Relevance of anisotropy in the multichannel Kondo effect: Comparison of conformal field theory and numerical renormalization-group results

Ian Affleck
Canadian Institute for Advanced Research and Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1

Andreas W. W. Ludwig
Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1 and Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5Y 1S6

H.-B. Pang and D. L. Cox
Department of Physics, The Ohio State University, Columbus, Ohio 43210
(Received 19 November 1991)

The multichannel Kondo model exhibits non-Fermi-liquid behavior in the overscreened case, when the number of channels, k, is greater than twice the size of the impurity spin, s. We show that, for overscreening, exchange anisotropy is irrelevant at the low-temperature fixed point for $s = 1/2$ or $s = k/2 - 1/2$, but relevant for all other values of s. However, an external field or channel asymmetry is relevant, producing crossover to Fermi-liquid fixed points with different phase shifts for each spin in the first case and for each channel in the second. These results are elucidated by explicit comparison of analytic finite-size spectra derived from conformal field theory with those obtained from numerical renormalization-group calculations. The relevance of the results (for $k = 2$ and $s = 1/2$) to the quadrupolar Kondo Hamiltonian, which has been proposed as a model for many uranium-based heavy-fermion materials, will be briefly discussed. Also, a larger, *symplectic* symmetry Sp($2k$) is shown to be present in the k-channel Kondo model.

I. INTRODUCTION

Recent experimental[1,2] and theoretical developments[3-12] have generated renewed interest in the multichannel Kondo model proposed by Nozières and Blandin.[13] The model describes antiferromagnetic coupling of k degenerate channels or flavors of spin-$\frac{1}{2}$ conduction electrons [with dispersion relation $\epsilon(\vec{k})$] to a quantum impurity spin $\vec{S}_I$ of arbitrary size s. Placing the impurity at the origin, the Hamiltonian is given by

$$\mathcal{H} = \sum_{\vec{k}} \epsilon(\vec{k}) c^{\alpha,i\dagger}_{\vec{k}} c_{\vec{k},\alpha\, i} - J\vec{S}_I \cdot \sum_{\vec{k},\vec{k}'} \frac{1}{2} c^{\alpha,i\dagger}_{\vec{k}} \vec{\sigma}^{\beta}_{\alpha} c_{\vec{k}',\beta,i}. \tag{1.1}$$

Here $c_{\vec{k},\alpha,i}$ annihilates electrons of wave vector $\vec{k}$ (running over the Brillouin zone), spin $\alpha = 1, 2$ and channel index $i = 1, 2, \ldots, k$; $\vec{\sigma}$ represents the three Pauli matrices for the spin degrees of freedom, and the exchange integral J is negative (antiferromagnetic). We use raised spin and flavor indices on creation operators and a repeated index summation convention.

Nozières and Blandin demonstrated that in the overscreened case, i.e., when the number of channels exceeds twice the impurity spin, this model will possess a non-trivial zero-temperature (T) fixed point with a *non-Fermi-liquid* excitation spectrum.[13] In particular, as was shown in subsequent work, for the case $k = 2$, $s = 1/2$, the specific heat and susceptibility increments due to the impurity diverge logarithmically as $T \to 0$, while the added $T = 0$ entropy is $(1/2)\ln(2)$.[14-16,5,6] Moreover, the resistivity was recently shown[7] to saturate to its residual zero temperature value with a non-trivial power law in T rather than T^2 as in the normal Kondo problem, derivable from Fermi-liquid theory.[17]

It has recently been discovered that for the dilute alloy system $Y_{1-x}U_xPd_3$ the specific heat, resistivity, and residual entropy appear to behave in the above fashion for $x \leq 0.2$.[1] Hence, for the first time there is concrete experimental evidence for the overscreened two-channel Kondo model, associated in this case with the uranium ions. The data make clear that this Kondo effect most likely arises from *quadrupolar* degrees of freedom on the uranium sites[1,2]—i.e., a non-Kramers Γ_3 state on the U^{4+} ions is orbitally quenched by the conduction states in two channels guaranteed degenerate by time reversal. It has been proposed that this two-channel quadrupolar Kondo model (when extended to the lattice) may also describe the heavy-fermion superconductors UBe_{13}, UPt_3, and URu_2Si_2.[10]

Independently of these developments, a conformal field theory (CFT) approach to the multichannel model has been developed, which allows for an exact evaluation of thermodynamic properties, static and dynamic correlation functions, and finite-size energy spectra in the asymptotic regime near the critical point.[3-9] This powerful approach allows a complete classification of all rel-

evant, marginal, and irrelevant perturbations about the critical point as well. This is of considerable phenomenological interest, since the quadrupolar Kondo effect will possess, generically, anisotropic exchange coupling, and may be perturbed by application of uniaxial stress (precisely analogous to a magnetic field in the usual Kondo effect) and magnetic field (which couples to the channel degrees of freedom in the quadrupolar Kondo effect). In what follows we shall avoid possible confusion by adhering to the usual spin-Kondo-effect terminology.

Many of these results can be obtained independently with numerical renormalization-group (NRG) calculations following the pioneering work of Wilson (for the single channel $s = 1/2$ model[18]) and Cragg, Lloyd, and Nozieres (for the $k = 2$, $s = 1/2$ model[19]). While the fixed-point spectra have been derived analytically from the CFT approach, it is useful to apply the NRG technique for two reasons: (i) The CFT approach rests upon a central "fusion rule" hypothesis, which has not been completely justified from first principles but may be tested against other approaches such as the NRG and (ii) within the NRG approach the various perturbations are written in terms of the original impurity and conduction-electron operators. This has intuitive appeal, although at low temperatures impurity and conduction electrons lose their identity, which, in the CFT approach, is reflected by the absorption of the impurity spin into the spectrum. Thus, it is of interest to compare the NRG spectra with the finite-size spectra derived from the CFT approach.

In this paper we shall demonstrate that for the overscreened model (i) exchange anisotropy is an *irrelevant* perturbation when $s = 1/2$ or $s = k/2 - 1/2$ but *relevant* in all other cases, (ii) a magnetic field is a relevant perturbation driving the system to a fixed point where the impurity spin is polarized and the conduction electrons form a Fermi liquid, (iii) as anticipated by Nozières and Blandin, for k=2, breaking of channel degeneracy drives the system to a fixed point, which is a product of two free fermion spectra, one with a $\pi/2$ phase shift and the other without phase shift—that is, one channel exhibits the ordinary Kondo effect and the other channel is decoupled, (iv) NRG spectrum and the analytic CFT spectrum agree well at the non-Fermi-liquid fixed point when k=2, $s = 1/2$, and (v) the NRG approach provides intuition complementary to the CFT method, which helps us understand in a different way the irrelevance of the exchange anisotropy. We shall also point out that the symmetry of the k-channel Kondo model, in continuum or lattice formulations, is larger than seems to have been previously noticed, namely, SU(2)×Sp($2k$). The (symplectic) Sp($2k$) band symmetry contains both the SU(k)×U(1) "flavor" and charge symmetries used previously in the CFT approach and the $\otimes$[SU(2)]^k "isospin" or "axial charge" symmetries used in the NRG approach. [For the case $k = 1$, Sp(2) is isomorphic to the SU(2) axial charge symmetry of Ref. 20. While this reference used the notation axial charge for the complete three-vector of symmetry generators, we reserve this name for the third component only and refer to the complete three-vector as isospin. For $k = 2$, Sp(4) is isomorphic to SO(5).] This paper is divided into the following sections: Section II discusses the (symplectic) Sp($2k$) symmetry (this section, even though rather fundamental, is not necessary for an understanding of the rest of the paper and may be skipped, at first reading). Section III discusses the mapping of Eq. (1.1) into a form amenable to the CFT approach, reviews this approach, presents all the CFT results relevant to this work, and discusses the effect of various symmetry breaking perturbations. Section IV summarizes briefly the NRG approach. Section V provides a comparison of CFT results with those of the NRG. Finally, Sec. VI summarizes our results and points out possible connections to experiment.

II. GENERAL SYMMETRY CONSIDERATIONS

The multichannel Kondo Hamiltonian of Eq. (1.1) has an "obvious" SU(2)×SU(k)×U(1) symmetry corresponding to the possibility of making unitary transformations, which mix the two spin components of the electron operators, the k flavor components, or multiply all components by a common phase. This symmetry was used extensively in the conformal field theory treatment.[3–8] In the NRG approach conserved axial charges and isospins have been used: for k channels there are k extra SU(2) symmetries that commute with ordinary spin. The ith axial charge is simply given by the total number of electrons in channel i. These isospins do not commute with flavor. Instead, as we show in the following, there is a larger symmetry group, namely, the symplectic group Sp($2k$), of which both SU(k)×U(1) *and* $\otimes$[SU(2)]^k are subgroups.

These symmetries exist under very general conditions: Consider a more general form of the k-channel Hamiltonian, Eq. (1.1):

$$\mathcal{H} - \mu N = \sum_n \epsilon(n) c_n^{\alpha,i\dagger} c_{n,\alpha,i} - J\vec{S}_I \cdot \sum_{n,n'} \frac{1}{2} c_n^{\alpha,i\dagger} \vec{\sigma}_\alpha^\beta c_{n',\beta,i} f(n,n'). \tag{2.1}$$

Here N is the particle number, n and n' run over a complete set of eigenstates of the noninteracting (single-particle) Hamiltonian with $J = 0$, having energy $\epsilon(n)$ ($c_n^{\alpha,i\dagger}$ creates eigenstate n of spin projection α in channel i). We will show in the following that the *symplectic symmetry* holds whenever the Hamiltonian in Eq. (2.1) is *particle-hole symmetric*.

This means more explicitly that there is a one-to-one map of the single-particle eigenstates into themselves, $n \to m = \check{n}$, such that $\epsilon(n) = -\epsilon(\check{n})$ and $\check{\check{n}} = n$ for an appropriate choice of the chemical potential μ (note that $\check{n}$ is a *function* of n). The particle-hole transformation is then defined as $c_{n,\alpha} \leftrightarrow \varepsilon_{\alpha\beta} c_{\check{n}}^{\dagger\beta}$ ($\varepsilon_{\alpha\beta}$ is the antisymmetric tensor). The Kondo interaction is particle-hole symmetric when the function f satisfies $f(n_1,n_2) = f(\check{n}_2,\check{n}_1)$.

When the noninteracting Hamiltonian is translationally invariant, n labels the momentum, $\vec{k}$, within the Brillouin zone. [Notice that for a *local* Kondo interaction the function $f(\vec{k},\vec{k}')$ is constant.] If, in this case, the energy-momentum dispersion relation is *linearized* around the Fermi-level (with a symmetric cutoff), particle-hole sym-

metry is automatic.

If the noninteracting Hamiltonian is nondiagonal, the particle-hole transformation is realized in general by $c_{n,\alpha} \leftrightarrow \varepsilon_{\alpha\beta} U_{n,m} c_m^{\dagger\beta}$, where U is unitary. The noninteracting Hamiltonian used in Wilson's NRG is a special case of not necessarily spatially uniform hopping (of arbitrary distance) between the two sublattices A and B of a bipartite lattice (in any dimension)

$$\mathcal{H} = \sum_{x,y} t_{x,y} \left(c_x^\dagger c_y + c_y^\dagger c_x\right) - J\vec{S}_I \cdot \frac{1}{2} c_{x=0}^{\alpha,i\dagger} \vec{\sigma}_\alpha^\beta c_{x=0,\beta,i}, \tag{2.2}$$

where $t_{x,y} = t_{y,x} = 0$ unless $x \in A$ and $y \in B$. This Hamiltonian is particle-hole symmetric as can be seen from the symmetry $c_{a,\alpha} \leftrightarrow \varepsilon_{\alpha\beta} c_a^{\dagger\beta}$, $c_{b,\alpha} \leftrightarrow (-1)\varepsilon_{\alpha\beta} c_b^{\dagger\beta}$, where $a \in A$, $b \in B$.

We now study the symmetries of the general Hamiltonian in Eq. (2.1), assuming particle-hole symmetry. The spin-symmetry generators are

$$\vec{S}_{\rm tot} = \sum_n c_n^{\alpha,i\dagger} (\vec{\sigma}_\alpha^\beta/2) c_{n,\beta,i} + \vec{S}_I, \tag{2.3}$$

the total charge is

$$Q = \sum_n c_n^{\alpha,i\dagger} c_{n,\alpha,i}, \tag{2.4}$$

and the flavor SU(k) generators are

$$J_f^A \equiv \sum_n c_n^{\alpha,i\dagger} (T^A)_i^j c_{n,\alpha,j}, \tag{2.5}$$

where the T^A's ($A = 1, 2, \ldots, k^2 - 1$) are a basis of traceless Hermitian $k \times k$ matrices.

