Integrable Two-Impurity Kondo Model

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The exact solution by means of Bethe's *Ansatz* of a variant of the two-impurity Kondo problem is presented. The occupation of the singlet and triplet states, the expectation value $\langle \vec{S}_1 \cdot \hat{S}_2 \rangle$, the homogeneous and staggered magnetic field susceptibilities, and the specific heat γ coefficient are studied for the ground state as a function of the Ruderman-Kittel-Kasuya-Yosida–coupling strength. [S0031-9007(98)06269-3]

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At least two competing energy scales, e.g., the single site Kondo temperature and the Ruderman-Kittel-Kasuya-Yosida (RKKY) intersite interaction, are frequently invoked to explain the nonuniversal behavior of heavy fermion compounds. While the single-impurity Kondo problem is by now well understood [1–3], the Kondo lattice model still remains unsolved. The simplest model showing the competition of these two energy scales is the two-impurity Kondo problem, which has been studied by numerous methods [4], in particular by the numerical renormalization group [5] and conformal field theory [6]. For strong ferromagnetic RKKY coupling between the impurities, their spins lock into a triplet state, which is spin compensated in analogy to the $S = 1$ two-channel Kondo problem. For strong antiferromagnetic RKKY coupling, on the other hand, the spins of the two impurities compensate each other. These two fixed points are in general joined by a line of fixed points [5,6] that yields nonuniversal behavior, except for a special electron-hole symmetry where the basins of attraction of these two stable fixed points are separated by an unstable fixed point with non-Fermi-liquid properties.

The analytic solution of a many-body problem is always of interest. In this Letter we present the exact solution of a model for two interacting Anderson impurities in the $U \to \infty$ limit. In this limit the ground state for each impurity is a linear superposition of two ionic configurations with zero and one localized (f) electrons, respectively. This excludes the particle-hole symmetry required for the unstable non-Fermi-liquid fixed point.

Some model assumptions and approximations are necessary to ensure the integrability. (i) Electrons are considered in pairs, such that the impurities have either one localized electron each or they are both in the empty configuration. States with one impurity in the f^1 and the other in the f^0 configurations are not allowed. Since we are interested in the magnetic integer-valent limit (both impurities in the f^1 configuration), this assumption is not expected to have dramatic consequences. (ii) In the Anderson model the impurity interacts with conduction electrons via a contact potential hybridization, i.e., only with states having s-wave symmetry about the impurity site. It is then necessary to introduce two channels for the conduction electrons, one for each impurity. These two channels are chosen to be even and odd parity states with respect to the midpoint between the impurity sites [5]. (iii) The two channels are sufficient to distinguish the impurities, so that now both impurities can be considered at the same site. The RKKY interaction, which is the interaction between the spins mediated by the conduction electrons, is introduced *a priori* as a parameter. This approximation is standard for numerical renormalization group approaches [5]. (iv) The hybridization matrix element is assumed to be independent of the spin and the channel. (v) It is further assumed that pairs of propagating electrons act like hard-core bosons (see below).

Without loss of generality we consider only forward moving particles along a ring with periodic boundary conditions and linearize the dispersion of the conduction states about the Fermi level. The Hamiltonian of the model with assumptions (i)–(iv) is $H = H_0 + H_1$,

$$H_0 = v_F \sum_{km\sigma} k c^\dagger_{mk\sigma} c_{mk\sigma} + 2\epsilon \sum_{\sigma\sigma'} |1\sigma, 2\sigma'\rangle\langle 1\sigma, 2\sigma'| + \frac{2V}{N} \sum_{k_1 k_2 \sigma\sigma'} (|1\sigma, 2\sigma'\rangle\langle 0| c_{2k_2\sigma'} c_{1k_1\sigma} + \text{H.c.}), \quad (1)$$

$$H_1 = \Delta \sum_{\sigma_1\sigma_2\sigma_1'\sigma_2'} |1\sigma_1', 2\sigma_2'\rangle \vec{S}_{\sigma_1'\sigma_1} \cdot \vec{S}_{\sigma_2'\sigma_2} \langle 1\sigma_1, 2\sigma_2|, \quad (2)$$

where $m = 1, 2$ labels the two impurities (channels), v_F is the Fermi velocity (to be equated to one) and the bra and kets denote the impurity states, $|0\rangle$ being the state without localized electrons and $|1\sigma, 2\sigma'\rangle$ the states in which each site has a localized electron. The parameter ϵ is the energy difference between the two ionic configurations relative to the Fermi energy, Δ is the RKKY coupling strength, and $\vec{S}$ is the vector of spin-1/2 matrices.

