A new non-Fermi liquid fixed point

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We study a new exchange interaction in which the conduction electrons with pseudo spin $S_c = 3/2$ interact with the impurity spin $S_I = 1/2$. Due to the overscreening of the impurity spin by higher conduction electron spin, a new non-trivial intermediate coupling strength fixed point is realized. Using the numerical renormalization group (NRG), we show that the low-energy spectra are described by a non-Fermi liquid excitation spectrum. A conformal field theory analysis is compared with NRG results and excellent agreement is obtained. Using the double fusion rule to generate the operator spectrum with the conformal theory, we find that the specific heat coefficient and magnetic susceptibility will diverge as $T^{-2/3}$, that the scaling dimension of an applied magnetic field is $5/6$, and that exchange anisotropy is always relevant. We discuss the possible relevance of our work to two-level system Kondo materials and dilute cerium alloys, and we point out a paradox in understanding the Bethe-Ansatz solutions to the multichannel Kondo model.

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I. INTRODUCTION

A number of Ce and U based heavy electron metals have recently been discovered to show “non-Fermi liquid physics,” in such anomalous properties as: i) a specific heat coefficient linear in $\log T$, $T$ the temperature; ii) resistivity which approaches its $T = 0$ value as $T^\alpha$ with $\alpha$ close to 1; iii) a magnetic susceptibility $\chi(T) \simeq \chi(0)|1 - A/\sqrt{T}|^{2/3}$. In the case of UBe$_{13}$ and CeCu$_2$Si$_2$, a superconducting instability arises within this exotic normal state \cite{12}. It is an open question whether these anomalous properties arise from distortions of Fermi liquid physics such as arise in the vicinity of a quantum critical point \cite{1,2} or due to a disordered distribution of Kondo scales \cite{3}. or whether the anomalies signal the appearance of an entirely new fixed point regulating the low temperature physics of these materials.

In this latter regard, it is prudent to study impurity models, such as the overcompensated multi-channel Kondo model \cite{4} which have very plausible relevance to Ce and U based systems \cite{5,6}. In this model, $M$ identical spin 1/2 conduction bands exchange couple to a single spin $S_I$ impurity with the condition $M/2 > S_I$, so that there is more conduction spin than needed to fully compensate the impurity, which leads to an instability of the strong coupling (exchange coupling $J \to \infty$) fixed point, as indicated in Fig. 1. Because the weak coupling ($J = 0$) fixed point is unstable always due the Kondo effect, this implies the presence of a non-trivial fixed point at intermediate coupling. This non-trivial fixed point corresponds to a degenerate ground state and non-Fermi liquid excitation spectrum—no 1:1 map exists of the states to a non-interacting fermion system. In particular, the charge and spin relations relevant for free fermions do not apply for these systems where spin/charge/channel separation occurs \cite{7}. For more than one impurity, this fixed point cannot remain stable at low temperatures \cite{8}, due to the overlap of the polarization clouds around each site which have diverging length scales as $T \to 0$. It is conceivable that the impurity models may regulate the physics of alloys with finite concentrations of Ce and U ions or even concentrated compounds over a finite range of temperatures before ultimately giving way to new fixed points as $T \to 0$. This picture is supported by recent results in infinite spatial dimensions \cite{1,2}.

Recently, impurity models containing a single high spin electron band have been derived which have been argued to show non-trivial physics. These models have been argued to describe various unstable fixed points of the two-level system Kondo model (describing electron assisted tunneling of atoms in a double well) \cite{9}, and a Ce impurity in a metal when finite Coulomb interaction is retained \cite{10,11}. The simplest example of this kind of model is for impurity spin $S_I = 1/2$ and conduction spin $S_c = 3/2$. Although only one channel of conduction electron is present, this model gives a nontrivial fixed point for the same reasons as the multi-channel model, as illustrated in Fig. 2. The point is that a single large spin $S_{\text{Cel}} = 2$ is coupled to the impurity as the lowest energy state in strong coupling. Again, strong coupling is unstable, and weak coupling is unstable, so that a non-trivial intermediate coupling fixed point
must exist. This kind of fixed point has been studied with a perturbative scaling analysis \cite{13–17}, and more recently with conformal field theory analysis \cite{16}.

In this paper we present a comprehensive numerical renormalization group analysis of the $S_I = 1/2, S_c = 3/2$ single channel Kondo model combined with a conformal field theory study of the energy and operator spectrum. We confirm the existence of a non-trivial fixed point with a non-Fermi liquid excitation spectrum. We find good agreement between finite size spectra predicted by the conformal theory with those obtained from the NRG, both from the group theoretic basis we use for our conformal theory and that of Ref. \cite{16} which uses a different basis. Using the double fusion rule of Affleck and Ludwig \cite{9}, we work out the spectrum of primary field operators for the model, and find that the magnetic susceptibility and specific heat coefficient in this model will diverge as $T^{-2/3}$ for $T \to 0$, that the scaling dimension of the applied magnetic field is 5/6, and that exchange anisotropy will always be relevant in this model. In concluding, we briefly discuss the possible relevance of this model to intermediate temperature regimes of two-level system Kondo materials and dilute cerium alloys. Finally, we discuss a separate point of theoretical interest concerning a paradox about the connection of this model to the Bethe-Ansatz solutions of the overcompensated multi-channel Kondo model \cite{17,18}.

Our paper is organized as follows: In Section II we discuss the model Hamiltonian and the numerical renormalization group methodology used to study it. We also discuss the results from the numerical renormalization group calculations. In Section III we develop the conformal field theory concepts required to study this model and calculate the finite size spectra and primary operator spectrum, and we compare the conformal theory results with the numerical renormalization group results. In Section IV we summarize and conclude.

II. NUMERICAL RENORMALIZATION GROUP

The numerical renormalization group (NRG) technique was invented by K. G. Wilson to study the Kondo problems. This method defines the renormalization group (RG) Hamiltonians and diagonalizes the RG Hamiltonian numerically. The essence of this method lies in the logarithmic discretization of the conduction band and in transforming the conduction electron Hamiltonian into a tridiagonal form. Hence we can visualize the NRG Hamiltonian as a linear array of sites with the hopping integrals between sites. The impurity lies at the $N = -1$ site and the conduction electrons sit at the sites $N = 0, 1, 2, \cdots$.

Since this method depends on direct numerical diagonalization, the numerical work requires a huge memory storage compared with, e.g., the NCA. The consideration of all the possible symmetry of the Hamiltonian is essential in reducing the computer memory. The NRG is defined by a set of energy eigenvalues and the reduced matrix elements of the electron operators between the energy eigenstates.

The NRG approach was the first to show the crossover physics of the Kondo effect from the high temperature regime to the low temperature fixed point. K. G. Wilson \cite{13} solved the simple Kondo exchange interaction model, calculated the magnetic susceptibility, and showed the RG flow from the high temperature fixed point to the low temperature fixed point. Later, the NRG was applied to the simple one-channel Anderson model with the conduction electron spins $S_c = 1/2$ interacting with the impurity system of $S_I = 1/2$ \cite{20}. The two-channel Kondo model was also studied using the NRG \cite{21}. The NRG method was able to show that the two-channel $S_c = S_I = 1/2$ Kondo model leads to the non-Fermi liquid ground state with a non-trivial finite exchange coupling at the fixed point. The one-channel two-impurity and two-channel two-impurity Kondo problems have been also studied using the NRG \cite{22,10} and the low energy levels from the NRG have been compared to the finite energy spectrum results of conformal field theory to verify the fusion rule hypothesis used in the CFT approach \cite{23}.

The NRG is a unique approach for studying stability of various fixed points of the Kondo problems. In contrast to other techniques, the NRG can provide the RG flow diagrams. In an earlier work, stability of the two-channel non-Fermi liquid fixed points were studied with the NRG against the channel anisotropy, the exchange coupling anisotropy, and the external magnetic field \cite{24}. This method was extended to the studies of the thermodynamics \cite{24} and the dynamical properties \cite{25,26} like the transport coefficients and the local spectral functions.

A. The conduction electrons with $S_c = 3/2$.

Here we apply the NRG method to the case that the conduction electrons with $S_c = 3/2$ interact with the impurity spin $S_I = 1/2$. Derivation of this exchange interaction is presented in Ref \cite{15}. Higher conduction electron pseudo spin can overcompensate the impurity spin leading to the non-Fermi liquid fixed point. In this section we are going to show that this model leads to new non-Fermi liquid fixed point using the NRG.
1. Logarithmic Discretization.

