

Undercompensated Kondo Impurity with Quantum Critical Point

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The low-temperature properties of a magnetic impurity of spin S interacting with an electron gas via *anisotropic* spin exchange are studied via Bethe's *ansatz*. For $S > 1/2$ the impurity is only partially compensated at $T = 0$, leaving an effective spin that is neither integer nor half integer. The entropy has an essential singularity at $H = T = 0$, and the susceptibility and the specific heat follow power laws of H and T with nonuniversal exponents, which are the consequence of a quantum critical point. The results for the generalization to an arbitrary number of channels are also reported.

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The deviations from the usual Fermi-liquid behavior observed in the specific heat, susceptibility, and resistivity of several heavy fermion compounds [1] are frequently attributed to the existence of a quantum critical point (QCP). One possible realization of such a QCP is the screening of each f electron site via the quadrupolar Kondo effect [2], which is a special case of an overcompensated multichannel Kondo impurity. In this Letter we show that a QCP can also be induced in an undercompensated Kondo impurity with *anisotropic* coupling to the conduction electrons.

In the multichannel Kondo problem [3] three qualitatively different situations have to be distinguished as a function of the number of channels n and the impurity spin S [4–7]: (i) If $n = 2S$ the channels are exactly sufficient to compensate the impurity spin into a singlet, giving rise to Fermi-liquid behavior at low T . This case is realized for Fe and Cr impurities in Cu and Ag [4,8]. (ii) If $n < 2S$ the impurity spin is only partially screened (undercompensated), since there are not enough channels to yield a singlet ground state, leaving an effective spin degeneracy of $(2S + 1 - n)$. As a function of T the remaining spin degeneracy gives rise to a Schottky anomaly at about $T \approx H$ and the zero-field susceptibility diverges following a Curie law. Impurities with two magnetic configurations such as Tm or Tb could be related to this situation [4,9]. (iii) If $n > 2S$ the number of channels is larger than required to compensate the impurity spin. Critical behavior with universal exponents dependent only on n is obtained as T and H tend to zero. The overcompensated non-Fermi-liquid fixed point is understood in terms of an essential singularity in the entropy of the impurity at $H = T = 0$, which corresponds to a fractional spin if $H = 0$ and to a singlet if $H \neq 0$ [4–7]. Possible applications for this case are the quadrupolar Kondo effect and electron-assisted tunneling of an atom in a double-well potential [2,10].

The *undercompensated fixed point* has received much less attention than the *overcompensated* one. In this Letter we show that exchange anisotropy drives the low- T fixed point from an asymptotically free spin to a QCP with nonuniversal exponents. Such a situation could arise in axial symmetry, where crystalline fields induce anisotropies. A possible experimental realization is an impurity (e.g.,

Tm or Tb) at the surface of a metallic film. As an example consider a mixed valent impurity with two magnetic configurations of spin $1/2$ and 1 , respectively. We denote the states according to their spin and z component, i.e., $|SS_z\rangle$. We assume that the configuration of spin 1 has one more electron and an energy ϵ relative to the Fermi level. The hybridization Hamiltonian is [9,11]

$$H_V = \sum_{\sigma} \left[V_1 c_{\sigma}^{\dagger} | \frac{1}{2} \sigma \rangle \langle 1(2\sigma) | + (V_2/\sqrt{2}) c_{\sigma}^{\dagger} | \frac{1}{2} - \sigma \rangle \langle 10 | + \text{H.c.} \right].$$

For $V_1 = V_2$ the model is isotropic in spin space. For $\epsilon \ll 0$ the configuration of spin $1/2$ can be eliminated via a Schrieffer-Wolff transformation, yielding an anisotropic exchange interaction of the form ($S = 1$)

$$H_{\text{ex}} = J_{\parallel} S^z \sigma^z + \frac{1}{2} J_{\perp} (S^+ \sigma^- + S^- \sigma^+) + \Delta (S^z)^2 I_{\sigma},$$

where I_{σ} , σ^z , and σ^{\pm} are the identity and the Pauli matrices (of eigenvalues $\pm \frac{1}{2}$) for the conduction states. Here $J_{\parallel} = V_1^2/|\epsilon|$, $J_{\perp} = V_1 V_2/|\epsilon|$, $\Delta = (V_1^2 - V_2^2)/2|\epsilon|$, and we neglected a normal scattering term. Kondo impurities with anisotropic exchange coupling have long been studied for the spin-compensated [12,13] and overcompensated [14] cases, but not for the undercompensated situation.

