Kondo Screening in a Magnetically Frustrated Nanostructure: Exact Results on a Stable, Non-Fermi-Liquid Phase

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Triangular symmetry stabilizes a novel non-Fermi-liquid phase in the three-impurity Kondo model with frustrating antiferromagnetic interactions between half-integer impurity spins. The phase arises without fine-tuning of couplings, and is stable against magnetic fields and particle-hole symmetry breaking. We find a conformal field theory describing this phase, verify it using the numerical renormalization group, and extract various exact, universal low-energy properties. Signatures predicted in electrical transport may be testable in scanning tunneling microscopy or quantum-dot experiments.

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The same many-body physics that is responsible for the Kondo screening of magnetic impurities in bulk metals 1 produces resonances in tunneling through a quantum dot 2 or an adatom on a metallic surface 3. Greater experimental control over the latter settings allows systematic study of multiple-impurity configurations in which the Kondo effect competes with ordering phenomena; indeed, it has been argued on the basis of weak-coupling RG 11 to describe the low-energy physics of the type-2 Cr trimer in 2. We make predictions for the conductance expected in STM experiments on trimer and in certain quantum-dot devices.

Model.—We start with a Hamiltonian $H_{\text{band}} + H_{\text{int}}$ describing a noninteracting conduction band coupled via

$$H_{\text{int}} = J \sum_{j,\alpha,\beta} \psi_j^{\dagger \alpha} (\vec{r}_j) \frac{1}{2} \vec{S}_{\alpha \beta} \psi_\beta (\vec{r}_j) \cdot \vec{S}_j \quad (J > 0) \quad (1)$$

to spin-$S$ impurities $\vec{S}_j$ ($j = 1, 2, 3$) at the vertices $\vec{r}_j$ of an equilateral triangle; $\psi_\alpha (\vec{r})$ annihilates an electron with spin $\alpha = \pm \frac{1}{2}$ at $\vec{r}$. We assume that the permutation group $S_3$ that maps the set $\{\vec{r}_j\}$ onto itself is a subgroup of the lattice symmetry group (as is the case, e.g., in 2). The impurities couple to just six orthonormal combinations of conduction states, annihilated by operators $\psi_{h,\alpha} \propto \sum_j e^{i2\pi jh/3} \psi_\alpha (\vec{r}_j)$, where $h = 0, \pm 1$ is the “helicity”; under a $2\pi/3$-rotation about the center of symmetry, a helicity-$h$ state is multiplied by $e^{i2\pi h/3}$. The combined states of the three impurities can also be constructed to have well-defined helicities, in which case the Hamiltonian conserves total helicity (modulo 3) and is invariant under interchange of all helicity labels 1 and $-1$. Then, Eq. (1) can be rewritten

$$H_{\text{int}} = \left[ J_{00} \hat{s}_{00} + J_{11} (\hat{s}_{11} + \hat{s}_{13}) \right] \cdot \vec{S}_0 + \left[ J_{01} (\hat{s}_{01} + \hat{s}_{10}) + J_{11} \hat{s}_{11} \right] \cdot \vec{S}_1 + \left[ J_{01} (\hat{s}_{01} + \hat{s}_{03}) + J_{11} \hat{s}_{11} \right] \cdot \vec{S}_1, \quad (2)$$

where $\vec{S}_h = \sum_j e^{i2\pi jh/3} \vec{S}_j$, $\hat{s}_{hh'} = \sum_{\alpha,\beta} \psi_j^{\dagger \alpha} \frac{1}{2} \vec{S}_{\alpha \beta} \psi_{h',\beta}$, and $\vec{S}_h \equiv -1$; $J_{hh'}$ equals $J$ times a non-negative factor that depends on the impurity separation and the conduction-band dispersion, as well as $h$ and $h'$. For $S = \frac{1}{2}$ the NRG shows 12 that over a large region of the parameter space of Eq. (2), the low-energy physics is governed by a “frustrated” fixed point at which the impurities are locked into the subspace of two doublets of combined spin $S_{\text{imp}} = \frac{1}{2}$, one each of helicity $h = \pm 1$. 

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Three spins of arbitrary half-integer $S$, coupled by
an additional Hamiltonian term $K \sum_{i<j} \vec{S}_i \cdot \vec{S}_j$ with $K \gg J$, also
lock into an $S_{\text{imp}} = \frac{1}{2}$, $h = \pm 1$ subspace. Weak-coupling RG analysis \[11\] of this augmented model, which
for $S = \frac{1}{2}$ provides a description of equilateral Cr trimers,
is consistent with flow to the same fixed point; for $S = \frac{3}{2}$,
moreover, the characteristic temperature $T_K$ for this
flow is found to greatly exceed the single-impurity Kondo
scale, in agreement with the Cr-trimer experiments \[3\].

