Supplemental Material for “Long-range entanglement near a Kondo-destruction quantum critical point”

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This document summarizes technical methods and presents results beyond those contained in the main paper. Section I analyzes the Wilson chain—the discretized representation of the conduction band used in numerical renormalization-group (NRG) calculations—in the absence of any impurity degree of freedom. Data are presented for the dependence of the entanglement entropy \( S_e \) on the overall chain length, the position of the cut across which the entanglement is computed, the exponent \( r \) entering the density of states

\[
\rho(\varepsilon) = \rho_0 |\varepsilon|^r \Theta(D - |\varepsilon|), \tag{S1}
\]

and the NRG discretization parameter \( \Lambda \). Section II addresses the many-body Kondo problem created by coupling a Wilson chain to a spin-\( \frac{1}{2} \) impurity. A description of the method that we use to calculate the entanglement entropy is followed by details of the entanglement results presented in the main text.

I. ENTANGLEMENT WITHIN THE WILSON CHAIN

This section focuses on the entanglement properties of isolated Wilson chains (without any coupling to an impurity degree of freedom). The quantity of interest is the entanglement entropy \( S_e(L) \) for a chain of length \( N \) sites that is split into subsystem \( A \) comprising sites 0 through \( L - 1 \) and subsystem \( B \) containing sites \( L \) through \( N - 1 \) [1]. Although the notation suggests that \( S_e \) is a function of \( L \) alone, it must be emphasized that in fact it also depends on \( N \), \( r \), and \( \Lambda \).

A. The Wilson chain

The NRG method [2, 3] uses a discretization parameter \( \Lambda > 1 \) to divide a conduction band having single-particle energies \( \varepsilon \) ranging from \( -D \) to \( D \) into an infinite set of logarithmic bins spanning \( D\lambda^{-(m+1)} < \varepsilon \leq D\lambda^{-m} \) for \( m = 0, 1, 2, \ldots \). Within each bin, the band is approximated by a single representative state, namely, the linear combination of the original band states that couples to the impurity. The band Hamiltonian is then mapped via the Lanczos method onto a tight-binding Hamiltonian for a semi-infinite “Wilson chain” of sites labeled \( n = 0, 1, 2, \ldots \), coupled to the impurity via site 0 only:

\[
H \rightarrow H_{\text{imp}} \left[ f_{0\sigma}, f^\dagger_{0\sigma} \right] + \sum_{n=1}^{\infty} t_n \left( f^\dagger_{n\sigma} f_{n-1,\sigma} + \text{H.c.} \right), \tag{S2}
\]

where \( t_n \sim D\lambda^{-n/2} \) for \( n \gg 1 \) [4]. The reader is referred to Ref. 5 for details of the calculation of the coefficients \( t_n \) and their large-\( n \) asymptotics for the power-law density of states specified in Eq. (S1).

The discretization-induced separation of energy scales \( t_n \) allows controlled approximation of the low-energy states of the full Hamiltonian \( H \) through iterative solution of finite-chain Hamiltonians

\[
H_M = H_{\text{imp}} \left[ f_{0\sigma}, f^\dagger_{0\sigma} \right] + H_{M}^{\text{chain}}, \tag{S3}
\]

\[
H_{M}^{\text{chain}} = \sum_{n=1}^{M-1} t_n \left( f^\dagger_{n\sigma} f_{n-1,\sigma} + \text{H.c.} \right), \tag{S4}
\]

with \( M = 1, 2, \ldots, N \). Here, \( N \) is chosen to be sufficiently large that \( t_N \) (the largest energy scale of the part of the semi-infinite chain that is omitted from \( H_N \)) is much smaller than all energy scales of physical interest.

The Wilson chain hopping coefficients converge for \( \lambda \rightarrow 1 \) to those for the exact Lanczos mapping of the continuum (“\( \lambda = 1 \)” Kondo model. For example, in the case of a metallic density of states [Eq. (S1) with \( r = 0 \)], \( t_n \) decreases
monotonically from $t_1 \approx 0.57D$ toward $t_\infty = D/2$. The log-log plot in Fig. S1 reveals an exponential decay of $t_n/D - 1/2$ with increasing $n$. This pattern distinguishes the exact tight-binding formulation of the Kondo model from a standard tight-binding (STB) chain corresponding to Eq. (S4) with $t_n = D/2$. The effect of this difference on the entanglement entropy will be discussed below. Figure S1 also plots $|t_n/D - 1/2|$ vs $n$ for the pseudogapped case $r = 0.2$. Here $t_n$ for $n$ odd (even) approaches $D/2$ from above (below).

**B. Calculation of the entanglement entropy**

The entanglement entropy of an isolated Wilson chain (without any impurity coupled to its end) can be computed within the NRG approach in the same manner as the corresponding quantity for the full Kondo problem (see Sec. II A). However, the quadratic nature of $H^\text{chain}_M$ allows use of a simpler method introduced in Ref. 6 to obtain the results presented in Sec. IC.