The k axial charge generators are

$$Q_i = (1/2) \sum_n [c_n^{\alpha i\dagger} c_{n,\alpha,i} - 1], \quad i = 1, \ldots, k. \tag{2.6}$$

(Note that i is not summed over in the above equation nor in the next few.) The Q_i's can be completed into k sets of SU(2) isospin generators in combination with

$$I_i^- = (1/2) \sum_n c_{n,i,\alpha} c_{\check{n},i,\beta} \varepsilon^{\alpha\beta}, \quad i = 1, \ldots, k \tag{2.7}$$

(recall that $\check{n}$ is to be thought of as a function of n.) It can be easily verified that (n and $\check{n}$ not summed)

$$[(\epsilon(n) c_n^{\dagger\alpha,i} c_{n,\alpha,i} + \epsilon(\check{n}) c_n^{\dagger\alpha,i} c_{\check{n},\alpha,i}), \varepsilon^{\gamma\delta} c_{n,\gamma,i} c_{\check{n},\delta,i}]$$

$$= [\epsilon(n) + \epsilon(\check{n})] \varepsilon^{\alpha\gamma} c_{\check{n},\alpha,i} c_{n,\gamma,i} = 0 \tag{2.8}$$

due to the particle-hole symmetry condition. This proves that I_i^- (and similarly I_i^+) does indeed commute with the *kinetic part* of the Hamiltonian, Eq. (2.1). The commutator with the *Kondo interaction* follows from

$$\sum_n \sum_{n_1,n_2} f(n_1,n_2) [\varepsilon^{\gamma\delta} c_{n,\gamma,j} c_{\check{n},\delta,j} \ , \ c_{n_1}^{\dagger\alpha,j} \vec{\sigma}_\alpha^\beta c_{n_2,\beta,j}]$$

$$= 2 \sum_{n_1,n_2} c_{\check{n}_1,\gamma,j} f(n_1,n_2) \left(\varepsilon^{\gamma\alpha} \vec{\sigma}_\alpha^\beta\right) c_{n_2,\beta,j}. \tag{2.9}$$

This is zero whenever $f(n_1,n_2) = f(\check{n}_2,\check{n}_1)$ because the matrix $\varepsilon^{\alpha\beta}\vec{\sigma}_\beta^\gamma$ is symmetric for all three components of $\vec{\sigma}$. It can be checked that $[I_i^-, Q_i] = I_i^-$, $[I_i^-, I_i^+] = -2Q_i$ [where $I_i^+ \equiv (I_i^-)^\dagger$], thus satisfying k mutually commuting copies of the SU(2) algebra. Note that while the axial charges Q_i are special cases of flavor generators, the $I_i^\pm$'s are not, and furthermore they do not commute with the flavor generators [Eq. (2.5)]. Clearly by calculating commutators of all these symmetry generators with the flavor generators, we can produce new ones, and eventually the algebra will close.

Let us look at this problem a little more systematically. The most general Hermitian fermion bilinear, which commutes with the ordinary spin operators [Eq. (2.3)] can be seen to be either of the form

$$\sum_n \left(c_n^{\dagger\alpha,i} M_i^j c_{n,\alpha,j} - {\rm tr} M\right)$$

or

$$\sum_n c_{n,\alpha,i} \varepsilon^{\alpha\beta} S^{ij} c_{\check{n},\beta,j} + {\rm H.c.}, \tag{2.10}$$

where M is Hermitian and S is a (complex) symmetric matrix (and i and j are summed). This can be proven in analogy to Eqs. (2.8) and (2.9). The total number of (Hermitian) symmetry generators is k^2 for the first set and $k(k+1)$ for the second, a total of $k(2k+1)$. It can be verified that these generators obey the commutation relations defining the symplectic algebra Sp($2k$): Explicitly the generators of Sp($2k$) can be defined as the set of $2k$ dimensional Hermitian matrices, $\mathcal{A}$, obeying

$$\mathcal{A}^T \Lambda + \Lambda \mathcal{A} = 0, \tag{2.11}$$

where Λ is the canonical antisymmetric matrix:

$$\Lambda \equiv \begin{pmatrix} \mathbf{0}_k & \mathbf{I}_k \\ -\mathbf{I}_k & \mathbf{0}_k \end{pmatrix}. \tag{2.12}$$

Here $\mathbf{I}_k$ and $\mathbf{0}_k$ represent k-dimensional unit and zero matrices. It can easily be seen that the most general matrix, $\mathcal{A}$, satisfying this condition is of the form

$$\mathcal{A} = \begin{pmatrix} -M^T & S \\ S^* & M \end{pmatrix}, \tag{2.13}$$

where M is Hermitian and S is symmetric. [The (Lie) algebra of generators $\mathcal{A}$ in Eq. (2.13) is commonly referred to[21] as C_k.] It can be checked explicitly that the commutation relations of the operators

$$\sum_n \left(c_n^{\alpha i\dagger} M_i^j c_{n,\alpha,j} - {\rm tr} M\right), \quad (1/2) \sum_n c_{n,\alpha,i} \varepsilon^{\alpha\beta} S^{ij} c_{\check{n}\beta,j},$$

and $(-1/2)\sum_n c_n^{\dagger\alpha,i} \varepsilon_{\alpha\beta} S_{ij}^* c_{\check{n}}^{\dagger\beta,j}$ are equivalent to those of the matrices

$$\begin{pmatrix} -M^T & 0 \\ 0 & M \end{pmatrix}, \quad \begin{pmatrix} 0 & S \\ 0 & 0 \end{pmatrix}, \text{ and } \begin{pmatrix} 0 & 0 \\ S^* & 0 \end{pmatrix},$$

respectively. This establishes the Sp($2k$) flavor symmetry of the Kondo problem.

In the special case of $k = 1$, Sp(2) is equivalent to SU(2), corresponding to the "axial-charge symmetry."[20,22] In the case $k = 2$, Sp(4) is equivalent

to SO(5). For Sp($2k$), SU(k)×U(1) (flavor and charge), and $\otimes$[SU(2)]^k (axial isospins) are subgroups as anticipated.

III. CONFORMAL FIELD THEORY APPROACH

A CFT approach has recently been developed for the Kondo effect effect.[3-7,9] For a pedagogical up-to-date review, see also Ref. 8. (Related work has been done independently in Refs. 12 and 23.) In this section we recapitulate the essential features of this approach and identify the relevant and irrelevant operators associated with the various physical symmetry-breaking terms, which may be added to the Hamiltonian of Eq. (1.1) (exchange anisotropy, spin field, and channel field). We shall divide this section into a discussion of the rewriting of Eq. (1.1) in the Sugawara form (Sec. III A), a discussion of the derivation of resulting spectra via conformal field theory (Sec. III B), and finally a discussion of various symmetry-breaking perturbations within the CFT approach (Sec. III C).

A. Sugawara form of the Hamiltonian

Due to the spherical symmetry of the problem specified by Eq. (1.1), we may eliminate all but the s-wave component of the electrons, leading to an effective one-dimensional quantum problem defined on the half line ($x \geq 0$). We introduce position space left and right moving (or equivalently incoming and outgoing) fermion fields ψ_L and ψ_R associated with the s-partial waves of the conduction states and having a Fermi velocity v_F (see Ref. 5 for details).

In terms of these fields, the Hamiltonian of Eq. (1.1) is thus rewritten as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\rm int}, \tag{3.1}$$

where the free Hamiltonian is

$$\mathcal{H}_0 = (v_F/2\pi)\int_0^\infty dx\left(i\psi_L^{i\alpha\dagger}(x)\frac{d\psi_{i\alpha L}(x)}{dx} - i\psi_R^{i\alpha\dagger}(x)\frac{d\psi_{i\alpha R}(x)}{dx}\right), \tag{3.2}$$

and the Kondo interaction is ($\lambda_K = -\nu J$, where ν is the density of states per spin per channel)

$$\mathcal{H}_{\rm int} = \frac{v_F\lambda_K}{4}\vec{S}_I\cdot[\psi_L^{i\alpha\dagger}(0)+\psi_R^{i\alpha\dagger}(0)] \times\frac{1}{2}\vec{\sigma}_\alpha^\beta[\psi_{i\beta L}(0)+\psi_{i\beta R}(0)]. \tag{3.3}$$

These fermion fields are normalized so that

$$\{\psi_L^\dagger(x),\psi_L(y)\} = 2\pi\delta(x-y) \tag{3.4}$$

(similar for ψ_R) and obey the boundary condition

$$\psi_L(0) = \psi_R(0). \tag{3.5}$$

This boundary condition allows us to define a left-moving field also at $x<0$ by $\psi_L(-x)\equiv\psi_R(x)$. The Hamiltonian can thus be written entirely in terms of left movers

$$\mathcal{H} = (v_F/2\pi)\int_{-\infty}^\infty dx\left(i\psi_L^{i\alpha\dagger}(x)\frac{d\psi_{i\alpha L}(x)}{dx} +\lambda_K\vec{S}_I\cdot\psi_L^{i\alpha\dagger}(0)\frac{1}{2}\vec{\sigma}_\alpha^\beta\psi_{i\beta L}(0)\right). \tag{3.6}$$

The Hamiltonian in the form of Eq. (3.6) is useful because it is then possible to write the free-fermion Hamiltonian in the so-called Sugawara form, which is a sum of three commuting terms, quadratic, respectively, in charge, spin, and channel (or flavor) currents. Indeed, the entire Hamiltonian $\mathcal{H}$ may be written in the Sugawara form at the low-temperature fixed point. To see this, note that the Kondo interaction involves only the spin current. Fourier transforming on a finite line segment $-l\leq x\leq l$ of length $2l$ (with, for convenience, antiperiodic boundary conditions) the spin part of the Hamiltonian (which contains the Kondo interaction) becomes

$$\mathcal{H}_s = \frac{v_F\pi}{l}\left(\sum_{n=-\infty}^{\infty}\frac{1}{2+k}:\vec{J}_{-n}\cdot\vec{J}_n: +\lambda_K\sum_{n=-\infty}^{\infty}\vec{J}_n\cdot\vec{S}_I\right). \tag{3.7}$$

Here the $\vec{J}_n$'s are Fourier modes of the spin current operator

$$\vec{J}_L(x) = \frac{1}{2}\psi_L^{i\alpha\dagger}(x)\vec{\sigma}_\alpha^\beta\psi_{i\beta L}(x) \tag{3.8}$$

and the ":" denotes normal ordering. The Fourier modes obey the SU(2)-"level"-k Kac-Moody commutation relations

$$[J_n^a,J_m^b] = i\epsilon^{abc}J_{n+m}^c + \frac{k}{2}n\delta^{ab}\delta_{n+m,0}. \tag{3.9}$$

The crucial point to derive from the above observations is as follows: When $\lambda_K = 2/(k+2)$ (which corresponds to the low-temperature fixed point), the interacting spin Hamiltonian of Eq. (3.7) becomes equivalent to the free-spin Hamiltonian when written in terms of the shifted current operators

$$\vec{\mathcal{J}}_n = \vec{J}_n + \vec{S}_I, \tag{3.10}$$

which obey the same Kac-Moody algebra as the free operators [specified by Eq. (3.9)]. (This point can be verified by writing out the Sugawara form spin term corresponding to $\vec{\mathcal{J}}$ and expanding the square.) Since the spectrum of the Hamiltonian is determined by the Kac-Moody commutation relations, it follows that, at the low-temperature fixed point we obtain simply a spectrum described by the same Kac-Moody algebra as the free fermions.

B. Spectra of the Hamiltonian: Fusion rules

The spectrum of a conformal field theory consists of sets of states with integer spaced energy levels (in units of $v_F\pi/l$ where l is the length of the system) known as "conformal towers." In the SU(2) case these conformal towers are labeled uniquely by the spin j of the lowest

energy state. At level k, there is one conformal tower for each $j = 0, 1/2, \ldots, k/2$. (Note that j is the spin of the lowest-energy state within a given conformal tower; in general, the higher energy states have different spin.)

In the U(1)×SU(2)×SU(k) case we will obtain a set of conformal towers as the levels deriving from the direct product of charge, spin, and flavor states. The structure of the conformal towers is completely determined by the Kac-Moody commutation relations. However, the *combinations* of spin, charge, and flavor towers, which actually occur in the physical spectrum are determined by auxiliary conditions that derive from the boundary conditions. In the free-fermion problem, selection rules determine which direct products of charge, spin, and flavor conformal towers occur. These rules can be derived from Fermi statistics as we show in Sec. V for $k = 2$ channels. At the low-temperature fixed point these selection rules are modified. Thus the low-energy spectrum will be completely determined if we can somehow find these modified selection rules.

