Phase boundaries of the pseudogap Anderson and Kondo models

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We use the poor man’s scaling approach to study the phase boundaries of a pair of quantum impurity models featuring a power-law density of states $\rho(\omega) \propto |\omega|^r$ that gives rise to quantum phase transitions between local-moment and Kondo-screened phases. For the Anderson model with a pseudogap (i.e., $r > 0$), we find the phase boundary for (a) $0 < r < 1/2$, a range over which the model exhibits interacting quantum critical points both at and away from particle-hole symmetry, and (b) $r > 1$, where the phases are separated by first-order quantum phase transitions. For the particle-hole-symmetric Kondo model with easy-axis or easy-plane anisotropy of the spin exchange, the phase boundary and scaling trajectories are obtained for both $r > 0$ and $r < 0$ (the later case describing a density of states that diverges at the Fermi energy). Comparison with nonperturbative results from the numerical renormalization group shows that poor man’s scaling correctly describes the shape of phase boundaries expressed as functional relations between model parameters.

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I. INTRODUCTION

The Kondo problem—the question of how an impurity local moment becomes screened at low temperatures by the conduction electrons of a host metal—was highly influential in stimulating the development of theoretical and numerical methods for treating strongly correlated condensed matter [1]. Perturbative treatments of the spin-flip scattering between local and delocalized spins necessarily break down below a characteristic Kondo temperature scale, giving rise to a complex many-body problem. Nonetheless, much valuable understanding of the Kondo problem has come from perturbative renormalization-group (RG) [2, 3] and perturbative scaling approaches [4, 5] approaches. These were distilled into their simplest form in the poor man’s scaling of Anderson [5].

In poor man’s scaling, electron states far from the Fermi energy are progressively eliminated as the effective bandwidth is reduced with a compensating adjustment of a dimensionless measure of the effective impurity-band exchange coupling. The evolution of this coupling to ever larger values with decreasing bandwidth is suggestive of approach to a fully screened strong-coupling fixed point, although the scaling approach breaks down once the effective bandwidth drops below the order of the Kondo temperature. More sophisticated but generally less intuitive methods (the first historically being the numerical renormalization group or NRG [6]) were devised to confirm that the infra-red fixed point indeed corresponds to infinite exchange [1]. Poor man’s scaling was subsequently extended to the Anderson model with impurity Coulomb interaction $U = \infty$ [7, 8], and the $n$-channel Kondo model [9], where it correctly predicts the existence of a stable RG fixed point at an intermediate value of the exchange coupling that lies within the perturbative domain for $n > 2$.

More recently, there has been much interest in Kondo physics in settings where the band density of states has a power-law variation $\rho(\omega) \propto |\omega|^r$ in the vicinity of the Fermi energy $\omega = 0$. Pseudogapped or soft-gap systems described by band exponents $r > 0$ can be found in a variety of materials including heavy-fermion unconventional superconductors [10, 11], zero-gap bulk [12] and engineered [13] semiconductors, and various (quasi) two-dimensional systems like graphite [14, 15] and graphene [16]. Several theoretical techniques that have proved powerful for describing quantum impurities in metallic hosts, including Bethe ansatz, bosonization, and conformal field theory, cannot be applied for a power-law density of states. However, power-law variants of the Kondo impurity model and the corresponding Anderson model have been extensively studied using a variety of techniques including perturbative scaling [17, 21], large-$N$ approaches [17, 22, 23], the NRG [20, 26, 33], the perturbative RG [34, 35], and the local-moment approach [37, 39]. Due to the depletion of the conduction-band density of states near the Fermi energy, these pseudogap models feature a quantum phase transition [17] between a local-moment phase for weak impurity-band couplings, in which the impurity spin survives unscreened down to zero temperature, and a Kondo or strong-coupling phase in which the impurity spin undergoes complete or partial many-body screening (depending on the presence or absence of particle-hole symmetry) [29].

This paper addresses the question of how well poor man’s scaling captures the phase boundaries in quantum impurity problems that feature both (i) more than one independent coupling that flows under the reduction of
the effective bandwidth, and (ii) unstable critical points arising from competing flows in the multi-dimensional parameter space of effective couplings. To this end, we extend the poor man’s scaling approach to treat the Anderson model (for arbitrary on-site repulsion $U$) and the particle-hole-symmetric Kondo model with easy-axis or easy-plane anisotropy of the impurity-band exchange coupling. In each case, the scaling equations are valid for any density of states $\rho(\omega) \propto |\omega|^r$, whether $r$ is positive, negative, or zero. We obtain analytical expressions for the locations of phase boundaries for different regimes of the pseudogap ($r > 0$) Anderson and power-law ($r \neq 0$) anisotropic Kondo models. Comparison with nonperturbative NRG results shows that poor man’s scaling correctly reproduces the power-law relations between model parameters along the phase boundaries and generally also reproduce the boundaries with good quantitative accuracy.

The rest of the paper is organized as follows. Section II treats the Anderson model with a power-law density of states. Section IIIA defines the model and summarizes the phase diagram that has been established through previous work. The poor man’s scaling equations are derived in Sec. IIIB. Section IIIC compares analytic approximations for the phase boundary with NRG results for superlinear ($r > 1$) densities of states and various regimes of the other model parameters, while Sec. IIDD does the same for $0 < r < 1$. Limitations of the poor man’s scaling approach are identified in Sec. IIID. The anisotropic Kondo model is the subject of Sec. IIIE. Section IIIF presents the poor man’s scaling equations along with a preliminary analysis. Phase boundaries are analyzed for $0 < r < \frac{1}{2}$ and $-1 < r < 0$ in Secs. IIIB and IIIC respectively. Section IV contains a brief summary.

II. POWER-LAW ANDERSON MODEL

A. Model Hamiltonian

The Anderson impurity model is described by the Hamiltonian [40]

$$\hat{H}_A = \hat{H}_{\text{band}} + \hat{H}_{\text{imp}} + \hat{H}_{\text{hyb}},$$

(1)

where

$$\hat{H}_{\text{band}} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma},$$

(2)

with $\sigma = \pm 1$ (or $\sigma = \uparrow$, $\downarrow$) describes a noninteracting conduction band having dispersion $\epsilon_{\mathbf{k}}$;

$$\hat{H}_{\text{imp}} = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow},$$

(3)

with $\hat{n}_d = \hat{n}_{d\uparrow} + \hat{n}_{d\downarrow}$ and $\epsilon_d = \epsilon_{\mathbf{k}}|_{\mathbf{k} = \mathbf{0}}$ describes an impurity having level energy $\epsilon_d$ and on-site Coulomb interaction $U$; and the hybridization term

$$\hat{H}_{\text{hyb}} = \frac{1}{\sqrt{N_k}} \sum_{\mathbf{k}, \sigma} (V_k \hat{d}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} + \text{H.c.})$$

(4)

accounts for impurity-band tunneling. $N_k$ is the number of unit cells in the host metal and, hence, the number of inequivalent $\mathbf{k}$ values. Without loss of generality, we take the hybridization matrix element $V_k$ to be real and non-negative. For compactness of notation, we drop all factors of the reduced Planck constant $\hbar$, Boltzmann’s constant $k_B$, and the impurity magnetic moment $g\mu_B$.

A mapping to an energy representation where

$$\hat{H}_{\text{band}} = \sum_{\sigma} \int d\epsilon \epsilon \hat{c}_{\epsilon\sigma}^\dagger \hat{c}_{\epsilon\sigma},$$

(5)

$$\hat{H}_{\text{hyb}} = \sum_{\sigma} \int d\epsilon \sqrt{\Gamma(\epsilon)/\pi} (\epsilon \hat{c}_{\epsilon\sigma}^\dagger \hat{d}_{\sigma} + \text{H.c.}),$$

(6)

shows that the conduction-band dispersion $\epsilon_{\mathbf{k}}$ and the hybridization matrix element $V_k$ affect the impurity degrees of freedom only in combination through the hybridization function [41]

$$\Gamma(\epsilon) \equiv \frac{\pi}{N_k} \sum_k V_k^2 \delta(\epsilon - \epsilon_{\mathbf{k}}).$$

(7)

To focus on the most interesting physics of the model, we assume a simplified form

$$\Gamma(\epsilon) = \Gamma|\epsilon/D|^r \Theta(D - |\epsilon|),$$

(8)

where $\Theta(x)$ is the Heaviside function. The primary focus of this work is cases $r > 0$ in which the hybridization function exhibits a power-law pseudogap around the Fermi energy. We will also briefly discuss $r = 0$, representing a conventional metallic host.

One way that a hybridization function of the form of Eq. (8) can arise is from a purely local hybridization matrix element $V_k = V \geq 0$ combined with a density of states (per unit cell, per spin orientation) varying as

$$\rho(\epsilon) \equiv N_k^{-1} \sum_k \delta(\epsilon - \epsilon_{\mathbf{k}}) = \rho_0 |\epsilon/D|^r \Theta(D - |\epsilon|),$$

(9)

with $\rho_0 = (1 + r)/(2D)$, in which case $\Gamma = \pi \rho_0 V^2$. However, all results below apply equally to situations in which the $\mathbf{k}$ dependence of the hybridization contributes to the energy dependence of $\Gamma(\epsilon)$.

The assumption that $\Gamma(\epsilon)$ exhibits a pure power-law dependence over the entire width of the conduction band is a convenient idealization. More realistic hybridization functions in which the power-law variation is restricted to a region around the Fermi energy exhibit the same qualitative physics, with modification only of nonuniversal properties such as critical couplings and Kondo temperatures.