To investigate under which conditions the Hamiltonian H_0 can be diagonalized exactly we consider first a pair of electrons (one in each channel) interacting with the impurities placed at the origin. The wave function is a linear superposition of a propagating plane wave and a localized state containing the two electrons. Hence, when the conduction electrons pass the impurities their wave function acquires a phase shift of $\phi_k = 2 \arctan[-(V^2/2)/(k - \epsilon)]$, where $2k$ is the momentum of their center of mass. This resonance occurs only if the two electrons arrive together as a pair with one electron in each channel. Individual electrons play then no role and pairs act like hard-core bosons, i.e., their double occupancy is forbidden.

Consider now four electrons, arranged as two pairs with one electron in each channel. The wave function for this case is the linear superposition of two propagating pairs with one propagating pair and a localized pair. Assuming that the pairs do not interchange individual electrons in the scattering process (i.e., pairs are not broken up and recombined in a different way), the scattering matrix between pairs is

$$\hat{X}(k_1 - k_2) = \frac{(k_1 - k_2)\hat{I} - iV^2\hat{P}}{(k_1 - k_2) - iV^2}, \tag{3}$$

where $k_1 - k_2$ is the momentum transfer, and $\hat{I}$ and $\hat{P}$ are the identity and permutation operators. The set of incoming and outgoing pairs is identical and these operators yield the amplitudes for the pairs remaining unchanged and interchanged, respectively [assumption (v)].

Using the same assumptions as for the four electron problem this solution is easily extended to N pairs of electrons. Since all pairs move forward with the same velocity, the relative distances $(x_i - x_j)$ are constants that do not change with time. Whenever a pair passes the origin it acquires a phase shift ϕ_k. There are $N!$ space arrangements of the coordinates of the pairs $\{x_i\}$. The wave functions in the $N!$ sectors are matched at adjacent boundaries by the scattering matrix (3). Nonadjacent sectors are related by a sequence of matched adjacent regions. The result is independent of the path through which two points in the N-dimensional space are joined (single-valued wave function) since (3) satisfies the triangular Yang-Baxter relation.

The above variant of the two-impurity Kondo problem is then integrable via nested Bethe *Ansatz*. The one and two particle scattering matrices are actually identical to those of the fourfold degenerate Anderson impurity in the $U \to \infty$ limit. The difference between the two models is that the pairs act like hard-core bosons rather than fermions. With two orbital channels and the spin we have four bosonic degrees of freedom and four impurity states, which can be redefined as a singlet and three triplet states, $m = S, T+, T0$, and $T-$. The effective Hamiltonian [including assumption (v)] is

$$H_{\text{eff}} = -2i \sum_{m=1}^{4} \int dx b_m^\dagger(x) \frac{\partial}{\partial x} b_m(x) + 2\epsilon \sum_{m=1}^{4} |m\rangle\langle m| + 2V \sum_{m=1}^{4} \int dx \,\delta(x) (|m\rangle\langle 0| b_m(x) + \text{H.c.}), \tag{4}$$

which differs from H_0 only by the condition that electrons appear and remain always in pairs. Equation (4) conserves the number of particles with given color m, $N_m = |m\rangle\langle m| + \int dx b_m^\dagger(x) b_m(x)$. Now the RKKY interaction, Eq. (2), (and the magnetic fields) are incorporated *a posteriori* by adding $\Delta[N_{T+} + N_{T0} + N_{T-} - 3N_S]/4$ to Eq. (4).

The model is diagonalized in terms of four nested Bethe *Ansätze* (one for the charges and three for the internal degrees of freedom), each giving rise to one set of rapidities. All rapidities within a given set have to be different (Fermi statistics of the rapidities). The discrete Bethe *Ansatz* equations and the classification of states (solutions in the thermodynamic limit according to the string hypothesis) are the same as for the SU(4) Anderson impurity in the $U \to \infty$ limit [3,7] and will not be repeated here. In the ground state there are free propagating charges and bound states of charges of up to four hard-core bosons (four internal degrees of freedom). These states correspond to charge rapidity strings of length l, $l = 0, \ldots, 3$. The distribution functions for the string states present in the ground state, $\sigma^{(l)}(\xi)$, and their respective holes, $\sigma_h^{(l)}(\xi)$, satisfy the coupled Wiener-Hopf integral equations