Additional crystalline field effects change the relative strengths of J_{\parallel} , J_{\perp} , and Δ . H_{ex} (for $S = 1$) is integrable (for a linear dispersion for the conduction states of density ρ) as a function of two real dimensionless parameters, μ and f , that determine J_{\parallel} , J_{\perp} , and Δ . For small anisotropy we obtain that $J_{\parallel} \rho = -2\mu/f$, $J_{\perp} = J_{\parallel}(1 - \delta/3)$, and $\Delta = -\frac{1}{3} J_{\parallel} \delta$ with $\delta = \frac{1}{2} f^2 + \frac{1}{8} \mu^2$. Note that the U(1) invariance restricts the model to two independent coupling parameters. The isotropic limit [15] is recovered for $f \rightarrow 0$ and $\mu \rightarrow 0$ with $\mu/f = -J/2$.

In this Letter we obtain the solution of a model with U(1) symmetry in which an impurity of spin S interacts with conduction electrons in one orbital channel (with linearized dispersion). The multichannel results are presented at the end of the Letter. For $S = \frac{1}{2}$ the Δ term in H_{ex} is irrelevant and the model reduces to the anisotropic Kondo model

($J_{\parallel} > J_{\perp}$) solved by Wiegmann [13]. For $S = \frac{1}{2}$ the impurity is exactly compensated and the ground state is a singlet. For $S = 1$ the model reduces to H_{ex} . For $S > 1$ there are additional U(1) invariants.

For N electrons in a box of length L with periodic boundary conditions the solution of H_{ex} is equivalent to the simultaneous diagonalization of N transfer matrices

$$\hat{T}_j \equiv \hat{P}_{j,j+1} \hat{P}_{j,j+2} \cdots \hat{P}_{j,N} \hat{R}_{j,S} \hat{P}_{j,1} \cdots \hat{P}_{j,j-1}, \quad (1)$$

$j = 1, \dots, N$, with eigenvalues $\exp(ik_j L)$, where k_j are the wave numbers of the electrons. Here $\hat{P}_{j,j'}$ permutes the electrons j and j' , and $\hat{R}_{j,S} = \exp(-iH_{\text{ex}})$ is the scattering matrix of the electron j off the impurity.

The model and its solution are constructed from the scattering matrices via the quantum inverse scattering method. The Yang-Baxter triangular relation (sufficient condition

for the integrability) has the following U(1)-invariant solution [16]:

$$R(\theta) = [\sinh(\theta + \frac{1}{2}\gamma + \gamma S^z \sigma^z) + \sinh(\gamma)(S^x \sigma^x + S^y \sigma^y)] / \sinh[\theta + \gamma(S + \frac{1}{2})],$$

where the Pauli matrices refer to an electron and the spin operators S^x , S^y , and S^z correspond to the impurity of spin S or to another conduction electron ($S = 1/2$). Here θ is the spectral parameter and γ is the anisotropy parameter (to be identified with $i\mu$). For $\theta \rightarrow 0$ and $\gamma \rightarrow 0$ with $\theta/\gamma = \lambda$ kept finite it reduces to the R matrix for isotropic exchange [impurity of spin S and SU(2) invariance]. For $\theta = f$ the R matrix corresponds to the scattering matrix of an electron off the impurity of spin S . For $\theta = 0$ and $S = 1/2$, on the other hand, the R matrix reduces to the spin permutation operator. Hence, all limits are properly contained.