In the metallic ($r = 0$) Anderson model, any value $\Gamma > 0$ places the system in its strong-coupling phase, where the impurity degrees of freedom are completely quenched at absolute temperature $T = 0$. The situation for pseudogapped hybridization functions ($r > 0$) is much richer, as summarized in the phase diagrams shown in Fig. IV for cases $U > 0$ of onsite Coulomb repulsion.
The most notable feature is the existence within a region $-U < \varepsilon_d < 0$, $\Gamma < \Gamma_c(r, U, \varepsilon_d)$ of a local-moment (LM) phase within which the impurity retains an unquenched spin degree of freedom down to $T = 0$. There are also three different strong-coupling phases, distinguished by their ground-state electron number $Q$ (measured from half filling): a symmetric strong-coupling (SSC) phase with $Q = 0$, reached only for $0 < r < \frac{1}{2}$ under the condition $\varepsilon_d = -\frac{1}{2}U$ for strict particle-hole symmetry; and a pair of asymmetric strong-coupling phases $\text{ASC}_+$ and $\text{ASC}_-$ with $Q = 1$ and $Q = -1$, respectively. For a compact summary of the ground-state properties in each phase of the pseudogap Anderson impurity model and the nature of the quantum phase transitions separating those phases, the reader is referred to Sec. II B1 of Ref. [12].

\section*{B. Derivation of poor man’s equations}

This section presents a poor man’s scaling treatment of the Anderson Hamiltonian with a power-law hybridization function. Jefferson \cite{Jefferson1999} and Haldane \cite{Haldane1999} provided scaling treatments of the metallic case $r = 0$ valid in the limit $U \gg D$. These were subsequently extended to general values of $U$ (Ref. \cite{Haldane1999}), although the analysis neglected the renormalization of $U$. Reference \cite{Jefferson1999} presented scaling equations for the pseudogap case $r > 0$ with $U = \infty$. Below, the scaling analysis is generalized to arbitrary values of $r$ and $U$. Two of us have previously presented a similar poor man’s scaling analysis of the Anderson-Holstein impurity model with a power-law hybridization \cite{Kotliar1999}. The treatment of the Anderson model is somewhat simpler, and as we will see, the resulting scaling equations are amenable to approximate integration is several physically interesting limits.

We start with the Anderson Hamiltonian written in the form

$$\hat{H}_A' = \hat{H}_{\text{band}} + \hat{H}_{\text{imp}} + \hat{H}_{\text{hyb}},$$

where $\hat{H}_{\text{band}}$ and $\hat{H}_{\text{imp}}$ are as defined in Eqs. (2) and (3), respectively, but with $\hat{H}_{\text{hyb}}$ in Eq. (4) replaced by

$$\hat{H}_{\text{hyb}}' = \frac{1}{\sqrt{N_k}} \sum_{k,\sigma} \left\{ V_{0,k}(1 - \delta_{d,-\sigma}) + V_{1,k} \delta_{d,-\sigma} \right\} d^\dagger_{\tau,k\sigma} c_{\kappa\sigma} + \text{H.c.},$$

with hybridization functions

$$\Gamma_{\tau}(\varepsilon) = \frac{\pi}{N_k} \sum_k V_{\tau,k}^2 \delta(\varepsilon - \varepsilon_k) = \Gamma_{\tau}\varepsilon/D \Theta(D - |\varepsilon|)$$

for $\tau = 0, 1$ having the same power-law dependence as $\Gamma(\varepsilon)$ defined in Eq. (5). At the bare Hamiltonian level, one expects the hybridization $V_{0,k}$ between the empty and singly occupied impurity configurations to be identical to that $V_{1,k}$ between the singly occupied and doubly occupied impurity configurations. However, this degeneracy might be broken under the scaling procedure.

Following Haldane \cite{Haldane1999}, we focus on many-body states $|0\rangle$, $|\sigma\rangle = d^\dagger_{\tau,0}\rho_{\tau,0}|0\rangle$, and $|2\rangle = \sigma d^\dagger_{\tau,0}|0\rangle$ formed by combining the conduction-band ground state (having $N_k$ electrons of energy $\varepsilon_k < 0$) with one of the four possible configurations of the impurity level. Neglecting for the moment the effect of the hybridization ($\hat{H}_{\text{hyb}}'$), the energies of these states are denoted $E_0$, $E_1 = E_0 + \varepsilon_d$, and $E_2 = E_1 + \varepsilon_d + U = 2E_1 - E_0 + U$.

We now consider the effect of an infinitesimal reduction in the half-bandwidth from $D$ to $\tilde{D} = D + dD$, where $dD < 0$. The goal is to write a new Hamiltonian $\hat{H}_A''$ similar in form to $\hat{H}_A'$ but retaining only conduction-band degrees of freedom having energies $|\varepsilon_k| < \tilde{D}$ and with parameters $\varepsilon_d$, $\tilde{U}$, and $\tilde{V}_{\tau,k}$ adjusted to account perturbatively for the band-edge states that have been eliminated.

Let $K^+$ be the set of wave vectors $k$ describing particle-like states having energies $\tilde{D} < \varepsilon_k < D$, and $K^-$ be the set of wave vectors describing hole-like state with energies $-D < \varepsilon_k < -\tilde{D}$. Virtual tunneling of an electron from a $K^-$ state into the empty impurity level transforms the state $|0\rangle$ to

$$|\tilde{0}\rangle = |0\rangle + \sum_{\sigma} \frac{1}{\sqrt{N_k}} \sum_{k \in K^-} \frac{V_{0,k}}{|\varepsilon_k| + E_1 - E_0} \sigma c_{\kappa\sigma} |\sigma\rangle + O(V^2)$$

with energy

$$\tilde{E}_0 = E_0 - \frac{2}{N_k} \sum_{k \in K^-} |\varepsilon_k| + E_1 - E_0 + O(V^3)$$

$$\approx E_0 - \frac{|dD|}{2D\varepsilon_d} + O(V^3).$$
Here, \( O(V^n) \) schematically represents all processes involving a product of at least \( n \) factors \( V_{\tau,k} \). Similarly, virtual tunneling of an electron from the doubly occupied impurity level into a \( K^+ \) state transforms \( |2\rangle \) to

\[
|2\rangle = |2\rangle + \sum_{\sigma} \frac{\sigma}{\sqrt{N_k}} \sum_{k \in K^+} \frac{V_{1,k}}{\varepsilon_k + E_1 - E_2} c_{k,\sigma}^\dagger |\sigma\rangle + O(V^2)
\]

with energy

\[
\tilde{E}_2 = E_2 - \frac{2}{N_k} \sum_{k \in K^+} \frac{V_{1,k}^2}{\varepsilon_k + E_1 - E_2} + O(V^3)
\]

\[
\approx E_2 - \frac{|dD|}{\pi} \frac{2\tilde{\Gamma}_1(D)}{D - U - \varepsilon_d} + O(V^3).
\]

Finally, virtual tunneling of an electron into the singly occupied impurity from a \( K^- \) state or from the singly occupied level into a \( K^+ \) state transforms \( |\sigma\rangle \) to

\[
|\tilde{\sigma}\rangle = |\sigma\rangle - \frac{\sigma}{\sqrt{N_k}} \sum_{k \in K^-} \frac{V_{1,k}}{\varepsilon_k + E_2 - E_1} c_{k,-\sigma} + |2\rangle
\]

with energy

\[
\tilde{E}_1 = E_1 - \frac{1}{N_k} \sum_{k \in K^-} \frac{V_{1,k}^2}{\varepsilon_k + E_2 - E_1} + O(V^3)
\]

\[
\approx E_1 - \frac{|dD|}{\pi} \left[ \frac{\tilde{\Gamma}_1(-D)}{D + U + \varepsilon_d} + \frac{\tilde{\Gamma}_0(D)}{D - \varepsilon_d} \right] + O(V^3).
\]

The \( O(V^2) \) terms in each of the above states \( |\tilde{\sigma}\rangle \) include terms to enforce normalization, i.e., \( \langle \tilde{\phi}|\tilde{\phi}\rangle = \langle \phi|\phi\rangle = 1 \).

The modified energies can be used to define effective Hamiltonian parameters \( \varepsilon_d = \tilde{E}_1 - E_0 \) and \( \tilde{\tilde{U}} = \bar{E}_2 + \bar{E}_0 - 2\tilde{E}_1 \). At the same time, for each \( k \) in the retained portion of the band (i.e., satisfying \( |\varepsilon_k| < \tilde{D} \)), \( V_{0,k} \) must be replaced by

\[
\tilde{V}_{0,k} = \begin{cases} \sqrt{N_k} \langle 0|c_{k\sigma} \hat{H}_A|\tilde{\sigma}\rangle & \text{for } \varepsilon_k > 0 \\ -\sqrt{N_k} \langle \tilde{\sigma}|c_{k,\sigma}^\dagger \hat{H}_A^\dagger|0\rangle & \text{for } \varepsilon_k < 0 \end{cases}
\]

and \( V_{1,k} \) must be replaced by

\[
\tilde{V}_{1,k} = \begin{cases} -\sigma \sqrt{N_k} \langle \tilde{\sigma}|c_{k,-\sigma} \hat{H}_A^\dagger |2\rangle & \text{for } \varepsilon_k > 0 \\ \sigma \sqrt{N_k} \langle 2|c_{k,-\sigma}^\dagger \hat{H}_A |\tilde{\sigma}\rangle & \text{for } \varepsilon_k < 0 \end{cases}
\]

It is straightforward to show that

\[
\tilde{V}_{\tau,k} = V_{\tau,k} + O(V^3).
\]

The leading corrections to \( \tilde{V}_{\tau,k} \) involve numerous terms arising from the \( V^2 \) terms in the states \( |\tilde{\phi}\rangle \). Since these corrections are too small to be of much practical importance, we shall not evaluate them here.