The formalism begins with a general fermionic tight-binding Hamiltonian

$$H = \sum_{m,n} t_{mn} c_m^\dagger c_n$$  \hspace{1cm} (S5)

having hopping $t_{mn}$ between sites $m$ and $n$ of a finite lattice. We split the system into subsystems $A$ and $B$, reserving labels $i$ and $j$ for sites within $A$. In any many-particle eigenstate $|\Psi\rangle$ of $H$, the single-particle correlation function for subsystem $A$ can be written

$$C_{ij} = \langle \Psi | c_i^\dagger c_j | \Psi \rangle = \text{Tr}_A (\rho_A c_i^\dagger c_j),$$  \hspace{1cm} (S6)

where $\rho_A = \text{Tr}_B (|\Psi\rangle \langle \Psi|)$ is the reduced density operator for subsystem $A$. Given the quadratic form of $H$, higher correlation functions within $A$ must factorize according to Wick’s theorem, and there must exist a Hermitian operator

$$\hat{H}_A = \sum_{i,j} \hat{H}_{ij} c_i^\dagger c_j$$  \hspace{1cm} (S7)

such that

$$\rho_A = Z_A^{-1} e^{-\hat{H}_A}, \hspace{1cm} Z_A = \text{Tr}_A (e^{-\hat{H}_A}).$$  \hspace{1cm} (S8)

The matrix $\hat{H}_{ij}$ has a set of eigenvalues $\tilde{\epsilon}_k$ and orthonormal eigenvectors $\mathbf{v}_k$ with components $v_{ik}$ that can be used to define new fermionic operators

$$a_k = \sum_i v_{ik}^* c_i \leftrightarrow c_i = \sum_k v_{ik} a_k$$  \hspace{1cm} (S9)
such that
\[ \mathcal{H}_A = \sum_k \tilde{\varepsilon}_k a_k^\dagger a_k, \quad \rho_A = Z_A^{-1} \exp \left( - \sum_k \tilde{\varepsilon}_k a_k^\dagger a_k \right), \quad Z_A = \prod_k (1 + e^{-\tilde{\varepsilon}_k}). \]  

(S10)

Substituting Eq. (S9) into Eq. (S7) yields
\[ \hat{H}_{ij} = \sum_k \tilde{\varepsilon}_k v_{ik} v_{jk}^\ast, \]  

(S11)

while substituting Eqs. (S8)–(S10) into Eq. (S6) gives
\[ C_{ij} = \sum_k \frac{v_{ik}^\ast v_{jk}}{e^{\tilde{\varepsilon}_k} + 1}. \]  

(S12)

Comparison of Eqs. (S11) and (S12) leads to the conclusion that matrices \( \hat{H} \) and \( C^T \) (the transpose of \( C \)) are diagonalized by the same similarity transformation. We therefore deduce that \( C^T \) (and hence \( C \)) has eigenvalues
\[ \gamma_k = \frac{1}{1 + e^{\tilde{\varepsilon}_k}} \quad \leftrightarrow \quad \tilde{\varepsilon}_k = \ln (1 - \gamma_k) - \ln \gamma_k. \]  

(S13)

The entanglement entropy for the partition of the system into subsystems \( A \) and \( B \) is
\[ S_e = -\text{Tr}_A(\rho_A \ln \rho_A) \]
\[ = \text{Tr}_A(\rho_A \ln Z_A) + \text{Tr}_A \left[ Z_A^{-1} \exp \left( - \sum_k \tilde{\varepsilon}_k a_k^\dagger a_k \right) \left( \sum_{k'} \tilde{\varepsilon}_{k'} a_{k'}^\dagger a_{k'} \right) \right] \]
\[ = \ln Z_A + \sum_k \frac{\tilde{\varepsilon}_k}{e^{\tilde{\varepsilon}_k} + 1} = \sum_k \ln (1 + e^{-\tilde{\varepsilon}_k}) + \sum_k \frac{\tilde{\varepsilon}_k}{e^{\tilde{\varepsilon}_k} + 1} \]
\[ = \sum_k \ln \left( 1 + \frac{\gamma_k}{1 - \gamma_k} \right) + \sum_k \gamma_k \left[ \ln (1 - \gamma_k) - \ln \gamma_k \right] \]
\[ = - \sum_k \left[ \gamma_k \ln \gamma_k + (1 - \gamma_k) \ln (1 - \gamma_k) \right]. \]  

(S14)

Equation (S14) provides a computationally fast and accurate method for calculating the entanglement of a spinless Wilson or STB chain from the eigenvalues of its single-particle correlation function. The entanglement entropy of a full (spin-\( \frac{1}{2} \)) Wilson or STB chain is twice that of its spinless counterpart.

C. Systematics of the Wilson chain entanglement entropy

The entanglement entropy of the Wilson chain exhibits even-odd alternation with increasing size \( L \) of partition \( A \). Such an alternation is present for a standard tight-binding chain, but it becomes more pronounced with increasing \( \Lambda > 1 \) and/or increasing \(|r|\). To filter out this alternation, which is a finite-size effect of little interest for our purposes, we consider a three-point average
\[ S_e^{\text{avg}}(L) = \frac{1}{4} \left[ S_e(L - 1) + 2S_e(L) + S_e(L + 1) \right]. \]  

(S15)

This section considers first the case of a metallic band with a density of states described by Eq. (S1) with \( r = 0 \). We identify a range of \( L \) values over which \( S_e^{\text{avg}} \) differs negligibly from the universal dependence exhibited by a standard tight-binding (STB) chain, and describe deviations found for small and large values of \( L \). We then turn to the effects of varying the band exponent \( r \) entering Eq. (S1).