The Model Hamiltonian reads

\[ H = H_{cb} + H_1, \]

\[ H_{cb} = \sum_{\alpha} \epsilon_{\alpha} c_{\alpha}^\dagger c_{\alpha}, \]  

\[ H_1 = J \vec{S}_{c}(0) \cdot \vec{S}_I. \]  

Here the conduction electron spin \( S_c = 3/2 \) and the impurity spin \( S_I = 1/2 \). We will assume the flat square DOS for the conduction band. Following the standard transformation using the logarithmic discretization [19], the NRG Hamiltonian reads

\[ H_{cb} = \frac{1}{2} \left[ 1 + \Lambda^{-1} \right] \sum_{\alpha} \sum_{n=0}^{\infty} \Lambda^{-n/2} \xi_n \left[ f_{n\alpha}^\dagger f_{n+1\alpha} + f_{n+1\alpha}^\dagger f_{n\alpha} \right], \]  

\[ H_1 = 2N(0)J \sum_{\alpha} f_{0\alpha}^\dagger \tilde{L}_{\alpha\beta} f_{0\beta} \cdot \vec{S}, \]  

\[ \xi_n = \frac{1 - \Lambda^{-n-1}}{\sqrt{(1 - \Lambda^{-2n-1})(1 - \Lambda^{-2n-3})}}, \]  

\[ f_{0\alpha} = \frac{1}{\sqrt{2}} \int_{-1}^{1} dc_{\alpha}. \]  

Here \( \tilde{L} \) is the canonical matrix representation of spin \( J = 3/2 \). This Hamiltonian can be envisaged as a linear array of sites with an impurity sitting at the site \( n = -1 \). Only the electrons at the origin \( (n = 0) \) interact with the impurity spin. This tight-binding form of Hamiltonian has a nearest neighbor hopping integral whose magnitude depends on the distance from the impurity site and is progressively reduced as the sites move away from the origin.

We may define the Hamiltonian up to \( N \)-th site by \( H_N \)

\[ H_N = \frac{1}{2} \left[ 1 + \Lambda^{-1} \right] \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n \left[ f_{n\alpha}^\dagger f_{n+1\alpha} + f_{n+1\alpha}^\dagger f_{n\alpha} \right] + H_0, \]  

\[ H_0 = 2N(0)J f_{0\alpha}^\dagger \tilde{L}_{\alpha\beta} f_{0\beta} \cdot \vec{S}. \]  

We can diagonalize this Hamiltonian step by step. The strategy is very simple. When the Hamiltonian upto the \( N \)-th site is assumed diagonalized, we add the \( N+1 \)-th electron site and diagonalize the extended Hamiltonian again. We continue this process until the structure of low lying energy levels does not change, or, when the stable fixed points are accessed. Since the hopping integral decreases exponentially with site number \( N \), rapid saturation is expected for a reasonable value of \( \Lambda \). To make the lowing lying energy of order one, we redefine the Hamiltonian,

\[ K_N \equiv \frac{2}{1 + \Lambda^{-1}} \Lambda^{(N-1)/2} H_N \]

\[ = \Lambda^{(N-1)/2} \left[ \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n \left[ f_{n\alpha}^\dagger f_{n+1\alpha} + f_{n+1\alpha}^\dagger f_{n\alpha} \right] + 2N(0)J f_{0\alpha}^\dagger \tilde{L}_{\alpha\beta} f_{0\beta} \cdot \vec{S} \right], \]  

\[ K_{N+1} = \Lambda^{1/2} K_N + \xi_N \sum_{\alpha} \left[ f_{N\alpha}^\dagger f_{N+1\alpha} + f_{N+1\alpha}^\dagger f_{N\alpha} \right]. \]

The last equation defines the renormalization group of the Kondo Hamiltonian.

\[ K_0 = \frac{2\Lambda^{-1/2}}{1 + \Lambda^{-1}} H_0 = \tilde{g} \sum_{\alpha \beta} f_{0\alpha}^\dagger \tilde{L}_{\alpha\beta} f_{0\beta} \cdot \vec{S}, \]  

\[ \tilde{g} = \frac{4\Lambda^{-1/2}}{1 + \Lambda^{-1}} JN(0). \]
2. Symmetries.

Now we show that the axial charge and the total spin operators commute with the Hamiltonian. We note that the axial charge may be more commonly called the isospin, and that this nomenclature is peculiar to the NRG literature.

The conduction band Hamiltonian is invariant under the unitary transformation $f_{n\alpha} \rightarrow U_{\alpha\beta} f_{n\beta}$. Including the exchange interaction, the total spin is conserved

$$\vec{J} = \sum_n f_{n\alpha}^\dagger \vec{L}_{\alpha\beta} f_{n\beta} + \vec{S}. \quad (14)$$

It can be easily shown that the total spin of the conduction electrons and the impurity spin commutes with the conduction band Hamiltonian

$$[H_{cb}, \vec{J}] = 0. \quad (15)$$

Also this spin operator commutes with the usual Kondo exchange interaction.

The Hamiltonian is invariant under the unitary transformation:

$$F_{n\alpha} \rightarrow UF_{n\alpha}F_{n\alpha} \equiv \left( f_{n\alpha} (-1)^n f_{n\alpha}^\dagger \right). \quad (16)$$

This invariance leads to the definition of axial charge symmetry operators [28]

$$Q^+ = k \sum_n (-1)^n \epsilon_{\alpha\beta} f_{n\alpha}^\dagger f_{n\beta}^\dagger, \quad (17)$$

$$Q^- = [Q^+]^\dagger = k \sum_n (-1)^n \epsilon_{\alpha\beta} f_{n\beta} f_{n\alpha}, \quad (18)$$

$$Q^z = \frac{1}{2} \sum_{n\alpha} \left[ f_{n\alpha}^\dagger f_{n\alpha} - \frac{1}{2} \right]. \quad (19)$$

Here $\epsilon_{\alpha\beta}$ is an antisymmetric tensor to be determined. These axial charge operators commute with the conduction band Hamiltonian

$$[H_{cb}, Q^i] = 0. \quad (20)$$

We will determine the prefactor $k$ and the antisymmetric tensor by demanding that these axial charge operators satisfy the angular momentum commutation relations. First they satisfy

$$[Q^z, Q^\pm] = \pm Q^\pm. \quad (20)$$

We demand

$$[Q^+, Q^-] = 2Q^z. \quad (21)$$

Then we find the following conditions to be satisfied

$$k^2 = \frac{1}{4}, \quad [\epsilon^2]_{\alpha\beta} = -\delta_{\alpha\beta}. \quad (22)$$

Hence we may choose, e.g., for $S_c = 3/2$,

$$k = \frac{1}{2}; \quad \epsilon = \sigma^x \otimes i\sigma^y. \quad (23)$$

Thus

$$Q^+ = \sum_{n=0}^\infty (-1)^n \left( f_{n3/2}^\dagger f_{n(-3/2)}^\dagger - f_{n1/2}^\dagger f_{n(-1/2)}^\dagger \right). \quad (24)$$

The above axial charge and angular momentum operators commute with each other and with the ordinary exchange interaction.
We can also generalize the axial charge operators for the conduction electron band with any half-integer spin. The angular momentum operators are self-evident.

\[
Q^+ = \frac{1}{2} \sum_{n\alpha} (-1)^n (1)^{s\alpha} f_{n\alpha}^\dagger f_{n\alpha},
\]

\[
Q^- = [Q^+]^\dagger,
\]

\[
Q^z = \frac{1}{2} \sum_{n\alpha} \left[ f_{n\alpha}^\dagger f_{n\alpha} - \frac{1}{2} \right] = \frac{1}{2} \sum_n (N_n - s - \frac{1}{2}).
\]

Thus the angular momentum operators and the axial charge operators commute with both the conduction band Hamiltonian and the ordinary Kondo exchange interaction. They also commute with each other, and hence provide good quantum numbers for our numerical calculations.

### 3. Irreducible symmetry tensor operators.

In this section, we will construct irreducible tensor operators at each site which are building blocks for new symmetry states in the NRG work.