The infinitesimal band-edge reduction described in the previous paragraphs can be carried out repeatedly to reduce the half-bandwidth by a finite amount from \( D \) to \( \tilde{D} < D \). Equations (14) and (15) indicate that during this process, the impurity level energy evolves according to the scaling equation

\[
\frac{d\tilde{\varepsilon}_d}{d\tilde{D}} = \frac{1}{\pi} \left[ \frac{\tilde{\Gamma}_{0,+}}{D - \varepsilon_d} - \frac{2\tilde{\Gamma}_{0,-}}{D + \varepsilon_d} + \frac{\tilde{\Gamma}_{1,-}}{D + U + \varepsilon_d} \right] + O(V^3),
\]

where \( \tilde{\Gamma}_{\tau,\pm} \) is the rescaled hybridization function at the reduced band edges \( \varepsilon = \pm \tilde{D} \). Taking into account Eq. (16), as well, one sees that the on-site repulsion follows

\[
\frac{d\tilde{U}}{d\tilde{D}} = \frac{2}{\pi} \left[ \frac{\tilde{\Gamma}_{0,+}}{D + \varepsilon_d} - \frac{\tilde{\Gamma}_{0,-}}{D - \varepsilon_d} - \frac{\tilde{\Gamma}_{1,-}}{D + U + \varepsilon_d} \right] + O(V^3).
\]

The band-edge values \( \tilde{\Gamma}_{\tau,\pm} \) of the hybridization functions \( \tilde{\Gamma}_{\tau}(\varepsilon) \) rescale both due to the replacement of \( D \) by \( \tilde{D} \) in Eq. (6) and due to the perturbative corrections to \( \tilde{V}_{\tau,k} \) in Eq. (21), leading to the scaling equation

\[
\frac{d\tilde{\Gamma}_{\tau,\pm}}{d\tilde{D}} = \gamma \tilde{\Gamma}_{\tau,\pm} + O(V^4).
\]

The scaling equations (22)–(24) have been derived to lowest order in nondegenerate perturbation theory, and are strictly valid only so long as \( |\tilde{D} \pm (\varepsilon_d + rU)| \gg \tilde{V}_{\tau,k} \) for each \( k \) such that \( \varepsilon_k = \pi \tilde{D} \).

Equation (24) shows that the band-edge values of the hybridization functions \( \tilde{\Gamma}_{\tau}(\varepsilon) \) are irrelevant (in the RG sense) for \( r > 0 \) and at most marginally relevant or marginally irrelevant for \( r = 0 \). For the particle-hole-symmetric bare hybridization functions considered in this work, it is an excellent approximation to set \( \tilde{\Gamma}_{0,\pm} = \tilde{\Gamma}_{1,\pm} = \tilde{\Gamma} \), leading to the simplified scaling equations

\[
\frac{d\tilde{\Gamma}}{d\tilde{D}} = \gamma \tilde{\Gamma},
\]

\[
\frac{d\tilde{\varepsilon}_d}{d\tilde{D}} \approx \frac{\tilde{\Gamma}}{\pi} \left[ \frac{1}{D - \varepsilon_d} - \frac{2}{D + \varepsilon_d} + \frac{1}{D + U + \varepsilon_d} \right],
\]

\[
\frac{d\tilde{U}}{d\tilde{D}} \approx \frac{2\tilde{\Gamma}}{\pi} \left[ \frac{1}{D + \varepsilon_d} - \frac{1}{D - \varepsilon_d} + \frac{1}{D - U - \varepsilon_d} - \frac{1}{D + U + \varepsilon_d} \right].
\]

Equations (25)–(27) with initial conditions \( \tilde{\varepsilon}_d = \varepsilon_d \), \( \tilde{U} = U \), and \( \tilde{\Gamma} = \Gamma \) represent the main results of this
section. The equations respect particle-hole symmetry in that
\[
\frac{d(\tilde{\varepsilon}_d + \frac{1}{2}\tilde{U})}{d\tilde{D}} \approx \frac{2\tilde{\Gamma}}{\pi} \frac{\tilde{\varepsilon}_d + \frac{1}{2}\tilde{U}}{(\tilde{D} - \frac{1}{2}\tilde{U})^2 - (\tilde{\varepsilon}_d + \frac{1}{2}\tilde{U})^2},
\]
so bare couplings satisfying \(\varepsilon_d = -\frac{1}{2}U\) inevitably lead to rescaled couplings that satisfy \(\tilde{\varepsilon}_d = -\frac{1}{2}\tilde{U}\). For \(r = 0\), Eqs. [25] to [27] reproduce the scaling equations for the metallic Anderson problem [1], while for \(r > 0\) in the limit \(U \to \infty\) of extreme particle-hole asymmetry, Eqs. [25] and [29] reduce to ones presented previously [19] for pseudogapped systems.

Equation [25] clearly has the solution
\[
\tilde{\Gamma} = (\tilde{D}/\tilde{D})^r \tilde{\Gamma}.
\]
Substituting this expression for \(\tilde{\Gamma}\) into Eqs. [26] and [27] creates a pair of coupled differential equations for \(\tilde{\varepsilon}_d\) and \(\tilde{U}\). Analytical or numerical integration of these differential equations allows one to follow the evolution of the rescaled couplings under reduction of \(\tilde{D}\) until one of the following conditions is met, signaling entry into a low-energy regime governed by a simpler effective model than the full pseudogap Anderson model:

1. If \(\tilde{\varepsilon}_d, \tilde{U} + 2\tilde{\varepsilon}_d > \tilde{D} > \tilde{\Gamma}\), the system enters the empty-impurity region of the ASC\_strong-coupling phase, in which the ground-state impurity occupancy approaches zero. In this case, \(T^* = \min(\tilde{\varepsilon}_d, \tilde{U} + 2\tilde{\varepsilon}_d)\) marks the crossover scale into a low-energy regime of (for \(r > 0\), generalized) Fermi-liquid behavior.

2. If \(-\tilde{U} + \tilde{\varepsilon}_d, -\tilde{U} + 2\tilde{\varepsilon}_d) > \tilde{D} > \tilde{\Gamma}\), the system enters the full-impurity region of the ASC\_strong-coupling phase, in which the ground-state impurity occupancy approaches two. Here, \(T^* = \min(-\tilde{U} + \tilde{\varepsilon}_d, -\tilde{U} + 2\tilde{\varepsilon}_d)\) marks crossover into the asymptotic Fermi-liquid regime.

3. If \(-\tilde{\varepsilon}_d, \tilde{U} + \tilde{\varepsilon}_d > \tilde{D} > \tilde{\Gamma}\), the system crosses over into an intermediate-energy local-moment regime. (This is distinct from the LM phase, in which an uncompensated spin-\(\frac{1}{2}\) degree of freedom survives at asymptotically low energies.) On entry to this regime, the empty and doubly occupied impurity configurations are effectively frozen out, and one can perform a generalization [29] of the Schrieffer-Wolff transformation [3] to map the pseudogap Anderson model to a pseudogap Kondo model.

\[
H_K = H_{\text{band}} + \frac{1}{N}\sum_{\kappa, \k', \sigma, \sigma'} C_{\kappa} \left[ \frac{J}{2} S_{\sigma' \sigma} + K \delta_{\sigma, \sigma'} \right] c_{\kappa' \sigma'},
\]
where \(H_{\text{band}}\) is as given in Eq. [2] with the power-law density of states specified in Eq. [9], \(\hat{S}\) is the spin-\(\frac{1}{2}\) operator for the impurity, \(\sigma\) is a vector of Pauli matrices, the (isotropic) exchange coupling \(J\) satisfies
\[
\rho_0 J = \frac{2\tilde{\Gamma}}{\pi} \left( \frac{1}{\varepsilon_d} + \frac{1}{\tilde{U} + \tilde{\varepsilon}_d} \right),
\]
and the potential scattering \(K\) satisfies
\[
\rho_0 K = \frac{\tilde{\Gamma}}{2\pi} \left( \frac{1}{\varepsilon_d} - \frac{1}{\tilde{U} + \tilde{\varepsilon}_d} \right).
\]
For metallic hosts (\(r = 0\)) the system always lies in the strong-coupling phase of the Kondo model, which constitutes another region of the strong-coupling phase of the Anderson model. In pseudogap cases, the asymptotic low-energy behavior depends on the values of \(J\) and \(K\): the system may lie in one of three Kondo phases that are associated with the SSC (for \(K = 0\)), ASC\_ (for \(K > 0\)), or ASC\_+ (for \(K < 0\)) phases of the Anderson model; or it may be fall in the LM phase of both the Kondo and Anderson models, in which the impurity retains a free two-fold spin degree of freedom down to absolute zero. In any of these cases, the energy scale \(T^*\) for crossover into the asymptotic low-energy regime is generally much smaller than the scale \(\min(-\varepsilon_d, \tilde{U} + \tilde{\varepsilon}_d)\) for entry into the local-moment regime. On approach to a strong-coupling ground state, \(T^*\) is just the Kondo temperature \(T_K\).

4. If \(\varepsilon_d, -\tilde{U} > \tilde{D} > \tilde{\Gamma}, \tilde{U} + 2\tilde{\varepsilon}_d\) (a situation that arises only if the bare \(U\) is negative), then the system enters the intermediate-energy local-charge regime. At this point, one can perform a generalized Schrieffer-Wolff transformation to a pseudogap charge-Kondo model. The system may lie in a strong-coupling phase of the charge-Kondo model (yet another region of an Anderson-model strong-coupling phase) or in the local-charge phase of both models, where the impurity retains a free two-fold charge degree of freedom down to absolute zero. Similarly to the situation in (3), \(T^* \ll \min(\varepsilon_d, -\tilde{U} + \tilde{\varepsilon}_d)\).

5. If \(\tilde{\Gamma} > \tilde{D} > |\varepsilon_d|\) and/or \(\tilde{\Gamma} > \tilde{D} > |\tilde{U} + \tilde{\varepsilon}_d|\), then the system enters a mixed-valence regime where the states \(|0\rangle, |\tilde{\sigma}\rangle\), and \(|2\rangle\) are no longer all well-defined. The scaling method is unable to determine whether further reduction of the effective half-bandwidth will bring the system into the mixed-valence regime of the strong-coupling phase or it will instead reach one or other of the phases with a residual localized degree of freedom [44].

In the remainder of Sec. II, we specialize to ranges of the band exponent \(r > 0\) and the bare parameters \(U\) (henceforth taken to be positive, representing on-site Coulomb repulsion), \(\varepsilon_d\), and \(\Gamma\) for which it possible to make analytical predictions for the location of boundaries between LM and strong-coupling phases. We compare these predictions with results obtained using the non-perturbative numerical renormalization group (NRG) method [35, 36], as adapted to treat systems containing a pseudogap density of states [28, 29]. Throughout the paper, we have used Wilson’s discretization parameter \(\Lambda = 3\) and kept up to 600 many body states after each iteration of the NRG.