We introduce a standard monodromy matrix [11,13,17]

$$L_{\{\sigma_1' \dots \sigma_N' S'\}}^{\{\sigma_1 \dots \sigma_N S\}}(\theta; \theta_1, \dots, \theta_{N+1}) = R_{\sigma_1' \sigma_1}^{\tau' \mu_1}(\theta - \theta_1) R_{\sigma_1' \sigma_2}^{\mu_1 \mu_2}(\theta - \theta_2) \cdots R_{\sigma_1' \sigma_N}^{\mu_{N-1} \mu_N}(\theta - \theta_N) R_{S' S}^{\mu_N \tau}(\theta - \theta_{N+1}), \quad (2)$$

with the implicit sum over all μ_j indices. The first N factors refer to conduction electrons and the last one corresponds to the impurity. With respect to the indices τ and τ' the monodromy matrix forms a 2×2 matrix, whose trace is the transfer matrix \hat{T} . For $\theta = 0$ and $\theta_j = -f \delta_{j,N+1}$ the transfer matrix is identical to (1). As a consequence of the triangular Yang-Baxter relation transfer matrices for different values of the spectral parameter commute and hence there exists a basis of states that diagonalizes the transfer matrices for all θ simultaneously. The derivatives of the logarithm of the transfer matrix with respect to θ yield the conserved quantities of the model, e.g., the Hamiltonian as $H = d \ln T(\theta) / d\theta|_{\theta=0}$.

The simultaneous diagonalization of the transfer matrices leads to the Bethe ansatz equations (BAE). Following a standard procedure [4–6,11,13] we obtain

$$e^{ik_j L} = e^{-i\varphi_{S\uparrow}} \prod_{\beta=1}^M g(\theta_{\beta}, \mu/2),$$

$$g(\theta_{\alpha} + f, \mu S) [g(\theta_{\alpha}, \mu/2)]^N = - \prod_{\beta=1}^M g(\theta_{\alpha} - \theta_{\beta}, \mu), \quad (3)$$

where $g(x, y) = \sinh(x + iy) / \sinh(x - iy)$, $\varphi_{S\uparrow}$ is the phase shift due to the scattering of an up-spin electron with the spin-polarized impurity, M is the number of flipped spins ($M \leq N/2$), $j = 1, \dots, N$ and $\alpha = 1, \dots, M$. The θ_{α} are the spin rapidities (related to the wave numbers of the spin excitations). The first factor on the left-hand side

of the second equation arises from the impurity. The remaining factors are identical to those of the [U(1)-symmetric] Heisenberg chain with planar anisotropy [18]. In the limit $f \rightarrow 0$ and $\mu \rightarrow 0$, keeping θ_{α}/μ and $f/\mu \propto 1/J$ fixed, we recover the isotropic case. The energy and the magnetization are $E = \sum_{j=1}^N k_j$ and $S_z = \frac{1}{2}N + S - M$.

In the thermodynamic limit the solutions of (3) are complex and form strings [19] of length $(n - 1)$, $n = 1, \dots, \infty$, $\theta_{\alpha}^{n,l} = \Lambda_{\alpha}^n + i\mu(n + 1 - 2l)/2$, $l = 1, \dots, n$, where Λ_{α}^n is real and represents the motion of the center of mass of the string. In contrast to the SU(2)-symmetric model [11,13,15,17] the BAE for the U(1)-invariant chain are twofold periodic in μ , so that a parity (even or odd) has to be associated with the order of the string state [19]. Limiting ourselves to low T (so that long strings do not contribute significantly) and to $2S\mu < \pi/2$, we have to consider only string states of even parity. This is satisfied if either the anisotropy or the impurity spin is not very large. We can restrict ourselves to string states so that $n\mu < \pi/2$, which substantially simplifies the thermodynamic BAE. The neglected strings with $n > n_{\text{max}}$ neither affect the ground state nor the low- T properties. If ξ_n is the number of strings of length $n - 1$, then $M = \sum_{n=1}^{n_{\text{max}}} n \xi_n$ must be satisfied.

