionless coupling, $j_0 = 0.286$. The associated Kondo correlation length is $\xi_K \approx 20$ lattice sites.

dimension. The procedure of Ref. [56] can also be carried out in a superconductor, and allows us to draw general conclusions in any dimension. For distances below the superconducting correlation length $r < \xi$ the superconducting gap does not play a major role, and at short distances $r < \xi_K$ one therefore recovers the scaling $C(r) \sim 1/r^D$, which follows from perturbation theory in j_0. For $\xi_K < r$ and $r < \xi$, on the other hand, one should find a behavior characteristic of a Fermi liquid, $C(r) \sim 1/r^{D+1}$, similar to the behavior of the spin-spin correlation function in a metal [57]. $C(r)$ seems to diverge at small distances, but its divergence is cancelled by subleading (high energy) contributions when $\mathbf{r} \to 0$. The asymptotic behavior of the spin-spin correlation function in the Kondo cloud is very similar to the spin-spin correlation function in a Fermi liquid. In three dimensions one has $\langle \mathbf{s}(\mathbf{r})\mathbf{s}(\mathbf{0})\rangle \sim [\sin(k_F r) - k_F r \cos(k_F r)]^2/r^6$. The apparent ultraviolet logarithmic divergency at the origin of the integral $\sim \int dr\, r^{D-1}(1/r^D)$ is regularized by the subleading terms. The scaling of $C(r)$ is only altered for $r > \xi$, where the gap of the superconductor introduces an exponential cutoff, $C(r) \sim e^{-2r/\xi}$, as typical in gapped systems.

Connection to experiments.—Our predictions could be tested experimentally with a device sketched in Fig. 4. 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. To generate a local field and observe the impurity's g factor, we propose to attach a ferromagnetic electrode to the quantum dot, and thereby create a local exchange field B_{eff}, as done in Ref. [58]. The strength of this field can be tuned efficiently by shifting the quantum dot's level [58–61]. To establish the exchange coupling to the superconductor, J, and to give rise to Kondo screening [58,62–66], one could tunnel couple the dot to a superconductor. Finally, a third, weakly coupled normal electrode could be used to perform bias spectroscopy [40] and to measure the exchange field induced splitting from the co-tunneling spectrum [60,61], and thus extract the g factor.

In the regime $\Delta \gtrsim 1.1 T_K \gg B_{\mathrm{eff}}$, corresponding to a weakly split doublet ground state, the Zeeman splitting between the doublet states can be extracted from the co-tunneling signal. The ground state Zeeman splitting is supposed to remain finite and directly proportional to g on the doublet side of transition, while it must vanish once the transition is crossed, and the ground state turns into a singlet.

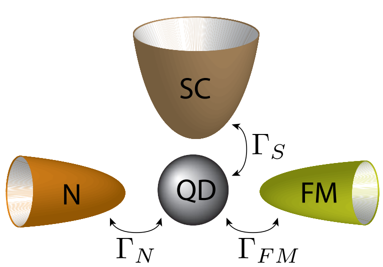

FIG. 4. Experimental setup for measuring the compensation κ. The quantum dot is coupled to a normal (N), a superconducting (SC), and a ferromagnetic (FM) lead.

We should emphasize that, although the proposed experiment is quite complex, all elements of the setup in Fig. 4 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 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/T_K, which we determined analytically and numerically, and which can be accessed experimentally by a proposed experimental setup.

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