The above transformation from $\vec{J}$ to $\vec{\mathcal{J}}$ [Eq. (3.10)] suggested the "fusion rule" hypothesis, which we now describe. Upon absorption of an impurity of spin s (by the shift of $\vec{J}$ to $\vec{\mathcal{J}}$), each conformal tower corresponding to a lowest-energy state of spin j, gets replaced by the set of conformal towers with spin

$$j' = |j - s|, |j - s| + 1, \ldots, \min\{j + s, k - j - s\}. \tag{3.11}$$

These "fusion rules"[24] are a generalization (actually a restriction) of the ordinary SU(2) angular-momentum addition rules. Note in particular that they ensure that we never obtain a conformal tower of spin $j > k/2$, consistent with the fact that such towers cannot exist in the level-k theory. Precisely these fusion rules have been shown[24] to govern the operator product expansion in the conformal field theory. Our new hypothesis of Ref. 4 was that they also govern the process of absorption of an impurity spin.

By now this fusion rule hypothesis has been rather convincingly verified. In the simple exactly screened case ($k = 2s$) the fusion rules imply[4] the standard local Fermi-liquid theory for the excitation spectrum associated with the low-temperature fixed point. In the simplest overscreened case $k = 2$, $s = 1/2$ they agree excellently with the approximate spectrum determined by Wilson's NRG method, as discussed in Ref. 5 and as we shall demonstrate more extensively later in this paper. Furthermore, the universal[6] ground-state entropy $\Delta S = \ln g$ inferred with the use of the fusion rule agrees exactly with the Bethe-ansatz result for all values of k and s. This is a nontrivial result given the generally noninteger value of g.[6]

C. Symmetry-breaking perturbations

While the spectrum, entropy, and asymptotic correlation functions are determined completely by this exact description of the low-temperature fixed point, many other properties, such as the specific heat, susceptibility and temperature-dependent scattering rate, are determined by the leading irrelevant operator. In this case, the effective Hamiltonian has the form of the free one (with impurity absorbed) plus an irrelevant term of the form

$$\delta\mathcal{H} = \lambda\mathcal{O}(0), \tag{3.12}$$

where $\mathcal{O}$ is a local operator in the Kac-Moody theory evaluated at the origin. Such operators are referred to as *boundary operators*. Note that the impurity spin has disappeared from our description of the low-temperature fixed point, being absorbed in the redefined spin current. Hence, the irrelevant boundary operators are simply those of the appropriate Kac-Moody theory.

The *boundary* operators that exist in the theory can be made to correspond to the various states in the conformal towers for a particular set of boundary conditions, and their scaling dimensions are thus completely determined by the Sugawara Hamiltonian. An elegant way of determining *these* boundary conditions is by making a conformal mapping. For the present problem we can map the Kondo problem on the semi-infinite plane (i.e., $-\infty < \tau < \infty$, $x \geq 0$) to a problem on a semi-infinite strip. The allowed operators in the first geometry are in one-to-one correspondence[25] with the allowed states in the second. The strip problem has "Kondo" boundary conditions at each end of a finite line segment, corresponding to an impurity spin of size s at each end of the line. This spectrum is obtained[5,8] by applying the fusion rules twice, once for each impurity spin. This procedure determines the complete spectrum of boundary operators ("the boundary operator content") at the low-temperature fixed point.

The set of boundary operators consists of primary fields and descendants, being in one-to-one correspondence with the lowest-energy states of the conformal towers and the higher-energy ones, respectively. Labeling the dimension of a primary field by Δ, the nth-order descendants have dimension $\Delta + n$. The primary fields of the spin sector are uniquely labeled by their spin, j. Their dimensions are $\Delta_j = j(j + 1)/(k + 2)$. Likewise we have charge and flavor primary fields (and their descendants). Which combinations of *spin, charge,* and *flavor* fields can occur, is determined by the free-fermion selection rules together with the modification corresponding to the double fusion process outlined above.

Let us determine, as a first example, the leading irrelevant operator, which describes corrections to scaling at the low-temperature fixed point (Ref. 5). It cannot be a primary field, since these all have nonzero spin, flavor, or charge quantum numbers. Rather it is a spin descendant of the primary field of spin $j = 1$ denoted by $\vec{\phi}$. A singlet first-order descendant of $\vec{\phi}$ is obtained by "raising" the primary field with the spin-current operator $\vec{\mathcal{J}}$, i.e., $\mathcal{O} = \vec{\mathcal{J}}_{-1} \cdot \vec{\phi}$. The operator $\mathcal{O}$ has dimension $\Delta = 1 + \Delta_1 = 1 + 2/(k + 2)$. This is the lowest-dimension singlet operator in the theory (apart from the identity operator). It exists for all $k \geq 2$. It is irrelevant, since $\Delta > 1$. Of course we must check that this operator is actually in the spectrum, as determined by the above fusion rules. This is shown as follows: The free-fermion

spectrum always contains the identity operator. Labeling arbitrary primary fields by spin (j), charge (Q), and flavor (ρ) quantum numbers (j,ρ,Q), the identity operator is $(0,0,0)$. The first application of the fusion rules for an impurity of size s, maps this operator into $(s,0,0)$. The second application of fusion gives the set of operators $(j,0,0)$ with $j=0,1,2,\ldots,\min\{2s,k-2s\}$. Thus, in all overscreened cases, $k>2s$, the $(1,0,0)$ operator is in the spectrum, and so its singlet descendant can appear as an irrelevant operator in the Hamiltonian. [Notice that in the Fermi-liquid situation, $k=2s$ (complete screening), only the identity occurs, and the leading irrelevant operator is in fact the second-order descendant $\vec{J}\cdot\vec{J}$ (see Refs. 3 and 5).]

We now wish to determine the effect of various types of anisotropy on the low-temperature fixed point, using the knowledge about the complete spectrum of boundary operators, which are possible at the Kondo boundary (as obtained from the double fusion rule, just described). Our strategy is simple. Breaking some symmetry in the underlying microscopic Hamiltonian may allow some other operator to appear at the fixed point. The set of possible operators is determined by the Kac-Moody structure and the double fusion rule, together with symmetry conditions. An example of the application of symmetry conditions occurred above. Even though the $j=1$ spin-primary field exists, it could not itself appear in the Hamiltonian, since it is not rotationally invariant, and thus only its singlet descendants appeared. In general, if an operator of dimension $\Delta<1$ is permitted, when the symmetry is broken, then this symmetry breaking is *relevant*. If all operators that are allowed when the symmetry is broken have $\Delta>1$, then symmetry breaking is *irrelevant*.

Apart from the spin-SU(2) and flavor-SU(k) symmetries it is time reversal, $\mathbf{T}$, which is important for this discussion. $\mathbf{T}$ is the anti-unitary operator, which maps the impurity spin operator into minus itself. It acts on the fermion fields at the origin as

$$\mathbf{T}:\psi_{i\alpha}(0)\rightarrow(\sigma^2)^{\beta}_{\alpha}\psi_{i\beta}(0). \tag{3.13}$$

The spin-rotation by σ^2 is neccessary so that

$$\psi^{i\alpha\dagger}\vec{\sigma}^{\beta}_{\alpha}\psi_{i\beta}\rightarrow\psi^{i\alpha\dagger}(\sigma^2)^{\gamma}_{\alpha}\vec{\sigma}^{*\delta}_{\gamma}(\sigma^2)^{\beta}_{\delta}\psi_{i\beta}\rightarrow-\psi^{i\alpha\dagger}\vec{\sigma}^{\beta}_{\alpha}\psi_{i\beta}. \tag{3.14}$$

In general, $\mathbf{T}$ changes the sign of (Hermitian) operators of odd-integer spin but leaves invariant Hermitian operators of even-integer spin.

We now discuss the interesting symmetry-breaking perturbations in turn: *flavor symmetry breaking, anisotropic Kondo interaction and external field* .

Flavor symmetry breaking (by flavor-anisotropic Kondo interaction or flavor-field): To take a simple example, consider $k=2$ channels and a $s=1/2$ impurity; the flavor symmetry group then is also SU($k=2$). Thus we add a symmetry-breaking perturbation to the Kondo interaction of the form

$$\delta\mathcal{H}=\lambda'\vec{S}_I\cdot[\psi^{i\alpha\dagger}_L(0)\tfrac{1}{2}(\sigma^3)^{j}_{i}\vec{\sigma}^{\beta}_{\alpha}\psi_{j\beta L}(0)]. \tag{3.15}$$

This anisotropy breaks the *flavor*-SU(2) symmetry down to a U(1) subgroup. No primary fields (other than the identity) from the *spin* sector are possible, since the SU(2)-spin symmetry remains unbroken; however, it is now possible to have a primary field from the flavor sector. For $k=2$ the set of flavor primary fields is the same as for spin, except that the selection rules are different. The flavor quantum number label, ρ becomes a "flavor-spin" label, j_f. The relevant operator, which may be allowed in the presence of the flavor anisotropy in Eq. (3.15) is the three-component of $(j,j_f,Q)=(0,1,0)$, of dimension 1/2. (Note that such a term arises in practice for quadrupolar Kondo systems because of the virtual polarization of excited magnetic configurations by an applied magnetic field—the exchange integral splitting is proportional to the field strength.)

We must check that this operator is indeed in the spectrum predicted by the double fusion rule. The free-fermion theory for $k=2$ contains the $(1,1,0)$ field, $\psi^{\alpha,i\dagger}(\sigma^a)^{\beta}_{\alpha}(\sigma^A)^{j}_{i}\psi_{\beta,j}$. The first fusion (with impurity spin $s=1/2$) maps the $j=1$ operator into $j=1/2$. The second fusion maps $j=1/2$ into $j=0$ and $j=1$. Thus the $(1,1,0)$ operator gets mapped into $(0,1,0)$ and $(1,1,0)$. The first of these is the pure flavor primary field mentioned above. Of course, it is not permitted by the SU(2) flavor symmetry in the flavor-symmetric case [i.e., when $\lambda'=0$ in Eq. (3.15)]; however, the flavor-anisotropic interaction breaks the SU(2)-flavor symmetry and the third component of the flavor triplet operator ϕ^3_f is allowed to appear. Moreover, this is not forbidden by time-reversal symmetry $\mathbf{T}$ [see Eq. (3.13)], since it transforms the same way as the fermionic bilinear: $\psi^{i\alpha\dagger}_L(\sigma^3)^{j}_{i}\psi_{L\alpha j}$, namely, it goes into itself, since σ^3 is real. In conclusion, flavor anisotropy is *relevant* in this case.

Nozières and Blandin pointed out the above result long ago.[13] The physical picture is that if one channel couples more strongly to the impurity, then the screening is fully accomplished by that channel. This leads to a one-channel, Fermi-liquid fixed point, with the second channel unaffected by the impurity in the low-temperature limit. The strongly coupled channel has a phase shift of $\pi/2$, while the weakly coupled one is not phase shifted in the low-temperature spectrum. We shall discuss this further when we explicitly compare energy levels with the numerical renormalization-group results. It is interesting to observe that the "ground-state degeneracy," i.e., $\lim_{T\rightarrow0}\lim_{l\rightarrow\infty}e^{S(T,l)}$, decreases from $\sqrt{2}$ to 1 upon addition of flavor symmetry breaking; this is an illustration of the "g theorem."[6]

As another example, we consider flavor anisotropy in the case $k=2$, $s=1$. Beginning again with the $(j,j_f,Q)=(1,1,0)$ operator, the first fusion gives $1\rightarrow0$ *only*, for an $s=1$ impurity and the second $0\rightarrow1$. Thus we do not obtain $(0,1,0)$ in this case. We do, however, obtain the identity operator, $(0,0,0)$ as always. The most relevant field is then a level-one descendant of the identity, the flavor-current operator $J^3_f(0)$, of dimension $\Delta=1$. This operator is marginal. Furthermore, it does not renormalize, since there are no connected n-point Green's functions with $n\geq3$ involving only J^3_f. This

corresponds to a potential scattering term with opposite signs for the two channels. It corresponds to the physical picture of the "two-stage" Kondo effect. The more strongly coupled channel first screens the impurity spin from $s = 1$ down to $s = 1/2$. At a lower temperature scale, the second channel screens the remaining $s = 1/2$. The phase shift in the two channels is $\pi/2 \pm \lambda'/T_K$. In this case the ground-state degeneracy remains unchanged at 1.

As another example we consider for $k = 2$ channels an external channel field applied directly at the impurity site, i.e.,

$$\delta\mathcal{H} = \lambda' \psi_L^{i\alpha\dagger} (\sigma^3)_i^j \psi_{j\alpha L}. \tag{3.16}$$

This breaks the symmetry in precisely the same way as the flavor-symmetry-breaking exchange term discussed above, so it has the same consequences. The physical picture is similar. Giving one channel a lower potential energy at the impurity site causes that channel to screen the impurity. We expect the resulting stable fixed point to be the same as for flavor-symmetry-breaking exchange. For $s = 1/2$, one channel suffers a $\pi/2$ phase shift and the other is unaffected by the interaction.

