Frustration-induced non-Fermi-liquid behavior in a three-impurity Kondo model

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A Kondo model for three spin-$\frac{1}{2}$ impurities placed at the vertices of an equilateral triangle is studied using the numerical renormalization-group method. The impurity spins can form two frustrated doublets which, because of the rotation symmetry, couple equally to the conduction band. Over a broad range of antiferromagnetic RKKY interaction strengths, this degeneracy drives the system to one of two novel, non-Fermi-liquid fixed points. Potential scattering is a relevant perturbation at one of these fixed points, but is marginal throughout the second regime.

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Much of the rich behavior of heavy-fermion compounds [1] is thought to stem from competition between ordering of local moments via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, and quenching of those moments due to the Kondo effect. Theoretical understanding of the subject is far from complete. It is widely believed that the essential physics is contained in the periodic Anderson Hamiltonian, but this model has been solved only at the mean-field level [2]. Insight has also been gained from exact solutions for one or two magnetic impurities in simple metals [3], and for lattices in the limit of infinite spatial dimensionality [4].

Recently, attention has focused on rare-earth and actinide systems which exhibit a specific heat coefficient C/T that diverges weakly with decreasing temperature T — rather than remaining constant, as in a (heavy) Fermi liquid — and a resistivity that is linear — instead of quadratic — in T [5]. Explanations proposed for these non-Fermi-liquid (NFL) properties include: (1) the single-impurity Kondo effect with a disorder-induced distribution of energy scales [6]; (2) isolated magnetic impurities coupled to two or more conduction bands [7]; and (3) proximity to a $T = 0$ magnetic-ordering transition [8].

A fourth possibility, overlapping with but not identical to (3) above, is that lattice effects, such as periodicity or geometric frustration, may induce NFL behavior where none exists in the one-impurity limit. Few-impurity systems may provide clues as to the plausibility of this scenario. The two-impurity Kondo problem yields NFL physics — but only at particle-hole symmetry and with fine-tuning of the RKKY coupling [9,10].

In this paper, a more robust form of NFL behavior is identified in a model for a single conduction band interacting with three identical spin-$\frac{1}{2}$ impurities arranged in an equilateral triangle. Magnetic frustration prevents even strong antiferromagnetic RKKY interactions from locking the impurities into a total spin singlet; instead, four degenerate spin-$\frac{1}{2}$ configurations remain. Using the numerical renormalization-group method, we find that over a wide range of RKKY couplings, Kondo screening of these impurity states is governed by two NFL fixed points. Particle-hole asymmetry destabilizes one of the regimes, but is a marginal perturbation in the other. Our results suggest that spatial symmetry might give rise to NFL behavior in more realistic models without the need for parameter tuning. (Similar considerations have led to the study of electron-assisted tunneling between three atomic sites [11] as a possible explanation for the anomalous conductance of certain point contacts [12].)

We start with a Hamiltonian, $H = H_{band} + H_{int}$, describing a non-interacting conduction band coupled locally to three spin-$\frac{1}{2}$ impurities, $\mathbf{S}_i$ ($i = 0, 1, 2$), which lie at the vertices $\mathbf{r}_i$ of an equilateral triangle. The band is assumed to be isotropic in momentum space, and to extend in energy over a range $\pm D$ about the Fermi level (taken to be energy $\epsilon = 0$). The interaction term is

$$H_{int} = \sum_{i=0}^{2} \left[V n(\mathbf{r}_i) - J \mathbf{s}(\mathbf{r}_i) \cdot \mathbf{S}_i \right], \tag{1}$$

where $n(\mathbf{r}_i)$ [$\mathbf{s}(\mathbf{r}_i)$] is the electron number [spin] at impurity site i. The exchange coupling J is assumed negative, whereas the potential scattering V can be of either sign.

Symmetry permits the impurities to couple to just six orthogonal, spatially localized conduction states, annihilated by operators $c_{h\sigma}$, where $\sigma = \pm\frac{1}{2}$ labels the spin z component, and $h \in \{0, 1, 2\}$ specifies the "helicity." Helicity is analogous to parity in a two-impurity problem, i.e., a helicity-h wave function acquires a multiplicative factor $e^{i2\pi h/3}$ under a rotation of $2\pi/3$ about the center of symmetry. The combined states of three spin-$\frac{1}{2}$ impurities decompose into a quartet having total spin $\frac{3}{2}$ and helicity $h = 0$, plus two doublets of total spin $\frac{1}{2}$. The doublets can be constructed so that one has $h = 1$ and the other $h = 2$, in which case the Hamiltonian conserves total helicity (modulo 3), and is invariant under interchange of helicity labels 1 and 2.