Results for \( r = 0 \): Fig. S2(a) shows the average entanglement entropy \( S_e^{\text{avg}} \) vs partition length \( L \) for a representative case \( \Lambda = 1.04 \) and for spinless chains of various lengths \( N \) specified in the legend. \( S_e^{\text{avg}}(L) \) is almost (but not quite) symmetric with respect to reflection about \( L = N/2 \) and peaks very close to \( L = N/2 \). The value \( S_e^{\text{max}} \simeq S_e^{\text{avg}}(N/2) \) initially increases with increasing chain length \( N \), but eventually saturates as a wide plateau forms in \( S_e^{\text{avg}}(L) \). No such plateau is observed in the data for \( \Lambda = 1 \) and \( N = 1200 \) (plotted with dashed lines).
FIG. S2. Spinless Wilson chain entanglement entropy $S^\text{avg}_e$ vs partition size $L$ for a metallic density of states described by Eq. (S1) with $r = 0$. (a) Data for discretization parameter $\Lambda = 1.04$ with different chain lengths $N$ (solid lines), and for $\Lambda = 1$, $N = 1200$ (dashed line). (b) Data for $N = 600$ with different values of $\Lambda$ (solid lines). Also shown (dashed line) is $S^\text{avg}_e$ vs partition size $L$ for a 600-site standard tight-binding (STB) chain. (c) Data from (b) replotted vs $\log L$. (d) Data for $N = 600$, $\Lambda = 1.04$ showing the definition of a partition size $L_A$ characterizing the crossover from a regime $S^\text{avg}_e \sim \log L$ for $L \ll L_A$ (red dashed line) to a regime $S^\text{avg}_e \simeq S^\text{max}_e$ for $L \gg L_A$ (blue dashed line). Inset: $L_A$ (calculated for $N = 1200$) vs $\Lambda^{-1}$ is well approximated by $L_A = 2/\left(\Lambda - 1\right)$ (red line).

Figure S2(b) plots (solid lines) $S^\text{avg}_e$ vs $L$ for spinless chains of fixed length $N = 600$ and different values of the discretization parameter on the range $1 \leq \Lambda \leq 1.1$. Also shown (dashed line) are the corresponding data for a spinless STB chain with $t_n = D/2$. The STB curve is exactly symmetric about $L = N/2$, while those for Wilson chains are slightly asymmetric. Curves for $\Lambda > 1$ exhibit a plateau similar to that seen in Fig. S2(a). As $\Lambda$ is increased, the plateau value $S^\text{max}_e$ decreases and is reached at smaller values of $L$.

For the fermionic STB chain with constant hopping coefficients between nearest neighbors, the entanglement entropy in the limit $L \ll N$ is equal to that of a critical conformal field theory (CFT) [7]. For a finite system with open boundary conditions,

$$S^\text{avg}_e = \frac{c}{6} \ln \left( \frac{N}{\pi} \sin \frac{\pi L}{N} \right) + b \quad \text{for} \quad L \ll N/2,$$

where $c$ is the central charge of the CFT and $b$ the boundary entanglement. For a spinless chain, the left-moving and right-moving fermions each carry a charge of $c = 1/2$, so the chain overall is described by $c = 1$. Fig. S2(c) replots the data for $L \leq N/2$ from Fig. S2(b) as $S^\text{avg}_e$ vs $\log L$. The Wilson chain results (solid lines) can be well approximated by

$$S^\text{avg}_e = \begin{cases} 
\frac{c}{6} \ln L + b & \text{for} \quad 10 \lesssim L \leq L_A, \\
\frac{c}{6} \ln L_A + b = S^\text{max}_e & \text{for} \quad L_A \ll L \leq N/2.
\end{cases}$$  

(S17)
Here, $c$ and $b$ are independent of $\Lambda$ and, when extrapolated to the infinite-limit $1/N \to 0$, are numerically indistinguishable from their respective STB-chain values: $c = 1$ and $b \approx 0.478$. For $L \lesssim 10$, all Wilson-chain data coincide with one another but clearly differ from those for the STB chain (dashed line), while the STB and $\Lambda = 1$ Wilson chain entanglement entropies converge for $L \gg 10$. These observations are quite natural given that the Wilson-chain hoppings $t_n$ break translational symmetry but the $\Lambda = 1$ Wilson chain hopping coefficients converge with increasing $n$ to the STB values $t_n = D/2$ (see Fig. S1).

The scale $L_\Lambda$ is the focus of Fig. S2(d). The main panel shows how $L_\Lambda$ can be defined as the horizontal coordinate of the intercept between the small-$L$ and large-$L$ asymptotes defined in Eq. (S17), i.e., $L_\Lambda = \exp[(6/c)(S_{\text{max}} - b)]$. The inset of Fig. S2(d) plots the variation of $L_\Lambda$ with $\Lambda$ (data points), demonstrating that for $\Lambda \lesssim 1.1$, the scale is well-described by the empirical relation $L_\Lambda = 2/(\Lambda - 1)$ (line). NRG many-body calculations are typically performed using a discretization parameter on the range $1.5 \leq \Lambda \leq 3$ chosen to balance discretization errors against truncation errors. In all such cases, $L_\Lambda \approx 1$, so $S_{\text{avg}}^L(L) \approx S_{\text{max}}^{\text{STB}}$ is almost independent of $L$.