C. Phase boundaries for \(r > 1\)

Analysis of band exponents in the range \(r > 1\) is simplified because Eq. [29] means that \(\tilde{\Gamma}/\tilde{D} = (\tilde{D}/\tilde{D})^{-1}(\Gamma/D)\) decreases monotonically under reduction of the half-bandwidth. In the physically most relevant regime \(\Gamma < D\), this decrease in \(\tilde{\Gamma}/\tilde{D}\) rules out the
possibility of entry into the mixed-valence regime under condition (5) of Sec. II B. Moreover, the decrease of $\Gamma$ is so rapid that any entry to the local-moment regime and subsequent mapping to the pseudogap Kondo problem \[via Eqs. (31) and (32)\] will yield a sub-critical exchange coupling \[29\].

Under these circumstances, the upper critical level energy $\tilde{\varepsilon}_d = \tilde{D}$ is satisfied at sufficiently low $\tilde{D}$) from the LM phase (in which one eventually reaches $\tilde{\varepsilon}_d = -\tilde{D}$) is effectively determined by the condition $\tilde{\varepsilon}_d(\tilde{D} = 0) = 0$ that places the fully renormalized impurity level precisely at the Fermi energy. This picture of the quantum phase transition as arising from a renormalized level crossing is consistent with the observation of first-order behavior for $r > 1$ \[31, 36\]. By particle-hole symmetry, the boundary between the LM and ASC$_-$ phases is at the lower critical level energy $\tilde{\varepsilon}_{d,c} = -U - \tilde{\varepsilon}_d$ [see Fig. 1(b)].

The aforementioned boundary between the LM and ASC$_-$ phases can be located by performing an approximate integration of Eqs. (26) and Eq. (27) using Eq. (29). For uniformity of presentation, we express our result in the form of a critical hybridization width $\Gamma_c(\tilde{U}, \tilde{\varepsilon}_d)$. We will consider bare parameters satisfying $0 < -\varepsilon_d \ll U$ and $-\varepsilon_d < 0$. The only exception occurs for a combination of bare parameters that places the system precisely on the boundary between the two phases, in which case $\tilde{\varepsilon}_d(\tilde{D} = 0) = 0$. Recalling that we are considering cases $r > 1$, Eq. (41) shows that the boundary location $\varepsilon_{d,c}(U, \Gamma)$ is primarily determined by initial phase of scaling $\tilde{D}_1 < \tilde{D}_2 < \tilde{D}$, and to leading order in $U/D$ and $\Gamma/D$ satisfies

\[ \tilde{\varepsilon}_{d,c} \simeq \varepsilon_d + \frac{\Gamma U}{(r-1)\pi D} \left[ \frac{1 - (\tilde{U}/\tilde{D})^{r-1}}{(r-1)\pi D} \right]. \]

In the case of present interest where $|\varepsilon_d| \ll U$, the level energy scales upward in absolute terms by one-quarter the amount that the on-site interaction scales down, but $\varepsilon_d$ experiences a much greater fractional shift than $U$.

Equations (33), (34), and (36) remain valid until $(\tilde{U} + \tilde{\varepsilon}_d)/\tilde{D}$ rises to approach unity, a condition that occurs for the assumed ordering of the bare parameters, and for the weak renormalization of $U$ that holds for $\Gamma \ll (r-1)D$ at $\tilde{D} = \tilde{D}_1 \simeq U$, at which point

\[ \tilde{\varepsilon}_{d,1} \equiv \tilde{\varepsilon}_d(\tilde{D}_1) \simeq \varepsilon_d + \frac{\Gamma U [1 - (U/D)^{r-1}]}{(r-1)\pi D}. \]  

In the regime $\tilde{D} < \tilde{D}_1$, the doubly occupied impurity configuration is essentially frozen out. Now Eq. (26) can be approximated by

\[ \frac{d\tilde{\varepsilon}_d}{d\tilde{D}} \simeq - \frac{\tilde{\Gamma}(\tilde{D} - 3\tilde{\varepsilon}_d)}{\pi D^2} = - \frac{\Gamma}{\pi D^2} (\tilde{D} - 3\tilde{\varepsilon}_d)^{r-2}, \]

which has the solution

\[ \tilde{\varepsilon}_d \simeq \tilde{\varepsilon}_{d,1} + \frac{\Gamma}{\pi D} \left[ \frac{D_1}{D} \right]^{r-1} \left[ 1 + O\left( \frac{\tilde{\varepsilon}_{d,1}}{U} \right) \right]. \]

Using Eq. (38), this gives

\[ \tilde{\varepsilon}_{d}(\tilde{D}) \simeq \tilde{\varepsilon}_{d,1} + \frac{\Gamma}{(r-1)\pi} \left[ \frac{U}{D} - \frac{1}{r} \left( \frac{U}{\tilde{D}} \right)^{r-1} - \frac{r-1}{r} \left( \frac{\tilde{D}}{\tilde{D}} \right) \right]. \]

A more careful treatment of scaling over the range of $\tilde{D}$ in which $|\tilde{D} - \tilde{U} - \tilde{\varepsilon}_d| \lesssim \tilde{\Gamma}$ [invalidating the nondegenerate perturbation theory used to derive Eqs. (25), (27)] would likely modify the numerical prefactor of $(U/D)\Gamma$ on the right-hand side of Eq. (41). With this caveat, the equation should capture the scaling of the impurity level energy until $|\varepsilon_d|/D$ grows to reach 1 at some reduced half-bandwidth $D_2$. For $\tilde{D} < \tilde{D}_2$, the system crosses over into the low-energy regime of the ASC$_-$ phase (for $\tilde{\varepsilon}_d > 0$) or that of the LM phase (for $\tilde{\varepsilon}_d < 0$). The only exception occurs for a combination of bare parameters that places the system precisely on the boundary between the two phases, in which case $\tilde{\varepsilon}_d(\tilde{D} = 0) = 0$. Recalling that we are considering cases $r > 1$, Eq. (41) shows that the boundary location $\varepsilon_{d,c}(U, \Gamma)$ is primarily determined by initial phase of scaling $\tilde{D}_1 < \tilde{D}_2 < \tilde{D}$, and to leading order in $U/D$ and $\Gamma/D$ satisfies

\[ \varepsilon_{d,c} \simeq \frac{\Gamma U}{(r-1)\pi D}. \]

This relation can be recast as

\[ \Gamma_c \simeq (r-1)\pi D |\varepsilon_d|/U \]

for $-U/2 \ll \varepsilon_d < 0$.

The phase boundary between the LM and ASC$_-$ phases at $\Gamma_c(U, \varepsilon_d)$ can be determined to the desired accuracy by performing successive NRG runs to refine the
value of $\Gamma_c$ using the method of bisection. At the end of
each run, the zero-temperature limit of $T_{\text{Ximp}}$ (tem-
perature times the impurity contribution to the static mag-
netic susceptibility) \cite{[17, 18]} is used to determine whether
the system is in the LM phase ($T_{\text{Ximp}} \rightarrow 1/4$) or in
the ASC\textsubscript{−} phase ($T_{\text{Ximp}} \rightarrow 0$), and thus to modify the range
of $\Gamma$ values within which $\Gamma_c$ must lie.

Figure 2 shows the critical hybridization width plotted as $\Gamma_c/|\varepsilon_d|$ vs
$U/D$, comparing NRG data (symbols) with the scaling predic-
tions of Eq. \eqref{eq:43} (dashed lines) and Eq. \eqref{eq:45} (dotted lines). Results are for $r = 1.1$ and 2 and for three values of $\varepsilon_d/U$
shown in the legend.

D. Phase boundaries for $0 < r < 1$

For $r < 1$, Eq. \eqref{eq:29} implies that $\tilde{\Gamma}/\tilde{D} = (D/\tilde{D})^{1-r}(\Gamma/D) \geq \Gamma/D$. The system flows to mixed
valence [under condition (5) in Sec. II B] at a reduced
half-bandwidth

$$\tilde{D}_r = \tilde{\Gamma}(\tilde{D}_r) = (\Gamma/D)^{1/(1-r)} D$$

providing that $|\tilde{\varepsilon}_d(\tilde{D}_r)|$ and $|\tilde{U}(\tilde{D}_r) + \tilde{\varepsilon}_d(\tilde{D}_r)|$ both remain
smaller than $\tilde{D}_r$. However, the system flows to a different
low-energy regime if $|\tilde{\varepsilon}_d(\tilde{D})|$ or $|\tilde{U} + \tilde{\varepsilon}_d(\tilde{D})|$ reaches 1 at
some $\tilde{D} > \tilde{D}_r$.

1. LM-SSC boundary for $\Gamma, U \ll D$

We first consider cases $\varepsilon_d = -\frac{1}{2}U$ where the system
exhibits strict particle-hole symmetry, and focus on the
universal (large-bandwidth) limit $\Gamma, U \ll D$.