Anisotropic exchange in spin space. Now, we consider anisotropic exchange in *spin* space, for *general values of* k *and* s, expressed through the perturbation

$$\delta\mathcal{H} = \lambda' [\psi_L^{\alpha i\dagger} (\sigma^3)_\alpha^\beta \psi_{L\beta i}] S_I^3. \tag{3.17}$$

This perturbation breaks the *spin*-SU(2) symmetry down to U(1) (rotations about the 3 direction in spin space). It might appear that the $j = 1$ spin-primary field, ϕ^3, is then allowed by symmetry. However, this is not the case because anisotropic exchange is *even* under time-reversal $\mathbf{T}$, whereas $\vec{\phi}$ is odd. The lowest dimension $\mathbf{T}$-even primary field is the $j = 2$ primary field, which transforms like a quadrupolar tensor of the spin variable. The corresponding $j = 2, m_j = 0$ component operator ϕ^{33} is allowed in the Hamiltonian by all remaining symmetries and appears as a likely candidate for the fixed-point perturbation corresponding to Eq. (3.17).

However, we must check to see if this primary boundary operator exists according to the double fusion rule. We first note that this operator is only present as a primary field in the Kac-Moody theory for $k \geq 4$. In this case we must check if the $(2,0,0)$ operator occurs from double fusion. It can be shown[26,4,5] that the only primary operator in the free-fermion spectrum of the form $(j,0,0)$ is the singlet, $j = 0$. At the first stage of the double fusion state $0 \rightarrow s$. At the next stage $s \rightarrow 1, 2, \ldots, \min\{2s, k-2s\}$. The $(2,0,0)$ primary field occurs if and only if

$$2 \leq 2s, \quad 2 \leq k - 2s. \tag{3.18}$$

These two inequalities can be written as $s > 1/2$ and $s < k/2 - 1/2$. Thus the $(2,0,0)$ primary field occurs in all overscreened multichannel cases, except in the two cases of minimal and maximal spin, $s = 1/2$ and $s = k/2 - 1/2$. It is a relevant field for all cases $k \geq 5$, $1/2 < s < k/2 - 1/2$, and is marginal for $k = 4$, $s = 1$. When $s = 1/2$ or $s = k/2 - 1/2$, the lowest-dimension operator generated by exchange anisotropy is the *irrelevant* boundary operator, $\mathcal{J}_{-1}^3 \phi^3$. This is part of $\vec{\mathcal{J}}_{-1} \cdot \vec{\phi}$, which occurs in the absence of anisotropy. It has dimension $\Delta = 1 + 2/(k+2)$.

Local magnetic field. As our next example, we consider a local magnetic field (acting on the impurity only), i.e.,

$$\delta\mathcal{H} = -h S_I^z. \tag{3.19}$$

This perturbation is similar to the case of exchange anisotropy [Eq. (3.17)] except that now time-reversal symmetry, $\mathbf{T}$, is broken. In this case the $(j, j_f, Q) = (1,0,0)$ primary field, of dimension $\Delta = 2/(k+2)$, is allowed by symmetry. As discussed above, this is always allowed by the double fusion rule in overscreened cases. Indeed, its descendant is the dominant irrelevant operator even without anisotropy. Therefore, h is a *relevant* perturbation, having scaling dimension $h \propto (\text{length})^{-k/(k+2)}$.

We can make a natural conjecture about the fixed point to which the system flows in this case, by considering the limit of very strong magnetic field $h \rightarrow \infty$: By Eq. (3.19), the impurity spin then becomes polarized in the z direction (i.e., its Hilbert space reduces to one state, spin up). The Kondo interaction with a polarized impurity then reduces to a simple potential scattering problem with a potential of opposite sign for spin up and spin down:

$$s\lambda_K \psi_L^{\alpha i\dagger} (\sigma^z/2)_\alpha^\beta \psi_{L\beta i}. \tag{3.20}$$

Note that the Kondo interaction λ_K is *finite* at the zero field (non-Fermi-liquid) fixed points, so that the effective local field off which the conduction electrons scatter has a finite magnitude. For very strong fields h the value of λ_K occurring in the effective field should be the bare value. There is thus a phase shift $\delta^\pm = \pm \tan^{-1}(\pi s \lambda_K/2)$ for up- and down-conduction electrons, respectively. For somewhat weaker fields, we must include renormalization of the Kondo interaction, λ_K, in order to determine the effective local field $s\lambda_{K,\text{eff}}(h)$ occurring in Eq. (3.20). This can be determined as follows: The infrared divergence of perturbation theory in λ_K is cut off at the energy scale $|h|^{k/(k+2)}$. Thus, reducing the cutoff further does not change λ_K any more as opposed to the zero-field case, $h = 0$, where λ_K approaches the fixed-point value upon further reduction of the cutoff. So $\lambda_{K,\text{eff}}(h)$ is essentially just the effective (i.e., renormalized) Kondo coupling at scale $|h|^{k/(k+2)}$, as determined from the renormalization group in the absence of the field h. Essentially, the coupling continues to renormalize as in the zero-field theory as we lower the ultraviolet cutoff until the latter reaches a value of order $|h|^{k/(k+2)}$. At this point further renormalization stops, and furthermore, spin-flip processes become unimportant because all states with the impurity spin polarized have large energies on the cutoff scale. Thus we may simply drop the spin-flip part of the Kondo interaction and replace λ_K by $\lambda_{K,\text{eff}}$ in the potential scattering part (z component). Actually, if h is too large,

$h \approx J$, the renormalized $\lambda_K(h)$ appearing in the phase shift becomes somewhat different than the one defined at zero field; see the discussion in Sec. V. It is very important that $\lambda_{K,\mathrm{eff}}(0)$ is not infinite, as in the Fermi-liquid Kondo fixed points, but takes on a finite value. Thus we expect some intermediate phase shift (i.e., neither zero nor $\pi/2$) in the limit $h \to 0$ taken at *zero temperature*. Adding an infinitesimal field provides a way of measuring $\lambda_{K,c}$, the value of λ_K at the nontrivial critical point. What value should we expect it to have? In general this is unclear, since this value is, in general, not universal. In particular, note that defining $\lambda_{K,c}$ from completing the square in the Sugawara Hamiltonian gives a finite value at the Fermi-liquid fixed points unlike the infinite value obtained from the phase shift definition. There are, however, two special cases where something can be said. In the large-k limit, the critical coupling can be calculated perturbatively, and has the value: $2/k$, so we obtain a small phase shift, $\pi s/k$. (The calculation of $\lambda_{K,c}$ in this case was first performed by Nozières and Blandin.[13] For a review of the calculation, correcting a factor of 2 error, see Ref. 5.) The other special case is $s = k/4$, which happens to include the case $k = 2$, $s = 1/2$ describing the quadrupolar Kondo effect. The unstable infinite-coupling fixed point, $\lambda_K = \infty$, has a decoupled[13] spin of magnitude $k - s/2 = s$ just as at the unstable zero-coupling fixed point. Indeed there appears to be a type of symmetry between zero and infinite coupling, when $s = k/4$, as was observed in Ref. 7. Thus it seems reasonable that the fixed-point value of λ_K should be exactly half way between zero and infinity. This corresponds to an effective field, which produces a phase shift of $\pm\pi/4$, of opposite sign for spin up and down. This is half way between the zero phase shift occurring at zero coupling and the $\pi/2$ phase shift at infinite coupling. (We note that a phase shift of $\pi/2k$ has been predicted in the context of the theory of electron assisted tunneling in two-level systems models, which map onto the k-channel $s = 1/2$ problem for conduction electrons with spin $k/2$.[27] The above arguments confirm this value for the two special cases: $k = 2$ and $k \to \infty$.) As we increase h, we expect $\lambda_{K,\mathrm{eff}}(h)$ to flow according to the renormalization group. At small h this initial flow is determined by the dimension of the coupling constant $(\lambda_{K,c} - \lambda_K)$ of the leading irrelevant operator, which, as discussed in the beginning of this section, is $-2/(k+2)$. Thus we predict $[\delta(0) - \delta(h)] \propto |h|^{2/k}$ (or $|h|ln|h|$ for $k = 2$) as $h \to 0$.

Explicitly, in the case $k = 2$, $s = 1/2$, for very weak field, we predict a spectrum, which corresponds to a Fermi liquid with a phase shift of $\pm\pi/4$ for spin up and down, i.e., an energy shift of $\pm(v_F\pi/l)j_c^z/2$, together with a shift of the total j^z quantum number reflecting the presence of the polarized impurity spin: $j^z = j_c^z + 1/2$, in the limit of zero applied field. Upon increasing the field, the magnitude of the phase shift changes, initially as $|h|\ln|h|$, saturating at a value of $\pm\tan^{-1}(\pi\lambda_K/4)$, where λ_K is the bare Kondo coupling. This is precisely what is observed numerically. (See Sec. V.)

The zero-temperature entropy is zero, since the impurity spin has a unique ground state, and a Fermi liquid has zero residual entropy regardless of the phase shift.

IV. NUMERICAL RENORMALIZATION-GROUP (NRG) APPROACH

In this section we briefly discuss the NRG method for treating the two-channel Kondo model with and without perturbation terms of the form discussed in the previous section. We also discuss how the effective single-particle levels in the applied magnetic field can be derived and how this information may be utilized to extract the field-dependent phase shifts discussed in the preceding section.

A. Overview of the NRG approach

In the NRG approach, Eq. (1.1) is first logarithmically discretized. For a more detailed discussion, see Sec. II of Ref. 28. Here is a brief outline of the discretization procedure: (i) Divide the conduction band into logarithmic intervals, e.g., $\Lambda^n D$ to $\Lambda^{n+1} D$, with D the bandwidth and $\Lambda > 1$; (ii) keep only the average states in each interval (those are the ones that couple to the impurity); (iii) for numerical convenience convert to a tridiagonal basis via the Lanczos algorithm with the initial state being the Wannier orbital about the impurity site. The Lanczos states correspond to electron annihilation operators $f_{0,\alpha,i}, f_{1,\alpha,i}, \ldots$ and have radial extent $\Lambda^{1/2}, \Lambda^{3/2}, \ldots$ times k_{Fermi}^{-1} about the impurity. The final Hamiltonian has the form

$$\mathcal{H}_{\mathrm{NRG}}/D = \sum_{n=0}^{\infty} t_n (f_n^{\alpha,i\dagger} f_{n+1,\alpha,i} + \mathrm{H.c.}) + (1/2)\lambda_K f_0^{\alpha,i\dagger} \vec{\sigma}_\alpha^\beta f_{0,\beta,i} \cdot \vec{S}_I, \tag{4.1}$$

where

$$t_n = \frac{\Lambda^{-n/2}(1+\Lambda^{-1})(1-\Lambda^{-(n+1)})}{2[(1-\Lambda^{-(2n+1)})(1-\Lambda^{-(2n+3)})]^{1/2}}. \tag{4.2}$$

Note that (a) one may view the t_n as measuring the hopping strength in the "onion-skin basis" of radial states between the state at radial position n and at $n+1$, (b) in a rather different way than discussed in the previous section one arrives at an effective $(1+1)$-dimensional problem, (c) in the limit of $\Lambda \to 1$, the approximation of (ii) in the above paragraph becomes exact—the full continuum of levels is recovered, and (d) at finite Λ there may be Λ-dependent renormalizations of various quantities, which one must attempt to determine for comparison with exact results from other methods. This point will be made clearer in the next section where the current algebra results are compared with those of the NRG.

The next step in the NRG is iterative diagonalization. Wilson has shown that one realizes a renormalization-group transformation of Eq. (4.1) by truncating the sum in that equation at a finite number of onion-skin shells, say N, and adding the hopping term to the next shell. More precisely, the addition of two hopping terms takes one from a system of radial extent $R_N \simeq \Lambda^{(N+1)/2} k_{\mathrm{Fermi}}^{-1}$ to one of size $\simeq \Lambda R_N$. It is necessary to distinguish between the spectra for even and odd N, since the fixed points are generically different, as we shall discuss further in the next section of the paper. Increasing N by iter-

atively diagonalizing the sequence of Hamiltonians specified by the transformation corresponds to lowering the temperature of the system. A fixed point of the transformation is obtained if the resulting spectrum of energy levels remains unchanged upon successive iterations of even or odd N. A well-defined procedure exists for constructing basis states of the enlarged Hamiltonian from those at the current iteration number, as discussed extensively in Refs. 28 and 20.