Results for $r \neq 0$: Figure S3 plots $S_{\text{avg}}^L$ vs $L$ (panel a) and vs log $L$ (panel b) for spinless chains of fixed length $N = 600$, for $\Lambda = 1$ (solid lines) and $\Lambda = 1.04$ (dashed lines), and for different values of the band exponent $r$ entering Eq. (S1) describing metallic ($r = 0$), pseudogapped ($r > 0$), and divergent ($r < 0$) densities of states. For $\Lambda = 1$, the main effect of increasing $|r|$ is a progressive increase in the asymmetry of $S_{\text{avg}}^L(L)$ about $L = N/2$. As $r$ increases (decreases) from zero, the peak in $S_{\text{avg}}^L(L)$ moves right (left) from $L \approx N/2$. For $10 \lesssim L \ll N/2$, the entanglement

![Fig. S3](image-url)  
**FIG. S3.** (a) $S_{\text{avg}}^L$ vs $L$ for spinless Wilson chains of length $N = 600$ with different band exponents $r$, for discretization parameters $\Lambda = 1.0$ (solid lines) and $\Lambda = 1.04$ (dashed lines). (b) Data for $L \leq N/2$ replotted on a logarithmic $L$ scale.

![Fig. S4](image-url)  
**FIG. S4.** Fitted coefficients $c$ and $b$ in Eq. (S17) for spinless Wilson chains with discretization $\Lambda = 1$ and band exponents $r = 0$, $0.2$, and $0.4$. (a) Log-log plot of $1 - c$ vs $1/N$, where $N$ is the chain length, showing apparent convergence to $c = 1$ for $1/N \to 0$. (b) $b$ vs $1/N$. Here, $c$ and $b$ are independent of $\Lambda$ and, when extrapolated to the infinite-size limit $1/N \to 0$, are numerically indistinguishable from their respective STB-chain values: $c = 1$ and $b \approx 0.478$. For $L \lesssim 10$, all Wilson-chain data coincide with one another but clearly differ from those for the STB chain (dashed line), while the STB and $\Lambda = 1$ Wilson chain entanglement entropies converge for $L \gg 10$. These observations are quite natural given that the Wilson-chain hoppings $t_n$ break translational symmetry but the $\Lambda = 1$ Wilson chain hopping coefficients converge with increasing $n$ to the STB values $t_n = D/2$ (see Fig. S1).

The scale $L_\Lambda$ is the focus of Fig. S2(d). The main panel shows how $L_\Lambda$ can be defined as the horizontal coordinate of the intercept between the small-$L$ and large-$L$ asymptotes defined in Eq. (S17), i.e., $L_\Lambda = \exp[(6/c)(S_{\text{max}}^{\text{STB}} - b)]$. The inset of Fig. S2(d) plots the variation of $L_\Lambda$ with $\Lambda$ (data points), demonstrating that for $\Lambda \lesssim 1.1$, the scale is well-described by the empirical relation $L_\Lambda = 2/(\Lambda - 1)$ (line). NRG many-body calculations are typically performed using a discretization parameter on the range $1.5 \leq \Lambda \leq 3$ chosen to balance discretization errors against truncation errors. In all such cases, $L_\Lambda \approx 1$, so $S_{\text{avg}}^L(L) \approx S_{\text{max}}^{\text{STB}}$ is almost independent of $L$.

Results for $r \neq 0$: Figure S3 plots $S_{\text{avg}}^L$ vs $L$ (panel a) and vs log $L$ (panel b) for spinless chains of fixed length $N = 600$, for $\Lambda = 1$ (solid lines) and $\Lambda = 1.04$ (dashed lines), and for different values of the band exponent $r$ entering Eq. (S1) describing metallic ($r = 0$), pseudogapped ($r > 0$), and divergent ($r < 0$) densities of states. For $\Lambda = 1$, the main effect of increasing $|r|$ is a progressive increase in the asymmetry of $S_{\text{avg}}^L(L)$ about $L = N/2$. As $r$ increases (decreases) from zero, the peak in $S_{\text{avg}}^L(L)$ moves right (left) from $L \approx N/2$. For $10 \lesssim L \ll N/2$, the entanglement
To calculate the entanglement entropy, we employ the full density-matrix NRG approach [8–10]. In order to explain our method, it is necessary first to briefly review aspects of the conventional NRG approach. If the impurity has \( d_i \) internal states (e.g., \( d_i = 2 \) for a spin \( S_{\text{imp}} = \frac{1}{2} \)) and each Wilson chain site has \( d \) possible states (e.g., \( d = 4 \) for the single, spinful conduction band considered in the present work), then \( H_M \) has a basis of dimension \( d_i d^M \). Due to the exponential growth of this dimension with increasing \( M \), starting at some NRG iteration \( M_0 \) (typically \( M_0 = 5 \)), the basis must be truncated to keep within acceptable bounds the computational time for setting up and diagonalizing a matrix representation of \( H_M \). The many-body eigenstates of \( H_M \) are divided into two sets: the high-energy states \( |l,M\rangle \), \( 1 \leq l \leq n_M^{\text{disc}} \) are discarded, and only the lowest-energy states \( |k,M\rangle \), \( 1 \leq k \leq n_M^{\text{kept}} \) are kept to set up the next Hamiltonian \( H_{M+1} \), which then has a truncated basis of dimension \( M^{\text{kept}}_M \equiv n^{\text{kept}}_{M+1} + n^{\text{disc}}_{M+1} \).