In the frustrated phase, $J_{12}$ in Eq. \[2\] scales to zero,
$J_{00}$ and $J_{11}$ can be neglected, and particle-hole asymmetry
is marginal \[12\]. Thus, we analyze the fixed point in a
restricted $S_{\text{imp}} = \frac{1}{2}$ space, replacing Eq. \[2\] by
\begin{equation}
H_{\text{int}} = -\sqrt{2} J_{01} [\langle \psi^\dagger \frac{1}{2} \sigma \Delta^+ \psi \rangle_{\text{imp}} + \text{H.c.}] \cdot \vec{S}.
\end{equation}

Here, $T^\pm$ and $T^z$ act on the electron helicity in the spin-1
representation of an “orbital-spin” $SU^{(1)}(2)$ \[13\], with
matrix elements $(T^z)_h = h$, $(T^z)_{0,-1} = \sqrt{2}$. The
Pauli matrices $\vec{\sigma}$, $2 \vec{S}_{\text{imp}} = 2 \vec{S}_0$ and $\vec{S}_{\text{imp}}$ act, respectively,
on the electron spin, impurity spin, and impurity helicity,
with $(\tau^z_{\text{imp}})_{h,-h} = -h$ for $h = \pm 1$.

It is important to note that setting $J_{11} = 0$ enlarges the
$S_3$ symmetry of Eq. \[2\] to a $U^{(1)}(1)$ symmetry in Eq. \[3\],
replacing total helicity (conserved only modulo 3) by a
conserved quantity $t_z$: the eigenvalue of $\psi^\dagger T^z \psi + \frac{1}{2} t_z$.

Now, $H_{\text{int}}$ commutes with $SU^{(1)}(2)$ spin, $U^{(1)}(1)$ orbital spin, and
also with $SU^{(1)}(2)$ isospin defined by $I^z = \frac{1}{2} \sum_{h,\alpha} \psi^\dagger h,\alpha,\Delta^+ \psi_{h,\alpha,\Delta}$ + \frac{1}{2} \sum_{h,\alpha,\beta} \epsilon_{\alpha\beta\gamma} \psi^\dagger h,\alpha,\Delta \psi_{h,\alpha,\Delta}$. It is
defined above, $P^\dagger$ commutes with isospin $\hat{I}$. The
free-fermion FSS can be decomposed into products of
$SU^{(1)}(2) \times SU^{(1)}(2) \times SU^{(1)}(2)$ conformal towers \[18\] as exemplified in Table \[I\] for boundary conditions that
yield a nondegenerate ground state. Here, $SU^{(1)}(2)_k$ is a
level-$k$ Kac-Moody CFT; see \[14\] and references therein.

We first construct a conformal embedding of the free
Dirac fermions $\psi_{h,\alpha}(x)$ in which the holonomies transform
in the spin-1 representation of an $SU^{(1)}(2)$ “pseudospin”
$\vec{P}$, where $P^+ = T^z$ and $P^+$ has matrix elements in the
helicity basis $(P^+)_{1,0} = -(P^+)_{1,0}$, $(P^+)_{0,-1} = -(P^+)_{0,-1}$. Unlike $\hat{I}$ defined above, $\vec{P}$ commutes with isospin $\hat{I}$. The
free-fermion FSS can be decomposed into products of
$SU^{(1)}(2) \times SU^{(1)}(2) \times SU^{(1)}(2)$ conformal towers \[18\] as exemplified in Table \[I\] for boundary conditions that
yield a nondegenerate ground state. Here, $SU^{(1)}(2)_k$ is a
level-$k$ Kac-Moody CFT; see \[14\] and references therein.

Since Eq. \[4\] lowers the $SU^{(1)}(2)$ symmetry of $H_{\text{band}}$
and to $U^{(1)}(1)$, we analyze the frustrated fixed