So long as $\frac{1}{2}\tilde{U} \ll \tilde{D}$, Eq. \eqref{eq:27} can again be approxi-
mated by Eq. \eqref{eq:33}, which can be integrated to yield

$$\tilde{U}(\tilde{D}) \simeq U \exp\left(-\frac{4}{(1-r)\pi}\left(\frac{\tilde{\Gamma}}{\tilde{D}} - \frac{\Gamma}{D}\right)\right).$$

Eq. \eqref{eq:47} can be re-expressed as

$$\left(U/2D\right)^{1-r} \simeq \tilde{x} e^{-\gamma \tilde{x}}$$

in terms of new variables

$$\tilde{x}(\tilde{D}) = \left(\frac{U}{2D}\right)^{1-r} \exp\left(\frac{4\Gamma}{\pi D}\right) \geq x \equiv \tilde{x}(D)$$

and

$$\gamma = \frac{2D}{U} \left(\frac{4\Gamma}{\pi D}\right) \exp\left(-\frac{4\Gamma}{\pi D}\right)$$

2. LM-ASC\textsubscript{−} boundary for $0 < -\varepsilon_d, \Gamma \ll D \ll U$

If the bare parameters of the Anderson Hamiltonian
instead satisfy $U \gg D$, then Eq. \eqref{eq:39} applies from the
outset of scaling, and $\tilde{\varepsilon}_d$ satisfies Eq. \eqref{eq:40} with $\tilde{D}_1 = D$ and $\tilde{\varepsilon}_{d,1} = \varepsilon_d$, i.e.,

$$\tilde{\varepsilon}_d(\tilde{D}) \simeq \varepsilon_d + \frac{\Gamma}{r\pi} \left[1 - \left(\frac{\tilde{D}}{\tilde{D}}\right)^r\right].$$

Now the condition $\tilde{\varepsilon}_d(\tilde{D} = 0) = 0$ places the LM-ASC\textsubscript{−}
phase boundary at

$$\Gamma_c \simeq r\pi|\varepsilon_d|.$$
that allow Eq. (29) to be recast exactly in the form
\[ \tilde{\Gamma}/\tilde{D} = \frac{\pi}{4} \gamma \tilde{x}. \]

Equation (48) shows that with increasing \( \tilde{x} \) (or decreasing \( \tilde{D} \)), \( \tilde{U}/2\tilde{D} \) initially rises, before peaking at \( \tilde{x} = 1/\gamma \), and then dropping off exponentially for \( \tilde{x} \gg 1/\gamma \). The system will enter its local-moment regime [under condition (3) in Sec. II B] if there exists a reduced half-bandwidth \( \tilde{D}_U > \tilde{D}_I \) such that \( \tilde{U}(\tilde{D}_U)/2\tilde{D}_U = 1 \). The approximate scaling equation (42) is valid only so long as \( \tilde{U}/\tilde{D} \lesssim 1 \). Equation (27) predicts that \( \tilde{U} \) experiences a stronger downward renormalization once \( \tilde{U}/\tilde{D} \) approaches 2, a range in which the nondegenerate perturbation theory used to derive Eqs. (25)–(27) also begins to break down. However, in this range of \( \tilde{U}/\tilde{D} \), physically one expects renormalization to slow to a halt as charge fluctuations are progressively frozen out. Therefore, in the spirit of Haldane [8], we apply Eq. (48) all the way to the point where \( \tilde{U}(\tilde{D})/2\tilde{D} = 1 \), and we seek \( \tilde{x}_U \) defined to be the smallest solution of
\[ \tilde{x} e^{-\tilde{y} \tilde{x}} = 1. \]

For \( \tilde{y} > 1/e \), Eq. (52) has no real solution, so the system necessarily crosses over to mixed valence for \( \tilde{D} \lesssim \tilde{D}_I \). For \( 0 \leq \tilde{y} \leq 1/e \), by contrast, Eq. (52) has a solution \( \tilde{x}_U(\tilde{y}) \) satisfying \( 1 \leq \tilde{x}_U \leq e \leq \gamma^{-1} \). Since \( \gamma \tilde{x}_U < 1 \), Eq. (51) gives \( \tilde{\Gamma}(\tilde{D}_U) < \tilde{D}_U \), meaning that at \( \tilde{D} = \tilde{D}_U \) the system satisfies condition (3) for crossover into its local-moment regime. Equation (49) gives
\[ \frac{\tilde{U}}{\tilde{U}} = \frac{2\tilde{D}_U}{\tilde{U}} = \left[ \frac{\exp(4\Gamma/\pi\tilde{D})}{\tilde{x}_U(\gamma)} \right]^{1/(1-r)} \geq e^{-1/(1-r)}. \]

since \( \tilde{x}_U \lesssim e \). This implies, at least for \( r \ll 1/2 \), that the rescaled on-site interaction \( \tilde{U}(\tilde{D}_U) \) remains of the same order as \( \tilde{U} \).

A Schrieffer-Wolff transformation performed at \( \tilde{D} = \tilde{D}_U \) yields a pseudogap Kondo model with [Eqs. (31) and (32)]
\[ \rho_0 J = 8\tilde{\Gamma}(\tilde{D}_U)\frac{\pi}{\tilde{U}(\tilde{D}_U)} = \gamma \tilde{x}_U, \quad \rho_0 K = 0. \]

It is known that for \( \rho_0 K = 0 \), the critical exchange coupling \( J_c \), separating the Kondo \( (J > J_c) \) and LM \( (J < J_c) \) phases satisfies \( \rho_0 J_c = f(r) \) where \( f(r) \approx r(1+r/2) \) for \( r \ll 1/2 \) [Refs. 17 and 18] and \( f(r) \to \infty \) for \( r \to 1^- \) [Ref. 27]. Combining this information with Eq. (54), one arrives at the prediction that the boundary between the LM and SSC phases is determined by the condition \( \gamma_c \tilde{x}_U(\gamma_c) = f(r) \). Then, Eq. (52) gives \( \tilde{x}_U \equiv \tilde{x}_U(\gamma_c) = \exp[f(r)] \) and, hence, \( \gamma_c = f(r)/\tilde{x}_U = f(r)\exp[-f(r)] \). This means that the LM phase occupies the parameter range \( U > U_c(\Gamma) \), where
\[ U_c = 2D \left\{ \frac{\exp[f(r)]}{f(r)} \frac{4\Gamma}{\pi\tilde{D}} \exp\left[ -\frac{4\Gamma}{\pi\tilde{D}} \right] \right\}^{1/(1-r)}. \]

For \( \Gamma \ll D \), one can invert Eq. (55) to deduce that the LM phase occupies the parameter range \( \Gamma < \Gamma_c(U) \), with
\[ \Gamma_c \approx D \frac{\pi f(r)}{4\exp[f(r)]} \left( \frac{U}{2D} \right)^{1-r}. \]

If one were to neglect the rescaling of the on-site Coulomb interaction and set \( \tilde{D}_U = U/2 \) in Eq. (54), one would instead obtain an equation for \( \Gamma_c \) identical to Eq. (56) apart from the omission of the factor of \( \exp[-f(r)] \) from the right-hand side. Thus, the leading effect of many-body renormalization of the on-site Coulomb repulsion is the reduction of \( \Gamma_c \) by a factor that can be approximated as \( 1 + r \) for \( r \ll 1/2 \).

Figure 3 plots the ratio of the critical hybridization width \( \Gamma_c, \text{NRG} \) found using NRG to the scaling prediction \( \Gamma_c, \text{scal} \) given by Eq. (56). For band exponents \( r = 0.1, 0.2, \) and 0.3, we find that this ratio is well converged for \( U/\tilde{D} \lesssim 0.1 \) which implies that the scaling analysis correctly captures the \( U^{1-r} \) dependence of \( \Gamma_c \) at the LM-SSC phase boundary. The absolute value of \( \Gamma_c, \text{NRG}/\Gamma_c, \text{scal} \) falls as \( r \) decreases, and seems likely to approach unity as \( r \to 0^+ \). We infer that Eq. (56) describes the NRG results apart from a correction factor that depends solely on the band exponent \( r \).

Poor man’s scaling can not only find the LM-SSC phase boundary at \( \Gamma = \Gamma_c \), but can also locate a crossover within the SSC phase at \( \Gamma = \Gamma_{\text{MV}} \) between a Kondo regime, in which only the singly occupied impurity configurations have significant occupation at low temperatures, and a mixed-valence regime having significant ground-state occupancy of the empty and/or doubly occupied impurity configuration(s). We have seen [after Eq.
fore, the system exhibits fully developed Kondo physics for \( \tilde{T} \) temperature or mixed-valent limiting value corresponding to a free spin-cutoff chosen to lie between the value \( \chi \) temperature dependence of the impurity contribution to the altogether \([28, 29]\).

Within the NRG approach, we can define the mixed-valence regime behavior for \( r \geq 0.2 \) \( |r| \geq 0.15 \).

The Kondo regime has a width \( \Delta \Gamma = \Gamma_{\text{MV}} - \Gamma_c \) that narrows rapidly with increasing \( r \) and turns out to be restricted to \( \Delta \Gamma \lesssim \Gamma_c/4 \) for \( r \gtrsim \frac{1}{2} \). For band exponents in the range \( \frac{1}{2} \lesssim r < \frac{1}{2} \), the SSC phase can be accessed only from mixed valence, while for \( r \geq \frac{1}{2} \) this phase disappears altogether \([28, 29]\).

Within the NRG approach, we can define the mixed-valence threshold hybridization by examining the temperature dependence of the impurity contribution to the magnetic susceptibility \( \chi_{\text{imp}} \). We can identify the Anderson model as being in its local-moment regime if \( T_{\text{XLM}} > T_{\text{XLM}} \) where \( T_{\text{XLM}} \) is a (somewhat arbitrary) cutoff chosen to lie between the value \( T_{\text{Ximp}} = 1/4 \) corresponding to a free spin-1/2 degree of freedom and the high-temperature or mixed-valent limiting value \( T_{\text{Ximp}} = 1/8 \). With this criterion, the system is in the Kondo regime of the SSC phase if with decreasing \( T \), \( T_{\text{Ximp}} \) first rises above \( T_{\text{XLM}} \) before dropping towards its SSC value \([29]\) of \( r/8 \). We therefore define \( \Gamma_{\text{MV},\text{NRG}} \) as the smallest hybridization prefactor for which \( T_{\text{Ximp}} < T_{\text{XLM}} \) at all temperatures.

Figure 4 shows the ratio \( \Gamma_{\text{MV, NRG}} / \Gamma_{\text{MV, scal}} \) of the mixed-valence threshold hybridization found using NRG and that given by poor man’s scaling. Results for fixed \( U = -2\varepsilon_d = 10^{-4}D \) are plotted vs band exponent \( r \) with \( \Gamma_{\text{MV, NRG}} \) defined using four different values of \( T_{\text{XLM}} \) (see text for details). For \( T_{\text{XLM}} = 3/16 \) \([21]\), it proves impossible to find Kondo-regime behavior for \( r \geq 0.2 \).

