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Non-Fermi-liquid behavior in quantum impurity models with superconducting channels

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Abstract

We study how the non-Fermi-liquid nature of the overscreened multi-channel Kondo impurity model affects the response to a BCS pairing term that, in the absence of the impurity, opens a gap. We find that the low-energy spectrum in the limit $\Delta \rightarrow 0$ actually does not correspond to the spectrum strictly at $\Delta = 0$. In particular, in the two-channel Kondo model the $\Delta \rightarrow 0$ ground state is an orbitally degenerate spin-singlet, while it is an orbital singlet with a residual spin degeneracy at $\Delta = 0$. In addition, there are fractionalized spin-1/2 sub-gap excitations whose energy in units of Δ tends towards a finite and universal value when $\Delta \rightarrow 0$; as if the universality of the anomalous power-law exponents that characterise the overscreened Kondo effect turned into universal energy ratios when the scale invariance is broken by $\Delta \neq 0$. This intriguing phenomenon can be explained by the renormalisation flow towards the overscreened fixed point and the gap cutting off the orthogonality catastrophe singularities. We also find other non-Fermi liquid features at finite Δ : the local density of states lacks coherence peaks, the states in the continuum above the gap are unconventional, and the boundary entropy is a non-monotonic function of temperature. The persistent sub-gap excitations are characteristic of the non-Fermi-liquid fixed-point of the model, and thus depend on the impurity spin and the number of screening channels.

I Introduction

The density of states (DOS) $\rho(\omega)$ of a conventional BCS s -wave superconductor has a gap and coherence peaks above it, $\rho(\omega) = \rho_0 \text{Re} \omega / \sqrt{\omega^2 - \Delta^2}$, where ρ_0 is the normal-state DOS. This remains true also in the presence of disorder and impurities that maintain time-reversal invariance¹. By contrast, magnetic impurities may induce additional states inside the gap by binding Bogoliubov quasiparticles through the exchange coupling^{2–6}. The bound-state energies depend on the interplay of Kondo screening, superconducting proximity effect, and spin-orbit coupling^{7–9}, and are measurable in hybrid superconductor-semiconductor nanostructures^{10–12} and adsorbed magnetic atoms or molecules^{13–15}. In

the limit of small gap, $\Delta \rightarrow 0$, the sub-gap states induced by impurities that are Kondo screened below the Kondo temperature T_K (and hence effectively non-magnetic) move towards the gap edges and merge with the coherence peaks^{16–23}, because the weak superconducting pairing ($\Delta \ll T_K$) perturbs a system that was formerly in a local Fermi liquid (FL) state²⁴. The effect of the impurity on the bulk electrons is thus fully accounted by the quasiparticle scattering phase shifts resulting from the Kondo effect ($\pi/2$ in the deep Kondo limit)²⁵. A similar scenario occurs in the case of underscreen local moments which have a residual local moment which is, however, asymptotically decoupled from the rest of the system; such systems are known as singular Fermi liquids^{26,27} and occur when the number of screening channels k is lower than twice the impurity spin, $2S$.

There is, however, a further class of quantum impurities that are Kondo overscreened because the number of screening channels exceeds twice the impurity spin, $k > 2S$ ^{28–33}. Such overcompensation has been experimentally demonstrated for the two-channel Kondo model ($k = 2$, $S = 1/2$) in artificial semiconductor quantum dot devices^{34–39}. The resulting states are non-Fermi liquids (NFL)^{29,40} with excitation spectra that deviate significantly from the FL paradigm, but can be still described in terms of appropriate boundary conformal field theories (CFT)^{41–46} and can be solved exactly using the Bethe Ansatz^{47–49}. When a small gap is opened in the contacts of such systems, the superconducting state thus emerges out of a non-Fermi liquid. Two related questions arise: 1) What is the nature of the excitations forming the continuum above the gap? 2) Can the sub-gap states be interpreted as bound states of NFL excitations?

In this work the problem is studied using the numerical renormalization group (NRG) technique^{16,50–54} and analytical arguments. For the two-channel Kondo (2CK) model⁵⁵ in the limit $\Delta \rightarrow 0$ we find surprisingly that the low energy spectrum does not reproduce that at $\Delta = 0$: the ground state (GS) is a doubly degenerate spin-singlet, while two $S = 1/2$ sub-gap Shiba states become degenerate with a *universal dimensionless energy ratio*

$$\epsilon^* \equiv E^*/\Delta \approx 0.5983. \quad (1)$$

In other words, even in the $\Delta \rightarrow 0$ limit these bound states do not merge with the continuum. The GS is connected with the excitations at the rescaled energy $1/8$ in the boundary CFT of the $\Delta = 0$ case, while the excited sub-gap states emerge out of the energy 0 and $1/2$ states^{41,42,56–59}. The excitations above the gap have NFL degeneracies and spacing, and there are no coherence peaks in the impurity DOS. When the NFL regime is disrupted by breaking the channel degeneracy^{29,56,60–62}, the sub-gap states do move toward the gap edge and the coherence peaks are restored when the FL-NFL cross-over scale T^* exceeds Δ .