The full density-matrix NRG approach is constructed around a complete basis of dimension \( d_i d^N \) for the longest Wilson chain (corresponding to \( M = N \)). This basis, introduced by Anders and Schiller [11, 12], comprises all states of the form \( |l,e,M\rangle = |l,M\rangle \otimes |e,M\rangle \) where \( M \) ranges from \( M_0 \) (the lowest-numbered iteration at which any eigenstate is discarded) to \( N \) (the highest-numbered iteration, and one at which we formally classify every eigenstate as discarded). Here, \( |l,M\rangle \) is one of the many-body eigenstates discarded after iteration \( M \) and \( |e,M\rangle \), called an “environmental state,” is any one of \( d^{N-M} \) different possible simple products of basis states for Wilson chain sites \( M \) through \( N-1 \). For any \( M < N \), \( |l,e,M\rangle \) is not an eigenstate of \( H_N \) but the full density-matrix NRG relies on a key approximation that \( H_N|l,e,M\rangle \approx H_M|l,M\rangle = E_{l,M}|l,M\rangle \) (where all energies are measured relative to the ground state of \( H_N \)).

Within the complete basis, the thermal equilibrium density matrix for the entire system composed of the impurity and \( N \) Wilson chain sites is diagonal and can be written (after tracing out the environmental states)

\[
\rho = \begin{pmatrix}
\rho_{M_0} & 0 & 0 & 0 \\
0 & \rho_{M_0+1} & 0 & 0 \\
0 & 0 & \ddots & 0 \\
0 & 0 & 0 & \rho_N
\end{pmatrix},
\]

where \( \rho_{M_0} \) represents the density matrix of the impurity in its ground state.

### II. ENTANGLEMENT ENTROPY FOR THE PSEUDOGAP KONDO PROBLEM

#### A. Numerical renormalization-group calculation of entanglement entropy

TABLE S-I. Values of the coefficients \( c \) and \( b \) defined in Eq. (S17) for the spinless STB and for spinless Wilson chains with different band exponents \( r \). A number in parentheses denotes the estimated nonsystematic error in the last digit.

<table>
<thead>
<tr>
<th>chain</th>
<th>( c )</th>
<th>( b )</th>
</tr>
</thead>
<tbody>
<tr>
<td>STB</td>
<td>1.0000(2)</td>
<td>0.4780(7)</td>
</tr>
<tr>
<td>( r = 0 )</td>
<td>1.0000(1)</td>
<td>0.47856(5)</td>
</tr>
<tr>
<td>( r = 0.2 )</td>
<td>1.0000(1)</td>
<td>0.43288(4)</td>
</tr>
<tr>
<td>( r = 0.4 )</td>
<td>1.0000(1)</td>
<td>0.39500(5)</td>
</tr>
</tbody>
</table>

The entanglement entropy is still described by Eq. (S16), as can be seen from Fig. S3(b). For \( \Lambda = 1.04 \) (dashed lines in Fig. S3), the entanglement entropy for all \( r \) values remains consistent with Eq. (S17), where \( L_\Lambda \) is independent of \( r \) and the value of \( S_\text{ent}^{\text{max}} \) tracks the \( r \) dependence of \( b \), i.e., \( S_\text{ent}^{\text{max}}(r) - S_\text{ent}^{\text{max}}(0) \propto b(r) - b(0) \).

Figure S4 plots the variation with inverse chain length \( 1/N \) of the fitted values of \( c \) and \( b \) for \( \Lambda = 1 \) and \( r = 0, 0.2 \), and 0.4. Table S-I lists the result of extrapolating \( c \) and \( b \) to the long-chain limit \( 1/N \to 0 \), along with the corresponding values for the STB chain. To within numerical accuracy, the slope remains \( c = 1 \) independent of \( r \), as demonstrated by a log-log plot of \( 1 - c \) vs \( 1/N \) [Fig. S4(a)], whereas the boundary entanglement \( b \) decreases (increases) as \( r \) is increased (decreased) from zero [Figs. S3(b) and S4(b)].

A density of states of the form of Eq. (S1) describes free fermions in one spatial dimension having a dispersion \( \varepsilon \propto |k-k_F|^{1/(1+r)} \text{sgn} (k-k_F) \). It is therefore quite surprising that, apart from a nonuniversal boundary term \( b(r) \), the \( L \) dependence of \( S_\text{ent}^{\text{max}} \) for \( 10 \lesssim L \ll N/2 \) is the same for \( r = 0 \) (where the host system exhibits conformal invariance) and for \( r \neq 0 \) (where the space and time axes are manifestly inequivalent). At present we do not fully understand the physical origin of this result. However, it suggests that the pseudogap host could in fact possess a “hidden” conformal symmetry with a central charge \( c = 1 \) (each \( c = \frac{1}{2} \) each for left- and right-movers).
\( \rho_M \) is an \( n_M^{\text{disc}} \times n_M^{\text{disc}} \) diagonal matrix having matrix elements
\[
(\rho_M)_{ll'} = \sum_{e,e'} (l,e,M | l',e',M) = \sum_{e,e'} \delta_{l,l'} \delta_{e,e'} e^{-\beta E_{l,M}} / Z = \delta_{l,l'} d^{-M} e^{-\beta E_{l,M}} / Z,
\]
with \( \hat{\rho} = Z^{-1} \exp(-\beta H_N) \), \( Z = \text{Tr} \exp(-\beta H_N) = \sum_{M=M_0}^{N} \sum_{l} d^{N-M} e^{-\beta E_{l,M}} \), and \( \beta = 1/k_B T \).