We now turn to the limit \( 0 < -\varepsilon_d \ll U \) and \( \Gamma, U \ll D \). For band exponents in the range \( 10^{-4} \), we therefore define \( \Gamma_{\text{MV, NRG}} / \Gamma_{\text{MV, scal}} \) of the mixed-valence threshold coupling found using NRG and the scaling prediction of Eq. \([57]\). The ratio is plotted vs band exponent \( r \) for fixed \( U/D = 10^{-4} \) and four different cutoffs: \( T_{\text{XLM}} = 0.15, 0.17, 3/16, 0.21 \). As one would expect, increasing the value of \( T_{\text{XLM}} \) creates a more stringent criterion for the identification of Kondo physics, reduces the range of exponents \( r \) over which Kondo-regime behavior is found, and for given \( r \) reduces the value of \( \Gamma_{\text{MV}} \). However, the ratio \( \Gamma_{\text{MV, NRG}} / \Gamma_{\text{MV, scal}} \) is nearly independent of \( r \) except in the case \( T_{\text{XLM}} = 0.15 \). This confirms that the condition for reaching mixed valence is correctly captured by Eq. \([57]\) apart from a multiplicative factor that depends on the value of the cutoff \( T_{\text{XLM}} \).

2. **LM-ASC boundary for** \( 0 < -\varepsilon_d \ll U \) **and** \( \Gamma, U \ll D \)**

Equations \([33], [47]\) remain valid until either \( \bar{\Gamma}/\tilde{D} \) reaches \( 1 \) at \( D = \tilde{D} \) or \( (\bar{\tilde{U}} + \bar{\varepsilon_d})/\tilde{D} \) reaches \( 1 \) at \( \tilde{D} = \bar{D} \). By writing \( \bar{\tilde{U}} + \bar{\varepsilon_d} = \left\{ \bar{\tilde{U}} + (\bar{\varepsilon_d} + \frac{1}{2}\tilde{U}) \right\} \), then employing Eqs. \([47], [48], \) and \([58]\), the latter condition can be recast as

\[
\bar{\varepsilon_d} + \frac{1}{2}\tilde{U} \simeq (\varepsilon_d + \frac{1}{2}U) \exp \left\{ -\frac{2}{(1-r)\pi} \sqrt{\frac{\bar{\Gamma}}{\tilde{D}} - \frac{\Gamma}{\tilde{D}}} \right\} .
\]  

Equations \([47]\) and \([58]\) imply that

\[
\bar{\varepsilon_d} + \frac{1}{2}\tilde{U} \simeq (\varepsilon_d + \frac{1}{2}U) \sqrt{\bar{\tilde{U}}/U} .
\]  

Given Eq. \([51]\), the conditions \( \bar{\Gamma}(\bar{D}_1) < \tilde{U}(\bar{D}_1) + \bar{\varepsilon_d}(\bar{D}_1) = \bar{D}_1 \) are satisfied provided that Eq. \([60]\) has a real solution \( \bar{x} = \bar{x}_1(\gamma) < 4/\pi\gamma \). Such solutions exist for \( \gamma \lesssim \gamma_{\text{max}}(r) = (4/\pi) e^{-2/\pi} \simeq 1 - r \) \( \gamma - \gamma_{\text{max}}(r) \). For \( \eta = 1 \), there is a monotonic decrease in \( \gamma_{\text{max}}(1) \) from \( \gamma_{\text{max}}(1) = 0.30 \) to \( \gamma_{\text{max}}(1) = 0.674 \).
while the solution to Eq. (60) satisfies $2^{-(1-r)} \leq \tilde{x}_1 \leq 4/\pi \gamma_{\text{max}} < 1.89$.

In the regime $\tilde{D} < \tilde{D}_1$, entered with $\tilde{\varepsilon}_d = \tilde{\varepsilon}_{d,1}$, the doubly occupied impurity configuration is essentially frozen out. Now Eq. (26) can be approximated by Eq. (39), again yielding Eq. (40). This second phase of the scaling continues until one of the following conditions is met:

(a) $\tilde{\varepsilon}_d = \tilde{D}$, signalling crossover into the empty-impurity region of the ASC$_{-}$ phase; (b) $\tilde{\Gamma} = \tilde{D}$, marking entry into the mixed-valence region of the ASC$_{-}$ phase; (c) $\tilde{\varepsilon}_d = -\tilde{D}$, marking entry into the local-moment regime. In case (c), the system may be mapped onto the pseudogap Kondo Hamiltonian described by Eqs. (30)–(32), which may lie in (c)(i) the ASC$_{-}$ phase, or (c)(ii) the LM phase. Integrating the poor man’s scaling equations with sufficient accuracy to distinguish among all these possibilities is in general a formidable challenge.

Progress on locating the LM-ASC$_{-}$ phase boundary can be made in the limit $\gamma \ll 1$ of very weak impurity-band hybridization, where $\tilde{D}_1 \simeq U + \varepsilon_d$ and $\tilde{x}_1 = (1 + \eta)^{-(1-r)}[1 + O(\gamma)]$. Focusing for simplicity on $\eta \to 1$, one finds

$$\tilde{\varepsilon}_{d,1} \simeq \varepsilon_d + \frac{\Gamma}{(1-r)\pi} \left( \frac{U}{\tilde{D}} \right)^r,$$

and hence [via Eq. (40)]

$$\tilde{\varepsilon}_d = \varepsilon_d + \frac{\Gamma}{r\pi} \left[ \frac{1}{1-r} \left( \frac{U}{\tilde{D}} \right)^r - \left( \frac{\tilde{D}}{\tilde{D}} \right)^r \right].$$

In this limit of small $\gamma$, one expects only a small fractional change in the bare level energy $\varepsilon_d$ to be required to drive the system from case (a) to case (c)(ii) of the previous paragraph. Under these circumstances, just as was done with greater rigor for $r > 1$, one can approximate the location of the phase boundary by the condition $\tilde{\varepsilon}_d(\tilde{D} = 0) = 0$, leading to

$$\varepsilon_d^+ \approx -\frac{\Gamma}{r(1-r)\pi} \left( \frac{U}{\tilde{D}} \right)^r.$$

Eq. (64) can be inverted such that the system is in the LM phase if $\Gamma < \Gamma_c$, where the critical coupling is given by

$$\Gamma_c = r(1-r)\pi |\varepsilon_d| \left( \frac{U}{\tilde{D}} \right)^r.$$

3. LM-ASC$_{-}$ boundary for $0 < -\varepsilon_d, \Gamma \ll D \ll U$

For $U \gg D$, the evolution of $\tilde{\varepsilon}_d$ with $\varepsilon_d$ is as described by Eq. (44). For $\gamma \ll 1$, arguments similar to those given at the end of the previous section lead to the conclusion that the LM-ASC$_{-}$ boundary is given by Eq. (45).

Figure 5 shows the critical hybridization width plotted as $\Gamma_c/|\varepsilon_d|$ vs $U/D$ for band exponents $r = 0.1, 0.2$ and 0.3 and for two values of the ratio $|\varepsilon_d|/U$ listed in legend. NRG data (symbols) are compared with the poor man’s scaling predictions of Eq. (65) for $U \ll D$ (dashed lines) and Eq. (45) for $U \gg D$ (dotted lines). These behaviors show that the poor man’s scaling approach provides a good account of the phase boundary in the limit of strong particle-hole asymmetry on the impurity site.

E. Limitations of the scaling approach

The results presented above demonstrate that poor man’s scaling successfully captures many aspects of the pseudogap Anderson model. However, it would be remiss to gloss over two limitations of the approach.

First, a reliable calculation of the critical hybridization based on poor man’s scaling alone is possible for all $r > 0$ only for $0 < -\varepsilon_d \ll U/2$ (on the ASC$_{-}$ side) or $0 < U + \varepsilon_d \ll U/2$ (on the ASC$_{+}$ side). Near the particle-hole symmetric point $\varepsilon_d = -\frac{U}{2}$, the method breaks down for $r > \frac{1}{3}$. This is clear to see for $r > \frac{1}{3}$ because $\Gamma_c(U, \varepsilon_d)$ diverges as $\varepsilon_d \to -\frac{U}{2}$ [see Fig. 1(b)] and therefore any phase boundary lies outside the perturbative regime. For $\frac{1}{3} \leq r < \frac{1}{2}$, $\Gamma_c(U, \varepsilon_d)$ remains finite for all $-U < \varepsilon_d < 0$ [see Fig. 1(b)] but, as discussed in Ref. 29 and in Sec. II D above, the strong-coupling phases are accessed directly from mixed valence, and in such cases we have been unable to find a scaling criterion for locating the phase boundaries.
Second, poor man’s scaling does not appear to be capable of reproducing the full RG fixed-point structure of the model as identified using the NRG [29]. Scaling Eq. (28) and its counterpart \(dK/dD = rK/D\) for the potential scattering in the pseudogap Kondo model both indicate that particle-hole asymmetry is an irrelevant perturbation about the symmetric plane \(\hat{z}_d = -\frac{1}{2}\hat{U}\). This is consistent with NRG results band exponents on the range \(0 < r < r^* \simeq 3/8\), where a single particle-hole-symmetric quantum critical point (QCP) governs the physics all over the phase boundary between the LM and strong-coupling phases shown in Fig. 1(a). However, there also exists a range \(r^* < r < \frac{1}{4}\) in which the boundaries between the LM phase and each strong-coupling phase (SSC, ASC\(_-\), and ASC\(_+\)) is governed by a different BCP. Within this second range of band exponents, poor man’s scaling cannot reproduce the fact that particle-hole asymmetry is a relevant perturbation that causes flow from the symmetric QCP to one or other of the two asymmetric QCPs [as illustrated schematically for the pseudogap Kondo model in Fig. 16(b) of Ref. 29]. This is a quite subtle aspect the pseudogap Kondo and Anderson models that even much more sophisticated RG treatments are unable to fully capture [30].

### III. ANISOTROPIC POWER-LAW KONDO MODEL

In this section, we present a poor man’s scaling analysis of the phase boundary between the Kondo and local-moment (LM) phases of the Kondo model with distinct longitudinal and transverse spin-flip couplings between the impurity and a power-law-vanishing or -divergent density of states. The model is described by the Hamiltonian

\[
\hat{H}_K = \hat{H}_{\text{band}} + J_{z}\hat{S}\hat{\delta}_z + \frac{1}{2}J_{\perp}(\hat{S}^+\hat{\delta}^- + \hat{S}^-\hat{\delta}^+),
\]

where \(\hat{H}_{\text{band}}\) is as given in Eq. (2) with the density of states specified in Eq. (9), and \(\hat{S}\) and \(\hat{\delta}\) = \(N^{-1}_k\sum_{\mathbf{k}, \mathbf{k}'}\sum_{\sigma, \sigma'} c_{\mathbf{k}, \sigma}^\dagger \frac{1}{2} \sigma_{\sigma'} c_{\mathbf{k}', \sigma'}\) (with \(\sigma\) being a vector of Pauli matrices) are, respectively, the spin-\(\frac{1}{2}\) operators for the impurity and for conduction band electrons at the impurity site. The properties of the model are invariant under \(J_{\perp} \rightarrow -J_{\perp}\), but for notational simplicity we will consider only \(J_{\perp} \geq 0\).