The rapidities satisfy Fermi statistics and their occupation is described in terms of dressed energies, $\epsilon_n(\Lambda)$, which enter the Fermi distribution. In thermal equilibrium they satisfy the integral equations [11,13,17,19]

$$\ln[1 + \exp(\epsilon_n/T)] = nH - \frac{N}{2L} f_n(\Lambda) + T \sum_{k=1}^{n_{\text{max}}} \int \frac{d\Lambda'}{2\pi} \times \ln\{1 + \exp[-\epsilon_k(\Lambda')/T]\} A_{n,k}(\Lambda - \Lambda'), \quad (4)$$

$$A_{n,k}(\Lambda) = f_{n+k}(\Lambda) + 2 \sum_{l=1}^{m_{n,k}} f_{n+k-2l}(\Lambda) + f_{|n-k|}(\Lambda), \quad f_n(\Lambda) = 2 \sin(n\mu) / [\cosh(2\Lambda) - \cos(n\mu)], \quad (5)$$

and $m_{n,k} = \min(k, n) - 1$. Equation (4) is the thermodynamic BAE, in this case restricted to $n < n_{\max}$. As $T \rightarrow 0$ only ϵ_1 can be negative; hence, only real rapidities are occupied in the ground state, while all string states are empty. In the limit $\mu \rightarrow 0$ these equations reduce to the thermodynamic BAE for isotropic Kondo coupling [15]. The impurity contributes only to order $1/N$ and does not drive the population of the bands.

The free energy of the impurity is given by

$$F_{\text{imp}}(H, T) = F_{\text{imp}}^0 - T \int d\Lambda G_0(\Lambda + f) \times \ln\{1 + \exp[\epsilon_{2S}(\Lambda)/T]\}, \quad (6)$$

where $G_0(\Lambda) = [2\mu \cosh(\pi\Lambda/\mu)]^{-1}$. F_{imp}^0 is the zero-field ground state energy, which is a nonuniversal constant.

The validity of Eqs. (4) and (6) is restricted to low T (due to the truncation at n_{\max}), where they yield the correct ground state and leading low- T properties. For special values of the anisotropy $\mu = \pi/\nu$ with $\nu = 3, 4, 5, \dots$, Takahashi and Suzuki [19] have shown that the recurrence relation for the exact thermodynamic BAE truncates and reduces to $\nu - 1$ integral equations. Here we consider the general case for which μ/π is an irrational number.

The ground state equations are obtained from (4) as $T \rightarrow 0$. Only the ϵ_1 band is populated, while all bands of stringed rapidities are empty. In zero field the band is completely filled and via Fourier transformation we obtain $\epsilon_1(\Lambda) = -(\pi N/L)G_0(\Lambda)$. With increasing field the large $|\Lambda|$ tails become depopulated. To leading order in the field (the bandwidth is assumed very large) the ground state integral equation is of the Wiener-Hopf type with the integration limit $B(H)$ determining the Fermi point. Its solution yields $B = (\pi/\mu) \ln(H/A)$, where A is a constant. Here $B \rightarrow -\infty$ corresponds to zero field.

The impurity changes the distribution of rapidities. The impurity density satisfies the Wiener-Hopf equation

$$\rho_h^{\text{imp}}(\Lambda) + \rho^{\text{imp}}(\Lambda) + \int_B^\infty \frac{d\Lambda'}{2\pi} f_2(\Lambda - \Lambda') \rho^{\text{imp}}(\Lambda') = (1/2\pi) f_{2S}(\Lambda + f), \quad (7)$$

where $\rho_h^{\text{imp}}(\Lambda)$ is the distribution of the rapidity holes. In zero field there are no holes and the solution is

$$\hat{\rho}^{\text{imp}}(\omega) = \frac{\sinh[(\pi - \mu 2S)\omega/2] e^{-i\omega f}}{2 \cosh(\omega\mu/2) \sinh[(\pi - \mu)\omega/2]}, \quad (8)$$

where the *hat* denotes Fourier transform. In zero field the impurity has a residual magnetization if $S > \frac{1}{2}$ (undercompensated impurity), $S_z^{\text{imp}} = \alpha(S - \frac{1}{2})$, where $\alpha = 1/(1 - \mu/\pi)$. For $\mu \rightarrow 0$ this reduces to the result for isotropic coupling. For anisotropic coupling we have that the remnant spin is neither integer nor half integer, but a fractional quantity. This feature is indicative of critical behavior even in the undercompensated limit.