The angular momentum operators are

\[
S_{N\alpha}^+ = \sum_{\alpha} \alpha f_{N\alpha}^\dagger f_{N\alpha},
\]

\[
S_{N\alpha}^- = \sqrt{3} f_{N3/2\alpha}^\dagger f_{N1/2\alpha} + 2 f_{N1/2\alpha}^\dagger f_{N-1/2\alpha} + \sqrt{3} f_{N-1/2\alpha}^\dagger f_{N3/2\alpha},
\]

\[
S_{N\alpha}^- = \sqrt{3} f_{N1/2\alpha}^\dagger f_{N3/2\alpha} + 2 f_{N-1/2\alpha}^\dagger f_{N1/2\alpha} + \sqrt{3} f_{N-3/2\alpha}^\dagger f_{N1/2\alpha}.
\]

And the axial charge operators are

\[
Q_{N\alpha}^z = \frac{1}{2} \sum_{\alpha} f_{N\alpha}^\dagger f_{N\alpha} - 1,
\]

\[
Q_{N\alpha}^z = (-1)^{N\alpha} (f_{N3/2\alpha}^\dagger f_{N-3/2\alpha} - f_{N1/2\alpha}^\dagger f_{N-1/2\alpha}),
\]

\[
Q_{N\alpha}^z = [Q_{N\alpha}^z]^\dagger.
\]

The electron operators \( f_{N\alpha}^\dagger \) and the hole operators \( h_{N\alpha}^\dagger \) are irreducible tensors of rank 3/2. That is,

\[
\begin{align*}
[ S_{N\alpha}^+, f_{N\alpha}^\dagger ] &= \alpha f_{N\alpha}^\dagger, \\
[ S_{N\alpha}^+, f_{N\alpha} ] &= L_{N\alpha + 1, \alpha}^+ f_{N\alpha + 1}^\dagger = \sqrt{s(s+1) - \alpha(\alpha+1)} f_{N\alpha + 1}^\dagger, \\
[ S_{N\alpha}^-, f_{N\alpha}^\dagger ] &= L_{N\alpha - 1, \alpha}^+ f_{N\alpha - 1}^\dagger = \sqrt{s(s+1) - \alpha(\alpha-1)} f_{N\alpha - 1}^\dagger, \\
[ S_{N\alpha}^-, h_{N\alpha}^\dagger ] &= \alpha h_{N\alpha}^\dagger, \\
[ S_{N\alpha}^+, h_{N\alpha}^\dagger ] &= L_{N\alpha + 1, \alpha}^- h_{N\alpha + 1} = \sqrt{s(s+1) - \alpha(\alpha+1)} h_{N\alpha + 1}^\dagger, \\
[ S_{N\alpha}^-, h_{N\alpha}^\dagger ] &= L_{N\alpha - 1, \alpha}^- h_{N\alpha - 1} = \sqrt{s(s+1) - \alpha(\alpha-1)} h_{N\alpha - 1}^\dagger.
\end{align*}
\]

Here \( L^+ \) and \( L^- \) are the standard \( S = 3/2 \) angular momentum matrices. Hence we can apply the Wigner-Eckart theorem when we calculate the matrix elements between two different angular momentum operator symmetry states. In the axial charge case, the electron operators and the hole operators satisfy the following commutation relations

\[
\begin{align*}
[ Q_{N\alpha}^z, h_{N\alpha}^\dagger ] &= -\frac{1}{2} h_{N\alpha}^\dagger, \\
[ Q_{N\alpha}^z, f_{N\alpha}^\dagger ] &= \frac{1}{2} f_{N\alpha}^\dagger, \\
[ Q_{N\alpha}^+, h_{N\alpha}^\dagger ] &= f_{N\alpha}^\dagger, \\
[ Q_{N\alpha}^+, f_{N\alpha}^\dagger ] &= 0, \\
[ Q_{N\alpha}^-, h_{N\alpha}^\dagger ] &= -h_{N\alpha}^\dagger, \\
[ Q_{N\alpha}^-, f_{N\alpha}^\dagger ] &= 0.
\end{align*}
\]
Thus we can see that the pair \( (f^\dagger_{N\alpha}, -h^\dagger_{N\alpha}) \) form a tensor of rank 1/2 in the axial charge sector. Thus we can apply the Wigner-Eckart theorem to these conjugate pair operators.

We now construct the irreducible symmetry operators, \( T_N(QR; JM) \), at the site \( N \) using the above operators. At each NRG site, the following three types of irreducible symmetry tensor operators can be developed and they generate 16 new symmetry states:

1. **\( Q = 1, J = 0 \):** We choose the vacuum state and operate the axial charge raising operator to find all states

\[
T_N(1\bar{1}; 0) = 1 \\
T_N(10; 0) = \frac{1}{\sqrt{2}} Q_N^+ T_N(1\bar{1}; 0) \\
= (-1)^N \left( f^\dagger_{N3/2} f^\dagger_{N-3/2} - f^\dagger_{N1/2} f^\dagger_{N-1/2} \right) \\
T_N(11; 0) = \frac{1}{\sqrt{2}} Q_N^+ T_N(10; 0) = -f^\dagger_{N3/2} f^\dagger_{N1/2} f^\dagger_{N-1/2} f^\dagger_{N-3/2}.
\]  

2. **\( Q = 1/2, J = 3/2 \):** First we define the \( Q = 1/2, R = -1/2 \) states and find the \( R = 1/2 \) states operating the axial charge raising operator on them

\[
T_N\left(\frac{1}{2}(-\frac{1}{2}); \frac{3}{2}m\right) = f^\dagger_{N^\prime m}.
\]

We already showed that these operators satisfy the proper commutation relations with the angular momentum operators. The \( R = 1/2 \) operators are found by operating the axial charge raising operator on the above operators

\[
T_N\left(\frac{11}{2}\frac{3}{2}; \frac{3}{2}m\right) = Q_N^+ T_N\left(\frac{1}{2}(-\frac{1}{2}); \frac{3}{2}m\right) = h^\dagger_{N^\prime m} T_N(11; 0),
\]

\[
h^\dagger_{N^\prime m} = (-1)^{N+3/2+m} f^\dagger_{N^\prime m}.
\]

As noted before, the hole operators \( h^\dagger_{N^\prime m} \) satisfy the tensor (of rank 3/2) commutation relations with the angular momentum operators.

3. **\( Q = 0, J = 2 \):** The irreducible operators can be found using the commutation relations

\[
T_N(0; 22) = f^\dagger_{N3/2} f^\dagger_{N1/2},
\]

\[
T_N(0; 21) = \frac{1}{2} \left[ S_N^-, T_N(0; 22) \right] = f^\dagger_{N3/2} f^\dagger_{N-1/2},
\]

\[
T_N(0; 20) = \frac{1}{\sqrt{6}} \left[ S_N^-, T_N(0; 21) \right] = \frac{1}{\sqrt{2}} \left( f^\dagger_{N3/2} f^\dagger_{N-3/2} + f^\dagger_{N1/2} f^\dagger_{N-1/2} \right),
\]

\[
T_N(0; 2\bar{1}) = \frac{1}{\sqrt{6}} \left[ S_N^-, T_N(0; 20) \right] = f^\dagger_{N1/2} f^\dagger_{N-3/2},
\]

\[
T_N(0; 2\bar{2}) = \frac{1}{2} \left[ S_N^-, T_N(0; 2\bar{1}) \right] = f^\dagger_{N-1/2} f^\dagger_{N-3/2}.
\]

4. **Construction of the NRG Hamiltonian and the reduced matrix elements of the discretized conduction electron operator**

16 new irreducible symmetry electron operators are generated at each NRG site. These new operators belong to one of three tensor operators \( T_N(QR; JM) \) with rank \( Q \) in the axial charge sector and with rank \( J \) in the angular momentum sector

\[
T_N(00; 2M), \; T_N\left(\frac{1}{2}R; \frac{3}{2}M\right), \; T_N(1R; 00).
\]
These irreducible tensor operators are basic building blocks for the construction of new symmetry sector.

In constructing the NRG Hamiltonian in each symmetry sector or in calculating the reduced matrix elements of the discretized conduction electron operators, we have to calculate the following matrix elements

\[
\begin{align*}
T_N^<(1R_1;00) & \quad T_N^<(1R_2;00) \\
T_N^<(00;2M_1) & \quad f_{N\alpha}^T \quad T_N^<(00;2M_2) \\
T_N^<>(1R_1;\frac{3}{2}M_1) & \quad T_N^<>(1R_2;\frac{3}{2}M_2)
\end{align*}
\]  

(58)

According to the Wigner-Eckart theorem, the non-vanishing combinations are

\[
\begin{align*}
T_N^<(\frac{1}{2}R_1;\frac{3}{2}M_1) f_{N\alpha}^T & \quad T_N^<(1R_2;00) \\
T_N^<(1R_1;00) & \quad T_N^<(00;2M_2) \\
T_N^>(\frac{1}{2}R_1;\frac{3}{2}M_1) & \quad T_N^>(00;2M_1)
\end{align*}
\]  

(59)

Guided by the Wigner-Eckart theorem, the explicit calculation gives

\[
T_N^<(\frac{1}{2}R_1;\frac{3}{2}M_1) f_{N\alpha}^T T_N^<(1R_2;00) = \sqrt{\frac{3}{2}} < \frac{1}{2}R_1 \frac{1}{2}R_2 > (M_1, \alpha),
\]