We seek to calculate the von Neumann entanglement entropy \( S_e \) with respect to the partition of the system into subsystems \( A \) of the impurity and Wilson chain sites \( n = 0, 1, \ldots, L-1 \) and a subsystem \( B \) made up of the remainder of the Wilson chain; see Fig. 1(b) of the main text. Tracing out the degrees of freedom in subsystem \( A \) results in the reduced density matrix
\[
\rho_A = \text{Tr}_B(\rho) = \left( \begin{array}{ccc} \rho_{M_0} & 0 & 0 \\ 0 & \rho_{M_0+1} & 0 \\ 0 & 0 & \rho_L \end{array} \right),
\]
where \( R^\text{red}_M \) is the partial reduced density matrix with elements \( R^\text{red}_M(k,k') \) indexed by states \( k \) and \( k' \) (not discarded) after iteration \( M \). \( R^\text{red}_M \) can be obtained from \( R^\text{red}_{M+1} \) via reverse iteration along the Wilson chain starting at \( M = N - 1 \), as detailed in Eq. (30) of Ref. 10. Diagonalization of \( R^\text{red}_L \) yields \( \lambda_{l,M} \) eigenvalues of \( \rho_A \) that can be combined with the values \( (\rho_M)_{ll'} \) for \( M_0 \leq M \leq L \) to construct the full set of eigenvalues \( \{\lambda_a\} \). Finally, one can compute the entanglement entropy
\[
S_e = -\text{Tr}_A(\rho_A \ln \rho_A) = -\sum_{a} \lambda_a \ln \lambda_a.
\]

To obtain the impurity contribution to the entanglement entropy, one subtracts from this \( S_e \) the entanglement of the isolated Wilson chain (computed in the manner described in Sec. I).

**B. Extraction of a characteristic temperature scale \( T^* \)**

Figure 4 of the main paper shows that for \( r > 0 \), the entanglement entropy in each phase (Kondo and local-moment) scales as a function of \( R/R^* \), where \( R^* = 1/(k_F T^*) \). For the purposes of this figure, we have extracted the characteristic scale \( T^* \) for any \( J \neq J_c \) from the temperature dependence of \( \chi_{\text{imp}}(T) \), the impurity contribution to the uniform magnetic susceptibility. We define \( 4T^* \) to be the temperature at which \( T_{\text{X} \text{imp}} \) reaches the midpoint between its critical value (the one that persists to \( T = 0 \) at \( J = J_c \)) and its zero-temperature limit [5] of 1/4 (for \( J < J_c \)) or \( r/8 \) (for \( J > J_c \)). This temperature is taken to be 4\( T^* \) (rather than \( T^* \), say) so that for \( r \to 0^+ \) where 4\( T^* \chi_{\text{imp}}(4T^*) \to 0.125 \), \( T^* \) smoothly approaches the metallic (\( r = 0 \) Kondo temperature, normally given the empirical definition \( T_K \chi_{\text{imp}}(T_K) = 0.0701 \) [13].

**C. Entanglement entropy as a function of Kondo coupling \( J \)**

The main paper presents results for \( S^\text{imp}_e(J,L) \), the smoothed (three-point-averaged) impurity contribution to the entanglement entropy as a function of the Wilson chain partition size \( L \ll N \) for different fixed Kondo couplings \( \rho_0 J \). Figure S6 instead plots \( S^\text{imp}_e \) vs \( \rho_0 J \) for the metallic case \( r = 0 \) with each data set representing a different fixed partition size \( L \). With increasing \( J \), each partition shows a monotonic decrease of \( S^\text{imp}_e \). For very weak Kondo couplings \( \rho_0 J \ll 1 \), the impurity spin is collectively screened by essentially the entire Wilson chain. The amount of screening that takes place within the first \( L \) sites of the Wilson becomes ever smaller as \( J \to 0^+ \), so the impurity’s entanglement with chain sites \( n \geq L \) approaches the full value \( \ln 2 \) for a spin singlet.

For the opposite limit \( \rho_0 J \gg 1 \), in the ground state of \( H_S \) given by Eqs. (S3) and (S4), the impurity is essentially locked into a spin singlet with the on-site combination of conduction electrons annihilated by the \( f_\sigma \) operator; chain sites \( 1, 2, \ldots, N-1 \) behave like a free Wilson chain partitioned into segments of length \( L-1 \) and \( N-L \). As a result, the impurity contribution to the entanglement entropy can be written \( S^\text{imp}_e(J,L,N) = S_e(J,L,N) - S^{(0)}_e(L,N) \simeq S^{(0)}_e(L-1,N-1) - S^{(0)}_e(L,N) \), where \( S^{(0)}_e \) is the entanglement entropy of a chain of length \( N \) partitioned into \( L \) and \( N-L \) sites. After making \( N \) very large and performing a three-point average, the smoothed impurity entanglement
FIG. S5. Extraction of the characteristic temperature scale $T^\ast$ from $\chi_{\text{imp}}(T)$, the impurity contribution to the uniform magnetic susceptibility. For each value of $J$, $4T^\ast$ is defined to be the temperature at which $T\chi_{\text{imp}}(T)$ (solid curves thin solid lines) reaches the midpoint (horizontal dashed line) between its $T \to 0$ limiting value for that $J$ (namely, $1/4$ for $J < J_c$, $r/8$ for $J > J_c$) and the corresponding limiting value for $J = J_c$ (solid line). Data shown are for band exponent $r = 0.4$ and $J = (1 \pm 10^x)J_c$ with the values of $x$ shown in the legend.

