Study of the Two-Impurity, Two-Channel Kondo Hamiltonian

Kevin Ingersent,[(1),(a)] Barbara A. Jones,[(2)] and John W. Wilkins[(1)]
[(1)]Department of Physics, The Ohio State University, Columbus, Ohio 43210
[(2)]IBM Research Division, Almaden Research Center, 650 Harry Road, San Jose, California 95120
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The two-channel Kondo Hamiltonian has recently been proposed as a description of several experimental systems. Our numerical renormalization-group treatment of a pair of magnetic impurities shows that at low temperatures, interimpurity interactions destabilize the "marginal-Fermi-liquid" behavior predicted by a single-impurity model. We find four stable zero-temperature regimes, three of which can be described by Fermi-liquid theory. The fourth possesses a complex many-body ground state and non-Fermi-liquid properties which are expected to be governed by nonuniversal critical exponents.

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The single-impurity, two-channel Kondo Hamiltonian describes the exchange interaction between a localized spin-$\frac{1}{2}$ moment and *two* degenerate channels (or bands) of conduction electrons. This Hamiltonian is notable for possessing a nontrivial critical point at temperature $T=0$ which is responsible for non-Fermi-liquid behavior at low temperatures [1], including such remarkable properties [2–5] as (i) a specific-heat coefficient C/T and a static susceptibility which diverge logarithmically as $T\rightarrow 0$, (ii) a residual entropy of $\frac{1}{2}\ln 2$ per impurity, (iii) a dynamical susceptibility of the form proposed as the basis for "marginal-Fermi-liquid" phenomenology [6], and (iv) a spin-spin correlation length diverging as $1/T$.

Considerable attention has recently been focused on possible experimental realizations of two-channel Kondo behavior. It has been proposed that certain uranium-based heavy-fermion materials [3,5], the cuprate superconductors [5,7] and electron-assisted tunneling in metallic glasses [8] can in various ways be mapped onto the two-channel Kondo Hamiltonian. Experiments on the heavy-fermion system $Y_{1-x}U_xPd_3$ (for $0.1\lesssim x\lesssim 0.2$) find impurity contributions to the specific heat, the residual entropy, and the resistivity of the appropriate form [9,10], although the response of the specific heat to an applied magnetic field has been argued to be inconsistent with a purely single-impurity description [10]. Resistivity measurements on $Pb_{1-x}Ge_xTe$ [11], on heavily doped polyacetylene and polypyrrole [12], and on structurally disordered metallic nanorestrictions [13], provide evidence for two-channel Kondo behavior arising from electron-assisted tunneling.

This paper reports the first theoretical study of interimpurity interactions in a two-channel Kondo system. The $1/T$ divergence of the single-impurity spin correlation length [4,5] hints at the importance of such interactions at low temperatures. Here we consider just two impurities, the simplest model featuring competition between ordering of the impurities via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction and formation of a critical state around each impurity through the two-channel Kondo effect. Our numerical renormalization-group (NRG) calculations indicate that the RKKY coupling destabilizes the single-impurity critical state and radically alters the low-energy physics. Three zero-temperature regimes exhibit Fermi-liquid behavior; a fourth is unlike any previously discovered in a Kondo system: We expect many of its properties to be described by nonuniversal critical exponents which depend on such parameters as the RKKY coupling strength and the shape of the conduction-band density of states.

Our formulation of the problem extends the treatment of the two-impurity, *one-channel* Kondo model by Jones *et al.* [14]. The interaction term in the Hamiltonian is

$$H_{\rm int}=J\{\mathbf{S}_l\cdot[\mathbf{s}_1(\mathbf{r}_l)+\mathbf{s}_2(\mathbf{r}_l)]+\mathbf{S}_r\cdot[\mathbf{s}_1(\mathbf{r}_r)+\mathbf{s}_2(\mathbf{r}_r)]\}\,, \quad (1)$$

where $\mathbf{S}_l$ and $\mathbf{S}_r$ are the "left" and "right" spin-$\frac{1}{2}$ impurity moments, residing at positions $\mathbf{r}_l$ and $\mathbf{r}_r$, respectively, and $\mathbf{s}_c(\mathbf{r})$ (for $c=1,2$) is the spin of the channel-c conduction electrons at position $\mathbf{r}$. The two conduction bands are assumed to have identical attributes, their electrons distinguished solely by the channel index c. The coupling J is positive in all cases of interest.

