Low-temperature physics of the two-impurity, two-channel Kondo model

Kevin Ingersent\textsuperscript{a,}\textsuperscript{*}, Barbara A. Jones\textsuperscript{b}

\textsuperscript{a} Department of Physics, University of Florida, 215 Williamson Hall, Gainesville, FL 32611, USA
\textsuperscript{b} IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, CA 95120 USA

Abstract

Numerical renormalization group calculations have shown that any nonzero RKKY coupling between a pair of spin-\(\frac{1}{2}\) impurities destroys the zero-temperature critical point responsible for the marginal-Fermi-liquid behavior of the single-impurity, two-channel Kondo model. Here we report recent progress on calculating the low-temperature properties of the two-impurity model.

1. Introduction

The multichannel Kondo Hamiltonian has received much recent attention as a possible description of a number of physical systems. The most intensive study has gone into a possible two-channel description \cite{1} of certain uranium- and cerium-based compounds which exhibit anomalous (non-Fermi-liquid) behavior at low temperatures \cite{2, 3}. While some properties of these systems seem to be well described by the two-channel Kondo model for a single impurity, several features cannot be accounted for within this framework. These include an up-turn in the specific heat below 0.2 K \cite{2}, the suppression of the specific heat in an applied magnetic field \cite{3}, and the linear temperature dependence of the resistivity at temperatures \(T\) much below the Kondo temperature \cite{2}. One factor which may contribute to these behaviors is interaction between impurities. The \(1/T\) divergence in the single-impurity spin correlation length \cite{4} hints at the importance of such interactions at low temperatures.

The simplest model that can be used to explore the competition between magnetic ordering of the impurities and the formation of a Kondo critical state around each impurity is one containing two impurities. In this paper we discuss ongoing work to understand the physical properties of this model.

The two-impurity, two-channel Kondo model is described by the Hamiltonian

\begin{equation}
    H = \sum_{c, i} \int d^3 k \epsilon_{c i} c_{k i}^\dagger c_{k i} - J \sum_{c, i} \mathbf{s}_i \cdot \mathbf{s}_i,
\end{equation}

where \(\mathbf{s}_i, i = l, r\) represents the "left", "right" spin-\(\frac{1}{2}\) impurity, located at position \(r_i\), and \(s_i(r), c = 1, 2\), represents the spin of channel-\(c\) conduction electrons at position \(r\). We are interested in negative values of \(J\).

Assuming the conduction bands to be isotropic, and utilizing the symmetry of the model, the Hamiltonian can

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\textsuperscript{*} Corresponding author; affiliated with the National High Magnetic Field Laboratory.
be rewritten in one-dimensional form,

\[ H/D = \sum_{c,p} \int d\varepsilon \varepsilon c_{\varepsilon p}^\dagger c_{\varepsilon p} \]

\[- \sum_{c} \int d\varepsilon \int d\varepsilon' \{ [\Gamma_e(c, c') c_{\varepsilon p e}^\dagger c_{\varepsilon' p o}],

\[ + \Gamma_o(c, c') c_{\varepsilon p o}^\dagger c_{\varepsilon' p e},

\[ + \Gamma_m(c', c') c_{\varepsilon p e}^\dagger c_{\varepsilon' p e}], \}

\[ \sigma_{\mu \nu} \cdot (\Sigma_i + \Sigma_o) \], \quad (2)\]

where \( \varepsilon \) is the reduced energy, measured from the Fermi level in units of \( D \), the conduction half-bandwidth, and the operators \( c_{\varepsilon p e}^\dagger, p = e, o, \) create states of even, odd parity about the mid-point between the impurities. The dimensionless couplings \( \Gamma_e, \Gamma_o \) and \( \Gamma_m \) depend on \( J/D \), on the separation between the impurities, and on the conduction band density of states evaluated at the energies \( \varepsilon, \varepsilon' \).

2. Solution of the particle-hole-symmetric problem

Following a previous treatment of the two-impurity, one-channel Kondo Hamiltonian [5], the couplings entering Eq. (2) can be averaged over their energy arguments, thereby reducing the problem to one with just three parameters, \( \Gamma_e, \Gamma_o \) and \( \Gamma_m \). In this "energy-independent couplings approximation" the Hamiltonian is particle-hole symmetric.

The parameters \( \Gamma_e, \Gamma_o \) and \( \Gamma_m \) can be replaced by an equivalent, but more intuitive, set: (i) the Kondo temperature, \( T_K \), the characteristic energy scale for the single-impurity Kondo effect; (ii) the RKKY coupling strength, \( I \), the coefficient of the effective Hamiltonian \( -I \hat{S}_i \cdot \hat{S}_o \), obtained by perturbatively integrating out all electronic degrees of freedom in Eq. (2); (iii) \( x \equiv (\Gamma_e - \Gamma_o)/(\Gamma_e + \Gamma_o) \), the relative asymmetry between the coupling of even- and odd-parity combinations of electrons to the net impurity spin.