(60)

\[
T_N^<(1R_1;00) f_{N\alpha}^T T_N^<(\frac{1}{2}R_2;\frac{3}{2}M_2) = (-1)^{N+3/2-\alpha} < \frac{1}{2}R_1 \frac{1}{2}R_2 > (M_2, \bar{\alpha}),
\]

(61)

\[
T_N^<(\frac{1}{2}R_1;\frac{3}{2}M_1) f_{N\alpha}^T T_N^>(00;2M_2) = (-1)^{N+1} \sqrt{\frac{5}{2}} (R_1, \frac{1}{2}) < \frac{3}{2}M_1 \frac{3}{2}M_2 >,
\]

(62)

\[
T_N^>(00;2M_1) f_{N\alpha}^T T_N^>(\frac{1}{2}R_2;\frac{3}{2}M_2) = \sqrt{2} (R_2, -\frac{1}{2}) < 2M_1 \frac{3}{2}M_2 >.
\]

(63)

Here \((x,y)\) is the shorthand notation for the Kronecker delta function \(\delta_{x,y}\). Using the above equations and the Wigner-Eckart theorem, we can construct the NRG Hamiltonian matrix elements at each symmetry sector which are expressed in terms of the reduced electron operator matrix and the \(6-j\) symbols.

As mentioned before, the numerical renormalization group is reduced to book-keeping of two sets of energy eigenvalues and reduced matrix elements in the Kondo problems. The reduced matrix elements are required for the construction of the NRG Hamiltonian in the next NRG site. Hence it is essential to keep track of two data sets. In the next section, we are going to present our NRG results, and give a physical interpretation.

**B. NRG results**

In this section, we are going to present the results of NRG calculation for the exchange interaction of the conduction electrons with spin \(S_c = 3/2\) with the impurity spin \(S_I = 1/2\).

First we show the low energy spectra in the weak coupling limit with the initial coupling \(g = 10^{-10}\) (free electron limit). We used the discretization parameter \(\Lambda = 5\) and the truncation energy 10. In this extremely weak coupling limit, the low lying excitation energy spectrum should be described by the free electrons. As shown in Fig. 3, the low lying energy levels are evenly spaced.

When we increase the bare exchange coupling, we should be able to observe the crossover from the weak coupling fixed point to a nontrivial non-Fermi liquid fixed point. In Fig. 4 we display the RG flow with initial exchange coupling \(g = 0.01\). We can observe the clear crossover from the weak coupling fixed point to new fixed point. The low lying excitation energy spectrum at this new fixed point is completely different from that of free electron at the weak coupling fixed point. That is, this new fixed point is non-Fermi liquid fixed point. From the Fig. 4, we can see that degeneracies at weak coupling fixed point are lifted after crossover at new non-Fermi liquid fixed point.

Now we present the three sets of figures with initial couplings ranging from weak coupling (see Figs. 3), coupling close to the fixed point \((g^* = 0.2\) form the third-order scaling analysis, see Figs. 4), and strong coupling(see Figs. 5). In
these cases, we used the same model parameters as above. The low energy structure is completely different from that in the zero coupling limit (free electron). That is, this interaction model generates new non-Fermi liquid fixed point. Three different initial couplings flow to the same fixed point as can be seen from the fixed point low energy spectra. The ground state is alternating between \((q = 0, j = 1/2)\) sector and \((q = 0, j = 3/2)\) sector with the conduction electron screening shell (NRG site \(N\)). For odd \(N\), the \((q = 0, j = 1/2)\) sector is the ground state and vice versa. Here \((q = \text{axial charge}, j = \text{angular momentum})\).

In summary, we have shown using the NRG that the one-channel \(S_c = 3/2, S_I = 1/2\) exchange interaction model generates non-trivial fixed point which is completely different from the Fermi liquid fixed point.

### III. CONFORMAL FIELD THEORY ANALYSIS: LOW-ENERGY SPECTRUM

In this section, we carry out a conformal field calculation \([30,9]\) determining the first few states and eigenvalues in the spectrum of the low-energy fixed-point. In contrast with the NRG procedure, the CFT approach starts out with the model Hamiltonian expressed in real-space coordinates. Following Affleck and Ludwig \([9]\), we introduce left-moving field operators \(\psi_\alpha(x) (\alpha = \pm 3/2, \pm 1/2)\) and rewrite Eqs. (2) and (3) as

\[
H_{ch} = \frac{i v_F}{2\pi} \int_{-\infty}^{\infty} dx \, \psi_\alpha(x) \partial_x \psi_\alpha(x),
\]

and

\[
H_1 = v_F \rho J \psi_0(0) \hat{L}_{\alpha\beta} \psi_\beta(0) \cdot \vec{S}_I,
\]

where \(\rho = 1/D\) is the density of states.

#### A. Free electrons

We must next find the Sugawara forms \([31]\) equivalent to Eqs. (64) and (65). These are harmonic oscillator-like Hamiltonians quadratic in certain “current” operators of the system whose spectrum can be determined by the relevant ladder-operator algebra. We follow the logic of Affleck and Ludwig \([9]\): first, decompose the free electron Hamiltonian in a Sugawara form which separates out the spin currents from other currents (e.g., charge) of the system. Then couple the electron spin to the impurity and generate the new spectra. The interaction with the impurity spin is “absorbed” into the spin sector of the Sugawara form Hamiltonian through a simple completing of the square. The excitations of the interacting system are found from those of the non-interacting system through application of the “fusion rule” \([3]\) which, loosely, corresponds to simple addition of the impurity spin to the conduction spins subject to the constraints of the Kac-Moody spin algebra.

We first consider the case of anti-periodic boundary conditions for the conduction states which corresponds to the odd-\(N\) NRG iterations, and gives rise to a non-degenerate free electron ground state. The Sugawara Hamiltonian is constructed from the Fourier components of the conserved currents—axial charge (or isospin) and spin. We therefore consider a segment of length \(2\ell\), with anti-periodic boundary conditions, and define a Fourier sequence for each component of the axial charge:

\[
Q_n^z = \sum_{\alpha} \int_{-\ell}^{\ell} \left[ \psi_\alpha(x) \bar{\psi}_\alpha(x) - \frac{1}{2} \right] \exp(-i\pi nx/\ell) \, dx,
\]

and

\[
Q_n^+ = (Q_n^-)^\dagger = \int_{-\ell}^{\ell} \left[ \psi_{3/2}^\dagger(x) \bar{\psi}_{3/2}^\dagger(x) - \psi_{1/2}^\dagger(x) \bar{\psi}_{1/2}^\dagger(x) \right] \exp(-i\pi nx/\ell) \, dx.
\]

Expressed as combinations of the conduction band operators \(c_{\epsilon}\), these components are

\[
Q_n^\pm = \sum_{\epsilon,\alpha} \left[ \epsilon_{\epsilon,\alpha} c_{\epsilon+\nu v_F \pi/2\ell,\alpha} - \frac{1}{2} \delta_{\epsilon,0} \right],
\]

and
Likewise, for the spin current, we have

$$\mathcal{J}_n = \sum_{\alpha\beta} \int_{-\ell}^{\ell} \psi_{\alpha}^*(x) \tilde{L}_{\alpha\beta} \psi_{\beta}(x) \exp(-i\pi nx/\ell), \, dx,$$

(70)

with $\mathcal{J}_0$ the total spin operator for the conduction system, referenced to the filled Fermi sea.

That the Fourier components $\tilde{Q}_n$ ($n = -\infty\ldots\infty$) obey the level-$k$ Kac-Moody commutation relations with $k = k_Q = 2$ is easily verified by direct substitution of Eqs. (66-69):

$$[Q_n^a, Q_m^b] = i\epsilon^{abc} Q_{n+m}^c + n\delta_{ab}\delta_{n,-m}.$$

(71)

Similarly, it is easily shown that the components $\mathcal{J}_n$ obey the level-$k$ Kac-Moody commutation relations with $k = k_J = 10$:

$$[J_n^a, J_m^b] = i\epsilon^{abc} J_{n+m}^c + 5n\delta_{ab}\delta_{n,-m}.$$

(72)

Note that although the level of the axial-charge algebra, $k = 2$ is equal to that for the two-channel impurity spin-1/2 Kondo problem, the level of the spin Kac-Moody algebra, $k = 10$ is substantially higher. Thus, although the single-channel conduction spin-3/2, impurity spin 1/2 model and the two-channel impurity spin-1/2 model have the same conduction-band degeneracy, their low-energy spectra are considerably different. As pointed out by Sengupta and Kim, the Kac-Moody algebra specified by Eq. (72) is an example of the general result for conduction spin $S_c$ which gives $k_J = 2S_c(S_c + 1)(2S_c + 1)/3$.