The field dependence of the impurity magnetization is obtained from the solution of the Wiener-Hopf equation

(7) [4,6,11,13]. We limit ourselves to state the results in small and large fields. In the low field limit we have to distinguish the cases $S = 1/2$ and $S > 1/2$. For $S = 1/2$ the ground state is a singlet, the susceptibility is finite, and all terms of the H/T_K expansion are analytic [15]. Here $T_K \propto \exp(-|f|\pi/\mu)$. This Fermi liquid fixed point is in agreement with Anderson's renormalization group result [12]. For $S > 1/2$, on the other hand,

$$S_z^{\text{imp}} = \alpha(S - \frac{1}{2}) + C(H/T_K)^{2\alpha\mu/\pi} + \dots, \quad (9)$$

where C is a constant and the dots stand for higher order analytic and nonanalytic terms in H . This proves the conjecture that a QCP is associated with the fractional remnant spin. In high field the saturation magnetization is S and as the field decreases S_z^{imp} is reduced by a power of T_K/H ,

$$S_z^{\text{imp}} = S - C'(T_K/H)^{2\mu/\pi} + \dots, \quad (10)$$

which replaces the logarithms of asymptotic freedom of the isotropic case. This result holds for all impurity spins. The impurity magnetization can also be obtained from the impurity free energy, Eq. (6), in the limit $T \rightarrow 0$.

Consider now (4) for low T , i.e., $T \ll 1$, and introduce a shift in the rapidities, $\Lambda = \lambda + (\mu/\pi) \ln[T\mu L/2\pi N]$. Defining $\eta_n(\lambda) = \exp[\epsilon_n(\Lambda)/T]$, Eq. (4) is written as

$\ln \eta_n = G_0 \star \ln[(1 + \eta_{n-1})(1 + \eta_{n+1})] - \delta_{n,1} e^{\pi\lambda/\mu}$, ($\eta_0 \equiv 0$) so that T has formally disappeared as a parameter. Here \star denotes convolution. As $\lambda \rightarrow -\infty$ it reduces to an algebraic equation and has the solution

$$1 + \eta_n = \{\sinh[(n + \kappa - 1)H/2T] / \sinh(\kappa H/2T)\}^2,$$

where κ is an arbitrary constant that tends to 1 as $\mu \rightarrow 0$. The constant κ cannot be determined from this set of equations because of its truncation for large n (n_{\max} , odd parity strings have been neglected). The impurity free energy, Eq. (6), now has the form

$$F_{\text{imp}} = F_{\text{imp}}^0 - T \int d\lambda \ln[1 + \eta_{2S}(\lambda)] \times G_0[\lambda + (\mu/\pi) \ln(T\mu L/2\pi N) + f]. \quad (11)$$

The function G_0 only contributes significantly around its maximum, i.e., $\lambda \approx (\mu/\pi) \ln(T_K/T)$, and inserting η_{2S} we obtain a residual entropy of

$$S_{\text{imp}}(T = H = 0) = \ln[1 + (2S - 1)/\kappa]. \quad (12)$$

Comparing to Eq. (9) we have that $\kappa = 1/\alpha = 1 - \mu/\pi$. If $H \neq 0$ the entropy vanishes at $T = 0$ for all spins.

Hence, for $S = 1/2$ the ground state is a singlet (Fermi liquid) and the entropy is a continuous function of H and T . If $S > 1/2$ a small H lifts the degeneracy and the entropy vanishes. Since the spin is fractional and the entropy has an essential singularity at $T = H = 0$, quantum critical properties arise, induced by the anisotropy. They are not existent in the $SU(2)$ -invariant model.