Of course, even with the approximation of the logarithmic discretization and tridiagonalization procedure discussed above taken together with maximal block diagonalizing of $\mathcal{H}_{\rm NRG}$, the sequence of Hamiltonians generates matrices far too large to diagonalize completely. A practical way of implementing this transformation, while keeping manageable numerics is to retain only the lowest few hundred states at each iteration. While there is no direct proof that this approximation is reliable, *a posteriori* confirmation by comparison with other exact methods has confirmed the overall reliability of the method. In numerical calculations discussed here run on a Sun-4 workstation, we have retained the lowest 250 states at each N value. (Data obtained with the lowest 1000 levels at each N value from runs on a Cray Y-MP48 supercomputer show no significant difference from the runs with fewer states.)

We have calculated our energy levels out to 14 significant figures, and when different symmetry labeled states are reported degenerate, that is typically to an accuracy of 12 decimal places.

We label our states in the NRG approach with the separate axial charges of the two channels and the total azimuthal spin quantum number j^z. There is a useful feature of the choice of the U(1)×U(1) axial charge subgroup of SO(5) with quantum labels $(\mathcal{I}_1^3, \mathcal{I}_2^3, j^z)$: application of impurity site spin fields, flavor fields, or exchange anisotropy will not lift the separate U(1) axial-charge symmetries of the two channels or break the total U(1) symmetry of j^z, so that the same classification scheme may be used in the presence of these perturbations. In contrast, either the full SU(2) spin or flavor symmetries will be broken by application of these perturbing fields. Thus, no modification of the basic code is required to treat these perturbations.

B. Free-particle levels in the NRG in the presence of potential scattering

As discussed in the preceding section, we anticipate that the finite-size spectra in the presence of an applied spin field corresponds to a phase-shifted free-particle spectra, with the phase shifts of up- and down-spin electrons being equal and opposite. The NRG results for phase-shifted single-particle spectra have been well studied in the context of the x-ray edge problem.[29] We summarize the results here.

Consider electrons with down spin in an applied local field along the $+z$ direction. As discussed in Sec. III C, we expect this to map onto the problem of spinless fermions in the presence of a potential scattering center with dimensionless coupling strength $\lambda_{K,\rm eff}(h)/4$ (for $s = 1/2$). For even number of onion-skin shells arising from odd iteration number N in the renormalization group, it is found that the energy for adding a single particle or hole in the mth excited level when $1 << m << N$ is given by

$$\eta_m^{(\pm)}(\delta_\Lambda) = \Lambda^{m-1\mp\delta_\Lambda/\pi}, \tag{4.3}$$

where the upper (lower) sign obtains for particles (holes). and η is a rescaled dimensionless quantity proportional to the energy, e:

$$\eta_m^{(\pm)}(\delta_\Lambda) = \frac{2\Lambda^{(N-1)/2} e_m^{(\pm)}(\delta_\Lambda)}{D(1+\Lambda^{-1})}. \tag{4.4}$$

The phase shift that appears in the exponent is determined by the strength of the potential scattering $\lambda_{K,\rm eff}(h)/4$ through the formula

$$\delta_\Lambda = \tan^{-1}\left(\frac{\pi\lambda_{K,\rm eff}(h)}{4A_\Lambda}\right), \tag{4.5}$$

where

$$A_\Lambda = \frac{(1+\Lambda^{-1})\ln(\Lambda)}{2(1-\Lambda^{-1})}. \tag{4.6}$$

Note that A_Λ tends rapidly to unity as $\Lambda \to 1$ so that the above equation simply reproduces the phase shift formula derived from the T matrix of a potential with strength $\lambda_{K,\rm eff}/4$. Experience shows that this form for $\eta_m^{(\pm)}$ typically holds at better than 1% accuracy for $3 \le m \le (N-3)/2$. Notice that an attractive phase shift pulls particle excitation energies down and pushes hole excitation energies up as one would expect. For odd number of onion-skin shells and even N, one has for $1 << m << N$

$$\eta_m^{(\pm)} = \Lambda^{m-1/2\mp\delta_\Lambda/\pi}, \tag{4.7}$$

which holds with comparable accuracy to the odd-N case.

In addition to this manifestation of the phase shift in the exponent of rather highly excited levels, we find numerically that the following relation holds for the first excited particle-hole levels when N is odd (even number of onion-skin shells)

$$\eta_1^{(\pm)}(\delta_\Lambda) = 2\eta_0\left(\frac{1}{2} \mp \frac{\delta_\Lambda}{\pi}\right) \tag{4.8}$$

provided δ_Λ is sufficiently smaller than $\pi/2$ in magnitude. Here η_0 is the first scaled excitation energy for odd N in the absence of potential scattering. For odd number of shells and even N, one state sits precisely at the Fermi energy for vanishing λ_K. We find from studying the spectra as a function of coupling strength, that for $\lambda_{K,\rm eff}$ sufficiently large, the first hole excitation occurs approximately at

$$\eta_1^{(-)}(\delta_\Lambda) \approx 2\eta_0\left(\frac{\{1+\mathrm{sgn}[\lambda_{K,\rm eff}(h)/4]\}}{2} + \frac{\delta_\Lambda}{\pi}\right) \tag{4.9}$$

and the first particle excitation occurs at

$$\eta_1^{(+)}(\delta_\Lambda) \approx 2\eta_0 \left(\frac{\{1 - \mathrm{sgn}[\lambda_{K,\mathrm{eff}}(h)/4]\}}{2} - \frac{\delta_\Lambda}{\pi} \right). \tag{4.10}$$

Note that in each case the lowest particle and hole excitations sum to $2\eta_0$, which identifies this scaled energy with $v_F\pi/L$ in the conformal theory. Thus any excitation processes involving the first excited particle or hole levels within conformal theory and NRG in the presence of finite potential scattering should agree within an overall scale factor, while any involving the second excited particle or hole levels will explicitly disagree.

The above relations (4.8)–(4.10) for the lowest excitations break down whenever there is a zero mode, i.e., for $\lambda_K = 0$ and even N, and for $\lambda_{K,\mathrm{eff}}(h) = \infty$ and odd N. On the other hand, the formulas (4.4)–(4.7) relating intermediate level particle and hole excitation energies to the phase shifts through exponentiation are accurate for all $\lambda_{K,\mathrm{eff}}(h)$. Unfortunately, due to the matrix truncation process, it is practically difficult to reliably estimate the intermediate energies where the formulas of Eqs. (4.4)–(4.7) hold. Thus, the procedure we have settled on is to match our η_0 values to those for a single-particle spectrum possessing the same overall phase shift and then apply Eqs. (4.8)–(4.10).

V. COMPARISON OF CFT AND NRG APPROACHES

In this section we compare finite-size spectra and scaling indices derived from the CFT approach discussed in Sec. III and the NRG method discussed in Sec. IV. The explicit comparisons are all for the model with $k = 2$, $s = 1/2$.

Free fermion spectrum. The low-energy excitations of a Fermi gas on a line of length l with some choice of boundary conditions and Fermi energy, can, of course, be obtained by elementary methods as we now show for $k = 2$ channels. The total energy E is the sum of the energies of the four species of fermions with quantum numbers $(j^z, j_f^z) = (\alpha, i) = (\pm 1/2, \pm 1/2)$. There are two different particle-hole symmetric spectra, depending on our choice of boundary conditions. When the free fermions are put on a lattice, a *nondegenerate* ground state arises for an even number of sites and the same boundary conditions on both ends: i.e., a vanishing wave function or a vanishing derivative of the wave function (Fig. 1). When different boundary conditions are chosen on the two ends, a vanishing wave function at one end and a vanishing derivative at the other, we obtain the other spectrum with a 16-fold degenerate ground state (Fig. 2), corresponding to a $\pi/2$ phase shift of the single-particle wave functions. The situation is reversed for an odd number of lattice sites, where the *nondegenerate* ground state appears for different boundary conditions on the two ends. Note that on a lattice there is an even-odd alternation of the free spectrum, when the boundary conditions are held fixed. Finally, we observe that a free boundary condition is equivalent to a vanishing boundary condition with one additional "phantom" site added. The coupling

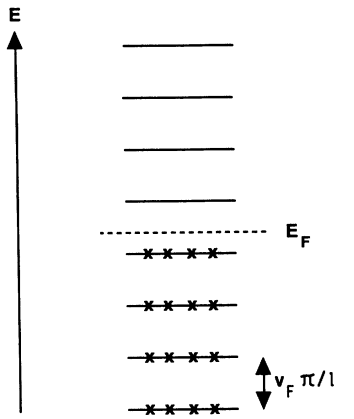

FIG. 1. Nondegenerate free-fermion ground state.

to this site has no effect because the fermion operator vanishes there. The NRG Hamiltonian corresponds to essentially this system, with free boundary conditions at both ends, at $\Lambda \to 1$. At the Nth iteration we have $N + 1$ sites so the degenerate ground state occurs for even iteration number. First focus on the spectrum with *nondegenerate* ground state (Fig. 1). The fermion levels near the Fermi energy have equal spacing, $v_F\pi/l$, and the zero of energy (Fermi level) lies symmetrically between two levels. The lowest excitations are one particle (or hole) excitations, having charge $Q = \pm 1$ and energy $lE/v_F\pi = 1/2$; there are four states (Fig. 3) forming a $(j, j_f) = (1/2, 1/2)$ multiplet of the direct product of spin and flavor SU(2) groups. (Note that we measure charge relative to that of the ground state.) The next excitations with $lE/v_F\pi = 1$ are two particle (or hole) excitations, having charge $Q = \pm 2$; by the Pauli principle there are $\binom{4}{2} = 6$ states (Fig. 4), forming a $(j, j_f) = (1, 0)$ and a $(0, 1)$ multiplet. At $lE/v_F\pi = 1$ there are in addition 16 particle-hole excitations, having $Q = 0$ (Fig. 5); they form $(j, j_f) = (0, 0), (1, 1), (0, 1), (1, 0)$ multiplets. Next, at $lE/v_F\pi = 3/2$ there are four three-particle (or hole) excitations, having charge $Q = \pm 3$ (Fig. 6), form-

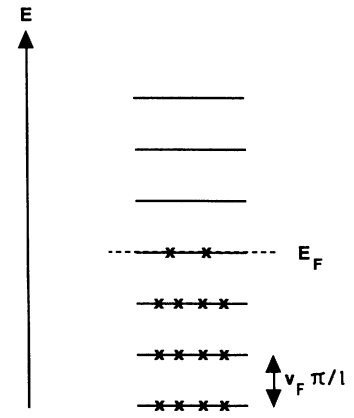

FIG. 2. Degenerate free-fermion ground states.

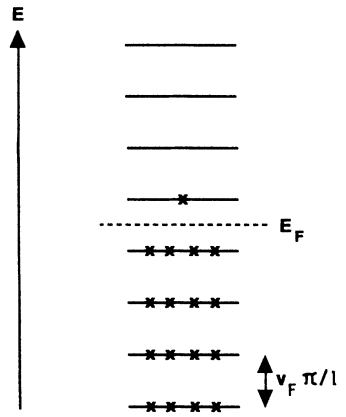

FIG. 3. One-electron excitation.

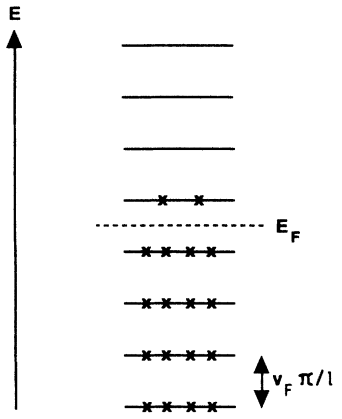

FIG. 4. Two-electron excitation.

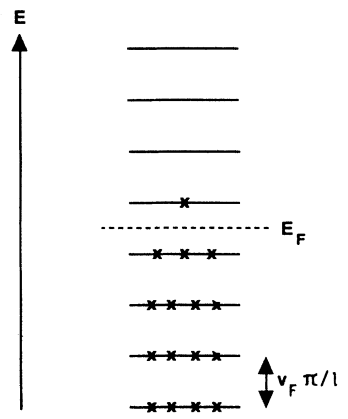

FIG. 5. One-electron, one-hole excitation.