The idea is now to write the Hamiltonian as a quadratic form in the axial charge (or isospin) currents and the spin currents. That this is possible is suggested by the Harmonic oscillator like structure of the commutation relation of, e.g., $J_m^a$ with $H_{cb}$. Specifically,

$$[H_{cb}, J_m^a] = -v_F m \frac{\pi}{\ell} J_m^a.$$

(73)

By assuming such a separation into quadratic forms, directly computing the commutation and matching the normalization of the quadratic forms to Eq. (74), we can construct the Sugawara hamiltonian. It turns out that the normalizations depend only on the levels of the Kac-Moody algebras in the problem.

The Kac-Moody levels determine the Sugawara form of the conduction Hamiltonian:

$$H_{cb} = \frac{v_F \pi}{\ell} \left[ \sum_{n = -\infty}^{\infty} \frac{1}{12} : J_{-n} : \mathcal{J}_n : + \sum_{n = -\infty}^{\infty} \frac{1}{4} : Q_{-n} : Q_n : \right],$$

(74)

where $A$ indicates normal-ordering of the operator $A$.

We wish to diagonalize this Hamiltonian. To this end, we consider first the primitive states (or highest-weight states), which are eigenstates devoid of particle-hole excitations and satisfying the conditions $q \leq k_Q/2 \equiv 1$ and $j \leq k_J/2 = 5$. We note that the combination of these constraints limits the primitive state spin values to $j \leq 7/2$. For $n > 0$, it follows from Eq. (68) that the $z$ component $Q_n^z$ annihilates particle-hole excitations, and hence $Q_{n>0}^z|\phi_0\rangle = 0$ for any primitive state $|\phi_0\rangle$. (For $n > 0$, by contrast, $Q_n^+|\phi_0\rangle$ need not vanish, for $Q_n^{++} > 0$ creates particle-hole excitations). Likewise, $Q_{n>0}^z|\phi_0\rangle = Q_{n>0}^z|\phi_0\rangle = 0$, since $Q_n^{++} (Q_n^-)$ (annihilates) electron pairs with one particle above the Fermi level and the other below. Finally, $\mathcal{J}_{n>0}^z$ annihilates particle-hole excitations and thus $\mathcal{J}_{n>0}^z|\phi_0\rangle = 0$. It results that, if $(q, j)_0$ is the primitive state with axial charge $q$ and spin $j$, then on the right-hand side of Eq. (74) only the $n = 0$ term contributes to its energy $E_0(q, j)$:

$$H_{cb}|q, j\rangle_0 = \frac{v_F \pi}{\ell} \left( \frac{1}{12} J_0^2 + \frac{1}{4} Q_0^2 \right) |q, j\rangle_0.$$

(75)

Since as Eqs. (68, 74) show, $Q_0$ and $\mathcal{J}_0$ are the conduction-band axial charge and spin operators, respectively, the primitive-state energies are given by

$$E_0(q, j) = \frac{v_F \pi}{\ell} \left[ \frac{q(q + 1)}{4} + \frac{j(j + 1)}{12} \right].$$

(76)
To determine the quantum numbers \( q \) and \( j \) associated with each primitive state, we have to construct it from the single-particle levels of the conduction-band Hamiltonian. Particle-hole symmetry disposes these levels symmetrically with respect to the Fermi energy \( \epsilon_F \). For even number of levels (The number of levels depends on the number of lattice sites and on the boundary conditions; for periodic boundary condition, for instance, the number of levels equal the number of sites.), then, half of them lie above \( \epsilon_F \) and half below, and the ground state of \( H_{cb} \) will be nondegenerate. This spectrum corresponds to an odd numbered iteration of the NRG, and to antiperiodic free-fermion boundary conditions. For odd number of energy levels, in contrast, one level—which can accommodate up to four electrons—must lie at the Fermi energy, and the ground-state degeneracy is \( 2^4 = 16 \). This corresponds to the even numbered NRG iterations and to free electrons with periodic boundary conditions.

For an even number of levels, the nondegenerate ground state has, therefore, quantum numbers \( q = j = 0 \). The other primitive states are generated by filling the first level above \( \epsilon_F \) with one or two electrons (or by vacating the first level below \( \epsilon_F \), corresponding to quantum numbers \((q,j)\) equal to \((1/2,3/2),(1,2),(0,3)\), and another primary state corresponding to three elementary excitations, which is \((1/2,7/2)\). All other excited states are not primary: since \( q \) increases as the energy levels are successively filled, the ones not containing elementary particle-hole excitations must have \( q > 1 \). The five primary multiplets appear in Table I.

The 16-fold degenerate ground state comprises three multiplets: (i) the triplet \((q,j) = (1,0)\), corresponding to a vacant (or fully occupied) level at \( \epsilon_F \), (ii) the octuplet \((q,j) = (1/2,3/2)\), corresponding to a single electron (or three electrons) at \( \epsilon_F \), and (iii) the quintuplet \((q,j) = (0,2)\), corresponding to a doubly occupied level at \( \epsilon_F \). Along with the states with two and three elementary excitations, \((q,j) = (1,3)\) and \((1/2,7/2)\), respectively, these are the only primitive states, since filling any level above the Fermi level (or vacating any level below \( \epsilon_F \)) makes \( q > 1 \). They are listed in Table I.

The eigenstates \( |\phi\rangle \) of \( H_{cb} \) containing one or more particle-hole excitations or with \( q > 1 \) are called descendant states; each such state can be obtained from a primitive state by successive applications of the raising operators \( \hat{Q}_n \) and \( \hat{J}_n \) \((n = 0,-1,-2,...)\). Disposed in order of increasing energy, a primitive state and its descendants form a conformal tower.

Two eigenstates belonging to a same tower may have different quantum numbers \( q \) or \( j \), and two energies on a same tower may have different degeneracies. The conformal towers are nonetheless important, for the commutation relations (73) and (72) make the energy spacing in each tower uniform, the splitting \( \Delta E = v_F \pi / \ell \) separating any two successive energies. It follows that, to calculate the low-energy spectrum of \( H_{cb} \), we need only construct the conformal towers associated with the lowest-lying primitive states. Eq. (73) gives the energy of the primitive state at the base of a tower, and the energies of the descendant states are given by

\[
E_m(q,j) = \frac{v_F \pi}{\ell} \left[ \frac{q(q+1)}{4} + \frac{j(j+1)}{12} + m \right],
\]

where \( m \) is a positive integer. Notice that the \( q \) and \( j \) are the quantum numbers of the primitive states at the base of the tower, in general different from the quantum numbers of the descendant states. The eigenvalues of the descendant states listed in Tables (I) and (II) were computed with Eq. (77).

B. Interacting system

We now consider the interaction term \( H_1 \). Expressed in terms of the spin Fourier components \( \hat{J}_n \), the right-hand side of Eq. (65) takes a particularly simple form:

\[
H_1 = \frac{v_F \pi}{\ell} \rho J \hat{S}_I \cdot \sum_{n=\infty}^{\infty} \hat{J}_n.
\]  (78)

To take advantage of the similarity between this expression and the one defining the Sugawara Hamiltonian, Eq. (74), it is convenient to introduce the shifted Fourier components

\[
\tilde{J}_n = \hat{J}_n + \hat{S}_I.
\]  (79)

Since the spins \( \tilde{J} \) and \( \hat{S}_I \) have the same \([SU(2)]\) symmetry, these shifted components follow the (level 10) commutation relations [Eq. (72)] obeyed by \( \hat{J}_n \). Moreover, for \( \rho J = 1/6 \), Eqs. (72) and (78) combine into a single expression for the model Hamiltonian (1) that is formally equivalent to the conduction Hamiltonian (1):
Identifying this special coupling constant with the low-temperature fixed point of the model Hamiltonian, we reduce the computation of the low-energy spectrum to the diagonalization of a quadratic Hamiltonian. This diagonalization follows the steps outlined in Section III A. There, however, the quantum numbers \( q \) and \( j \) of the conformal towers were determined by the free-electron single-particle levels. Here, to determine the quantum numbers \( q' \) and \( j' \) of the interacting system, we refer to Affleck’s and Ludwig’s fusion rule \( [6] \).

According to that rule, the embedding of the impurity spin \( S_I = 1/2 \) in the conduction-band spin dictated by Eq. 74 leaves the conformal tower axial charge unchanged, \( q' = q \) and yields a sequence of spins \( j' \) ranging from \( |j - 1/2| \) to the minimum of \( j + 1/2 \) and \( k_I - j - 1/2 \). Thus, for \( j \leq 9/2 \), i.e., for the spins we are interested in, the fusion rule is equivalent to the angular momentum addition law.