II Model

We consider the Hamiltonian $H = \sum_{i=1}^k J_i \mathbf{s}_i \cdot \mathbf{S} + H_i$, where

$$H_i = \sum_{k\sigma} \epsilon_k c_{i,k\sigma}^\dagger c_{i,k\sigma} + \sum_k \left(\Delta c_{i,k\uparrow}^\dagger c_{i,k\downarrow}^\dagger + \text{H. c.} \right), \quad (2)$$

i.e., a k -channel Kondo model²⁹ with each channel described by a BCS mean-field Hamiltonian with fixed J_i . J_i is the exchange coupling, s_i is the spin density of channel- i electrons at the position of the impurity, $\mathbf{S}$ is the impurity spin- S operator, and finally $c_{i,k\sigma}^\dagger$ creates an electron in channel- i with momentum k , spin σ , and energy ϵ_k . The continuum has a flat DOS with half-bandwidth D , i.e., $\rho_0 = 1/2D$. The Kondo scale for small exchange coupling is $T_K \approx \exp(-1/\rho_0 J_{\text{avg}})$, where $J_{\text{avg}} = \sum_i J_i/k$.⁶³ If J_i are non-equal, there is further relevant scale T^* that grows as a power law with the difference between the two largest J_i .⁵⁵ For $\gamma = 0$, the system has NFL properties for $T^* < T < T_K$ and crosses over to a FL GS for $T < T^*$. For $\gamma > 0$, we use the NRG to compute the finite-size excitation spectra, thermodynamic properties, and the T -matrix spectral function (impurity DOS).

III Persistent Sub-Gap States

A Two-channel Kondo model

The discrete (sub-gap) part of the excitation spectrum for the 2CK model with $J_1 = J_2 = J$ is shown in Fig. 1(a) at constant gap γ as a function of the dimensionless coupling constant $g = \rho_0 J$. To better understand the origin of these states, we introduce a simplified zero-bandwidth model where each screening channel is represented by a single orbital f_i with pairing

$\left(\Delta f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger + \text{H. c.} \right)$, and $2s_i = \sum_{\alpha\beta} f_{i\alpha}^\dagger \sigma_{\alpha\beta} f_{i\beta}$. The lowest four eigenstates, shown in Fig. 1(b), are in qualitative correspondence with those of the full model. The even-parity $S = 1/2$ state represents a decoupled impurity spin. (The parity refers to the channel inversion symmetry.) This is the GS for low g and corresponds to the local-moment phase at $\gamma > T_K$. Each spin-singlet state corresponds to the impurity spin coupled into an $S = 0$ state to a singly-occupied orbital, the other orbital being instead in the configuration $(|0\rangle - |\uparrow\downarrow\rangle) / \sqrt{2}$. There are evidently two such spin-singlet states, depending on which orbital screens the impurity. This is actually the doubly degenerate GS for intermediate values of g . Finally, in the large- g limit the GS is an odd-parity strong-coupling state: both orbitals are singly occupied and coupled into an odd-parity spin-triplet configuration, which is in turn coupled to the impurity into a $S = 1/2$ state.

The low- g and high- g limits are related through a duality mapping which interchanges the parity of the $S = 1/2$ states and which also occurs in the $\gamma = 0$ model^{60,63}. At $g = g^* \approx 0.7$ these states cross and thereby define the self-dual point. This occurs at a particular value of the excitation energy ϵ^* defined in Eq. (1). This value is actually universal: for any g the two doublet levels converge in the $\gamma \rightarrow 0$ limit toward the same value ϵ^* , see Fig. 1(c). In Fig. 2 we plot the sub-gap $S = 1/2$ states as a function of the dimensionless exchange coupling constant $g = \rho_0 J$ for a range of values for the gap γ . All curves cross in the self-dual point at $g^* \approx 0.7$. For values of J close to the self-dual point, where the Kondo temperature is of

magnitude comparable to the bandwidth, the universal limit is reached already at high values of Δ .

The self-dual point thus defines the universal non-trivial fixed point of the theory in the small-gap limit, as well as at $\Delta = 0$. The approach toward this limit is a square-root function of Δ :

$$E_{o,e}/\Delta \sim \epsilon^* + c_{o,e}(g) \Delta^{1/2}. \quad (3)$$

Magnetic anisotropy $J_{\perp} - J_z$ is irrelevant, as in the normal state, and does not affect the value of ϵ^* . We have also verified that the presence or absence of the particle-hole symmetry plays no role.

In Fig. 3 we show the finite-size excitation spectrum (NRG flow diagram) as a function of the Wilson chain length N , corresponding to the energy scale $\epsilon_N = \Lambda^{-N/2}$. Specifically, Fig. 3(a) reports the energies scaled as $\epsilon = E/\epsilon_N$, and demonstrates the cross-over from the local-moment to the 2CK NFL fixed point for $N \gtrsim 30$, with characteristic fractional energies $\epsilon_N = 0, 1/8, 1/2, 5/8, 1, \dots$ and degeneracies 2, 4, 10, 12, 26, $\dots$, respectively, that reflect the peculiar $SU(2)_2 \times SO(5)$ conformal field theory (CFT) that describes the asymptotic behaviour of the model at $\Delta = 0.41, 46, 55$. We observe that a finite Δ lowers the $SO(5)$ symmetry down to $SU(2) \times U(1)$, which corresponds to an $SU(2)_2$ CFT times the Z_2 orbifold of a compactified $c = 1$ CFT. The latter allows for a marginal boundary operator able to split the $SO(5)$ multiplets; for instance the degeneracy 4 of the $1/8$ state into $4 \rightarrow 2 + 2$, or the degeneracy 10 of the $1/2$ state into $10 \rightarrow 2 + 6 + 2$ (see Sec. VI). Such splitting is already evident in Fig. 3(a) for $40 \lesssim N \lesssim 45$. However, for $N \gtrsim 45$, the BCS gap exceeds ϵ_N and induces flow toward a new fixed point which is better characterized by scaling the energies as E' , see Fig. 3(b). The lowest doublet of the split $\epsilon = 1/8$ multiplet becomes the doubly degenerate spin-singlet GS, while the $\epsilon = 0$ $S = 1/2$ -state and the lowest $S = 1/2$ state of the split $\epsilon = 1/2$ multiplet meet into the $S = 1/2$ sub-gap doublet. The continuum of excitations for $E > \Delta$, which is dense close to the gap edge, is best shown scaled as $(E - \Delta)/\Lambda^{-N}$, Fig. 3(c). The energies are spaced by the ratio of Λ , rather than Λ^2 as in the gapped single-channel FL case²³. Such progression results from a combination of FL states with one channel having $\delta = 0$ and the other $\delta = \pi/2$ quasiparticle phase shift, as expected for a GS where the Kondo effect is formed with one channel, the other being decoupled. This does not imply, however, that FL behavior is recovered. The degeneracy of states above the gap is twice the number for a FL. More remarkably, when the matrix elements are evaluated to compute the impurity DOS, there are no coherence peaks in the $\Delta \ll T_K$ limit (see Sec. V).