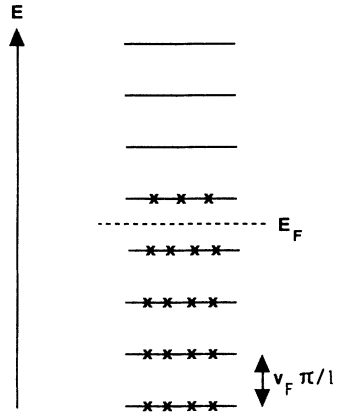

FIG. 6. Three-electron excitation.

ing a $(1/2,1/2)$ multiplet. In addition there four single-particle (or hole) states (Fig. 7), having $Q = \pm 1$, which form a $(1/2,1/2)$ multiplet. Furthermore, at $lE/v_F\pi = 3/2$, there are, $24 = 4\binom{4}{2}$ two-particle–one-hole states (Fig. 8) (or two-hole–one-particle), having $Q = \pm 1$, which form two $(j, j_f) = (1/2,1/2)$ and a $(3/2,1/2)$ as well as a $(1/2,3/2)$ multiplet. All other states have energy $lE/v_F\pi \geq 2$. All states of free fermions with $lE/v_F\pi \leq 3/2$ are listed in Table I for the case of non-degenerate ground state. As discussed in Sec. II these theories have an SU(2)× SO(5) symmetry. [Actually, in the free fermion case the full symmetry is SO(8), but only the SU(2)×SO(5) subgroup survives the Kondo interaction.] Thus we may reclassify levels according to SO(5) representations. The decomposition of SO(5) reps into $SU(2)_f \times U(1)$ reps is given in Table II labeling SO(5) representations by their dimensions. [4 is the spinor, 5 the vector, 10 the antisymmetric tensor, etc.] In Table III we give the free fermion spectrum using SO(5) reps.

This free fermion excitation spectrum can also be labeled using the CFT classification. In this case states come in conformal towers with energy spacing

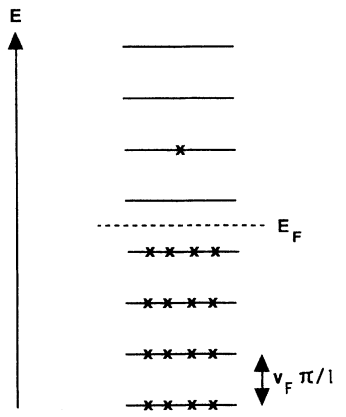

FIG. 7. Higher-energy one-electron excitation.

TABLE I. Spectrum of free fermions (nondegenerate ground-state case) for $El/v_F\pi \leq 3/2$ (descendant states denoted by ′).

Q	j	j_f	$El/v_F\pi$	D
0	0	0	0	1
±1	1/2	1/2	1/2	8
±2	0	1	1	6
±2	1	0	1	6
0	1	1	1	9
0′	0	0	1	1
0	1′	0	1	3
0	0	1′	1	3
±3	1/2	1/2	3/2	8
±1′	1/2	1/2	3/2	8
±1	1/2	(1/2)′	3/2	8
±1	(3/2)′	1/2	3/2	16
±1	1/2	(3/2)′	3/2	16
±1	(1/2)′	1/2	3/2	8

$\Delta lE/v_F\pi = 1$. The lowest state in each tower is known as a "primary" (or "highest weight") state and the rest as "descendants." Furthermore, the states are represented as products of charge, spin, and flavor states, with additive energies. Each of the three factors can be a primary or descendant. In Tables I and III we have denoted descendants by a ′. These results, together with the double fusion rule discussed in Sec. III C, provide the basis for understanding the energy levels of the strongly coupled system.

Now consider the free fermions with the other spectrum having a *degenerate* ground state. The low-lying spectrum, depicted in Table IV, can be obtained similarly to Table III. The ground state consists (Fig. 2) of

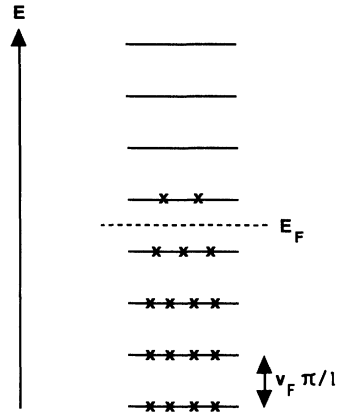

FIG. 8. Two-electron, one-hole excitation.

particle hole symmetric $(j, j_f) = (0,1),(1,0)$ multiplets of charge $Q = 0$, a $Q = \pm 2$ singlet $(j, j_f) = (0,0)$ and a $Q = \pm 1$ multiplet $(1/2, 1/2)$. [All charges are redefined by $Q \rightarrow (Q - 2)$, i.e., we take the zero of charge to be the symmetric choice where two of the four zero-energy fermion states are occupied.] All states with energy $lE/v_F\pi \leq 2$ are listed in Table IV using SO(5) reps and distinguishing primaries and descendants.

Non-Fermi liquid spectrum. The finite size results at the non-Fermi-liquid fixed point are presented in Table V. The first two columns give the spin j and SO(5) state labels. The third column lists the energy predicted by conformal theory in units of $v_F\pi/l$, and the fourth column lists the numerically derived NRG levels, scaled so the first excited splitting matches that of the conformal theory. The CFT predicts the same spectrum at the non-Fermi-liquid fixed point beginning with either a degenerate or a nondegenerate free-fermion spectrum, in agreement with the NRG observation.

TABLE II. Branching rules of SO(5) representations into representations of SU(2)×U(1) (flavor×charge) and SU(2)×SU(2) (isospin of each separate channel). As discussed in the text, SO(5) is an exact symmetry of the lattice Hamiltonian, which is preserved in the numerical renormalization-group calculations. We find that the lowest states to be compared between the conformal theory finite-size scaling and the NRG belong to the lowest-dimensionality SO(5) representations (excluding the 14-fold degenerate representation, which is absent from the lowest-energy spectra). We index the SO(5) representations by their dimensionality. For the SU(2)×U(1) labeled states, the first number in parentheses represents the flavor spin j_f and the second the charge Q. For the SU(2)×SU(2) isospin labeled states, the first number is the isospin $\mathcal{I}_1$ of channel 1 and the second is the isospin $\mathcal{I}_2$ of channel 2.

SO(5)=Sp(2)	SU(2)×U(1)	SU(2)×SU(2)
(Dimension)	(j_f, Q)	$(\mathcal{I}_1, \mathcal{I}_2)$
1	(0,0)	(0,0)
4	$(1/2, \pm 1)$	$(1/2,0) \oplus (0,1/2)$
5	$(1,0) \oplus (0, \pm 2)$	$(0,0) \oplus (1/2,1/2)$
10	$(0,0) \oplus (1,0) \oplus (1, \pm 2)$	$(0,1) \oplus (1,0) \oplus (1/2,1/2)$
14	$(2,0) \oplus (1,0) \oplus [2(0,0)] \oplus (0, \pm 2) \oplus (0, \pm 4)$	$(0,0) \oplus (1/2,1/2) \oplus (1,1)$
16	$(3/2, \pm 1) \oplus (1/2, \pm 3) \oplus (1/2, \pm 1)$	$(1/2,0) \oplus (0,1/2) \oplus (1,1/2) \oplus (1/2,1)$

TABLE III. Spectrum of free fermions (nondegenerate ground-state case) using SO(5) reps for $El/v_F\pi \leq 3/2$ (descendant states denoted by ′).

j	SO(5)	$El/v_F\pi$
0	1	0
1/2	4	1/2
1	5	1
0	(10)′	1
(1)′	1	1
1/2	(16)′	3/2
1/2	(4)′	3/2
(1/2)′	4	3/2
(3/2)′	4	3/2

Clearly the overall agreement is excellent. We note the following features: (i) Agreement with the conformal theory is better at lower energy scales. There are two contributing factors here—first, the logarithmic discretization provides an approximate uniform spacing of free-fermion levels at low-energy scales, but becomes less uniform the higher the energy. The second is the state truncation mentioned in Sec. IV A. This removes states of the same symmetry at high energies, which can mix with some of the low states. This problem is expected to be most severe as the discretization parameter tends to unity, which point we shall discuss further below. (ii) The NRG preserves degeneracies of SO(5) multiplets to 12 decimal places of numerical precision. This is to be expected because none of the approximations inherent in the NRG break SO(5). In particular, the truncation of the spectrum is always done at a gap between levels so it never breaks up SO(5) multiplets. On the other hand, it is particularly clear looking at the $1+1/8$ levels that the splitting between different SO(5) representations can be more substantial (10% precision). We note that the overall symmetry of the asymptotic low-energy spectrum in the continuum limit is much larger than SO(5)×SU(2); it is the infinite-dimensional Kac-Moody symmetry. This additional symmetry fully accounts for the degeneracies of states derived from the conformal approach.

TABLE IV. Spectrum of free fermions (degenerate ground-state case) using SO(5) reps for $El/v_F\pi \leq 1$ (descendant states denoted by ′).

j	SO(5)	$El/v_F\pi$
0	5	0
1/2	4	0
1	1	0
(0)′	1	1
0	(5)′	1
0	(10)′	1
(1/2)′	4	1
1/2	(4)′	1
1/2	(16)′	1
(1)′	1	1
(1)′	5	1
1	(10)′	1
(3/2)′	4	1

TABLE V. Comparison of (first 76 states of) conformal field theory finite-size spectra with NRG spectra at the non-Fermi-liquid fixed point. For convenience we label states with the SO(5) designations (in terms of their degeneracies only) and total spin j. For the labeling in terms of flavor spin and charge or isospin see Table II. Numerical levels have been reported for Λ=3.0 and are multiplied by a constant factor of 1.60 to make the first splitting agree with the finite-size scaling value. Note that the same $SU(2)_{spin}$ and SO(5) representations arise for the NRG states as for the conformal theory. The discrepancies between NRG and conformal theory levels grow with the energy and are attributed to the combined factors of logarithmic discretization plus matrix truncation. See the text and Figs. 9 and 10 for further discussion.

j	SO(5) rep	$El/v_F\pi$	E_{num}
1/2	1	0	0
0	4	1/8	0.125
1/2	5	1/2	0.505
1	4	5/8	0.637
(1/2)′	1	1	1.053
1/2	(10)′	1	1.035
(3/2)′	1	1	1.013
0	(4)′	1+1/8	1.232
0	(16)′	1+1/8	1.147
(1)′	4	1+1/8	1.179

We have attempted to isolate the origin of the breaking of conformal symmetry by the NRG approach by extrapolating the discretization parameter towards 1. As a particular measure, we check to see if the splittings between the $1+1/8$ levels tend to zero with some power of $\Lambda-1$. These results are summarized in Figs. 9 and 10. For $\Lambda \geq 2$, the extrapolation procedure appears to work. However, the splitting takes a sudden upturn as Λ is reduced below 2. We suspect that this is due to the truncation of states required within the NRG. Because large Λ spreads the states out more in energy, corrections from mixing with excited states of the same symmetry is likely to be less severe when Λ is sufficiently large. However, the problem becomes more acute as one approaches the continuum limit.

Exchange anisotropy. The NRG approach allows a somewhat different picture of the irrelevance of exchange anisotropy for $s=1/2$, $s=k/2-1/2$ than the conformal theory. The basic argument is illustrated in Fig. 11. For these particular spin choices, at least one of the odd-even iterations will possess a $j^z=\pm 1/2$ ground state. Time reversal ensures the degeneracy of the doublet ground state. For a given iteration with the $j^z=\pm 1/2$ ground state, one finds the first few states to also be $j^z=\pm 1/2$ or $j^z=0$, which smoothly connect to $j=1/2,0$ as the

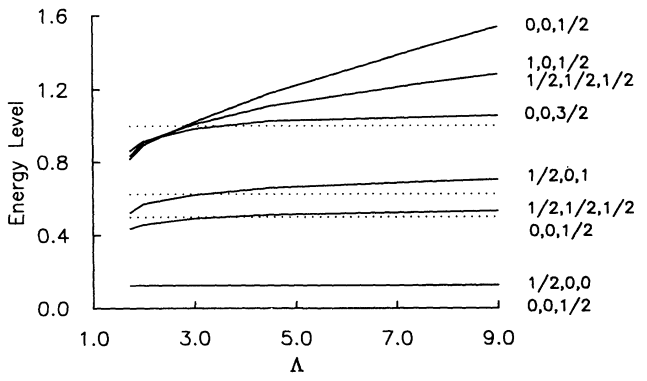

FIG. 9. Λ dependence of NRG levels at the isotropic non-Fermi-liquid fixed point of the $k = 2$, $s = 1/2$ model. The lowest level is scaled to 0.125, with the scale factor attaining a nearly Λ independent value of 1.58–1.62 for the range of Λ shown. In the absence of systematic error due to the truncation of states in the NRG, the levels should tend to the continuum limit as $\Lambda \to 1$.

anisotropy is removed. Since $j = 0$ states do not couple linearly to the anisotropy, and since the first few states at one iteration produce the lowest states at the next iteration, the anisotropy should damp out. On the other hand, for $k \geq 4$ and $s \neq 1/2, k/2 - 1/2$, the lowest state at any iteration will have at least $j = 1$ in the absence of anisotropy. Turning on the anisotropy will always split the $j = 1$ manifold and thus must be relevant or at least marginal.