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
$(s)_\Delta$ & $(t)_\Delta$ & $(p)_\Delta$ \\
\hline
$(0)_0$ & $(0)_0$ & $(0)_0 + (4)_2$ \\
$(\frac{1}{2})_{3/4}$ & $(\frac{1}{2})_{3/4}$ & $(0)_0 + (4)_2$ \\
$(\frac{1}{2})_{3/20}$ & $(\frac{1}{2})_{3/20}$ & $(1)_{1/5} + (3)_{6/5}$ \\
$(1)_{2/5}$ & $(1)_{2/5}$ & $(1)_{1/5} + (3)_{6/5}$ \\
$(0)_0$ & $(1)_{2/5}$ & $(2)_{3/5}$ \\
$(1)_{2/5}$ & $(0)_0$ & $(2)_{3/5}$ \\
$(\frac{1}{2})_{3/20}$ & $(\frac{1}{2})_{3/20}$ & $(2)_{3/5}$ \\
$(\frac{1}{2})_{3/4}$ & $(\frac{1}{2})_{3/4}$ & $(2)_{3/5}$ \\
\hline
\end{tabular}
\caption{Finite-size spectrum of free fermions decomposed into products of spin, isospin, and pseudospin conformal
towers, labeled by $s$, $i$, and $p$, respectively. The subscript $\Delta$ gives
each tower’s contribution to the excitation energy \[13\].}
\end{table}
TABLE II: Finite-size spectrum at the frustrated fixed point.

\begin{tabular}{|c|c|c|c|c|}
\hline
\( (s)_{\Delta} \) & \( (i)_{\Delta} \) & \( (t_{z})_{\Delta} \) & \( (p,m)_{\Delta} \) & \( E \) & \( E_{\text{NRG}} \) \\
\hline
(0) & (0) & (0) & (0) & 0 & 0 \\
\hline
(1) & (1) & (1) & (1) & 0.1 & 0.1001 \\
\hline
(2) & (2) & (2) & (2) & 0.2 & 0.2000 \\
\hline
(3) & (3) & (3) & (3) & 0.3 & 0.2996 \\
\hline
(4) & (4) & (4) & (4) & 0.5 & 0.4968 \\
\hline
(5) & (5) & (5) & (5) & 0.5 & 0.5020 \\
\hline
(6) & (6) & (6) & (6) & 0.6 & 0.5971 \\
\hline
(7) & (7) & (7) & (7) & 0.6 & 0.6040 \\
\hline
(8) & (8) & (8) & (8) & 0.6 & 0.6001 \\
\hline
(9) & (9) & (9) & (9) & 0.7 & 0.7004 \\
\hline
(10) & (10) & (10) & (10) & 0.7 & 0.7004 \\
\hline
(11) & (11) & (11) & (11) & 0.7 & 0.7043 \\
\hline
(12) & (12) & (12) & (12) & 0.7 & 0.6982 \\
\hline
(13) & (13) & (13) & (13) & 0.7 & 0.6982 \\
\hline
(14) & (14) & (14) & (14) & 0.8 & 0.8038 \\
\hline
(15) & (15) & (15) & (15) & 0.8 & 0.8045 \\
\hline
(16) & (16) & (16) & (16) & 0.8 & 0.8116 \\
\hline
\end{tabular}

again be decomposed using Eq. (3) into \( U^{(1)}(1)_{s} \times Z_{s} \).

Boundary operators entering the effective low-energy Hamiltonian for the frustrated fixed point must respect the \( SU^{(3)}(2) \times SU^{(3)}(2) \times U^{(1)}(1) \) symmetry of the full Hamiltonian [5]. Such operators appear in the first row of Table III. Only \((s,i,t_{z},Z_{s}) = (0,0,0,(\psi_{1,1}^{0})_{1,5})\) is relevant (in the RG sense). It cannot appear because it is odd under the \( Z_{2} \) subgroup of \( S_{3} \): \( \psi_{s} \rightarrow -\psi_{s} \), \( t_{\text{imp}} \rightarrow t_{\text{imp}}^{-} \), which is representable as a \( \pi \)-rotation about the \( x \)-axis in orbital-spin space [23]. The least-irrelevant operator also respecting this discrete \( Z_{2} \) symmetry of Eq. (6) is the corresponding \( SU^{(5)}(2)_{s} \)-descendant of dimension \( \Delta = 1 + 1/5 \), which yields a correction-to-scaling exponent 1/5 in excellent agreement with the value 0.200 \( \pm 0.002 \) observed in the NRG spectrum.

**Physical results.**—We now present exact properties that can be deduced from the CFT description. Details, including analysis of the conditions required for observation of these properties, will appear elsewhere [23].

(a) Fixed-point properties.—The frustrated fixed point has an irrational “ground-state degeneracy” [24] \( g = (\sqrt{5} + 5)/4 \). Moreover, in a quantum-dot device of triangular symmetry, where biases \( V_{j} \) in leads \( j = 1,2,3 \) produce in lead \( i \) a current \( I_{i} = \sum G_{ij} V_{j} \), the T = 0 zero-bias conductance is \( G_{0} = 4e^{2}/3h \). By contrast, the “isospin two-channel” regime [13], in which \( J_{11} \) dominates Eq. (4), is unstable against particle-hole asymmetry and at low energy exhibits the Fermi-liquid behavior of the \( SU(4) \) fixed point of [12] a), with \( g = 1 \) and (in the limit of small particle-hole asymmetry) \( G_{0} \sim e^{2}/2h < 4e^{2}/3h \). The other stable fixed point of [13], at which inter-impurity correlations are irrelevant and the standard Kondo effect is recovered, has \( g = 1 \) and \( G_{0i} = 0 \).