B Three-channel Kondo model

We now turn to the three-channel Kondo (3CK) models with $k = 3$ which also have NFL ground states for $2S < k$ ^{64–67}. The three-channel Kondo models with $S = 1/2$ and $S = 1$ exhibit cross-duality: the small- g limit of the $S = 1/2$ model corresponds to the large- g limit of the $S = 1$ model, and vice versa. This occurs because the overscreening of a spin-1/2 by three channels produces a spin-1 residual object, while overscreening of a spin-1 produces a

spin-1/2 residual object. Accordingly, the two models share essentially the same intermediate-coupling NFL fixed point, only shifted by one Wilson shell, i.e., the even and odd system sizes are interchanged; for $S = 1/2$, the level progression is 0, 1/8, 2/8, 5/8, 6/8, 7/8, ... with degeneracies 3, 12, 14, 28, 42, 24 for odd lengths and 0, 2/8, 6/8, 10/8, ... with degeneracies 2, 6, 46, 90, ... for even lengths (for both small and large g), and vice-versa for the $S = 1$ model. The Kondo temperature peaks for $g \sim 1$. For finite g , the even-odd alternation no longer occurs and the cross-duality becomes more obvious. For $g \sim 1$, the spin-singlet ground state is triply degenerate, and there are two spin-doublet energy levels, one non-degenerate and one triply degenerate, again with *universal energy ratios*:

$$\epsilon_1^* \equiv E_1^*/\Delta \approx 0.19, \quad \epsilon_3^* \equiv E_3^*/\Delta \approx 0.72. \quad (4)$$

A spin-triplet sub-gap state is also present and becomes the ground state in the small- g limit of the $S = 1$ model and in the large- g limit of the $S = 1/2$ model.

The sub-gap states can be interpreted in the zero-bandwidth limit. For the $S = 1/2$ case, the following holds:

- the three spin-singlet states correspond to the Kondo states formed between the impurity spin and one of the three channels, the other two remaining decoupled;
- the non-degenerate spin-doublet 1 is the local-moment state;
- the triply degenerate spin-doublet 3 is composed of spin-1/2 “Heisenberg-chain” states formed between the impurity spin and two of the neighboring orbitals, the third channel being decoupled;
- the spin-triplet is a “Heisenberg-star” state formed by the impurity and all three orbitals.

For the $S = 1$ case, we find:

- the three spin-singlet states correspond to the exactly screened Kondo states formed between the impurity spin and two of the three channels, the third one remaining decoupled;
- the non-degenerate spin-doublet 1 is a “Heisenberg-star” state formed between the impurity spin and the three neighboring orbitals;
- the triply degenerate spin-doublets 3 can be thought of as underscreened Kondo states where the impurity spin binds to one of the neighboring orbitals, the other two channels remaining decoupled;
- the spin-triplet is the local-moment state.

Because of the duality, the sub-gap spectra shown in Fig. 4 are essentially mirror-images of each other. The non-trivial regime corresponds to the flat parts for intermediate-coupling $g^* \sim 1$. For any g , the $g \rightarrow 0$ fixed point is the same. The approach is now

$$E_{1,3}/\Delta \sim \varepsilon_{1,3}^* + c_{1,3} \Delta^{1/3}. \quad (5)$$

Compared to the 2CK case, the two sub-gap states now approach two different values, and the exponent is $1/3$ rather than $1/2$.

IV Anomalous Thermodynamics

The reshuffling of states when the gap opens leads to peculiar thermodynamics. In Fig. 5 we plot the impurity magnetic susceptibility, χ_{imp} , and impurity (boundary) entropy s_{imp} for the two-channel Kondo model. For $T \gg T_K$, the temperature dependence equals that of the $S = 0$ model: the effective local moment goes to zero and the impurity entropy reaches the $\ln 2/2$ plateau. At $T \sim T_K$, the effective degeneracy of the impurity-generated states *increases*, leading to peaks in both χ_{imp} and s_{imp} . The boundary entropy thus increases from $\sim \ln 2/2$ to $\ln 2$. The g -theorem⁶⁸ does not hold here because T_K breaks the conformal invariance. Rising impurity entropy at low temperatures is also found in other related impurity models^{69–71}.