It is therefore a simple matter to construct the conformal towers for the interacting system, the low-energy spectrum being given by Eq. 80. Results for the cases of a nondegenerate and of a degenerate free-electron ground state appear in Tables III and IV, respectively.

Finally, we briefly address an issue raised by Sengupta and Kim [16], who suggest that for arbitrary \( S_I, S_c \), since the spin current Kac-Moody algebra is the same as for a multichannel model with \( k_j = 2S_c(S_c + 1)/(2S_c + 1)/3 \) channels that overcompensation will occur for impurity spins obeying \( S_I < k_j/2 \). This is based upon the result for the multichannel model which says overcompensation occurs for \( S_I < k, k \) the number of channels. We disagree with this claim. To see why, we note that based upon the single fusion rule the maximal ground state spin which is obtained considering both non-degenerate and degenerate free spectra is \( S_I'(\text{degenerate}) \) and \( S_c' - S_I'(\text{non-degenerate}) \) where

\[
S_c^* = \sum_{m>0} m = \frac{S_c(S_c + 1)}{2} \quad [2S_c \text{ even}] \tag{81}
\]

or

\[
S_c^* = \frac{(S_c + 1/2)^2}{2} \quad [2S_c \text{ odd}] \tag{82}
\]

In view of this, we believe the maximum overcompensated spin value is determined by the condition \( S_c^* > S_I \), not \( k_j/2 > S_I \). This checks with the generalization of the strong coupling picture presented in Fig. 2, since the largest conduction spin you can form from the single band in this picture is in fact \( S_c^* \), which restricts overcompensated impurity spins to \( S_I \leq S_c - 1/2 \).

C. Boundary Operator Spectra and Physical Properties

The conformal theory may also be used to generate the spectra of boundary operators about the non-trivial fixed point by evaluating the spectrum for a different set of boundary conditions, as noted by Affleck and Ludwig [6]. Specifically, one considers the situation where a Kondo impurity is placed at each end of the system. Then one applies a double fusion rule to identify the spectrum, because the impurity spin must be absorbed at each end. Denoting the impurities at either end by \( S_I, S_I' \) the double fusion rule that yields allowed \( S \) values of this double impurity system is, for a parent state with spin \( S' \)

\[
0 \leq S \leq \min\{S' + S_I + S_I', k_J - S' - S_I - S_I'\} . \tag{83}
\]

The quantum numbers of the states with these boundary conditions then identify the quantum numbers of allowed boundary operators. These operators are so called because the critical behavior is limited solely to the boundary of the system. The normalized energy levels \( \delta E/\nu_F \pi \) give the scaling dimensions \( \Delta_\phi \) of the operators, which enter into time dependent correlation functions of the boundary operators through the long time expression

\[
< O(\tau)O(0) > \sim \frac{1}{\tau^{2\Delta_\phi}} . \tag{84}
\]

We present the spectrum of primary field boundary operators in Table V as determined by the double fusion rule. From this table we can glean immediately a number of facts about the physical properties of the model:

1) Low Temperature Behavior of the Specific Heat and Magnetic Susceptibility. The field with quantum numbers \( q = o, j = 1 \) is a triplet of primary spin field operators \( \Phi_{x,y,z}^o \), which has scaling index of \( \Delta_\phi = 1/6 \). In the manner of
Affleck and Ludwig, we may identify the leading irrelevant operator about the fixed point Hamiltonian as \( \mathcal{J}^{-1} \cdot \Phi \). If we carry out second order perturbation theory to compute the impurity contribution to the specific heat coefficient \( C/T = \gamma \) and magnetic susceptibility \( \chi \), as did Affleck and Ludwig for the multichannel Kondo model, we will obtain \( \gamma, \chi \sim T^{2\Delta_\phi - 1} = T^{-2/3} \). This conclusion was also reached by Sengupta and Kim. The scaling dimension of the magnetic field \( h \) is \( 1 - \Delta_\phi = 5/6 \) and the crossover scale \( T_h = h^{6/5}/T_K^{1/5} \). To see this, consider adding the local Zeeman term

\[
S_{\text{Zeeman}} = h^2 \int_0^\beta d\tau \Phi^2(\tau)
\]  

(85)

to the action. Upon rescaling time by \( \Lambda \), the prefactor becomes \( h^2 \Lambda^{1 - \Delta_\phi} \) due to the singular behavior of \( \Phi^2 \) for long times. This must be a constant to preserve the form of the action. Hence \( (h)^{1/(1 - \Delta_\phi)} = (h^2)^{6/5} \sim \Lambda \) and the physical properties will be universal functions in \( x = h^{6/5}/T \).

2) **Crossover in Applied Magnetic Field** Application of a magnetic field is a relevant perturbation which, in analogy with the multichannel model, will drive the system to a Fermi liquid fixed point associated with a polarized scatterer. The scaling dimension of the magnetic field \( h \) is \( 1 - \Delta_\phi = 5/6 \) and the crossover scale \( T_h = h^{6/5}/T_K^{1/5} \). To see this, consider adding the local Zeeman term

(85)

to the action. Upon rescaling time by \( \Lambda \), the prefactor becomes \( h^2 \Lambda^{1 - \Delta_\phi} \) due to the singular behavior of \( \Phi^2 \) for long times. This must be a constant to preserve the form of the action. Hence \( (h)^{1/(1 - \Delta_\phi)} = (h^2)^{6/5} \sim \Lambda \) and the physical properties will be universal functions in \( x = h^{6/5}/T \).

3) **Relevance of Exchange Anisotropy** The operator \( Q \) with quantum numbers \( q, j = 2 \) is a local quadrupolar field. Because its scaling index is \( 1/2 \), this suggests that application of a uniaxial stress or electric field gradient conjugate to the quadrupolar field will be a relevant perturbation. This is even the case for \( S_I = 1/2, 3/2 \) in contrast to the multichannel Kondo model. The reason is straightforward: exchange anisotropy in this model will split the conduction band degeneracy between \( |S^z| = 3/2, 1/2 \) states which is responsible for the nontrivial ground state. This is analogous to the lifting of channel degeneracy which is always relevant in the multi-channel Kondo model. In the event that we generalize from impurity spin \( 1/2 \) to impurity spin \( 1 \), the exchange anisotropy will also crystal field split the impurity spin and further alter the fixed point structure.

4) **Presence of Fermion Operators** The operators with \( q = 1/2, j = 3/2 \) have appropriate quantum numbers and scaling indices to be identified with fermion fields. As in the two-channel model, there are two such fields here, and the interpretation of this is unclear, though it appears to be a generic result for overcompensated Kondo models with \( S_I = 1/2 \).

**D. Comparison between NRG and Conformal Theory**

In the last columns of Tables and [15] are NRG eigenvalues normalized such that the first excited state energy relative to the ground state is forced to agree with the conformal theory finite size spectra. The scaled Energies are then multiplied by a factor of 24 to multiply out the lowest common denominator of the conformal theory spectra. NRG iterations for odd number of sites correspond to even number of levels and so should be compared with the conformal theory spectra for non-degenerate free electrons. NRG iterations with even numbers of sites correspond to odd number of levels and thus should be compared with the conformal theory spectra for degenerate free electrons.

We can readily see from the tables that with few exceptions the agreement is quite satisfactory. When discrepancies arise, there are three sources, identified in Ref. [23]; (i) the logarithmic discretization of the NRG conduction band breaks conformal invariance, and will lead to detailed deviations between NRG and conformal theory spectra as the energy is raised; (ii) the conformal theory spectra themselves are generated at the fixed point, and corrections to scaling can arise as the energy is raised due to the irrelevant operators about the fixed point (the NRG takes these into account); (iii) the truncation of states in each \( q, j \) sector of the NRG will lead to systematic errors in the eigenvalues as one moves the excitation energy towards the cutoff value.

It is satisfactory that in each sector (degenerate vs. non-degenerate free states) we not only have good agreement on the energies but also find all the states generated by the conformal theory up to the energies considered. Hence we have little doubt that the non-trivial fixed point identified by absorption of the impurity spin in the conformal theory is precisely the same as the fixed point identified by the NRG analysis.