Our focus is primarily on pseudogap cases \(r > 0\), which can arise, for example, due to the low-temperature freeze-out of charge fluctuations in the Anderson-Holstein model with a power-law density of states [12]. However, in Sec. III C we briefly consider the range \(-1 < r < 0\) describing bands with a generalized van Hove singularity at the Fermi energy [20] [21].

#### A. Poor man’s scaling equations

By generalizing Anderson’s poor man’s scaling treatment of the conventional \((r = 0)\) Kondo problem [5], it is straightforward to extend Withoff and Fradkin’s analysis of the pseudogap Kondo problem to anisotropic exchange. Under progressive reduction of the half-bandwidth from \(D\) to \(D = De^{-l}\), the exchange couplings \((J_z, J_{\perp})\) evolve to \((\tilde{J}_z, \tilde{J}_\perp)\) according to

\[
\frac{d\tilde{J}_z}{dl} = -r\tilde{J}_z + \rho_0\tilde{J}_\perp^2, \quad (67a)
\]

and

\[
\frac{d\tilde{J}_\perp}{dl} = -r\tilde{J}_\perp + \rho_0\tilde{J}_z\tilde{J}_\perp. \quad (67b)
\]

On the right-hand side of each of these equations, the first term reflects the change in the density of states at the band edge (a single-particle effect) while the second term reflects the lowest-order many-body effects. These equations neglect all contributions beyond second-order in the exchange, and are therefore restricted in validity to the regime where \(|\rho_0 J_z| \ll 1\) and \(\rho_0 J_{\perp} \ll 1\).

Equations (67) can be combined to obtain

\[
\frac{d}{dl}(\tilde{J}_z^2 - \tilde{J}_\perp^2) = -2r(\tilde{J}_z^2 - \tilde{J}_\perp^2), \quad (68)
\]

which can be integrated to yield

\[
\tilde{J}_z^2 - \tilde{J}_\perp^2 = (J_z^2 - J_{\perp}^2)e^{-2rl}, \quad (69)
\]

One sees that exchange anisotropy is irrelevant for \(r > 0\) (pseudogapped systems), marginal for \(r = 0\) (conventional metals), and relevant for \(r < 0\) (describing a power-law divergence of the host density of states at the Fermi energy). Equation (69) can be inserted into Eq. (70) to obtain

\[
\frac{d\tilde{J}_z}{dl} = -r\tilde{J}_z + \rho_0\tilde{J}_\perp^2 - \rho_0(J_z^2 - J_{\perp}^2)e^{-2rl}. \quad (70)
\]

After the completion of the work reported in this paper, we learned of a recent poor man’s scaling formulation of the power-law Kondo model with a more general anisotropic exchange coupling \(J_x\hat{S}_x\hat{\delta}_x + J_y\hat{S}_y\hat{\delta}_y + J_z\hat{S}_z\hat{\delta}_z\) [49]. For the case \(J_y = J_z\) considered here, the scaling equations of Ref. [49] reduce to Eqs. (67) and yield scaling trajectories fully equivalent in appearance to those plotted in Figs. 6 and 11 of this paper.

#### B. Pseudogapped density of states

For \(r > 0\), Eqs. (67) have two stable fixed points, both isotropic as expected from Eq. (69): the weak-coupling or LM fixed point \(\tilde{J}_z = \tilde{J}_\perp = 0\), and the strong-coupling or Kondo fixed point \(\tilde{J}_z = \tilde{J}_\perp = \infty\) (which lies beyond the
regime of validity of the equations but is known to exist from nonperturbative studies). There is also a critical fixed point \( \rho_0 J_z = \rho_0 J_\perp = r \) that lies on the boundary between the basins of attraction of the stable fixed points. The goal of this subsection is to map out the location of this boundary away from the point of SU(2) spin symmetry. In light of Eq. (69), it is clear that any location of this boundary away from the point of SU(2) fixes the isotropic critical point, which therefore governs the spin symmetry. In light of Eq. (69), it is clear that any location of this boundary away from the point of SU(2) fixes the isotropic critical point, which therefore governs the spin symmetry.

For \( J_z \neq 0 \), one can factorize out the variation of \( J_z \) arising from pure density-of-states effects [i.e., the effect of the \( -rJ \) term on the right-hand-side of Eq. (70)] through the substitution

\[
\tilde{J}_z = f(l) J_z e^{-rl},
\]

which converts Eq. (70) to

\[
\frac{df}{dl} = \left[ f^2 - 1 + (J_\perp / J_z)^2 \right] \rho_0 J_z e^{-rl}
\]

with the initial condition \( f(0) = 1 \). For any antiferromagnetic bare exchange \( J_z > 0 \), Eq. (72) yields \( df/dl \geq 0 \) and \( f \geq 1 \) for all \( l \geq 0 \). If \( f \) remains finite as \( l \to \infty \), then \( J_z \) vanishes as \( D \to 0 \) and the system must lie in the LM phase. On the other hand, we can associate the divergence of \( f \) at some value \( l = l_K \) with entry into the Kondo regime around temperature \( T_K = D e^{-l_K} \). The boundary between the two phases is determined by the divergence of \( f(l) \) only at \( l = \infty \). For a ferromagnetic bare exchange \( J_z < 0 \), \( J_\perp \neq 0 \) is sufficient to ensure that \( f < 1 \) for all \( l > 0 \). In this case, the system enters the Kondo regime if \( f \) changes sign and reaches \( -\infty \) for some finite \( l_K \).

For the purposes of more detailed analysis, it proves convenient to parameterize the anisotropy of the bare exchange couplings in terms of the variable

\[
\alpha = \sqrt{J_\perp / J_z^2 - 1} \quad \text{sgn}(J_\perp / J_z^2 - 1),
\]

which can range from \(-1 \) (for \( J_\perp = 0 \)) to \(+1 \) (for \( J_\perp = |J_z| \)) to \(+\infty \) (for \( J_\perp \gg |J_z| \)). Then Eq. (72) can be rewritten

\[
\frac{df}{dl} = (f^2 + \alpha |\alpha|) \rho_0 J_z e^{-rl}.
\]

Solutions of this equation will be examined in the next two subsections.

1. Easy-plane anisotropy

In cases where \( J_z > |J_\perp| > 0 \), \( \alpha \) defined in Eq. (73) is positive and Eq. (74) has the solution

\[
f(l) = \alpha \tan \left[ \cot \alpha + \frac{\alpha \rho_0 J_z}{r} (1 - e^{-rl}) \right].
\]

For antiferromagnetic bare exchange \( (J_z > 0) \), the Kondo phase occupies the region of parameter space in which there is a solution \( 0 \leq l_K < \infty \) of the equation

\[
f(l_K) = \infty, \text{i.e.,} \quad \cot \alpha + \frac{\alpha \rho_0 J_z}{r} > \frac{\pi}{2}
\]

Thus, the Kondo phase extends over \( J_z > J_{z,c}(\alpha) \) where

\[
\rho_0 J_{z,c}(\alpha) = r \frac{\tan \alpha}{\alpha}.
\]

For \( \alpha \ll 1 \) (weak anisotropy),

\[
\rho_0 J_{z,c} \approx r \left(1 - \frac{1}{3} \alpha^2 \right),
\]

which reduces for \( \alpha \to 0 \) to the standard result

\[
\rho_0 J_{z,c} = \rho_0 J_{\perp,c} = r \quad \text{for} \quad \alpha \gg 1 \quad \text{(strong anisotropy)},
\]

\[
\rho_0 J_{\perp,c} \approx \frac{r \pi}{2} \left(1 - \frac{2}{\pi \alpha}\right).
\]

For ferromagnetic bare exchange \( (J_z < 0) \), the condition for entry into the Kondo regime becomes \( f(l_K) = -\infty \), which is met for some finite \( l_K \) provided that

\[
\cot \alpha + \frac{\alpha \rho_0 J_z}{r} < -\frac{\pi}{2}.
\]

Therefore, the Kondo phase extends over the region \( J_z < J_{z,c}(\alpha) \) where

\[
\rho_0 J_{z,c}(\alpha) = -\frac{r}{\alpha} \left(\pi - \tan \alpha\right).
\]

For \( 0 < \alpha \ll 1 \) (weak anisotropy),

\[
\rho_0 J_{z,c} \approx -\frac{r \pi}{\alpha} \left(1 - \frac{\alpha}{\pi}\right),
\]

while for \( \alpha \gg 1 \) (strong anisotropy),

\[
\rho_0 J_{z,c} \approx -\frac{r \pi}{2 \alpha} \left(1 + \frac{2}{\pi \alpha}\right),
\]

so the Kondo phase spans \( J_z > J_{\perp,c}(\alpha) \) where

\[
\rho_0 J_{\perp,c}(\alpha) \approx \frac{r \pi}{2} \left(1 + \frac{2}{\pi \alpha}\right).
\]

2. Easy-axis anisotropy

For \( |J_z| > J_{\perp} > 0 \), \( \alpha \) defined in Eq. (73) is negative and the solution of Eq. (74) is

\[
f(l) = \alpha \coth \left[ \tanh \alpha - \frac{\alpha \rho_0 J_z}{r} (1 - e^{-rl}) \right].
\]
For antiferromagnetic bare exchange \( J_z > 0 \), the Kondo phase spans the region in which
\[
\text{atanh} \alpha - \frac{\alpha \rho_0 J_z}{r} > 0,
\]
for \( |\alpha| < 1 \) (weak anisotropy),
\[
\rho_0 J_{z,c} = r \frac{\text{atanh} \alpha}{\alpha}.
\]
For \( J_z < -J_L < 0 \), \( f(l) \) is a monotonically decreasing function of \( l \) and the system always lies in the LM phase.