V Absence of Coherence Peaks

The FL properties are restored when the channel symmetry in overscreened Kondo models is broken^{38,56,60–62,72}. The sub-gap spectrum, shown in Fig. 6(a) as a function of $J = (J_1 - J_2)/2$ for constant J_{avg} such that $T_K \gg T^*$, now depends on the relative value of J and the NFL-FL crossover scale T^* . For small J such that $T^* \ll T_K$, the sub-gap spectrum is “NFL-like” with the $S = 1/2$ doublet close to ε^* . As J increases, the degeneracy between the spin-singlet states is lifted. The Kondo state in the dominant channel remains the GS, while the other Kondo state rapidly rises in energy and enters the continuum. The sub-gap $S = 1/2$ doublet asymptotically approaches the gap edge in the large J limit where $T^* \gg T_K$, and the spectrum becomes “FL-like” with no sub-gap states (because $T_K \ll T^*$). The NFL-FL crossover has a characteristic signature also in the impurity DOS, see Fig. 6(b): with increasing J , the δ -peaks move toward the continuum edges and the spectral weight is transferred from the sub-gap region into the continuum to form the coherence peaks characteristic of the FL regime.

VI CFT Approach to the 2CK

In this section we will briefly sketch how the conformal field theory (CFT) can be applied to the two-channel Kondo (2CK) model. We will throughout make great use of the results in the book *Conformal Field Theory* by P. Di Francesco, P. Mathieu and D. Sénéchal⁷³. We will not pretend to be as rigorous and as detailed as they are, we will just limit to list some results whose derivation can be relatively easily obtained through that book. Therefore in this section we implicitly give for granted that the reader is a bit familiar with the CFT.

First of all we assume that the low-energy physics of the model can be equally reproduced by a simple tight-binding model on a semi-infinite chain, with the impurity spin sitting at the edge. The Hamiltonian thus reads

$$\begin{aligned}
H = & -t \sum_{x \geq 1} \sum_{a=1}^2 \sum_{\sigma} \left(c_{x a \sigma}^{\dagger} c_{x+1 a \sigma} + c_{x+1 a \sigma}^{\dagger} c_{x a \sigma} \right) \\
& - \Delta \sum_{x \geq 1} \sum_{a=1}^2 \left(c_{x a \uparrow}^{\dagger} c_{x a \downarrow}^{\dagger} + c_{x a \downarrow} c_{x a \uparrow} \right) \\
& + J \sum_{a=1}^2 \sum_{\alpha \beta} S \cdot c_{1 a \alpha}^{\dagger} S_{\alpha \beta} c_{1 a \beta}
\end{aligned} \quad (6)$$

$$\equiv H_0(\Delta) + H_{\text{Kondo}}. \quad (7)$$

In order to identify in a simple way the symmetries of the Hamiltonian, it is convenient to perform the unitary transformation

$$\begin{aligned}
c_{x a \uparrow} &= \frac{1}{\sqrt{2}} \left(d_{x a \uparrow} - (-1)^x d_{x a \downarrow}^{\dagger} \right), \\
c_{x a \downarrow} &= \frac{1}{\sqrt{2}} \left(d_{x a \downarrow} + (-1)^x d_{x a \uparrow}^{\dagger} \right),
\end{aligned}$$

which leaves H_{Kondo} invariant, while $H(\Delta)$ transforms into a tight-binding Hamiltonian with a staggered on-site potential:

$$\begin{aligned}
H_0(\Delta) \rightarrow & -t \sum_{x=1}^{2L} \sum_{a=1}^2 \sum_{\sigma} \left(d_{x a \sigma}^{\dagger} d_{x+1 a \sigma} + d_{x+1 a \sigma}^{\dagger} d_{x a \sigma} \right) \\
& - \Delta \sum_{x=1}^{2L} \sum_{a=1}^2 \sum_{\sigma} (-1)^x d_{x a \sigma}^{\dagger} d_{x a \sigma}.
\end{aligned} \quad (8)$$

In this representation it becomes evident that the full Hamiltonian $H = H_0(\Delta) + H_{\text{Kondo}}$ is invariant under spin $SU(2)$, channel flavour $SU(2)$ and charge $U(1)$.

A transparent way to build the correct CFT for this model is to equate partition functions via the so-called character decomposition. When $J = 0$, the model possesses a large symmetry. As pointed out by Maldacena and Ludwig⁴⁶ it is convenient to represent the degrees of freedom of the model in terms of eight chiral Majorana fermions, thus through an $SO(8)$ CFT. We start from the partition function of the $H_0(0)$, namely of two spinful channels, which reads

$$Z = \sum_{n_1, n_2=0}^1 \left(\chi_{n_1}^{(1)} \chi_{n_2}^{(1)} \right)_{\text{charge}} \left(\chi_{n_1}^{(1)} \chi_{n_2}^{(1)} \right)_{\text{spin}}, \quad (9)$$

where $\chi_n^{(k)}$ with $n = 0, \dots, k$ are the characters of the $SU(2)_k$ CFT, where k is the level, and are related to primary fields $\phi_n^{(k)}$, of spin $S = n/2$ and dimension $S(S+1)(k+2)$. In Eq. (9)

the $SU(2)_1$ primary fields occur. Since an electron brings both spin 1/2 and charge isospin 1/2, the label $n_a = 0, 1$ in each channel is the same in the spin and charge sectors, being $n_a = 0$ the contribution to Z of states with even number of electrons in channel $a = 1, 2$, and $n_a = 1$ that of states with odd electron number. It is known that