**IV. DISCUSSION AND CONCLUSION.**

We have analyzed the \( S_I = 1/2, S_z = 3/2 \) single band Kondo model with the Numerical Renormalization Group (NRG) and conformal field theory. Our work confirms that the model displays a non-trivial intermediate coupling fixed point which is unstable to the relevant perturbations of an applied magnetic field and spin exchange anisotropy. In particular, we have obtained detailed numerical agreement between the finite size spectra generated by the conformal theory with those of the NRG, both for degenerate and non-degenerate free electron spectra. From the conformal
theory, we infer that the impurity contributions to the specific heat coefficient and magnetic susceptibility will diverge as $T^{-2/3}$ and that in the presence of a magnetic field the system will crossover to a Fermi liquid with a polarized scatterer, with crossover scale $T_h = h^{6/5}/T_K^{1/5}$ and that thermodynamic properties will be universal functions of $x = h^{6/5}/T$. We have argued that when the model is generalized to arbitrary $S_I, S_c$ that non-trivial intermediate coupling fixed points corresponding to over-compensation will arise for $S_I < S_c^*$ with $S_c^*$ defined by Eqs. S1 and S2. We have also generated the operator primitive boundary operator spectrum of the model employing the double fusion rule. Our conformal theory results agree with those of Sengupta and Kim [14] for the finite size spectra and low temperature thermodynamics despite the different choice of basis for the Sugawara hamiltonian in our work.

We wish to close by discussing the experimental relevance of our work and further theoretical issues raised by it.

Our work may be of relevance at intermediate temperature scales in two-level system Kondo impurity materials as an unstable fixed point. An experimental example of this may have been realized in metallic point contact devices [32]. Such fixed points were first studied by Zaránd [13]. Similarly, this fixed point may be relevant at intermediate temperature scales for dilute alloys of Ce$^{3+}$ ions, such as $La_{1-x}Ce_xCu_2Si_2$ [33], such as argued by Kim [14] and Kim and Cox [15].

On the theoretical front, two key issues are raised. First, we are unable to compute the residual entropy and residual resistivity of this model using the same methods of Affleck and Ludwig [1] because as far as we are aware no generalization of the Kac-Peterson [34] and Verlinde [35] formulæ for the spin $1/2$ representations other than spin $1/2$. The computation of the residual entropy and residual resistivity rests upon knowledge of the Kac-Peterson [34] and Verlinde [35] formulæ for the spin $1/2$ representation of SU(2). Such a generalization would be of theoretical interest at least for working out the general properties of this model for arbitrary $S_I, S_c$, though it is unlikely to be of great experimental relevance.

Second, and of greater interest is the connection of this model to the Bethe-Ansatz solutions of the multi-channel Kondo model, which point was first made by Zaránd [13] in his $1/k$ expansion solution to the $k$-channel two-level system Kondo model. In the approach of Tsvelik and Wiegman [17] to the $k$-channel Kondo model, it is shown that a model with a single band of spin $k/2$ conduction electrons possessing an interaction to the impurity spin of a certain polynomial $P(x)$ in $x = S_I \cdot S_c^{(0)}$ is in fact an integrable model. It is claimed that this model has the same Bethe-Ansatz spectrum in the compensated case as the corresponding $k$-channel impurity Anderson model in the local moment limit where a Kondo description applies. It is then conjectured that in the overcompensated case the single band spin $k/2$ model has the same spectrum as the $k$-channel Kondo model. In the case $S_I = 1/2$, $P(S_I \cdot S_c^{(0)})$ reduces to a simple Heisenberg exchange form. This claim has obvious physical appeal as illustrated in Fig. 1, since the strong coupling limit of the model indeed “fuses” the conduction electrons into a single large spin complex with magnitude $k/2$. However, some doubt about the conjecture arises when one considers the non-interacting limit. In that case, there are $2k$ free fermion branches to the $k$ channel model, whereas the single channel spin $k/2$ band has $k + 1$ free fermion branches. Namely, in the noninteracting limit, the number of degrees of freedom of the two models simply do not match.

Andrei and Destrei [18] solved the Bethe-Ansatz directly on the multichannel model. In their approach, a dynamical fusing of conduction electrons into a spin $k/2$ object describes the ground state. This again would appear to nicely match the strong coupling picture of Nozières and Blandin [1]. The Bethe-Ansatz equations obtained by Andrei and Destrei [15] are identical to those obtained by Tsvelik and Wiegman [17] on the basis of the conjecture described in the preceding paragraph. Indeed, both Bethe-Ansatz solutions yield thermodynamics and finite size spectra in excellent agreement with NRG and conformal theory results on the $k$ channel models, giving great confidence in the final Bethe-Ansatz equations, arrived at through completely different routes. An interpretation of the correspondence is that the Tsvelik and Wiegman [17] conjectured mapping amounts to an effort to match the dynamical fusion of Andrei and Destrei [15] to a local Hamiltonian. This conjecture leads us to expect that the $k = 3$ channel $S_I = 1/2$ model should have the same spectrum as the single band $S_c = 3/2, S_I = 1/2$ model, but this is clearly not the case as shown here and by Sengupta and Kim [16]. We regard this discrepancy between the Tsvelik and Wiegman Bethe-Ansatz approach [17] and NRG/conformal theory approaches presented here and in Sengupta and Kim [16] as an interesting paradox to be resolved.

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**TABLE I.** Low-energy spectrum of the free conduction-band Hamiltonian for a nondegenerate ground state. Energies E (measured from the ground state) less than 2υFπ/ℓ are shown. The fourth column distinguishes primary states (p) from descendant ones (d).
TABLE II. Low-energy spectrum of the free conduction-band Hamiltonian for a degenerate ground state. Energies \( E \) (measured from the ground state) less than \( v_F \pi/\ell \) are shown. The fourth column distinguishes primary states (p) from descendant ones (d).

| \( q \) | \( j \) | \( \ell \) \( v_F \pi \) | \( p/d \) |
|-------|-------|-----------------|-------|
| 0     | 0     | 0               | p     |
| 1/2   | 3/2   | 1/2             | p     |
| 1     | 2     | 1               | p     |
| 0     | 3     | 1               | p     |
| 0     | 1     | 1               | d     |
| 1     | 0     | 1               | d     |
| 1/2   | 7/2   | 3/2             | p     |
| 3/2   | 3/2   | 3/2             | d     |
| 1/2   | 5/2   | 3/2             | d     |
| 1/2   | 3/2   | 3/2             | d     |
| 1/2   | 1/2   | 3/2             | d     |
| 0     | 2     | 1               | d     |
| 0     | 1     | 1               | d     |
| 0     | 0     | 1               | d     |
| 3/2   | 3/2   | 1               | d     |
| 1/2   | 5/2   | 1               | d     |
| 1/2   | 3/2   | 1               | d     |
| 1/2   | 3/2   | 1               | d     |
| 1/2   | 1/2   | 1               | d     |
TABLE III. Low-energy spectrum of the interacting model Hamiltonian for a nondegenerate conduction-band ground state (even iteration in NRG). Energies of the states derived from the ones in Table I by the fusion-rule procedure described in the text are shown. The fourth column distinguishes primary states (p) from descendant ones (d). The fifth column lists some NRG low energy spectra normalized such that the energy difference between the ground state and the first excited state agree with the conformal theory. Overall the agreement is excellent. The lack of perfect numerical agreement is due to the combination of the breaking of conformal symmetry by the NRG logarithmic discretization scheme and the truncation of states above a particular energy necessary to render the NRG block Hamiltonian matrices finite. Note the reversal of the pairing of integer(half-integer) \(q\) to integer(half-integer) \(j\) compared to Table I which indicates the non-Fermi liquid character of this spectrum in conjunction with the fractional energy spacings.

| \(q\) | \(j\) | \(\frac{q}{p}\) | p/d | \(E_{NRG}(\pi/24)\) |
|-------|-------|----------------|-----|------------------|
| 0     | 1/2   | 0              | p   | 7.000            |
| 1/2   | 1     | 7/24           | p   | 15.166           |
| 1     | 5/2   | 2/3            | p   | 16.018           |
| 0     | 3/2   | 3/4            | p   | 18.051           |
| 0     | 1     | 1              | d   | 24.000           |
| 0     | 1/2   | 1              | d   | 24.358           |
| 1     | 1/2   | 1              | d   | 24.262           |
| 1     | 5/2   | 7/6            | p   | 28.443           |
| 0     | 7/2   | 5/4            | p   | 30.309           |
| 3/2   | 2     | 31/24          | d   | 31.165           |
| 1/2   | 1     | 31/24          | d   | 31.486           |
| 1/2   | 1     | 31/24          | d   | 31.198           |
| 3/2   | 2     | 13/8           | d   | 39.637           |
| 1/2   | 1     | 13/8           | d   | 35.077           |
| 1/2   | 0     | 13/8           | d   | 31.133           |
| 0     | 7/2   | 5/3            | d   | 40.443           |
| 0     | 5/2   | 5/3            | d   | 45.446           |
| 0     | 3/2   | 5/3            | d   | 40.581           |
| 1     | 5/2   | 5/3            | d   | 41.154           |
TABLE IV. Low-energy spectrum of the model Hamiltonian for a degenerate conduction-band ground state (odd iteration in NRG). Energies of the states derived from the ones in Table II by the fusion-rule procedure described in the text are shown. The fourth column distinguishes primary states (p) from descendant ones (d). The fifth column lists some NRG low energy spectra normalized such that the energy difference between the ground state and the first excited state agree with the conformal theory. Overall the agreement is excellent. The lack of precise numerical agreement is due to a combination of the breaking of conformal symmetry by the NRG logarithmic discretization procedure and the truncation of energy levels to render the NRG block Hamiltonian matrices finite for diagonalization. Note the reversal of the binding of integer(half-integer)\(q\) to integer(half-integer)\(j\) in comparison with Table II, which, along with the fractional energy spacings, indicates the inapplicability of Fermi liquid theory to this spectrum.