When exchange anisotropy is introduced, as discussed in Sec. II, we anticipate that it is irrelevant in this case of $k = 2$, $s = 1/2$ with a scaling dimension of $-1/2$ for the coupling constant. We have checked this idea numerically by examining the splitting of the ±1 and 0 levels in the lowest $j = 1$ multiplet as well as the ±3/2 and ±1/2 levels in the lowest $j = 3/2$ multiplet. In each case, we attempt to see when the splitting falls below a fixed small value and find what number of iterations we need to go to reach the same small splitting as we double the anisotropy $\Delta\lambda_K$. We find that $\Delta\lambda_K$ scales linearly with the inverse system size rather than as a square root in each instance. For the $j = 1$ manifold, this is readily explained on the basis of the fusion rules. The argument is as follows: The splitting, to linear order in the irrelevant coupling, is proportional to the matrix element of $\mathcal{J}^3_{-1}\phi^3$ in the $j = 1$ primary states. This matrix element is also governed by the fusion rules. Since the product of two $j = 1$'s does not contain $j = 1$ in the case $k = 2$, according to Eq. (3.11), this matrix element vanishes. Therefore the splitting is of second order in the irrelevant coupling constant and hence scales linearly with the system size. For the $j = 3/2$ manifold, more

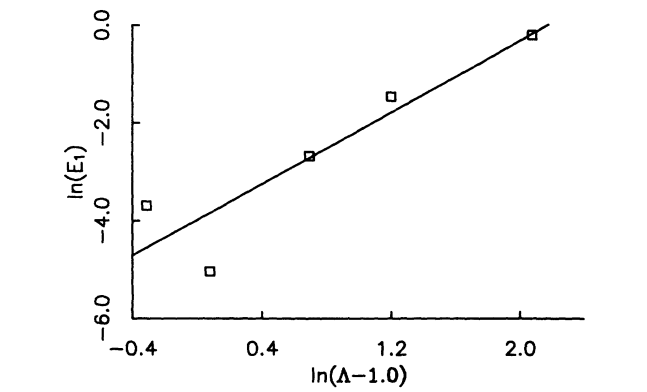

FIG. 10. Extrapolation of discretization induced splitting to the $\Lambda \to 1$ limit. Plotted is the magnitude of the splitting between the $j = 3/2$ SO(5) singlet and the $j = 1/2$ SO(5) decaplet at nominal unit energy for $\lambda_K = 0.7$ as a function of $(\Lambda - 1)$. Clearly above $\Lambda \approx 2$ the extrapolation appears to be towards zero as would be expected. We tentatively ascribe the growth of the splitting magnitude below $\Lambda = 2$ to the systematic error made in the truncation of states within the NRG.

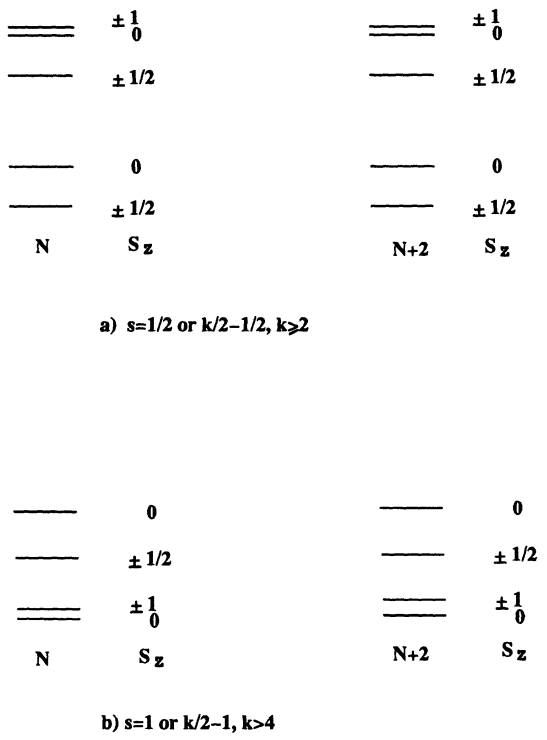

FIG. 11. Heuristic visualization of the irrelevance of anisotropy for $k > 2s$, $s = 1/2$, or $k/2 - 1/2$ in the NRG scheme. (a) For the overcompensated case with $s = 1/2$ (or $k/2 - 1/2$), odd (or even) iteration number ground states will have $j_{\text{tot}} = 1/2$. Within the NRG, the lowest few levels will always be either singlets or doublets for that iteration. The singlet is clearly insensitive to anisotropy, and the doublet is also, since time reversal guarantees its degeneracy (and it possesses no quadrupole moment to couple to the anisotropy). Since the lowest states at the next iteration have significant parentage from these low-lying doublets and singlets, the anisotropy must damp out with increasing iteration number irrespective of the magnitude of k. In contrast, in (b) we see that for $s = 1$ (or $k/2 - 1$) the ground state for odd (or even) iteration will always be a triplet, which will be split by the anisotropy.

work is needed to explain the linear scaling with system size.

Relevance of applied spin and channel fields. By applying the same arguments to the application of exchange integral splitting and spin field, we find each perturbation is relevant with an exponent of 1/2. The plot of crossover temperature scale (at which a fixed energy splitting of levels is exceeded) vs applied spin field is shown in Fig. 12. A corresponding plot for the split exchange integral case appears in Fig. 11 of Ref. 11.

When a magnetic field h is applied at the the two-channel ($s = 1/2$) fixed point, the system crosses over (on a scale $T_s \propto h^2$) to a *Fermi-liquid* fixed point, corresponding to a polarized impurity and an effective local field acting on the conduction electrons at the origin of magnitude $\lambda_{K,\mathrm{eff}}(h)/2$, 1/2 the effective Kondo coupling at energy scale h^2. Such a local field produces an energy shift of $[2\delta(h)/\pi]j^z$ in the spectrum, where the phase shift δ is given by Eq. (4.5). The spectrum at this fixed point is obtained from Tables III and IV by shifting the energies of all states by $[2\delta(h)/\pi]j^z$ and then redefining the total z component of spin to be $j^z \equiv j_c^z + 1/2$, to include the impurity spin. A suitable choice of $\delta(h)$ reproduces excellently the numerical spectrum (after a trivial redefinition of the energy scale). Tables VI and VII show

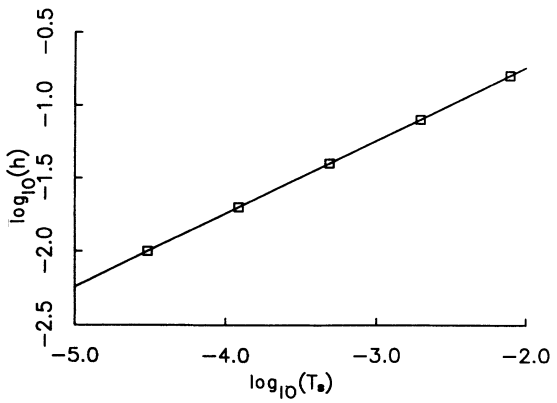

FIG. 12. Crossover scaling in the NRG spectrum as a function of applied spin field. As described in Sec. III, the fixed point for a Fermi liquid with a polarized impurity scatterer will develop below a crossover temperature scale proportional to h^2. Here we identify the crossover scale by monitoring the iteration number N_s where a particular level splitting [between the lowest SO(5) quintet and singlet with $j^z = -1/2$ of Table VI] drops below a fixed magnitude of 0.001. in a given applied field. The crossover temperature is then given by $T_s = (1+\Lambda^{-1})\Lambda^{-(N_s-1)/2}/2$. Our log-log plot of T_{spin} vs. h yields a slope of 2 as expected. For this figure, $\lambda_K = 1$ and $\Lambda = 4$ were used.

TABLE VI. Comparison of finite-size spectra for continuum free fermions with a nondegenerate ground state and a polarized impurity scatterer with NRG levels of the two-channel Kondo model for odd N in an applied field at the impurity site. The ground-state spin reflects only the +1/2 polarization of the impurity. The energy is determined by shifting the zero-field spectra up or down by $2j_c^z\delta/\pi$, where a field-dependent phase shift δ/π parameterizes the scattering. Here the logarithmic discretization parameter Λ=3, the dimensionless field strength $h_z = 0.08$, $\lambda_K = 0.5$ and the fitted phase shift is δ/π=0.206. For a comparison with the NRG levels, all dimensionless continuum levels have been multiplied by a factor of 1.613, which is the spacing of the lowest two scaled NRG single particle levels for Λ=3, as explained in the text, Sec. IV B. The anomalous quartet level on the last line, expected to be degenerate with the other levels in its grouping, corresponds to a second excited particle-hole state where the logarithmic discretization scheme deviates from the linear spaced spectrum of the continuum theory substantially. Charge and flavor quantum numbers are grouped under the single SO(5) representation label; refer to Table II to convert to flavor-charge or isospin labels. j_z is the total spin $j_c^z + 1/2$.

SO(5)	j_c^z	j^z	$\frac{lE}{v_F\pi}$	$\frac{lE(\delta)}{v_F\pi}$	$r^*\frac{lE(\delta)}{v_F\pi}$	E_{num}
1	0	+1/2	0	0	0	0
4	−1/2	0	1/2	$(1-2\delta/\pi)/2$	0.474	0.475
1	−1	−1/2	1	$1-2\delta/\pi$	0.948	0.949
5	−1	−1/2	1	$1-2\delta/\pi$	0.948	0.949
4	+1/2	+1	1/2	$(1+2\delta/\pi)/2$	1.139	1.139
4	−3/2	−1	3/2	$(1-2\delta/\pi)3/2$	1.423	1.424
5	0	+1/2	1	1	1.613	1.613
10	0	+1/2	1	1	1.613	1.613
1	0	+1/2	1	1	1.613	1.614
1	−1	−3/2	2	$2(1-2\delta/\pi)$	1.897	1.899
4	−1/2	0	3/2	$(3-2\delta/\pi)/2$	2.087	2.088
16	−1/2	0	3/2	$(3-2\delta/\pi)/2$	2.087	2.088
4	−1/2	0	3/2	$(3-2\delta/\pi)/2$	2.087	2.089
4	−1/2	0	3/2	$(3-2\delta/\pi)/2$	2.087	2.398

the cases where the zero-coupling, zero-field spectra have nondegenerate or degenerate ground states, respectively, for a field of $h = 0.08$, and $\lambda_K = 0.5$.

Figure 13(a) displays δ vs h for a large field range and two different bare λ_K values, one weak coupling and one strong coupling. As discussed in Sec. III, we expect the renormalized Kondo coupling $\lambda_{K,\mathrm{eff}}(h)$, to approach the bare coupling, λ_K, at large h. The agreement is quite good, once we take into account the Λ-dependent correction of Eq. (4.5) as shown in Table VIII.

For weak bare coupling, λ_K, we find that $\delta(h)$ simply decreases monotonically from the value of $\pi/4$ at low field to the bare value, modulo a discretization-dependent renormalization. For strong bare coupling, $\delta(h)$ displays a nonmonotonic rise *above* $\pi/4$, falling eventually to the bare phase shift at infinite fields. We interpret this unusual result for strong coupling in the following way: As in the single-channel Kondo model, the phase shift must grow as the field is diminished from infinity due to second-order spin-flip processes—at second order, since channel index is conserved, there can be no difference between the single-channel and two-channel models. We expect second-order perturbation theory to be valid, even for strong bare coupling, provided that h is even larger ($h >> \lambda_K$). In the single-channel model the phase shift continues to increase towards the zero-field value of $\pi/2$. However, in the two-channel model, this growth cannot continue indefinitely because the zero-field coupling strength corresponds to a phase shift of $\pi/4$ as argued in Sec. III. Thus, the growth must be arrested at some crossover field scale and the phase shift must then decrease with further reduction of the field towards $\pi/4$. Clearly, the critical bare λ_K value, which divides the monotonic and nonmontonic behavior is that which sits at the fixed point, $\lambda_{K,c} \approx 0.7$. This is the point where the leading irrelevant operator, $\vec{J}_{-1} \cdot \vec{\phi}$, has vanishing coupling constant. Note that for the critical coupling λ_K=0.7 the infinite field phase shift is 0.16π, which is clearly smaller than $\pi/4$. It is interesting that a similar situation arises in the leading frequency and/or temperature dependence of the one-electron scattering rate $1/\tau(\omega, T)$ for scattering from the impurity.[7] At $\lambda_K = \lambda_{K,c}$, the sign of the leading $\omega^{1/2}, T^{1/2}$ dependence in $1/\tau(\omega, T) - 1/\tau(0,0)$ reverses, since this quantity is linear in the leading irrelevant coupling constant. (The situation is different at the Fermi-liquid point where the scattering rate is quadratic in the leading irrelevant coupling constant.) Regardless of the sign of $\delta(h) - \pi/4$, as illustrated in Fig. 13(b) the low-field deviations of $\delta(h)$ from $\pi/4$ are proportional to $|h|\ln|h|$ as anticipated in Sec. III.