$$\chi_0^{(1)} \chi_0^{(1)} = (\chi_0^I)^4 + (\chi_{1/2}^I)^4 + 6(\chi_0^I)^2 (\chi_{1/2}^I)^2, \quad (10)$$

$$\chi_0^{(1)} \chi_1^{(1)} = 4(\chi_0^I)^3 + (\chi_{1/2}^I) + 4(\chi_0^I) (\chi_{1/2}^I)^3, \quad (11)$$

$$\chi_0^{(1)} \chi_1^{(1)} = 2(\chi_{1/16}^I)^4, \quad (12)$$

where χ_x^I are the characters of an Ising CFT with primary fields of dimension 0, 1/16 (σ) and 1/2 (ϵ). Substituting equations (10)–(12) in Eq. (9), one can rewrite the original partition function in terms of the characters of eight Ising CFT, i.e. eight Majorana fermions, and as a benefit get immediately the degeneracy of the states of each conformal tower.

However, three of the eight Majorana fermions merge together into the spin operators that are coupled with the impurity, realising an $SU(2)_2$ CFT. By means of the known results

$$\begin{aligned} \chi_0^{(1)} \chi_0^{(1)} &= \chi_0^I \chi_0^{(2)} + \chi_{1/2}^I \chi_2^{(2)} \\ \chi_0^{(1)} \chi_1^{(1)} &= \chi_{1/16}^I \chi_1^{(2)}, \\ \chi_1^{(1)} \chi_1^{(1)} &= \chi_0^I \chi_2^{(2)} + \chi_{1/2}^I \chi_0^{(2)}, \end{aligned}$$

that describe the combination of two $SU(2)_1$ CFTs into an $SU(2)_2$ plus an Ising, we finally obtain the partition function of the $SO(5) \times SU(2)_2$ CFT, where the $SU(2)_2$ refers to the spin degrees of freedom,

$$\begin{aligned} Z = & \left[(\chi_0^I)^5 + 10(\chi_0^I)^3 (\chi_{1/2}^I)^2 + 5(\chi_0^I) (\chi_{1/2}^I)^4 \right] \chi_0^{(2)} \\ & + 4(\chi_{1/16}^I)^5 \chi_1^{(2)} \\ & + \left[5(\chi_0^I)^4 (\chi_{1/2}^I) + 10(\chi_0^I)^2 (\chi_{1/2}^I)^3 + (\chi_{1/2}^I)^5 \right] \chi_2^{(2)}, \end{aligned}$$

which therefore represents the partition function in terms of a spin $SU(2)_2$ and 5 Ising CFTs.

Following the fusion hypothesis⁴¹, the NFL fixed point is obtained after fusion with an $SU(2)_2$ primary field of spin-1/2, and it is characterised by the partition function

$$Z_{\text{NFL}} = 4 \left(\chi_{1/16}^I \right)^5 \left(\chi_0^{(2)} + \chi_2^{(2)} \right) + \left(\chi_0^I + \chi_{1/2}^I \right)^5 \chi_1^{(2)}. \quad (13)$$

The ground state belongs to the tower $\left(\chi_0^I \right)^5 \chi_1^{(2)}$ with energy $E_0 = 3/16$. The next lying state corresponds to $4 \left(\chi_{1/16}^I \right)^5 \chi_0^{(2)}$. It is fourfold degenerate and its energy with respect to the ground state one $E_{1,8} = 5/16 - 3/16 = 1/8$. Above it there are several states with energy difference from the ground state of $E_{1,2} = 1/2$. These correspond explicitly to the terms $5 \left(\chi_0^I \right)^4 \left(\chi_{1/2}^I \right) \chi_1^{(2)}$, hence a tenfold degeneracy since $\chi_1^{(2)}$ has spin $S=1/2$. One can proceed further and obtain all levels and their degeneracies.

When $\ell = 0$ it is more convenient to extract out of the 5 Majorana fermions those 3 that combine to produce a flavour $SU(2)_2$. This is readily done by observing that

$$\begin{aligned} \left(\chi_0^I + \chi_{1/2}^I \right)^5 &= \left(\chi_0^I + \chi_{1/2}^I \right)^2 \left(\chi_0^{(2)} + \chi_2^{(2)} \right), \\ 4 \left(\chi_{1/16}^I \right)^5 &= 2 \left(\chi_{1/16}^I \right)^2 \chi_1^{(2)}, \end{aligned}$$

so that we can rewrite Eq. (13) as

$$\begin{aligned} Z_{\text{NFL}} &= \mathbf{2} \left(\chi_{1/16}^I \right)^2 \left(\chi_1^{(2)} \right)_{\text{flavour}} \left(\chi_0^{(2)} + \chi_2^{(2)} \right)_{\text{spin}} \\ &+ \left(\chi_0^I + \chi_{1/2}^I \right)^2 + \mathbf{2} \chi_0^I \chi_{1/2}^I \left(\chi_0^{(2)} + \chi_2^{(2)} \right)_{\text{flavour}} \left(\chi_1^{(2)} \right)_{\text{spin}}. \end{aligned} \quad (14)$$

The two Ising CFTs can in turn be recombined in a $c = 1$ CFT on compactification radius $R = \sqrt{2p'} = 2$, which has primary fields

- $\phi_{1,8}$ with dimension $1/8$;
- a doubly degenerate field $\phi_{1/2}^{(a)}$, $a = 1, 2$, with dimension $1/2$;
- the twist operators $\sigma^{(a)}$ and $\tau^{(a)}$ with dimensions $1/16$ and $9/16$, respectively;
- the dimension 1 operator θ .