For simplicity, we take the conduction bands to be isotropic in momentum space, and to be symmetric in energy space about the Fermi level with a width $2D$. Real-space symmetries of $H_{\rm int}$ allow the impurities to couple to just four conduction states at each energy ε—states created by operators $a^\dagger_{\varepsilon cp\mu}$, where $\mu=\pm\frac{1}{2}$ is the spin and $p=e,o$ is the spatial parity under reflection in the plane midway between the impurities. Then Eq. (1) becomes

$$H_{\rm int}=\int d\varepsilon\int d\varepsilon'\sum_c\{(\mathbf{S}_l+\mathbf{S}_r)\cdot[\Gamma_e a^\dagger_{\varepsilon ce\mu}\boldsymbol{\sigma}_{\mu\mu'}a_{\varepsilon' ce\mu'}+\Gamma_o a^\dagger_{\varepsilon co\mu}\boldsymbol{\sigma}_{\mu\mu'}a_{\varepsilon' co\mu'}]+(\mathbf{S}_l-\mathbf{S}_r)\cdot[\Gamma_m a^\dagger_{\varepsilon ce\mu}\boldsymbol{\sigma}_{\mu\mu'}a_{\varepsilon' co\mu'}+\text{H.c.}]\}\,, \quad (2)$$

where $\Gamma_{e,o,m}=g_{+,-,+}(\varepsilon)g_{+,-,-}(\varepsilon')$, with $g^2_\pm(\varepsilon)=(J/4)\rho(\varepsilon)[1\pm\sin k_\varepsilon R/k_\varepsilon R]$. Here $R\equiv|\mathbf{r}_l-\mathbf{r}_r|$ is the separation between the impurities, k_ε describes the electron dispersion, and $\rho(\varepsilon)$ is the conduction-band density of states.

Two energy scales emerge from Eq. (2): the single-impurity, two-channel Kondo temperature [15], $T_K \approx D\Gamma\exp(-1/\Gamma)$, where $\Gamma \equiv J\rho(0)$, and the RKKY coupling—the coefficient of the effective term $I(R)\mathbf{S}_l\cdot\mathbf{S}_r$ arising in $H_{\rm int}$ due to exchange of virtual electrons between the impurities.

We follow Ref. [14] in averaging Γ_e, Γ_o, and Γ_m over ε and ε' in such a way that the couplings are functions of R only. In the limit $\Gamma \ll 1$, these three couplings can be reexpressed in terms of a more intuitive set of dimensionless parameters, Γ, I/T_K, and $(\Gamma_e-\Gamma_o)/(\Gamma_e+\Gamma_o)$ which, respectively, measure the electron-impurity exchange coupling, the relative energy scales for interimpurity and intraimpurity effects, and the asymmetry between the coupling of even- and odd-parity conduction states to the net impurity spin.

Thus simplified, Eq. (2) can be solved via Wilson's NRG method [14,16], which allows one to follow the renormalization of the "bare" parameters Γ, I/T_K, and $(\Gamma_e-\Gamma_o)/(\Gamma_e+\Gamma_o)$ via many-body interactions as the temperature is reduced. The renormalized parameters eventually flow to a fixed point which describes the zero-temperature properties of the system.

Our calculations reveal a rich variety of behaviors, which are summarized in the phase diagram shown in Fig. 1. Table I lists the locations and properties of the NRG fixed points.

There are four types of *stable* fixed points, each with a spin-singlet ground state, and each determining the low-temperature behavior within a region of parameter space delineated by thick lines in Fig. 1 [17].

(a) Even-parity Kondo.—For $\Gamma_e > \Gamma_o$, and ferromagnetic or sufficiently weak antiferromagnetic RKKY interactions (i.e., bare parameters lying above, and to the right of all thick lines in Fig. 1), the impurity spins are completely quenched by condition electrons of the more strongly coupled parity. As the temperature is lowered, Γ_e diverges while the quantities Γ_o and I/T_K renormalize to zero. One even-parity electron from each channel effectively binds to the impurities to form a spin singlet. The remaining even-parity electrons form a Fermi liquid with a $\pi/2$ phase shift due to strong scattering from the impurities, whereas the odd-parity conduction states decouple and undergo no phase shift. Although the screening at each impurity site is reminiscent of one-channel Kondo behavior, the two Kondo effects are not independent; there are correlations between the impurity spins in the ground state unless the bare RKKY coupling is identically zero [18].