FIG. S6. Impurity entanglement entropy $S_{e,\text{imp}}$ vs dimensionless Kondo coupling $\rho_0J$ for band exponent $r = 0$, discretization parameter $\Lambda = 3$ and different partition sizes $L$. The inset shows the collapse of curves for different $L$ values when the data spanning $\rho_0J \leq 0.3$ are replotted as $S_{e,\text{imp}}$ vs $R/R_K$.

Entropy $S_{e,\text{imp}}(J, L)$ defined in the main paper is negative for $L \lesssim L_\Lambda$—over which range $S_{e,\text{imp}}(L, N \gg L/2)$ grows with increasing $L$—and rapidly approaches zero for $L \gtrsim L_\Lambda$. For the value $\Lambda = 3$ used to produce Fig. S6, $L_\Lambda \approx 1$ and negative $S_{e,\text{imp}}$ values are found only for $L \lesssim 3$.

As $L$ is increased, the crossover in $S_{e,\text{imp}}$ from $\ln 2$ toward zero takes place more sharply and centered around a smaller value of $\rho_0J$. This is another manifestation of the notion presented in the main text that $S_{e,\text{imp}}$ drops once the radius $R$ of subsystem $A$ exceeds the characteristic size $R_K$ of the Kondo screening cloud. The inset of Fig. S6 replots the data for $\rho_0J \leq 0.3$ as a function of $R/R_K$, where each $L$ curve corresponds to fixed value of $R = c\Lambda^{L/2}/k_F$ (with $k_F$ being the Fermi wave vectors and $c$ a constant of order unity) and points within a curve arise from a decrease with increasing $J$ of $R_K \sim 1/(k_F T_K)$.

Whereas in the main paper, the Kondo temperature $T_K$ was deduced from the impurity contribution to the magnetic susceptibility via the conventional definition $T\chi_{\text{imp}}(T_K) = 0.0701$ [13], in Fig. S6 we instead employed the perturbative definition [14]

$$k_B T_K \sim D \sqrt{\rho_0 J} \exp[-1/(\rho_0 J) + O(\rho_0 J)].$$

The collapse of all curves except those for $L = 1$ and 2 (which are anomalous for reasons discussed in the preceding
FIG. S7. Impurity entanglement at the quantum critical point and the Kondo fixed point: (a) Kondo fixed-point value of $S_{\text{imp}}^e$ (symbols) vs $\Lambda$ (on a log scale) for band exponent $r = 0.1$. A polynomial fit (solid line) is used to extrapolate $S_{\text{imp}}^e$ to the continuum limit $\Lambda = 1$. (b) Extrapolated $\Lambda = 1$ values of $S_{\text{imp}}^e$ at the critical point (squares) and at the Kondo fixed point (circles) vs band exponent $r$, along with a heuristic fit $S_{\text{imp}}^e = \frac{3}{2} r \ln 2$ (dashed line).

paragraph) is consistent with the existence of a universal scaling function $S_{\text{imp}}^e(J, R) = f_0(R/R_K)$, as also argued on the basis of the data presented in the main paper.

Similar behavior can be seen in plots (not shown) of $S_{\text{imp}}^e$ vs $\rho_0 J$ at fixed $L$ for pseudogapped hosts (i.e., $r > 0$). The data in each phase (Kondo or local-moment) can be collapsed by plotting $S_{\text{imp}}^e$ against $R/R^*$, where the crossover length scale $R^* = 1/k_F T^*$. While $T^*$ can be determined from $\chi_{\text{imp}}(T)$ via the operational procedure laid out in Sec. II B, for values of $J$ sufficiently close to $J_c$, good collapse can be achieved by instead using the asymptotic expression

$$T^* \propto |J - J_c|^\nu,$$

where the numerical value of the correlation length exponent $\nu$ has a nontrivial dependence on the band exponent $r$ [15].

D. Fixed-point entanglement entropy vs $r$

This section provides more details of the $r$ dependence of the impurity entanglement entropy at each renormalization-group fixed point, as well as the manner in which $S_{\text{imp}}^e$ approaches its value at each of the stable fixed points.

The results in the main paper show that, whereas $S_{\text{imp}}^e = 0$ at the weak-coupling fixed point, the impurity entanglement takes nontrivial, $r$-dependent values at the Kondo-destruction quantum critical point and at the Kondo fixed point. The fixed-point values of $S_{\text{imp}}^e$ can be obtained from many-body NRG calculations by taking the limit $R \ll R^*$ (for the unstable critical point) or $R \gg R^*$ (for the stable Kondo and local-moment fixed points). The Kondo fixed-point value of $S_{\text{imp}}^e$ can also be calculated using the single-particle method outlined in Sec. I B as the difference of $S_{\text{avg}}^e$ for a free Wilson chain with and without the first site frozen due to the formation of a local spin singlet with the magnetic impurity. That the many-body and single-particle approaches yield numerical values in excellent agreement provides a valuable check on the accuracy of the full NRG results.