$$\sigma_h^{(l)}(\xi) + \sigma^{(l)}(\xi) + \sum_{q=0}^{3} \sum_{p=0}^{p_{lq}} \int_{-\infty}^{B_q} d\xi' \sigma^{(q)}(\xi') a_{l+q-2p}(\xi - \xi') = \frac{l+1}{2\pi} + \frac{1}{L} a_{l+1}(\xi - \epsilon), \tag{5}$$

where $a_q(\xi) = (qV^2/2\pi)/[\xi^2 + (qV^2/2)^2]$, L is the length of the box, and $p_{lq} = \min(l, q) - \delta_{l,q}$. The integration limits B_q correspond to the Fermi points of each class of states and are determined by the number of particles of each "color" N_q through

$$\int_{-\infty}^{B_q} d\xi \sigma^{(q)}(\xi) = N_{q+1} - N_{q+2},$$

where the levels are arranged such that $N_1 > N_2 > N_3 > N_4$ with $N_5 = 0$. The energy of the system is given by

$$E = \sum_{l=0}^{3} (l+1) \int_{-\infty}^{B_l} d\xi \xi \sigma^{(l)}(\xi). \tag{7}$$

The two driving terms of Eqs. (5) correspond to the host and the impurities, respectively. Since the integral equations are linear, the densities can be separated into a host and an impurity part.

Assuming that the bandwidth is much larger than the Kondo temperature and the RKKY splitting, the valence of the impurities is completely determined by $\sigma^{(3)}(\xi)$. Although the valence is not of great physical interest [because of the construction of model (1)], it is important to study this quantity to understand how the integer valent limit is reached. Setting $B_l = -\infty$ for $l = 0, 1, 2$ but keeping B_3 finite, Eqs. (5) reduce to a single Wiener-Hopf integral equation. Its solution yields n_f, the number of localized electrons per impurity,

$$n_f = \frac{1}{2} + \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x}(-ix+0)^{3ix/2} \times \exp[ix\tilde{\epsilon} - 2\pi|x|]\,\frac{\Gamma(1-2ix)}{\Gamma(1-ix/2)},$$

$$\tilde{\epsilon} = \frac{\pi}{V^2}(\epsilon - B_3) + 4\ln 2 + \frac{3}{2}\ln(4D/eV^2), \quad (8)$$

where 0 is a positive infinitesimal and D is a cutoff for the electronic excitations introduced *a posteriori* into the Bethe ansatz [3,7]. It is easy to verify that n_f varies smoothly between 0 for $\tilde{\epsilon} \gg 0$ to 1 for $\tilde{\epsilon} \ll 0$. The magnetic integer valent limit is then obtained suppressing the charge fluctuations by taking the limit $\tilde{\epsilon} \to -\infty$.

The RKKY interaction changes the relative population of the singlet and triplet states of the pair of impurities. The same procedure as for the Anderson impurity with crystalline fields [8] can now be followed. We have to distinguish the cases $\Delta > 0$ and $\Delta < 0$. For $\Delta > 0$ the singlet has lower energy than the triplet and in the absence of magnetic fields the splitting is given by the density $\sigma^{(0)}(\xi)$ with $B_1 = B_2 = -\infty$ and B_0 parametrizing the splitting. Equations (5) consist then of two coupled equations for $\sigma^{(0)}(\xi)$ and $\sigma^{(3)}(\xi)$. Since the band width is much larger than Δ, the feedback of $\sigma^{(0)}(\xi)$ onto $\sigma^{(3)}(\xi)$ can be neglected. This decouples the two equations, leaving the Wiener-Hopf equation for $\sigma^{(0)}(\xi)$ with two driving terms, one arising from the Kondo effect and the other one from the valence fluctuations through $\sigma_h^{(3)}$. The latter tends to zero as the integer valent limit is approached and can be neglected. Similarly, for $\Delta < 0$ the triplet has lower energy and the splitting is given by $\sigma^{(2)}(\xi)$ with $B_0 = B_1 = -\infty$. Neglecting the valence fluctuations (integer valent limit), in both cases the splitting $sp^{(l)}$ is obtained by solving one Wiener-Hopf equation ($l = 0, 2$)

$$sp^{(l)} = -\frac{1}{2\pi i}\int \frac{dt}{t + i0}\,G_l(t),$$

$$G_l(t) = \exp\left[-i\,\frac{\pi}{V^2}(B_l - \epsilon)t\right] \times \left[\frac{-it+0}{2ec}\right]^{-it/2}\frac{\Gamma(1+2it)}{\Gamma(1+3it/2)}\,F_l(t), \quad (9)$$