Applying these observations, Eq. (1) can be rewritten

$$\begin{aligned} H_{int} = {} & V_0 n_0 + V_1 (n_1 + n_2) - J_{00}\, \mathbf{s}_{00} \cdot \tilde{\mathbf{S}}_0 \\ & - J_{11} (\mathbf{s}_{11} + \mathbf{s}_{22}) \cdot \tilde{\mathbf{S}}_0 - J_{12} (\mathbf{s}_{12} \cdot \tilde{\mathbf{S}}_1 + \mathbf{s}_{21} \cdot \tilde{\mathbf{S}}_2) \\ & - J_{01} [(\mathbf{s}_{01} + \mathbf{s}_{20}) \cdot \tilde{\mathbf{S}}_1 + (\mathbf{s}_{10} + \mathbf{s}_{02}) \cdot \tilde{\mathbf{S}}_2], \end{aligned} \tag{2}$$

where $n_h = \sum_\sigma c^\dagger_{h\sigma} c_{h\sigma}$ is the number of helicity-h electrons at the impurity sites, $\mathbf{s}_{hh'} = \sum_{\sigma\sigma'} c^\dagger_{h\sigma} \frac{1}{2} \boldsymbol{\sigma}_{\sigma\sigma'} c_{h'\sigma'}$

gives the spin of an electron scattering from helicity h' to h, and $\tilde{\mathbf{S}}_{\Delta h} = \sum_{j=0}^{2} e^{i2\pi j \Delta h} \mathbf{S}_j$ is the spin of the impurities as their helicity is raised by Δh. The couplings

$$V_h = V F_h^2, \quad J_{hh'} = J F_h F_{h'} \tag{3}$$

depend on the band dispersion $k(\epsilon)$, the density of states $\rho(\epsilon)$, and the impurity separation R, through form factors $F_h^2 = \frac{1}{3} \int d\epsilon \, \rho(\epsilon) \left[1 + (3\delta_{h,0} - 1) \sin(kR)/(kR)\right]$.

This problem can be solved using a generalization of the non-perturbative renormalization-group method developed for the one-impurity Kondo model [13]. The continuum of electronic energies is replaced by a discrete set, $\pm D\Lambda^{-n}$, $n = 0, 1, \ldots$, where $\Lambda > 1$. The Hamiltonian is then mapped, via the Lanczos method, onto a tight-binding model for a one-dimensional chain with the impurities coupled to one end. The discretization introduces a separation of energy scales which allows the Hamiltonian to be solved iteratively, starting with a single site. At each subsequent step, one site is added to the chain, while the effective temperature T falls by a factor of $\Lambda^{1/2}$. This continues until the energy spectrum becomes scale-invariant, i.e., a stable fixed point is reached.

The discretized Hamiltonian contains an infinite set of parameters which depend on the band shape and the impurity separation R. We argue, along lines advanced for the two-impurity Kondo problem [14], that these band parameters can be replaced by standard values calculated for $\rho(\epsilon) =$ constant and $R = \infty$. All possible low-temperature regimes of the original model can be explored provided that one treats the couplings entering Eq. (2) as independent parameters, freed from the constraints implied by Eqs. (3). In particular, J_{11} and J_{12}, although equal as originally defined, should be regarded as separate couplings because no symmetry of the problem prevents them from renormalizing independently.

We have solved the discretized version of this problem for different initial values of the couplings V_0, V_1, J_{00}, J_{11}, J_{12}, and J_{01}. Even taking advantage of conserved quantities to break the Hamiltonian matrix into block-diagonal form and thereby to reduce CPU time, we have generally found it practical to retain no more than 1200 states after each iteration. This corresponds to keeping all energies $E \lesssim 5T$, which allows identification of fixed points, but is insufficient for direct computation of physical properties as thermodynamic traces. The good quantum numbers are total helicity, H; total spin and its z component, S and S_z; and total "isospin" [10] or "axial charge" [9] and its z component, I and I_z [15]. Total isospin is only conserved at particle-hole symmetry, so most runs were performed with $V_0 = V_1 = 0$ in order to benefit from the additional quantum number.