| \(q\) | \(j\) | \(\frac{\nu}{\nu_F^2}\) | p/d | \(E_{NRG}/(24)\) |
|---|---|---|---|---|
| 0 | 3/2 | 0 | p | 0.000 |
| 1/2 | 1 | 1/24 | p | 1.000 |
| 1 | 1/2 | 1/4 | p | 6.004 |
| 1/2 | 2 | 3/8 | p | 9.014 |
| 0 | 5/2 | 5/12 | p | 10.018 |
| 1/2 | 3 | 7/8 | p | 21.782 |
| 1 | 5/2 | 11/12 | p | 22.759 |
| 0 | 5/2 | 1 | d | 24.715 |
| 1 | 3/2 | 1 | d | 24.942 |
| 0 | 3/2 | 1 | d | 25.245 |
| 0 | 1/2 | 1 | d | 24.879 |
| 3/2 | 1 | 25/24 | d | 25.593 |
| 1/2 | 2 | 25/24 | d | 26.114 |
| 1/2 | 1 | 25/24 | d | 25.550 |
| 1/2 | 1 | 25/24 | d | 26.608 |
| 1/2 | 0 | 25/24 | d | 26.938 |
| 1 | 1/2 | 5/4 | d | 30.765 |
| 1 | 1/2 | 5/4 | d | 33.357 |
| 1 | 1/2 | 5/4 | d | 31.789 |
| 0 | 1/2 | 5/4 | d | 31.967 |
| 3/2 | 2 | 11/8 | d | 35.504 |
| 1/2 | 3 | 11/8 | d | 34.977 |
| 1/2 | 2 | 11/8 | d | 34.969 |
| 1/2 | 2 | 11/8 | d | 36.339 |
| 1/2 | 1 | 11/8 | d | 34.889 |
| 1 | 5/2 | 17/12 | d | 36.459 |
| 0 | 7/2 | 17/12 | d | 35.918 |
| 0 | 5/2 | 17/12 | d | 37.471 |
| 0 | 3/2 | 17/12 | d | 35.823 |
TABLE V. Primary Field Boundary Operator Spectrum for the $S_c = 3/2, S_I = 1/2$ model. We obtain this spectrum by applying the double fusion rule of Affleck and Ludwig [9] to the spectrum of Table III. This rule assumes an impurity at each end of the finite size chain of length $\ell$. The scaling dimensions $\Delta_o$ are simply the scaled energies $\ell E/v_F \pi$ for this double impurity boundary condition. The $Q = 0, j = 0$ operator is simply the local charge of the site. The physical interpretation of the $q = 0, j = 1$ operator is the primary spin field at the impurity site. With the scaling dimension of $1/6$, this indicates that the specific heat coefficient and susceptibility will diverge as $T^{-2/3}$ as argued in the text. The $q = 1/2, j = 3/2$ field is a fermionic operator, which always must have scaling index $1/2$ in any model. Fields with $q = 1$ include pair fields ($q_z = \pm 1$), which clearly do not provide singular pair field susceptibilities here. The $q = 0, j = 2$ field is a quadrupolar tensor, which given scaling index $1/2$, indicates the relevance of exchange anisotropy for this model. See the text for further discussion.

| $q$ | $j$ | $\Delta_o$ |
|-----|-----|-------------|
| 0   | 0   | 0           |
| 0   | 1/2 | 1/6         |
| 1/2 | 1/2 | 1/4         |
| 1/2 | 3/2 | 1/2         |
| 1/2 | 3/2 | 1/2         |
| 0   | 2   | 1/2         |
| 1   | 1   | 2/3         |
| 1/2 | 5/2 | 11/12       |
| 1   | 2   | 1           |
| 0   | 3   | 1           |
| 0   | 3   | 1           |
| 1   | 2   | 1           |
| 1   | 3   | 3/2         |
| 0   | 4   | 5/3         |
FIG. 1. **Strong coupling limit of the two-channel $S_f = 1/2$ Kondo model** At strong coupling (zero kinetic energy) in the two-channel spin 1/2 Kondo model, two units of conduction spin (labeled $c_1$ and $c_2$) bind to form a net spin 1 complex that lines up antiparallel to the impurity spin. The resulting spin of the ground state is $S_{tot} = 1/2$. The strong coupling fixed point is unstable to the introduction of the kinetic energy because antiferromagnetic superexchange will be generated to electrons off the impurity site as argued by Nozières and Blandin \[6\] of order $t^2/J$, where $t$ is the intersite hopping, which maps the effective model back to the weak coupling limit where the exchange interaction must grow. Since both weak coupling and strong coupling limits are unstable, a non-trivial fixed point must exist at intermediate coupling.

FIG. 2. **Strong coupling limit of the single channel $S_c = 3/2, S_I = 1/2$ model** In the strong coupling limit of this model, two conduction electrons with $S_z = 3/2, 1/2$ will bind to form a spin 2 object that aligns antiparallel with the impurity spin. This strong coupling fixed point is unstable to the introduction of the kinetic energy which will generate an antiferromagnetic superexchange with the $S_{tot} = 3/2$ bound object of order $t^2/J$, which then maps it back to a weak coupling Kondo problem with growing exchange interaction. Since both strong- and weak-coupling limits are unstable, a non-trivial fixed point must exist at intermediate coupling.

FIG. 3. **RG flow diagram in the free electron limit for $S_c = 3/2, S_I = 1/2$ exchange interaction model.** The RG flow diagram is displayed for bare coupling $g = 10^{-10}$. This bare coupling correspond to the free electron limit. The low lying excitation energy spectrum is that of free conduction electrons. Note that low lying energy levels are evenly spaced. Labeling the first five lowest lying symmetry sectors are as follows throughout all the RG flow diagrams presented here. (1) $N = \text{odd case.}$ the ground energy symmetry sector is (0,1/2): the solid line; (1/2,1): the dashed line; (1/2,2): the dash-dotted line; (0,3/2): the dash-dot-dotted line; (1,3/2): the dash-dash-dotted line. (2) $N = \text{even case.}$ the ground energy symmetry sector is (0,3/2): the solid line; (1/2,1): the dashed line; (1,1/2): the dash-dotted line; (1/2,2): the dash-dot-dotted line; (0,5/2): the dash-dash-dotted line.

FIG. 4. **RG flow diagram displaying the crossover from the weak coupling to non-trivial finite coupling fixed point for $S_c = 3/2, S_I = 1/2$ exchange interaction model.** The RG flow diagram is displayed for initial exchange coupling $g = 0.01$. With this weak coupling, we can observe the clear crossover from the weak coupling fixed point to new fixed point which is completely different from the former. Before the crossover, the low lying excitation energy spectrum is close to that of free conduction electrons. After the crossover, the low energy excitation spectrum is described by non-Fermi liquid. See Figs. 3, 4, and 5.

FIG. 5. **RG flow diagram with the initial weak coupling for $S_c = 3/2, S_I = 1/2$ exchange interaction model.** The RG flow diagram is displayed for bare coupling $g = 0.1$. This bare coupling corresponds to the weak coupling regime. The low lying excitation spectrum is quite different from those of free electrons in Fig. 4.

FIG. 6. **RG flow diagram with with the initial coupling close to the fixed point for $S_c = 3/2, S_I = 1/2$ exchange interaction model.** The RG flow diagram is displayed for bare coupling $g = 0.2$. This bare coupling is close to the fixed point. Note that the third-order scaling analysis gives $g^* = 0.2$ at the fixed point.
FIG. 7. RG flow diagram with the initial strong coupling for $S_e = 3/2$, $S_f = 1/2$ exchange interaction model. The RG flow diagram is displayed for bare coupling $g = 0.5$. This bare coupling corresponds to the strong coupling regime.