3. **XY exchange anisotropy**

In the special case \( J_z = 0 \) of pure-XY bare exchange coupling, the scaling in Eq. (74) can be replaced by
\[
\tilde{J}_z = g(l) J_L e^{-rl},
\]
which converts Eq. (70) to
\[
\frac{dg}{dl} = (g^2 + 1) \rho_0 J_L e^{-rl}
\]
with initial condition \( g(0) = 0 \). The equation has solution
\[
g(l) = \tan \left[ \frac{\rho_0 J_L}{r} \left( 1 - e^{-rl} \right) \right].
\]
In the Kondo phase, there must be an \( l_K \) (\( 0 < l_K < \infty \)) such that \( g(l_K) = \infty \), a condition that is satisfied for \( J_L > J_{L,c} \), where
\[
\rho_0 J_{L,c} = \frac{r \pi}{2}.
\]
As one would expect, this result coincides with the limits \( \alpha \to \infty \) of Eqs. (80) and (85).

4. **Comparison with NRG**

The preceding results for the location of the phase boundary as a function of \( \alpha \) and the sign of \( J_z \) can be re-expressed as the statement that for any value of \( J_z \), the Kondo phase occupies the region \( J_L > J_{L,c}(J_z) \), where \( J_{L,c} \) is a monotonically decreasing function of \( J_z \) that has the following limiting forms:
\[
\begin{align*}
\rho_0 J_{L,c} &\simeq \rho_0 |J_z| \left[ 1 + \frac{1}{2} \left( \frac{r \pi}{\rho_0 J_z} \right)^2 \right] \text{ for } 1 \gg -\rho_0 J_z \gg r \pi, \\
\rho_0 J_{L,c} &\simeq r \pi / 2 - 2 \rho_0 J_z / \pi \text{ for } |\rho_0 J_z| \ll r, \\
\rho_0 J_{L,c} &\simeq r / 2 (\rho_0 J_z - r) \text{ for } |\rho_0 J_z - r| \ll r / 3, \\
\rho_0 J_{L,c} &\simeq 2 \rho_0 J_z \exp(-\rho_0 J_z / r) \text{ for } r \ll \rho_0 J_z \ll 1.
\end{align*}
\]
In the limit \( r \to 0 \), these expressions reproduce the standard result \([5]\) \( J_{L,c} = |J_z| \theta(-J_z) \). The purpose of this section is to test these statements based on poor man’s scaling against nonperturbative NRG calculations.

Scaling trajectories for the pseudogap Kondo model, calculated via numerical iteration of Eqs. (67) with different starting parameters, are plotted in Figs. 6(a) and 6(b) for \( r = 0.1 \) and \( r = 0.3 \), respectively. Solid lines show trajectories that flow to the fixed points of the model. Arrows on some of the trajectories show the direction of flow of the couplings under reduction of the half-bandwidth \( D \). The phase boundary (solid line) separating the basins of attraction of the LM fixed point (\( \rho_0 J_z = \rho_0 J_L = 0 \)) and the Kondo fixed point (\( \rho_0 J_z = \rho_0 J_L = \infty \)) was found by (a) reversing the flow of Eqs. (67) and (b) choosing starting parameters very close to the critical coupling \( \rho_0 J_{z,c} = \rho_0 J_{L,c} = r \) and lying on either side of the the trajectory \( J_z = J_L \). For comparison, NRG data for the phase boundary (circles) are shown, with all values of \( J_z \) and \( J_{L,c} \) rescaled by the multiplicative factor that places the isotropic critical point at \( \rho_0 J_z = \rho_0 J_L = r \). This \( r \)-dependent multiplicative factor is introduced to account both for a known reduction in hybridization arising from the NRG discretization \([29, 35]\) and for the effect of higher-order terms omitted from the poor man’s scaling equations \([7]\), which shift the isotropic critical point from \( \rho_0 J_c = r \) to \( \rho_0 J_c = f(r) \simeq r(1 + r / 2) \) \([33]\). Figure 6 shows that poor man’s scaling does an excellent job of reproducing the shape of the phase boundary over the entire region of couplings \( \rho_0 |J_z| < 1, \rho_0 J_L < 1 \).

A more rigorous test of the poor man’s scaling is provided by Figs. 7[10] which compare \( \rho_0 J_{L,c} \) vs \( \rho_0 J_z \) calculated for one of the limiting cases in Eqs. (95) (solid lines) with their NRG counterparts (symbols). The NRG results are again scaled so that the isotropic critical point is at \( \rho_0 J_z = \rho_0 J_{L,c} = r \).

Figure 7 plots the critical coupling \( \rho_0 J_{L,c} \) for \( r = 0.1 \) over a range of ferromagnetic exchange couplings \( \rho_0 J_z < 0 \). Although the perturbative scaling analysis is not strictly valid for \( \rho_0 J_z \lesssim -1 \), Eq. (95a) captures surprisingly well the variation of \( \rho_0 J_{L,c,\text{NRG}} \) at least as far as \( \rho_0 J_z = -1.7 \). For \( r = 0.3 \), the restriction \( \rho_0 J_z \ll -r \pi \) rules out the applicability of Eq. (95a) anywhere within
that the NRG results closely follow the asymptotic form as given in Eq. (95b) over its entire range of validity. The overall conclusion from Figs. 6–10 is that the poor man’s scaling approach provides an excellent account of the location of the boundary between the Kondo and local-moment phases of the spin-anisotropic pseudogap Kondo model under conditions of strict particle-hole symmetry.

Lastly, Fig. 10 plots the critical coupling as $r \ln(J_{\perp,c}/2J_z)$ versus $\rho J_z$ for $0 \leq \rho J_z \leq 1$. We find that the NRG results closely follow the asymptotic form as given in Eq. (95d), dotted lines] over the range $0.2 \leq \rho J_z \leq 0.7$ for $r = 0.1$ and over $0.6 \leq \rho J_z \leq 1$ for $r = 0.3$. There are minor deviations from the asymptotic form as $\rho J_z$ nears 1 due to perturbative effects beyond second order. We have also plotted the poor man’s scaling prediction obtained via numerical solution of Eq. (88) (solid lines), which can be seen to describe correctly the deviation of $J_{\perp,c,NRG}$ near $J_z = 0$ from its $\rho J_z \gg r$ asymptote.

The overall conclusion from Figs. 6–10 is that the poor man’s scaling approach provides an excellent account of the location of the boundary between the Kondo and local-moment phases of the spin-anisotropic pseudogap Kondo model under conditions of strict particle-hole symmetry.
FIG. 9. Pseudogap Kondo model phase boundary plotted as $\rho_0 J_{\perp, c} - r$ vs $3(\rho_0 J_z - r)/r$ for $r = 0.1$ and $r = 0.3$, comparing NRG results (symbols) with the poor man’s scaling prediction for $\rho_0 |J_z - r| \ll r/3$ as given in Eq. (95c) (lines).

FIG. 10. Pseudogap Kondo model phase boundary plotted as $r \ln(J_{\perp, c}/2 J_z)$ vs $\rho_0 J_z$ for $r = 0.1$ and $r = 0.3$, comparing NRG results (symbols) with the poor man’s scaling prediction obtained via numerical solution of Eq. (88) (solid lines) and the asymptotic form for $\rho_0 J_z \gg r$ from Eq. (95d) (dashed line).

C. Divergent density of states

The poor man’s scaling analysis of the anisotropic Kondo model can also be applied to cases $r < 0$ where the density of states in Eq. $9$ diverges in power-law fashion at the Fermi energy. Examination of Eqs. (67) show that the poor man’s scaling trajectories for $r < 0$ can be obtained from those for band exponent $|r| > 0$ through the simple replacements $r \rightarrow -r$, $J_z \rightarrow -J_z$. This mapping implies that the scaling trajectories for $r < 0$ should be reflections of those for $r > 0$ about the axis $J_z = 0$ with reversal of the direction of flow arrows. This is illustrated Fig. 11 which plots the scaling trajectories for a representative case $r = -0.1$ over the range of exchange couplings $-1 < \rho_0 J_z < 1$ and $0 < \rho_0 J_\perp < 1$. Arrows indicate the direction of flow of couplings with decreasing effective half-bandwidth. The model has three stable fixed points: a ferromagnetic fixed point at $(\rho_0 J_z, \rho_0 J_\perp) = (-\infty, 0)$ where the impurity is locked into a many-body spin triplet with the conduction band, the symmetric strong-coupling fixed point at $(\rho_0 J_z, \rho_0 J_\perp) = (\infty, \infty)$, and an intermediate coupling fixed point at $(\rho_0 J_z, \rho_0 J_\perp) = (-|r|, |r|)$. The phase boundary (thick lines) separating the ferromagnetic and strong-coupling phase is given by the condition $J_z = -|J_\perp|$, which is consistent with NRG studies of the model.

FIG. 11. Scaling trajectories for the power-law Kondo model with $r = -0.1$, representing a divergence of the density of states at the Fermi energy. Arrows indicate the direction of flow under reduction of the half-bandwidth $D$. Thick lines show trajectories that flow to the critical point, defining the phase boundary between the ferromagnetic and Kondo phases.

IV. SUMMARY

In this work, we have extended the poor man’s scaling method to analyze phase boundaries in variants of the Anderson and Kondo impurity models that feature a power-law vanishing or divergence of the host density of states at the Fermi energy. The predicted locations of the phase boundaries are generally in excellent qualitative and good quantitative agreement with those obtained using the numerical renormalization group (NRG), which remains the most reliable technique for treating power-law quantum impurity problems. The scaling approach has the advantages that it is much more intuitive than the NRG and it can clarify algebraically the functional dependence of the critical impurity-host coupling on other model parameters. Thus, poor man’s scaling retains
The hybridization function is denoted by the symbol $\bar{\Gamma}$ to distinguish it from the hybridization prefactor $\Gamma$ appearing on the right-hand side of Eq. (8).

\[ \bar{\Gamma} \]

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