In order to remove discretization effects, fixed-point values of $S_{\text{imp}}^e$ were calculated for values of $\Lambda$ between 1.01 and 3, then fitted with a polynomial function of $\ln \Lambda$, allowing extrapolation of $S_{\text{imp}}^e$ to the continuum limit $\Lambda = 1$, as illustrated in Fig. S7(a).

Extrapolated values of $S_{\text{imp}}^e$ are shown in Fig. S7(b). As $r$ increases from 0, the critical value of $S_{\text{imp}}^e$ decreases from $\ln 2$ while the Kondo fixed-point value increases almost linearly from 0. The two fixed-point values meet at $r = \frac{1}{2}$, the band exponent at which the quantum critical point merges with the Kondo fixed point. (No quantum critical point exists for $r > \frac{1}{2}$ [5].) A weak superlinear variation can be seen when the Kondo entanglement entropy is compared...
TABLE S-II. Values of the exponent $\alpha$ defined in Eq. (S24) for different band exponents $r$, as determined in the local-moment (LM) and Kondo (K) phases. A number in parentheses denotes the estimated nonsystematic error in the last digit. Values without error estimates are assumed rather than computed.

<table>
<thead>
<tr>
<th>$r$</th>
<th>$\alpha$(LM)</th>
<th>$\alpha$(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0</td>
<td>1.000(3)</td>
</tr>
<tr>
<td>0.2</td>
<td>0.38(3)</td>
<td>0.800(5)</td>
</tr>
<tr>
<td>0.25</td>
<td>0.58(5)</td>
<td>0.693(8)</td>
</tr>
<tr>
<td>0.3</td>
<td>0.750(4)</td>
<td>0.630(7)</td>
</tr>
<tr>
<td>0.33</td>
<td>0.79(4)</td>
<td>0.399(5)</td>
</tr>
<tr>
<td>0.4</td>
<td>0.89(5)</td>
<td>0.199(2)</td>
</tr>
<tr>
<td>0.5</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

FIG. S8. Values of the exponent $\alpha$ defined in Eq. (S24) for different band exponents $r$, as determined in the local-moment (LM, circles) and Kondo (K, squares) phases, along with lines showing the functions $\alpha = 2r$, $1 - r$, and $2(1 - 2r)$.

with a heuristic fit $S_{\text{imp}}^e = 3^2r \ln 2$ [dashed line in Fig. S7(b)]. This superlinear behavior is somewhat unexpected since thermodynamic properties at strong coupling have been shown to exhibit a strictly linear variation with $r$ [5].

Insets in Fig. 4 of the main paper demonstrate that $S_{\text{imp}}^e$ has a power-law-decaying tail in both the local-moment and Kondo phases, namely,

$$S_{\text{imp}}^e(J,R) - S_{\text{imp}}^e(J_c,\infty) \propto (R/R^*)^{-\alpha} \quad \text{for } R \gg R^*.$$  \hspace{1cm} \text{(S24)}

Fitted values of $\alpha$ are listed in Table S-II and plotted in Fig. S8. To within the estimated numerical uncertainty, the extracted exponents are consistent with $\alpha = 2r$ for $J < J_c$ and $\alpha = \min(1 - r, 2 - 4r)$ for $J > J_c$. These expressions coincide with twice the exponent of the leading irrelevant operator at the local-moment and Kondo fixed points, respectively; see Eqs. (4.7) and (4.10) in Ref. 5. This is consistent with the natural interpretation that the power-law tails are associated with the renormalization-group flow toward the stable fixed point in either phase, leading to the expectation that the exponent $\alpha$ is a characteristic of that fixed point.

It is probable that the departure of $S_{\text{imp}}^e$ from its value on the critical plateau is also described by a power-law behavior, i.e.,

$$S_{\text{imp}}^e(J,R) - S_{\text{imp}}^e(J_c,\infty) \propto (R/R^*)^{-\alpha'} \quad \text{for } R \ll R^*,$$  \hspace{1cm} \text{(S25)}

where one would expect $\alpha'$ to be positive and a characteristic property of the Kondo destruction critical point (and, hence, likely to have a nontrivial $r$ dependence). However, numerical uncertainty in the value of the critical value $S_{\text{imp}}^e(J_c,\infty)$ impedes reliable determination of $\alpha'$.

[1] For notational simplicity, in this section we drop the superscript “(0)” used elsewhere to distinguish the entanglement entropy of the isolated chain from its counterpart when site 0 of the chain is coupled to an impurity.
In the presence of particle-hole asymmetry [i.e., if it is not true that $\rho(\varepsilon) = \rho(-\varepsilon)$ for all $\varepsilon$], then the right-hand side of Eq. (S2) must be supplemented by on-site term $\sum_{n=0}^{N} \sum_{\sigma} \varepsilon_{n} f_{n\sigma}^\dagger f_{n\sigma}$, where $|\varepsilon_{n}|$ decays exponentially with $n$ for $n \gg 1$. 