(b) Odd-parity Kondo.—Since the Hamiltonian (2) is invariant under exchange of parity labels, $e \leftrightarrow o$, the

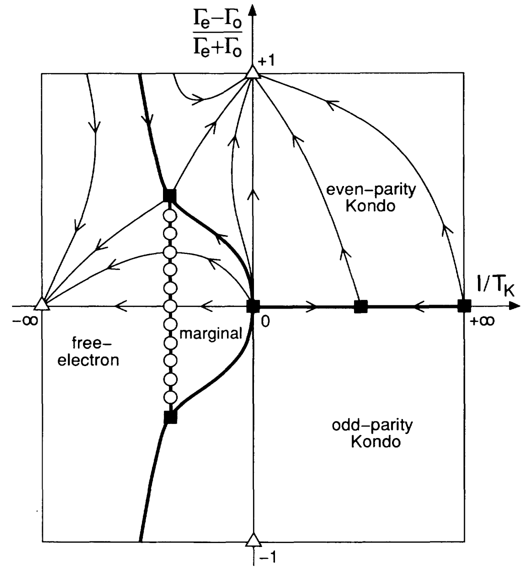

FIG. 1. Schematic renormalization-group (RG) phase diagram for the two-impurity, two-channel Kondo Hamiltonian, parametrized by I/T_K, the ratio of the interimpurity coupling to the single-impurity Kondo temperature, and $(\Gamma_e-\Gamma_o)/(\Gamma_e+\Gamma_o)$, the fractional difference between the coupling of the total impurity spin to even- and odd-parity conduction states [17]. Thin curves represent RG flows (drawn only in the upper half plane—the flows are mirror symmetric about the horizontal axis). Triangles, squares, and circles denote stable, unstable, and marginal fixed points, respectively. Thick lines demarcate four distinct regimes of low-temperature behavior. A continuous line of fixed points separates the marginal and free-electron regimes.

TABLE I. Renormalization-group fixed points of the two-impurity, two-channel Kondo Hamiltonian; see also Fig. 1. At fixed points exhibiting Fermi-liquid (FL) behavior, even- and odd-parity conduction states are scattered with phase shifts δ_e and δ_o, respectively. (Note that these shifts are independent of the channel index.)

Fixed point	I/T_K	$(\Gamma_e-\Gamma_o)/(\Gamma_e+\Gamma_o)$	Stability	Physical behavior
(a) Even-parity Kondo	0	$+1$	Stable	FL ($\delta_e=\pi/2, \delta_o=0$)
(b) Odd-parity Kondo	0	-1	Stable	FL ($\delta_e=0, \delta_o=\pi/2$)
(c) Free electron	$-\infty$	0	Stable	FL ($\delta_e=\delta_o=0$)
(d) Marginal line	$O(-1)$	~ -0.5 to $+0.5$	Marginal	Critical (nonuniversal)
(e) Even, odd antiferromagnetic	$O(-1)$	$\sim \pm 0.5$	Unstable	Critical
(f) Single impurity	0	0	Unstable	Critical
(g) Strong ferromagnetic	$+\infty$	0	Unstable	Critical
(h) Intermediate ferromagnetic	$O(+1)$	0	Unstable	Critical

NRG flows are mirror symmetric about the horizontal axis of Fig. 1. At the odd-parity Kondo fixed point, the counterpart of (a) for $\Gamma_o > \Gamma_e$, only odd-parity electrons quench the impurities.

(c) Free electron.— For strong antiferromagnetic RKKY interactions (i.e., bare parameters lying to the left of all thick lines in Fig. 1, or $I/T_K \lesssim -1$), there is no Kondo effect. The low-energy electrons completely decouple from the impurities; both even- and odd-parity electrons form Fermi liquids with zero phase shifts. Higher-energy electrons still play an important role in the formation of the spin-singlet ground state [18].

(d) Marginal.— The three preceding regions surround a fourth, characterized by weak antiferromagnetic RKKY couplings, within which the renormalized parameters flow towards a continuous line of fixed points which are only marginally stable (being stable to the right of the thick vertical line in Fig. 1, but unstable to the left). Each marginal fixed point exhibits a different non-Fermi-liquid spectrum: Certain energy splittings vary smoothly along the line, passing through zero precisely at $\Gamma_e = \Gamma_o$. As a consequence, we expect many of the low-temperature physical properties to be nonuniversal, governed by critical exponents that vary continuously with the bare parameters.