The three-impurity Kondo problem has a rich phase diagram, as might be expected given the large number of independent parameters. In this paper, we focus on the stable low-temperature regimes of the particle-hole-symmetric model. Figure 1 shows a schematic phase diagram for this case, projected onto the plane spanned by two dimensionless combinations of the four exchange couplings entering Eq. (2): The first, $K = (J_{00}^2 + 2J_{11}^2 - J_{12}^2 - 2J_{01}^2)/(J_{00}^2 + 2J_{11}^2 + 2J_{12}^2 + 4J_{01}^2)$, measures the strength of the RKKY interaction. As K ranges from $-\frac{1}{2}$ through 0 to $+1$, the static impurity correlation function $\langle \frac{1}{3} \sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ varies smoothly from $-1/4$ through 0 to $+1/4$. The second combination, $\alpha \equiv (J_{01} - J_{12})/(J_{01} + J_{12})$, measures the difference between the two couplings that dominate the region of antiferromagnetic RKKY interactions, $K < 0$.

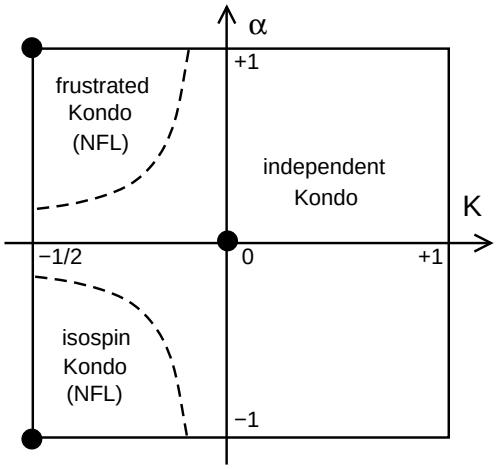

FIG. 1. Schematic phase diagram for the three-impurity Kondo model at particle-hole symmetry. Here K is a measure of the RKKY interaction, and α measures the relative strengths of the couplings J_{01} and J_{12} in Eq. (2). Circles represent stable fixed points, and dashed lines mark the borders between different regimes of low-temperature behavior.

There are three distinct regions in Fig. 1:

Independent-Kondo regime: For ferromagnetic and weakly antiferromagnetic RKKY couplings, the system renormalizes to a stable fixed point at which interactions between the impurities are essentially irrelevant. The ground state is a spin singlet, and all electrons at the Fermi level undergo a phase shift $\delta_h(\epsilon = 0) = \pi/2$. Thus, the low-energy excitations are those for three impurities at infinite separation, each independently undergoing a Kondo effect. Particle-hole asymmetry is exactly marginal in this regime, just as it is in the one-impurity Kondo model.

Frustrated-Kondo regime: In a region of medium-to-strong antiferromagnetic RKKY interactions where J_{01} is the dominant coupling, the system flows to a novel, stable NFL fixed point at which electrons of all three helicities screen the frustrated spin-$\frac{1}{2}$ impurity configurations.

Table I gives the finite-size spectrum at this fixed point, computed for $\Lambda = 3$, a value that represents a near-optimal compromise between discretization errors (which grow with Λ) and numerical rounding errors (which become larger as Λ approaches unity) [13]. The energies

L odd			L even		
E	(S,I,H)		E	(S,I,H)	
0	$(0,0,0)$	$\times 2$	0	$(0,\frac{1}{2},*)$	$(\frac{1}{2},0,*)$
0.100	$(\frac{1}{2},\frac{1}{2},*)$		0.400	$(\frac{1}{2},1,*)$	$(1,\frac{1}{2},*)$
0.200	$(0,1,*)$	$(1,0,*)$	0.500	$(0,\frac{1}{2},0)$	$\times 2$
0.299	$(\frac{1}{2},\frac{1}{2},0)$	$\times 2$	"	$(\frac{1}{2},0,0)$	$\times 2$
0.499	$(0,0,*)$	$\times 2$	0.501	$(0,\frac{1}{2},*)$	$(\frac{1}{2},0,*)$
0.599	$(\frac{1}{2},\frac{1}{2},*)$		0.603	$(\frac{1}{2},1,0)$	$\times 2$
0.601	$(1,1,*)$		"	$(1,\frac{1}{2},0)$	$\times 2$
0.604	$(\frac{1}{2},\frac{1}{2},0)$	$\times 2$	0.799	$(0,\frac{3}{2},0)$	$(\frac{3}{2},0,0)$
0.699	$(0,1,0)$	$(1,0,0)$	0.800	$(0,\frac{3}{2},0)$	$(\frac{3}{2},0,0)$
0.700	$(0,1,0)$	$(1,0,0)$	0.904	$(\frac{1}{2},1,0)$	$(1,\frac{1}{2},0)$
0.701	$(\frac{1}{2},\frac{3}{2},*)$	$(\frac{3}{2},\frac{1}{2},*)$	0.905	$(\frac{1}{2},1,0)$	$(1,\frac{1}{2},0)$
0.704	$(0,1,*)$	$(1,0,*)$	0.913	$(\frac{1}{2},1,*)$	$(1,\frac{1}{2},*)$
0.804	...		1.00	...	