Ingersent et al. [6] used Wilson's numerical renormalization-group (NRG) method [7] to solve the particle-hole-symmetric version of the model. Figure 1 provides a schematic phase diagram for cases where the RKKY interaction is antiferromagnetic - the situation of greatest relevance to heavy-fermion compounds. The three-dimensional parameter space has been collapsed onto two dimensions by plotting the ratio \( I/T_K \) versus \( x \). The NRG results can be interpreted in terms of the renormalization of \( I/T_K \) and \( x \) from their "bare" values as the temperature \( T \to 0 \). There are four types of stable zero-temperature ground states:

(a) Even-parity Kondo: For \( \Gamma_e > \Gamma_o \) and weak antiferromagnetic RKKY interactions, the impurity spins are completely quenched by even-parity conduction electrons, while odd-parity electrons near the Fermi energy are totally decoupled from the impurities (i.e. \( \Gamma_e \) renormalizes to infinity, \( \Gamma_o \) renormalizes to zero). The low-energy behavior can be described by local Fermi-liquid theory with the even \([odd]-parity electrons undergoing a phase shift \( \delta_e = \pi/2 \) \([\delta_o = \pi] \) at the Fermi surface.

(b) Odd-parity Kondo: A region analogous to (a) is obtained by exchanging even- and odd-parity labels.

(c) Free-electron: For large antiferromagnetic RKKY interactions, the impurity spins undergo no Kondo effect. The low-energy electrons completely decouple from the impurities, corresponding to a local Fermi liquid with phase shifts \( \delta_e = \delta_o = 0 \).

(d) Marginal: The three regions (a)–(c) surround a fourth, within which the low-temperature behavior is not that of a Fermi liquid. Each set of initial conditions within the marginal region seems to flow to a distinct fixed point. The RKKY interaction and the asymmetry between the coupling of even- and odd-parity electrons to the impurities act as marginally relevant operators connecting these fixed points. The fixed point corresponding to two completely independent impurities lies at \( I = 0 \), \( x = 0 \), on the border...
between the marginal region and the even- and odd-parity Kondo regions. Thus, there is no finite domain of stability for single-impurity behavior [8].

3. Low-temperature properties

The local deviations from any stable Fermi-liquid fixed point can be expressed in terms of an effective Hamiltonian of the form

$$H_{\text{eff}}(T) = H_0 + \sum_i c_i (T/D)^{\lambda_i} \hat{O}_i,$$

where operator $\hat{O}_i$ respects all symmetries of the full Hamiltonian but breaks the higher symmetry of the fixed-point Hamiltonian $H_0$. The exponents $\lambda_i$ are positive, i.e., all the operators $\hat{O}_i$ are irrelevant in the renormalization-group sense. At temperatures $T \ll D$, only the leading irrelevant operators -- those with the smallest exponents -- are physically important. The coefficients $c_i$ vary with the bare parameters $T_K$, $I$, and $\alpha$.

The NRG Hamiltonian can be solved exactly at any Fermi-liquid fixed point, and expressions obtained for the eigenenergies in terms of the coefficients of the leading irrelevant operators. The $c_i$'s can be extracted by fitting energies obtained numerically. The resulting coefficients can then be inserted into analytical (perturbative) expressions for thermodynamic quantities in the vicinity of the fixed point.

For the present problem we have identified seven leading irrelevant operators that preserve the full spin, axial-charge [7] and Sp (4) [9] symmetries of the two-channel Kondo Hamiltonian. Two of these are simple operators that allow for hopping of electrons on and off the impurity sites. The remaining five operators mix channels 1 and 2 in a nontrivial way, e.g.

$$\hat{O}_p = |s_{1p} + s_{2p}|^2, \quad p = e, o,$$

and

$$\hat{O}_m = (s_{1e} + s_{2e}) \cdot (s_{1o} + s_{2o}),$$

where $s_{cep}$ is the net spin of channel-$c$, parity-$p$ conduction electrons localized about the impurity sites.

For the particle-hole-symmetric version of the problem, most of the coefficients $c_i$ entering Eq. (3) diverge as the bare parameters $I/T_K$ and $\alpha$ approach the borders of the marginal region. This is to be expected, since the marginal region is non-Fermi-liquid-like and hence cannot be related perturbatively to any Fermi-liquid fixed point.

One thermodynamic quantity of interest is the Wilson (or Sommerfeld) ratio, $R$. For single-impurity Kondo models, $R$ is a universal quantity, taking the values 2 and $8/3$ for one and two channels, respectively. Figure 2 shows the variation of $R$ with $I/T_K$ in the free-electron regime. The plot is for $\alpha = 0$, but similar results are obtained for nonzero $\alpha$ throughout the free-electron regime. For large antiferromagnetic RKKY couplings, $R$ tends to unity, the value appropriate for a free-electron gas. As the bare parameters approach the left boundary of the marginal region in Fig. 1, the Wilson ratio decreases. However, since calculation of $R$ involves taking the small difference of diverging coefficients, errors grow rapidly in this region of the parameter space. Further work is in progress to determine $R$ more accurately all round the borders of the marginal region.

In the particle-hole-symmetric version of the two-impurity, one-channel Kondo model, there is an unstable, marginal-Fermi-liquid fixed point reached from one critical value of $I/T_K$ on the antiferromagnetic side of the phase diagram [7]. This fixed point is completely wiped out by potential scattering [11]. It is natural to ask whether the same is true for the marginal region of the two-channel model. Calculations are presently being carried out to address this question.

A more general treatment of Eq. (2) is also under way. This involves the reformulation of Wilson's NRG procedure [7] to permit an essentially exact solution of Eq. (2) without relying on the energy-independent couplings approximation for an isotropic, but otherwise arbitrary, electronic dispersion.

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References