It is just the latter operator θ that becomes allowed at the boundary and which lifts the degeneracy indicated in Eq. (14) by a bold **2**. In table I we tabulate the NRG finite-size spectrum at $\Lambda = 2$ in the presence of a small local ℓ term on the first site of the chain.

VII Anderson-Yuval Approach in the Presence of a Staggered Potential

We now sketch an analytical argument that explains qualitatively and to some extent also quantitatively the NRG results for the two-channel Kondo model in the presence of the super-conducting gap. We consider the model defined by Eq. (8), i.e., a tight-binding model

in the presence of a staggered potential, and apply a simplified version of the Anderson-Yuval approach to the Kondo effect^{74–76}. The unperturbed spectrum is $\pm E_k = \pm \sqrt{\epsilon_k^2 + \Delta^2}$, and we shall assume a constant DOS ρ for $\epsilon_k \in [-D, D]$ with $D \gg \Delta$. The first step is to consider the scattering problem for a frozen impurity (no spin-flip term). Suppose the impurity spin is down, then the spin up electrons will feel an attractive potential $-J_Z/4$, whereas the spin down a repulsive one $+J_Z/4$. We will shortly define the potential V , including both possibilities $V = \pm J_Z/4$. The variation of the DOS for a single spin species due to the impurity is

$$\Delta\rho(\epsilon) = -\frac{1}{\pi} \frac{\partial}{\partial \epsilon} \text{Arg} \ln(1 - VG(\epsilon)).$$

We define $\Gamma(\epsilon) = 1 - VG(\epsilon)$. $G(z)$ is the unperturbed local Green's function depending on the complex frequency z ,

$$G(z) = -2\rho(z + \Delta) \int_0^D d\omega \frac{1}{\omega^2 - z^2 + \Delta^2},$$

while $G(\epsilon) = G(z = \epsilon + i0^+)$. We hereafter take $\Delta > 0$, which actually corresponds to the case in which at the impurity site the staggered potential is $+ > 0$. We find that

$$(1) \quad \epsilon^2 < \Delta^2;$$

$$G(\epsilon) = -2\rho \frac{\epsilon + \Delta}{\sqrt{\Delta^2 - \epsilon^2}} \tan^{-1} \frac{D}{\sqrt{\Delta^2 - \epsilon^2}} \\ \simeq -\pi\rho \frac{\epsilon + \Delta}{\sqrt{\Delta^2 - \epsilon^2}}.$$

In the second line we took the $D \rightarrow \infty$ limit. In this case

$$\Gamma(\epsilon) = 1 + \pi\rho V \sqrt{\frac{\Delta + \epsilon}{\Delta - \epsilon}}.$$

If $V > 0$, then $\Gamma(\epsilon) > 0 \forall \epsilon \in [-\Delta, \Delta]$. If $V < 0$, then $\Gamma(\epsilon) > 0$ for $\epsilon \in [-\Delta, \epsilon_*]$, it changes sign at ϵ_* , and $\Gamma(\epsilon) < 0$ for $\epsilon \in [\epsilon_*, \Delta]$. Here

$$\epsilon_* = \Delta \frac{1 - (\pi\rho V)^2}{1 + (\pi\rho V)^2}.$$

In vicinity of ϵ_* , $\Gamma(\epsilon) = -(\epsilon - \epsilon_*)/ \dots$

The self-dual point is actually identified by⁷⁶

$$(\pi\rho V)^2 = 1,$$

so that $\epsilon^* = 0$. It corresponds to a genuine bound state just in the centre of the gap.

$$(2) \quad \epsilon^2 < D^2 + \Delta^2;$$

$$G(\epsilon) = -i\pi\rho \operatorname{sign}(\epsilon) \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}} + \rho \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}} \ln \frac{D + \sqrt{\epsilon^2 - \Delta^2}}{D - \sqrt{\epsilon^2 - \Delta^2}}.$$

It follows that

$$\begin{aligned} \operatorname{Re} \Gamma(\epsilon) &= 1 - V\rho \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}} \ln \frac{D + \sqrt{\epsilon^2 - \Delta^2}}{D - \sqrt{\epsilon^2 - \Delta^2}}, \\ \operatorname{Im} \Gamma(\epsilon) &= \pi\rho V \operatorname{sign}(\epsilon) \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}}. \end{aligned}$$

$$(3) \quad \epsilon^2 > D^2 + \Delta^2;$$

$$G(\epsilon) = \rho \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}} \ln \frac{\sqrt{\epsilon^2 - \Delta^2} + D}{\sqrt{\epsilon^2 - \Delta^2} - D}.$$

Then $\operatorname{Im} \Gamma(\epsilon) = 0$, while

$$\operatorname{Re} \Gamma(\epsilon) = 1 - V \frac{\epsilon + \Delta}{\sqrt{\epsilon^2 - \Delta^2}} \ln \frac{\sqrt{\epsilon^2 - \Delta^2} + D}{\sqrt{\epsilon^2 - \Delta^2} - D}.$$

It follows that, if $D \gg \Delta$ and $\epsilon^2 \ll D^2$,

$$\Gamma(\epsilon) = \begin{cases} 1 + \pi\rho V \sqrt{\frac{\Delta + \epsilon}{\Delta - \epsilon}} & \epsilon^2 < \Delta^2 \\ 1 + i\pi\rho V \operatorname{sign}(\epsilon) \sqrt{\frac{\epsilon + \Delta}{\epsilon - \Delta}} & \Delta^2 < \epsilon^2 \ll D^2 \end{cases}$$