To obtain the leading low- T dependence of the specific heat in zero field we distinguish $S = \frac{1}{2}$ from $S > \frac{1}{2}$. For $S = \frac{1}{2}$ the Sommerfeld expansion of the Fermi functions

yields the usual Fermi-liquid behavior. For $S > \frac{1}{2}$, on the other hand, we consider

$$\begin{aligned} \delta F_{\text{imp}}(T) = & -T \int \frac{d\omega}{2\pi} \exp[i(\omega\mu/\pi) \ln(T/T_K)] \\ & \times \frac{\sinh[\omega(\pi - 2S\mu)/2]}{\sinh(\omega\pi/2)} \\ & \times \ln\{1 + \exp[-|\epsilon_1(\lambda)|/T]\}, \end{aligned}$$

where ϵ_1 is the $T = 0$ solution. The leading term arises from the zero of $\sinh(\omega\pi/2)$ at $\omega = -2i$, yielding $C_{\text{imp}} \propto (T/T_K)^{2\mu/\pi}$. The critical exponent depends on the anisotropy, but not on S , and it is different from the exponent of the magnetization. The QCP disappears as $\mu \rightarrow 0$. From the scaling dimensions of the field and temperature we have $T\chi_{\text{imp}} \propto (T/T_K)^{2\mu/\pi}$.

Finally, we summarize our results for the anisotropic n -channel Kondo problem. As in the isotropic case the conduction electron spins of the n channels glue together to form a composite of spin $n/2$. The BAE for the U(1)-invariant model are similar to (3), but with $\sinh(\theta \pm i n\mu/2)$ replacing $\sinh(\theta \pm i\mu/2)$ in the first equation and in the driving factors in the second. The general structure of the integral equations is then the same as for $n = 1$, except for the driving terms. We limit ourselves to the low- T and small field properties of (i) compensated ($n = 2S$), (ii) undercompensated ($n < 2S$), and (iii) overcompensated ($n > 2S$) impurity spins.

A completely *compensated* impurity has Fermi-liquid properties, i.e., the ground state is a singlet, the susceptibility is finite, and the specific heat is proportional to T . The anisotropy does not affect the low- T fixed point.

In the *undercompensated* case the impurity spin is partially compensated leaving a fractional remnant spin of $\alpha'(S - \frac{n}{2})$, where $\alpha' = 1/(1 - n\mu/\pi)$. The entropy has an essential singularity at $H = T = 0$ jumping from $\ln[1 + \alpha'(2S - n)]$ to zero when $H \neq 0$. The specific heat and χ_{imp} follow power laws as $H \rightarrow 0$ and $T \rightarrow 0$

$$\begin{aligned} S_{\text{imp}}^z - \alpha'(S - n/2) & \propto (H/T_K)^{2\alpha'\mu/\pi}, \\ C_{\text{imp}} & \propto T\chi_{\text{imp}} \propto (T/T_K)^{2\mu/\pi}. \end{aligned} \quad (13)$$

The fractional character of the remnant spin is induced by the anisotropy and drives a QCP, which is the main new feature of this model. The exponents depend on the anisotropy parameter μ and the critical behavior disappears in the isotropic exchange limit.

The low- T properties of an *overcompensated* impurity are governed by a QCP with singular ground state entropy, which is $\ln\{\sin[\pi(2S + 1)/(n + 2)]/\sin[\pi/(n + 2)]\}$ in zero field and zero if $H \neq 0$. The magnetization and specific heat follow power laws as $H \rightarrow 0$ and $T \rightarrow 0$

$$S_{\text{imp}}^z \propto (H/T_K)^{2/n}, \quad C_{\text{imp}} \propto T\chi_{\text{imp}} \propto (T/T_K)^{4/(n+2)}.$$

The critical exponents depend on the number of channels, but not on the anisotropy. For $n = 2$ the dependence on H and T is logarithmic. This non-Fermi-liquid behavior is identical to that for isotropic exchange.

In summary, the exchange anisotropy does not affect the compensated and overcompensated fixed points, but it is a relevant variable for the undercompensated Kondo impurity. For $n \neq 2S$ the system has a QCP, with universal exponents for $n < 2S$, but nonuniversal ones (they depend on the anisotropy) for $n > 2S$.

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