(b) Differential conductance.—The leading irrelevant operator of dimension \( \Delta = 1 + 1/5 \) governs many properties near the fixed point. In particular, the differential tunneling conductance into the impurities from a metallic lead (e.g., an STM tip located symmetrically with respect to the impurities) in the regime \( k_{B} T, |eV| \ll k_{B} T_{K} \) (\( V \) being the bias voltage) has the form \( G_{0}^{-1} dI/dV \sim 1 - B(T/T_{K})^{1/5} g[AeV/k_{B}T] \), where \( G_{0} \) is the T = 0 linear-response conductance; \( A \) and \( B \) are constants that can be fitted to experiment. For \( x \rightarrow 0 \), \( g[x] \rightarrow \text{const.} \), so \( G_{0}^{-1} dI/dV \sim 1 - B(T/T_{K})^{1/5} g[0] \); whereas \( g[x] \sim c x^{2/5} \) (with \( c \) a constant) for \( x \rightarrow \infty \), yielding \( G_{0}^{-1} dI/dV \sim 1 - cB(AeV/k_{B}T_{K})^{1/5} \). To lowest (quadratic) order in the tunneling matrix element between the impurities and the lead [20], the universal scaling function \( g[x] \) equals the exact function given in [13] b]. Similar (and in linear response, identical) behavior is expected in transport through triangular quantum-dot devices [23].

(c) Breaking of particle-hole symmetry.—This lowers the isospin \( SU(2) \) symmetry to the \( U(1) \) subgroup that conserves global charge \( 2I \), while preserving the discrete \( S_{3} \) symmetry. The spectrum in Table III is reclassified by applying Eq. (4) to \( SU^{(3)}(2)_{3} \supset U^{(1)}(1) \times Z_{s} \). The most-relevant operators that become allowed in the low-energy Hamiltonian are marginal: the charge current operator \( 2IF \), which is exactly marginal and corresponds to a simple phase shift [13]; and a degenerate pair \((s,I^{z},Z_{s},t_{z},Z_{s}) = ((0,0),(0,0), (\psi_{1,1}^{0})_{2,5},(0,0), (\psi_{1,1}^{0})_{3,5})\) arising from Table III row 5. The last two operators...
are the boundary limits of the left- and right-moving bulk currents $J_{L,R} = \psi_{L,R}^\dagger(\tau^z)^2 - \frac{2}{3}\psi_{L,R}$ (Table III, row 5) \cite{27}. $J_{L,R}$ generate a $U(1)$ symmetry of the free-fermion bulk theory not preserved by the boundary condition. The boundary limits of such operators are exactly marginal \cite{24}, consistent with NFL results in the presence of particle-hole asymmetry \cite{13}. Like a phase shift, the three exactly marginal deformations of the boundary conditions affect the FSS (and the boundary limits of $J_{L,R}$ affect the $T = 0$ zero-bias conductance), but not the operator spectrum in Table III \cite{23}. Thus, the NFL fixed point and its signatures, including the ground-state degeneracy and power laws in the conductance, persist away from particle-hole symmetry (unlike, e.g., the NFL behavior of the two-impurity Kondo model \cite{26}).

(d) Other symmetry-breaking perturbations.—It can be deduced from Table III that (i) spin-orbit coupling is relevant, with dimension $3/5$ \cite{28}, (ii) breaking of $S_\theta$ symmetry (e.g., through distortion of the equilateral triangular impurity geometry) is relevant with dimension $1/5$ \cite{28}, (iii) spin-exchange anisotropy is irrelevant, (iv) a Zeeman field acting only on the impurity spins is exactly marginal, and (v) the coupling $J_{11}$ in Eq. 7 is irrelevant. The implications of these results will be discussed elsewhere \cite{23}.

In summary, we have found the exact low-energy behavior of a non-Fermi-liquid phase arising from the interplay of magnetic frustration and Kondo physics in the three-impurity Kondo model. The phase is stable against particle-hole asymmetry, exchange anisotropy, and magnetic fields. It should be detectable in tunneling into magnetic adatoms on metallic surfaces and in electrical transport through triangular quantum-dot devices.

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