TABLE I. Low-lying states from the finite-size spectrum at the frustrated-Kondo fixed point. Energies E are given for odd- and even-length chains. States are labeled by their spin S, isospin I, and helicity H; an asterisk stands for one state each of helicity 1 and 2. See the text for further details.

have been multiplied by a factor of 0.625, chosen to map the smallest splitting in the spectrum of the free conduction band (without any impurity) onto its value in the continuum limit, $\Lambda \to 1$. The scaled energies E are expressed in units of $\pi v_F/L$, where L is the number of sites in the chain, and v_F is the Fermi velocity.

The regularity of the levels in Table I is reminiscent of a Fermi liquid, but several details — particularly the absence of states in the odd-L spectrum at $E \approx 0.4$, and the ordering of the even-L states for $E < 0.7$ — prove impossible to explain within this framework.

The rate at which the eigenenergies approach their fixed-point values also points to an NFL description: By examining the L-dependence of the spectrum, and using the relation $T \sim D\Lambda^{-L/2}$ [13], we deduce that the leading irrelevant operator at this fixed point varies like T^λ, with $\lambda = 0.21 \pm 0.03$ (c.f. $\lambda = 1$ for a Fermi liquid). This exponent should be reflected in anomalous temperature dependences of physical properties.

An NFL interpretation of the frustrated-Kondo regime is supported by evidence that the fixed point occurs at finite, non-zero exchange couplings. Empirically, one can eliminate all spin-$\frac{3}{2}$ impurity configurations, and set $J_{00} = J_{11} = J_{12} = 0$ in Eq. (2), to arrive at a one-parameter model which, for all $-D < J_{01} < +D$ (at least), reproduces the fixed-point spectrum in Table I. It can be shown using poor-man's scaling [16] that the J_{00} and J_{11} terms in Eq. (2) are regenerated under renormalization; however, J_{12} remains identically zero. In principle, one should be able to locate the fixed point by adjusting J_{00}, J_{11}, and J_{01} until the energy spectrum does not change at all as the tight-binding chain is extended. In practice, the band discretization introduces irrelevant operators which renormalize the spectrum at small values of L. We therefore associate the fixed point with the couplings which yield the smallest deviation from the asymptotic spectrum at some standard chain length, usually $L = 20$. This procedure gives $J^*_{00} = J^*_{01} = -0.8D$ and $J^*_{11} = +0.4D$ (all to within $\pm 0.1D$), and $J^*_{12} \equiv 0$.

Throughout the frustrated-Kondo regime, potential scattering is found to act as a marginal perturbation about the particle-hole symmetric limit, shifting the energy of each state by an amount proportional to its charge quantum number, I_z. Thus, for moderate values of V_0 and V_1 [see Eq. (2)], this regime retains its NFL character. Very strong potential scattering suppresses the Kondo interaction, however, and drives the system to a weak coupling Fermi liquid. The crossover between these extremes is hard to analyze given the limited number of states we can retain in our calculations, but this issue merits future attention.

The evidence presented above demonstrates that the frustrated-Kondo regime has an NFL fixed point which is stable with respect to the RKKY interaction and is marginal under particle-hole asymmetry. (However, breaking the real-space symmetry of the impurity locations will lead to the recovery of Fermi-liquid behavior below some crossover temperature.) This fixed point does not seem to map onto any fixed point known from previous studies of impurity models. One likely candidate, the overscreened limit of the 3-channel Kondo model for a spin-$\frac{1}{2}$ impurity, is ruled out because it predicts a ground state spin $S = 1$ for L odd, and $S = \frac{1}{2}$ for L even.

Isospin-Kondo regime: In a second region of the parameter space — characterized by antiferromagnetic RKKY interactions, but dominated by J_{12} rather than J_{01} — the system flows to a stable NFL fixed point which is related, by interchange of spin and isospin degrees of freedom, to the one-impurity, two-channel Kondo model.

Table II gives the finite-size spectrum at this fixed point, once again computed for $\Lambda = 3$ and scaled by a factor of 0.625. The energies and quantum numbers of all the low-lying states can be reproduced by convoluting the free-fermion spectrum for decoupled helicity-0 electrons with a spectrum derived from the NFL fixed point of the one-impurity, two-channel model [17]: For each state at the two-channel fixed point, labeled by spin J, flavor J_f and charge Q [17,18], one constructs a three-impurity state with the same energy, having quantum numbers $S = J_f$; $I = S$; and $H = 0$, 1 or 2, depending on whether $Q = 0$, $Q > 0$ or $Q < 0$.