VI. CONCLUSIONS AND SUMMARY

This paper has reached the significant conclusion that exchange anisotropy is irrelevant for overcompensated

TABLE VII. Comparison of the continuum field theory spectrum of free fermions with degenerate ground state and a polarized impurity scatterer with NRG calculations for the two-channel s=1/2 Kondo model for even N and a field at the impurity site. Here, as in Table VI, $h = 0.08$, $\lambda_K = 0.5$, and again a single choice for the phase shift $\delta/\pi = 0.198$ provides an excellent fit to the NRG levels through the first several SO(5) multiplets. Note, however, a slight difference for the phase shift between even and odd spectra. (For comparison of continuum and NRG levels, the ground-state energy has been set to zero.) The anomalous splitting of the last quartet in the NRG relative to the continuum theory arises from the position of the second excited particle-hole level in the logarithmic discretization scheme. Here $\Lambda = 3$ and all continuum levels have been rescaled by the factor of r^*=1.630 to agree with the NRG results, which represents the splitting of the two lowest levels in the scaled, nondegenerate NRG free particle spectrum as discussed in the text (Sec. IV B).

SO(5)	j_c^z	j^z	$\frac{lE}{v_F\pi}$	$\frac{lE(\delta)}{v_F\ pi}$	$r^*\frac{l\Delta E(\delta)}{v_F\pi}$	E_{num}
1	−1	−1/2	0	$-2\delta/\pi$	0	0
4	−1/2	0	0	$-\delta/\pi$	0.322	0.322
1	0	+1/2	0	0	0.644	0.644
5	0	+1/2	0	0	0.644	0.644
4	+1/2	+1	0	$+\delta/\pi$	0.966	0.966
1	+1	+3/2	0	$+2\delta/\pi$	1.288	1.288
4	−3/2	−1	1	$1-3\delta/\pi$	1.308	1.308
5	−1	−1/2	1	$1-2\delta/\pi$	1.630	1.630
10	−1	−1/2	1	$1-2\delta/\pi$	1.630	1.630
1	−1	−1/2	1	$1-2\delta/\pi$	1.630	1.631
4	−1/2	0	1	$1-\delta/\pi$	1.952	1.952
16	−1/2	0	1	$1-\delta/\pi$	1.952	1.952
4	−1/2	0	1	$1-\delta/\pi$	1.952	1.953
4	−1/2	0	1	$1-\delta/\pi$	1.952	2.152

Kondo models when $s = 1/2$ or $k/2 - 1/2$. Since it is expected that the quadrupolar Kondo effect (and two-level systems Kondo analog models[27]), which is described by the case $k = 2, s = 1/2$, will generically possess anisotropic exchange couplings, the irrelevance of the anisotropy is important in ensuring the local marginal Fermi-liquid behavior of the model. This analytic result of the conformal theory is completely borne out by the NRG analysis. Thus, the description of the apparent non-Fermi-liquid properties of the alloy system $Y_{1-x}U_xPd_3$ by the two-channel Kondo model attributed to the quadrupolar Kondo effect is supported by our analysis. This picture of the quadrupolar Kondo effect may extend to concentrated Kondo systems as well, such as UBe_{13}.

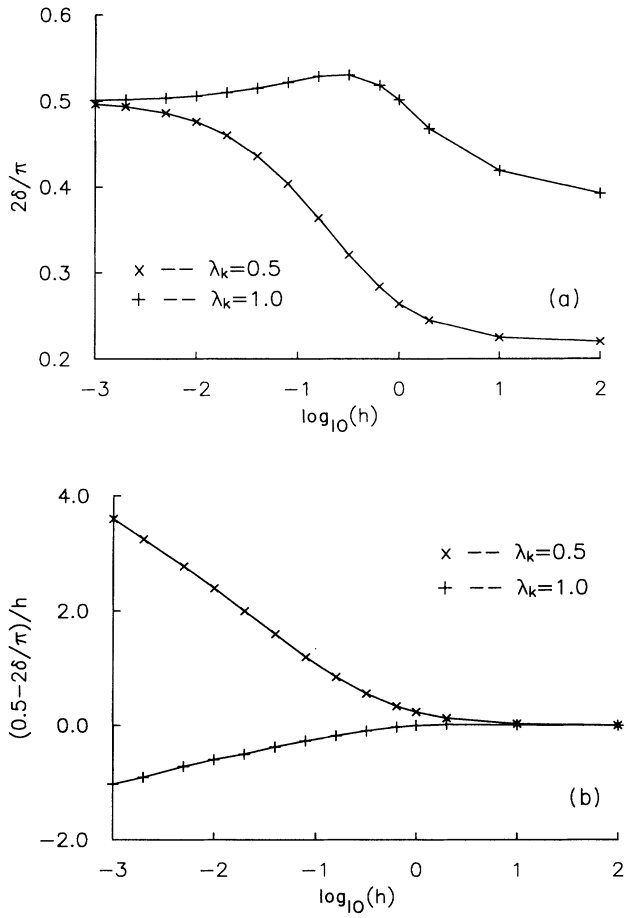

FIG. 13. Phase shift at the polarized scatterer fixed point as a function of field. (a) Using the phase shift measurement described in Sec. IV. and Tables VI and VII, we have computed the phase shift for down-spin electrons within the NRG for $\lambda_K = 0.5, 1$ and $\Lambda = 3$ as a function of applied spin field h coupling only to the impurity. As anticipated, for initial weak coupling (λ_K=0.5) the phase shift decreases from a low field value of $\pi/4$ to a high field value given by $\tan^{-1}(\pi\lambda_K/4A_\Lambda)$, where A_Λ is a Λ-dependent renormalization factor of approximately unit value explained in Sec. IV B. In contrast, for initial strong coupling, the phase shift is nonmonotonic, first rising from $\pi/4$ and then falling as transverse spin fluctuations are frozen out to the high field value. (b) In the low field limit, for both weak and strong coupling choices for λ_K, the deviation of the phase shift from $\pi/4$ follows an $|h|\ln|h|$ form, as illustrated by this plot of $|1/2 - 2|\delta(h)|/\pi|/|h|$ vs $\ln|h|$. Note that the single-particle $\eta_0 = 0.800$ value for a $\pi/4$ phase shift scatterer has been used for the analysis here in conjunction with Eqs. (4.8)–(4.10).

TABLE VIII. Phase shift δ/π in high field limit for several initial exchange λ_K values. In the high field limit, the spin-flip scattering is frozen out and the phase shift is described in terms of the simple t-matrix based relation of Eq. (4.5). The factor of A_Λ arises from the logarithmic discretization and is described in Sec. IV B.

λ_K	$\frac{\delta}{\pi}$ h=5.0	h=100.0	$\frac{1}{\pi}\tan^{-1}(\frac{\pi}{4A_\Lambda}\lambda_K)$
2.0	0.339	0.312	0.306
1.0	0.219	0.204	0.198
0.7	0.163	0.153	0.148
0.5	0.116	0.112	0.110
0.3	0.074	0.070	0.068

In summary, we have used CFT and NRG methods to demonstrate the irrelevance of exchange anisotropy for overcompensated multichannel Kondo models with $s = 1/2, k/2-1/2$, and the relevance of channel asymmetry and applied spin field (on site) in the same models. Explicit comparison of NRG and CFT finite-size level spectra for the $k = 2$, $s = 1/2$ model are in excellent agreement at the non-Fermi-liquid fixed point, and the applied field NRG spectrum agrees with that of a Fermi liquid. Small discrepancies arise at higher energies, which can be attributed to the logarithmic discretization and numerical state truncation of the NRG method. At all stages, the NRG and CFT approaches retain the exact SO(5) symmetry of the single impurity problem embedded in a lattice.

Our result that the overall symmetry of k-channel models is $SU(2)_{spin}\times Sp(2k)$ may be of significance to future numerical studies. The reason is that the high symmetry of the $Sp(2k)$ group could allow efficient block diagonalization of matrices reducing the storage overhead in, e.g., NRG calculations on multisite Kondo models. Generally, the $SU(2)_{spin}\times Sp(2k)$ symmetry is also enjoyed by a full k-channel Kondo lattice so long as the Hamiltonian and chemical potential respect particle-hole symmetry.

ACKNOWLEDGMENTS

We acknowledge useful conversations with K. Ingersent. Two of us (H.-B.P. and D.L.C.) were supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Research. D.L.C. also acknowledges a grant from the A.P. Sloan Foundation. Some of the NRG calculations were carried out with computer time furnished by the Ohio Supercomputer Center. The research of I.A. and A.W.W.L. was supported in part by NSERC of Canada. All authors acknowledge the hospitality of the Aspen Center for Physics, where part of this work was completed.

[1] C.L. Seaman, M.B. Maple, B.W. Lee, S. Ghamaty, M.S. Torikachvili, J.-S. Kang, L.Z. Liu, J.W. Allen, and D.L. Cox, Phys. Rev. Lett. **67**, 2882 (1991); J. Less. Common Metals (to be published).
[2] B. Andraka and A. Tsvelik, Phys. Rev. Lett. **67**, 2886 (1991).
[3] I. Affleck, Nucl. Phys. **B336**, 517 (1990).
[4] I. Affleck and A.W.W. Ludwig, Nucl. Phys. **B352**, 849 (1991).
[5] I. Affleck and A.W.W. Ludwig, Nucl. Phys. **360**, 641 (1991).
[6] I. Affleck and A.W.W. Ludwig, Phys. Rev. Lett. **67**, 161 (1991).
[7] A.W.W. Ludwig and I. Affleck, Phys. Rev. Lett. **67**, 3160 (1991).
[8] A.W.W. Ludwig, in *Quantum Field Theory and Condensed Matter Physics*, Proceedings of Trieste Conference ICTP–Trieste, 1991, edited by E. Brézin, Yu Lu, and S. Randjbar-Daemi (World Scientific, Singapore, in press).
[9] I. Affleck and A.W.W. Ludwig (unpublished).
[10] D.L. Cox, Phys. Rev. Lett. **59**, 1240 (1987); (unpublished).
[11] H.-B. Pang and D.L. Cox, Phys. Rev. B **44**, 9454 (1991).
[12] A. Tsvelick, J. Phys. Condens. Matter **2**, 2833 (1990); (unpublished).
[13] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).
[14] N. Andrei and C. Destri, Phys. Rev. Lett. **52**, 364 (1984).
[15] P.B. Wiegmann and A.M. Tsvelick, Z. Phys. B **54**, 201 (1985); A.M. Tsvelick, J. Phys. C **18**, 159 (1985).
[16] P.D. Sacramento and P. Schlottman, Phys. Lett. A **142**, 245 (1989); Phys. Rev. B **43**, 13 294 (1991).
[17] P.Nozières, J. Low Temp. Phys. **17**, 31 (1974).
[18] K.G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[19] D.M. Cragg, P. Lloyd, and P. Nozières, J. Phys. C **13**, 803 (1980).
[20] B. Jones and C.M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B. Jones, C.M. Varma, and J.W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988); B. Jones, Ph.D. thesis, Cornell University, 1988 (unpublished).
[21] See, e.g., H. Georgi, *Lie Algebras in Particle Physics* (Benjamin/Cummings, Menlo Park, 1982).
[22] S.C. Zhang, Phys. Rev. Lett. **65**, 120 (1990).
[23] E. Fradkin, C. von Reichenbach, and F.A. Schaposnik, Nucl. Phys. **B316**, 710 (1989); **B340**, 692 (1990).
[24] A.B. Zamolodchikov and V.A. Fateev, Yad. Fiz. **43**, 1031 (1986) [Sov. J. Nucl. Phys. **43**, 657 (1986)].
[25] J.L. Cardy, Nucl. Phys. **B275**, 200 (1986).
[26] D. Altschüler, M. Bauer, and C. Itzykson, Commun. Math. Phys. **132**, 349 (1990).
[27] K. Vladar, G. Zimanyi, and A. Zawadowski, Phys. Rev. Lett. **56**, 286 (1986). A Friedel sum-rule argument requiring charge balance (no net charge polarization at the impurity) produces the $\pi/4$ phase shift as well as shall be discussed elsewhere in detail.
[28] H.R. Krishna-murthy, J.W. Wilkins, and K.G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).
[29] L.N. Oliveira and J.W. Wilkins, Phys. Rev. B **24**, 4863 (1981); L.N. Oliveira, Ph.D. thesis, Cornell University, 1981 (unpublished).