At the self-dual point $\pi\rho V = \operatorname{sign}(V)$, thus we rewrite the above as

$$\Gamma(\epsilon) = \begin{cases} 1 + \operatorname{sign}(V) \sqrt{\frac{\Delta + \epsilon}{\Delta - \epsilon}} & \epsilon^2 < \Delta^2 \\ 1 + i\operatorname{sign}(V) \operatorname{sign}(\epsilon) \sqrt{\frac{\epsilon + \Delta}{\epsilon - \Delta}} & \Delta^2 < \epsilon^2 \ll D^2 \end{cases}$$

The retarded local Green's function reads

$$\mathcal{G}_R(\epsilon) = \frac{G(\epsilon)}{\Gamma(\epsilon)}.$$

In the limit of very large bandwidth so that $\epsilon^2 \ll D^2$ we find for $\epsilon^2 < \Delta^2$

$$\mathcal{G}_R(\epsilon) = -\pi\rho \frac{\sqrt{\Delta+\epsilon}}{\sqrt{\Delta-\epsilon} + \pi\rho V \sqrt{\Delta+\epsilon}}.$$

For $V < 0$, at the self-dual point with $\epsilon^* = 0$, its DOS has a mid-gap bound state

$$\mathcal{A}(\epsilon) = -\frac{1}{\pi} \text{Im} \mathcal{G}(\epsilon) = \pi\rho \Delta \delta(\epsilon).$$

The scattering phase shift is defined as

$$\delta_V(\epsilon) = \arg[\Gamma(\epsilon)] \quad (15)$$

which implies in this case

$$\tan \delta_V(\epsilon) = \text{sign}(V) \sqrt{\frac{\epsilon+\Delta}{\epsilon-\Delta}}.$$

Indeed, if $\epsilon = 0$ or $\epsilon^2 \gg \Delta^2$ we recover the value at the self-dual point

$$\delta_V(\epsilon) = \text{sign}(V) \frac{\pi}{4}.$$

On the contrary, if $\epsilon^2 \rightarrow \Delta^2$, we find that for $V > 0$

$$\delta_V(\epsilon \rightarrow \Delta) = \frac{\pi}{2}, \quad \delta_V(\epsilon \rightarrow -\Delta) = 0.$$

Indeed, for any $\eta > 0$

$$\delta_+(\Delta + \eta) = \frac{\pi}{2} - \delta_+(-\Delta - \eta).$$

We now include in the consideration also the transverse exchange

$$H_{\perp} = \frac{J_{\perp}}{2} \sum_{a=1,2} \left(S^- \Psi_{a\uparrow}^{\dagger}(0) \Psi_{a\downarrow}(0) + \text{H. c.} \right),$$

where

$$\Psi_{\sigma}(0) = \sum_{\epsilon} \psi_{\epsilon\sigma}(0) c_{\epsilon\sigma},$$

with $\psi_\epsilon(0)$ the amplitude of the eigenfunction of energy ϵ at the impurity site. In particular, at the self-dual point the bound state $c_{\epsilon=0\sigma} \equiv d_\sigma$ has

$$\psi_0(0) = \sqrt{\rho\Delta},$$

so that, if the impurity is down,

$$\begin{aligned}\Psi_\uparrow(0) &= \sqrt{\rho\Delta} d_\uparrow + \sum_{\epsilon^2 > \Delta^2} \psi_{\epsilon\uparrow}(0) c_{\epsilon\uparrow}, \\ \Psi_\downarrow(0) &= \sum_{\epsilon^2 > \Delta^2} \psi_{\epsilon\downarrow}(0) c_{\epsilon\downarrow},\end{aligned}$$

while if the impurity is up,

$$\begin{aligned}\Psi_\uparrow(0) &= \sum_{\epsilon^2 > \Delta^2} \psi_{\epsilon\downarrow}(0) c_{\epsilon\uparrow}, \\ \Psi_\downarrow(0) &= \sqrt{\rho\Delta} d_\downarrow + \sum_{\epsilon^2 > \Delta^2} \psi_{\epsilon\uparrow}(0) c_{\epsilon\downarrow}.\end{aligned}$$

Suppose we just consider the contribution to the spin-flip of the bound state, namely within the subspace of the four states

$$\begin{aligned}|a, \downarrow\rangle &= |\downarrow\rangle \times d_{a\uparrow}^\dagger |\Phi_\downarrow\rangle, \\ |a, \uparrow\rangle &= |\uparrow\rangle \times d_{a\downarrow}^\dagger |\Phi_\uparrow\rangle,\end{aligned}$$

where $|\Phi_\sigma\rangle$ is the Slater determinant where the valence band is fully occupied and the conduction one empty, which depends on the impurity spin since the single particle wavefunctions have different phase shifts. One trivially finds that

$$\langle a, \downarrow | H_\perp | a, \uparrow \rangle = \frac{J_\perp}{2} \rho \Delta \langle \Phi_\downarrow | \Phi_\uparrow \rangle,$$

where the overlap

$$\begin{aligned}\langle \Phi_\downarrow | \Phi_\uparrow \rangle &\sim \exp \left[-\frac{8}{\pi^2} \int_{-\Delta}^{\Delta} d\epsilon d\epsilon' \frac{\delta(\epsilon) \delta(\epsilon')}{(\epsilon + \epsilon')^2} \right] \\ &\simeq \sqrt{\frac{\Delta}{D}},\end{aligned}$$