where $F_0 = 1$, $F_2(t) = \sinh(\pi t/2)/\sinh(3\pi t/2)$, and $c = 27/256$. For $\Delta > 0$ the level populations are $n_S = \frac{1}{4} + \frac{3}{4}sp^{(0)}$, $n_T = \frac{1}{4} - \frac{1}{4}sp^{(0)}$, while for $\Delta < 0$ we have $n_S = \frac{1}{4} - \frac{3}{4}sp^{(2)}$, $n_T = \frac{1}{4} + \frac{1}{4}sp^{(2)}$. B_l is related to Δ through

$$\exp\left[\frac{\pi(B_l - \epsilon)}{2V^2}\right] = \frac{|\Delta|}{T_K}\,\Gamma(1/4)\,(4ec)^{1/4}, \qquad l = 0, 2, \quad (10)$$

where T_K is the Kondo temperature for the $S = 3/2$ Coqblin-Schrieffer model.

The occupation of the singlet and triplet states as a function of the RKKY-coupling strength is displayed in Fig. 1(a). n_S varies between 0 and 1, while n_T decreases from 1/3 to 0. Both are analytic functions of Δ. For $|\Delta| \gg T_K$ they approach their asymptotic values on a logarithmic scale. The logarithmic dependence arises from the factor $(-it+0)^{-it/2}$ in Eq. (9), and can be obtained by closing the contour through the lower complex half-plane. Another quantity of interest is the ground state expectation value $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = \frac{3}{4}(n_T - n_S)$, shown as the dashed line in Fig. 1(a).

The susceptibility is obtained as the linear response of the impurities to a small homogeneous field. The magnetic field lifts the degeneracy of the triplet states, so that now all integration limits B_l are finite. We assume that $H \ll |\Delta| \ll D$, so that for $\Delta > 0$ we have $B_1, B_2 \ll B_0 \ll B_3$, where B_1 and B_2 parametrize the magnetic field. In

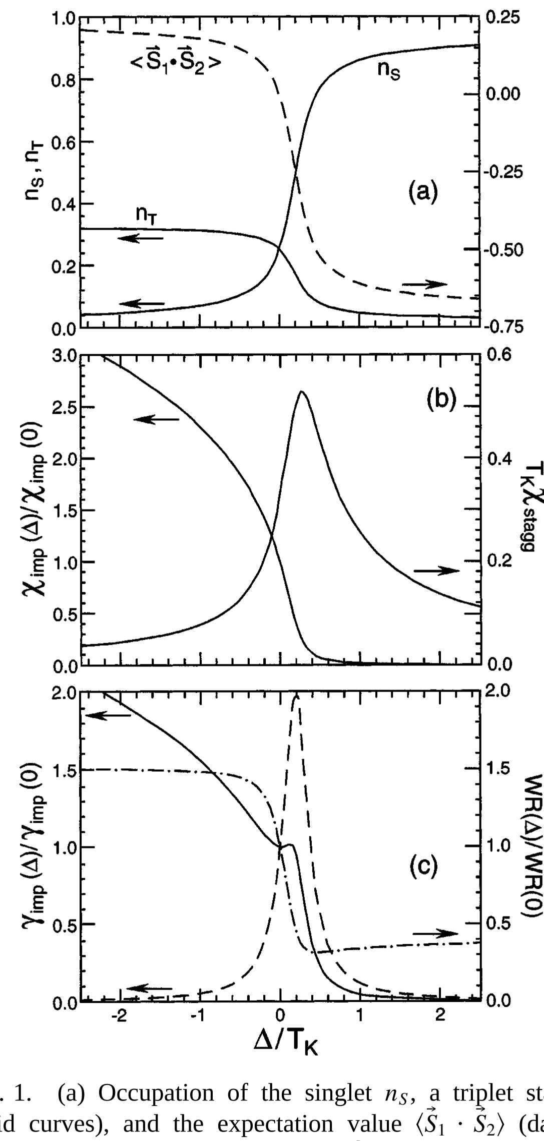

FIG. 1. (a) Occupation of the singlet n_S, a triplet state n_T (solid curves), and the expectation value $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle$ (dashed), (b) the homogeneous and staggered field susceptibilities, and (c) the specific heat γ (solid), S to T fluctuations contribution to γ (dashed) and the Wilson ratio (dash-dotted) as a function of Δ/T_K for the ground state.