Insight into these observations can be gained from another one-parameter model. Spin-$\frac{3}{2}$ impurity configurations are eliminated, just as for the frustrated-Kondo fixed point, but here J_{12} is the only non-zero coupling. For all $-D < J_{12} < +D$, this model flows to the fixed-point listed in Table II. Since $J_{00} = J_{01} = 0$, the helicity-

L odd			L even		
E	(S,I,H)		E	(S,I,H)	
0	$(0,0,0)$	$(0,1,0)$	0	$(0,\frac{1}{2},0)$	
"	$(\frac{1}{2},\frac{1}{2},0)$		0.124	$(\frac{1}{2},0,*)$	
0.125	$(0,0,*)$	$(1,0,*)$	0.498	$(0,\frac{1}{2},*)$	$(1,\frac{1}{2},0)$
"	$(\frac{1}{2},\frac{1}{2},*)$		0.501	$(\frac{1}{2},0,0)$	$(\frac{1}{2},1,0)$
0.500	$(0,0,*)$	$(0,1,*)$	0.625	$(0,\frac{1}{2},*)$	$(1,\frac{1}{2},*)$
"	$(\frac{1}{2},\frac{1}{2},0)$	$(\frac{1}{2},\frac{1}{2},*)$	0.628	$(\frac{1}{2},1,*)$	
"	$(1,0,0)$	$(1,1,0)$	0.997	$(0,\frac{3}{2},0)$	
"	$(\frac{3}{2},\frac{1}{2},0)$		1.000	$(\frac{1}{2},0,0)$	$(\frac{1}{2},1,0)$
0.629	$(0,1,*)$	$(1,1,*)$	"	$(\frac{1}{2},0,*)$	$(\frac{1}{2},1,*)$
"	$(\frac{1}{2},\frac{1}{2},*)$	$(\frac{1}{2},\frac{3}{2},*)$	"	$(\frac{3}{2},0,0)$	$(\frac{3}{2},1,0)$
1.001	...		1.003	...	

TABLE II. Low-lying states at the isospin-Kondo fixed point. See Table I for an explanation of the entries.

0 electrons must be decoupled at the fixed point. The interaction between the remaining degrees of freedom can be written

$$H_{\rm int} = \frac{1}{4}\sum_{\mu,\nu=1}^{3}\sum_{h,h'=1}^{2}\sum_{\sigma,\sigma'} J_{\mu\nu} c^{\dagger}_{h\sigma}\sigma^{\mu}_{\sigma\sigma'}\sigma^{\nu}_{hh'}c_{h'\sigma'}S_{\mu}H_{\nu}, \quad (4)$$

where $\mathbf{S}$ and $\mathbf{H}$ are commuting SU(2) operators acting on the impurity spin and helicity, respectively. An isotropic ($J_{\mu\nu} = J$) version of Eq. (4) has been considered in combination with pure spin and flavor interactions in a generalized two-channel model [19], but we are aware of no study of the case $J_{\mu\nu} = J(1-\delta_{\nu,3})$ which arises here.

Unlike the other two fixed points, the isospin-Kondo fixed point is unstable with respect to particle-hole asymmetry. Specifically, V_1 entering Eq. (2) plays the role of the magnetic field in the standard two-channel Kondo model, driving the system to a Fermi-liquid state. Since there is no reason to expect V_1 to be zero in any real system, this instability implies that the isospin-Kondo regime is unlikely to be observed in practice.

In the preceding discussion, we have not specified the precise positions of the boundaries between the three regimes shown in Fig. 1. These depend in a fairly complicated fashion on the two combinations of exchange couplings orthogonal to K and α. We note, though, that the frustrated-Kondo and isospin-Kondo regimes expand as the Kondo coupling J decreases in magnitude, i.e., as the RKKY coupling grows to dominate the single-impurity Kondo effect. We suspect that in the limit $J \to 0$, each NFL regime occupies an entire quadrant of Fig. 1.

We have presented numerical renormalization-group results for a model of three magnetic impurities interacting with a non-magnetic metal. For ferromagnetic and weakly antiferromagnetic RKKY interactions, the impurities undergo essentially independent Kondo effects. For stronger antiferromagnetic RKKY couplings, the threefold spatial symmetry of the model leads to two novel low-temperature regimes of non-Fermi-liquid behavior, one of which is marginally stable against particle-hole asymmetry. Further work is required to identify the physical properties of the stable non-Fermi-liquid regime, and to determine whether or not it can be reached starting from any realistic band structure.

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