which does not vanish despite the orthogonality catastrophe because the gap cuts off the singularity. Therefore the antisymmetric combination of the two states, which is a spin singlet but doubly degenerate since the bound state is occupied in one channel but empty in the other, has energy lower by $E \sim J_\perp (\rho)^{3/2}$ than the states where the bound state is occupied in each channel or when they are not occupied at all, both states being actually degenerate. Evidently this is just the first order in perturbation theory. One needs higher

order terms. In the spirit of Ref. 75, see also Ref. 44, the spin-flip grows by integrating out the high-energy degrees of freedom and asymptotically its dimension lowers to 1/2. However, in the presence of a gap, one cannot push the renormalisation down to zero frequency but must stop at an energy of the order of Δ . We thus expect that the net effect is an upward renormalisation of $J_{\perp}$:

$$J_{\perp} \rightarrow J_{\perp*} \sim \frac{J_{\perp}}{\sqrt{\rho\Delta}},$$

so that the energy of the aforementioned doubly degenerate singlet changes into

$$\Delta E_* \sim -\frac{J_{\perp}}{2} \rho \Delta,$$

followed by the $S = 1/2$ states in which each channel has the bound state either empty or occupied, at energy 0, and by the doubly degenerate triplet at energy $-\Delta E_*$. If the model is spin isotropic, $J_{\perp} = J_z = J$, and the Kondo exchange is at the dual point

$$\pi \rho \frac{J}{4} = 1,$$

then

$$\Delta E_* \simeq -\frac{2}{\pi} \Delta \simeq -0.63662 \Delta.$$

In other words, within such very rough approximation the ground state is indeed the even/odd spin singlet with charge $Q = 1$, followed at energy $\simeq 0.63662 \Delta$ by two $S = 1/2$ states with charge $Q = 0$ or $Q = 2$. Above energy Δ the continuum starts.

The sub-gap many-particle states computed with the NRG for the 2CK with $g = 0.25$ and $D = 10^{-6}$ are tabulated in Table II.

VIII Conclusion

We speculate that impurity models with Kondo overscreening generically flow in the small-gap limit to fixed points with characteristic persistent bound states of NFL character. More generally, let us imagine to add the mass term first at the impurity site. This term does not correspond to any of the relevant boundary operators at the NFL fixed point, nevertheless it lowers the symmetry and allows for a marginal boundary operator. If this is the case, we argue that an arbitrarily weak mass term of that kind added at the impurity site as well as in the bulk will induce sub-gap states with universal ratios.

The predicted universal spectra could be tested in experimental setups involving semiconductor nanowire quantum dots coupled to superconducting electrodes. Such setups have been refined in recent years due to the search for Majorana zero-modes which are

predicated to occur in such systems. One possibility would be building a mesoscopic superconducting island serving the same role as the ‘metallic grain’ in the setup in Refs. 35 and 36.

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Figure 1.

(a) Sub-gap many-particle states in the two-channel Kondo (2CK) model with fixed gap as a function of $g = \rho_0 J$. The energies are given with respect to the ground-state energy. (b) Eigenstates in the zero-bandwidth limit. (c) Approach toward the asymptotic universal spectrum in the zero-gap limit.

Figure 2.

Sub-gap $S = 1/2$ many-particle states in the two-channel Kondo (2CK) model for a range of Δ/D forming a geometric sequence with ratio $\sqrt{10}$.

Figure 3. Renormalization flow diagram with different scalings of the energy axis for the two-channel Kondo (2CK) model. N is the iteration number and $\Lambda = 2$ is the NRG discretization parameter.

Figure 4. Sub-gap many-particle states in the three-channel Kondo (3CK) models with (a) $S = 1/2$ and (b) $S = 1$. Here $\Lambda = 5$.

Figure 5. Temperature dependence of (a) impurity magnetic susceptibility and (b) impurity entropy in the two-channel Kondo (2CK) model.

Figure 6.

Channel symmetry breaking, $J_1 \neq J_2$, in the two-channel Kondo (2CK) model. (a) Evolution of the sub-gap states vs. J ; the cross-over point $T^* \sim \Delta$ occurs for $J \approx 10^{-3}$. (b) Impurity spectral function (Im part of T -matrix) for a range of J .

Table I

Energy levels of the two-channel Kondo (2CK) model upon including a local ϵ term on the first site of the Wilson chain. The small deviation from exact values in the progression $0, 1/8, 1/2, 5/8, \dots$ at $\epsilon = 0$ is a discretization effect.

Q	S	P	deg	$\epsilon(0)$	$\epsilon(\infty)$
0	1/2	even	2	0	0
-1	0	even,odd	2	0.125	0.1206
1	0	even,odd	2	0.125	0.1290
-2	1/2	odd	2	0.498	0.4897
0	1/2	2×odd,even	6	0.498	0.4980
2	1/2	odd	2	0.498	0.5063
-1	1	even,odd	6	0.621	0.6165
1	1	even,odd	6	0.621	0.6247

Table II

Quantum numbers and the energies of the lowest-lying many-particle states in the two-channel Kondo model with $g = 0.25$ and $\hbar/D = 10^{-6}$

Q	S	P	$E/$
1	0	odd	0
1	0	even	0
2	1/2	even	0.59
0	1/2	odd	0.60