The bare parameters which select between the above regimes depend on the impurity separation R and the density of states $\rho(\varepsilon)$. For flat conduction bands, the bare parameters vary with increasing R in such a way that the low-temperature regime repeatedly cycles through the sequence: even-parity Kondo, marginal, odd-parity Kondo, marginal. For sufficiently small Γ, the bare parameters may also pass through the free-electron region. Thus, in principle, the regimes (a)–(d) are all accessible.

There are also five *unstable* fixed points in the problem, which in general affect the behavior only at high temperatures. Starting from the leftmost solid squares in Fig. 1, they are as follows:

(e) Even and odd antiferromagnetic.— At each end of the marginal line is an unstable fixed point, beyond which the energy splittings diverge and the NRG flows head towards either the Kondo or the free-electron fixed point.

(f) Single impurity.— A fixed point at $I/T_K = 0$ and $\Gamma_e = \Gamma_o$ corresponds to the limit of infinite separation between the impurities. The ground state, a product of single-impurity critical states, contains spin-singlet and -triplet components with equal weight. *A principal result of this work is the instability of this "single-impurity" fixed point with respect to any nonzero RKKY coupling or any difference between the coupling of the net impurity spin to even- and odd-parity conduction states.* For bare parameters lying close to the fixed point, a single-impurity approximation may be valid down to low energies. However, there must eventually be a crossover at some finite temperature to one of the stable regimes (a), (b), or (d).

(g) Strong ferromagnetic.— There exists a novel fixed point that can be reached only by starting with $\Gamma_e = \Gamma_o$ and $I = I_{\max}(\Gamma)$, where $I_{\max}(\Gamma)$ is the strongest possible ferromagnetic RKKY coupling that can be generated from Eq. (2), obtained by setting $\Gamma_m = 0$ [14]. We conjecture that this fixed point, which has a spin-triplet ground state and a non-Fermi-liquid excitation spectrum, is equivalent to the nontrivial fixed point of *four* channels of conduction electrons interacting equally with a *single, spin-one* impurity.

(h) Intermediate ferromagnetic.— For $\Gamma_e = \Gamma_o$ and $0 < I < I_{\max}(\Gamma)$ [see (g)], the NRG flows are towards another novel fixed point, which also possesses a spin-triplet ground state and a non-Fermi-liquid excitation spectrum. The slightest difference between Γ_e and Γ_o drives the NRG flows off to one or another of the Kondo fixed points. However, this intermediate fixed point would be stable if some additional symmetry were to maintain equality between the even- and odd-parity couplings. None of the realizations of the two-channel Kondo Hamiltonian proposed to date exhibits such a symmetry.

It is instructive to compare the above results with those from the NRG treatment of the two-impurity, *one-channel* Kondo model [14], most of which have recently been confirmed using conformal field theory [19]. Although Kondo and free-electron regimes figure prominently in both the one- and two-channel problems, there are significant differences between the two cases.

(i) In the one-channel model, any asymmetry between the even- and odd-parity couplings always renormalizes to zero, so $(\Gamma_e - \Gamma_o)/(\Gamma_e + \Gamma_o)$ is an irrelevant parameter.

(ii) In the one-channel case, weak RKKY interactions produce only small perturbations around the single-impurity behavior. In the two-channel case, by contrast, any interimpurity interaction drives one away from the single-impurity regime and radically alters the physics.

(iii) An isolated, unstable fixed point, at $I/T_K \simeq -1$ [15] and $\Gamma_e = \Gamma_o$, separates the one-channel Kondo and free-electron regimes. This non-Fermi-liquid fixed point disappears if the Hamiltonian's particle-hole symmetry is broken (by the introduction of potential scattering, for instance) [20]. We suspect that the two-channel marginal regime— which occupies a finite region of phase space, rather than a single point— is a more robust feature.

In summary, the behavior of the two-impurity, two-channel Kondo model is more complex than that of any Kondo system studied previously. We find that any interaction between the impurities, however weak, dominates the physics at sufficiently low temperatures. A novel regime of non-Fermi-liquid behavior which occurs for weak antiferromagnetic RKKY interactions is probably associated with nonuniversal critical properties.

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[a]Present address: Department of Physics, University of Florida, Gainesville, FL 32611.

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