linear response the feedback of $\sigma^{(1)}$ and $\sigma^{(2)}$ on the other two distributions can be neglected, so that the ratio of the susceptibilities of the impurity and the host is given by the $\xi \to -\infty$ asymptotic of the driving terms for $\sigma^{(1)}$ and $\sigma^{(2)}$. In general there are three contributions, namely, a Kondo term, an RKKY-splitting contribution, and one due to valence fluctuations. As before we consider the magnetic integer valence limit, i.e., we suppress the valence fluctuations. For $\Delta > 0$ the singlet has lower energy than the triplet, so that no Kondo term arises. On the other hand, for $\Delta < 0$ we have $B_0, B_1 \ll B_2 \ll B_3$, where B_0 and B_1 parametrize the magnetic field. The susceptibility is now given by the $\xi \to -\infty$ asymptotics of the driving terms for $\sigma^{(0)}$ and $\sigma^{(1)}$. In this case the triplet has the lower energy so that there is a Kondo term and the RKKY-splitting contribution. With $\alpha = (3ec)^{1/3}\Gamma(4/3)$ we obtain

$$\chi_{\rm imp}^{(l)}/\chi_{\rm host}^{(l)} = [\delta_{l,2}e^{2\pi(B_l-\epsilon)/3V^2} - \alpha \int dt G_l(t)/(t - 2i/3)]/(3\alpha|\Delta|/D), \qquad (11)$$

where $l = 0$ refers to $\Delta > 0$ and $l = 2$ to $\Delta < 0$.

The homogeneous field susceptibility for the impurity normalized to $\chi_{\rm imp}(\Delta = 0) = 2/T_K$ is shown in Fig. 1(b). For $\Delta > 0$ the singlet state dominates and the susceptibility rapidly falls off with Δ. There is no van Vleck contribution, since the field does not couple the singlet and triplet states. The dependence on Δ is more exciting for $\Delta < 0$ (triplet has lower energy). For large $|\Delta|$ the spin triplet is spin compensated into a singlet via the Kondo effect. This is analogous to the two-channel Kondo problem, where the channels form composites of spin one which compensate an impurity of $S = 1$ into a singlet. In this limit $\chi_{\rm imp}^{(l)}(\Delta) = (\Delta/T_K)^{4/3}/T_K$, i.e., the effective Kondo temperature is renormalized by $(\Delta/T_K)^{4/3}$ (4/3 is the ratio of the degeneracy of the S and T states over that of the triplet). This effect was found previously in the context of orbital quenching by crystalline fields in the Coqblin-Schrieffer model [8,9]. The dependence of Eq. (11) on Δ is analytic.

The response to a staggered field is also of interest. A staggered field couples the $T0$ and S states. The staggered susceptibility is given by $\chi_{\rm stagg} = (n_S - n_T)/(\pi\Delta)$ and is shown in Fig. 1(b). The staggered susceptibility has a large peak for a small positive RKKY splitting Δ.

The low temperature specific heat is proportional to T with the γ coefficient given by [10]

$$\gamma_{\rm imp} = \frac{\pi}{6}\sum_{l=0}^{3}\frac{\sigma_{\rm imp}^{(l)}(B_l)}{\sigma_{\rm host}^{(l)}(B_l)}. \qquad (12)$$

If the valence fluctuations are suppressed the term for $l = 3$ does not contribute. In zero magnetic field the remaining terms can be written as

$$\gamma_{\rm imp}^{(l)} = \frac{\pi}{3}\frac{\chi_{\rm imp}^{(l)}}{\chi_{\rm host}^{(l)}} + \frac{\pi}{6}\frac{\sigma_{\rm imp}^{(l)}(B_l)}{\sigma_{\rm host}^{(l)}(B_l)}, \qquad (13)$$

where $l = 0$ for $\Delta > 0$ and $l = 2$ for $\Delta < 0$. The second term arises from the RKKY splitting (S to T fluctuations) and is given by the resonance (dashed curve) shown in Fig. 1(c). The γ coefficient normalized to its value for $\Delta = 0$ is given by the solid line; for large negative Δ, γ is determined by the susceptibility, while for large positive Δ the S to T fluctuations are dominating. The dash-dotted curve in Fig. 1(c) is the Wilson ratio, $WR = \chi_{\rm imp}/\gamma_{\rm imp}$, normalized to the $\Delta = 0$ value. Its Δ dependence evidences the nonuniversal nature of the interplay between RKKY and Kondo interactions.

In summary, we mapped a variant of the two-impurity model onto the SU(4) Anderson impurity with large U. There are no particle-hole symmetries from the start, so that the unstable fixed point with non-Fermi-liquid properties is bypassed. Instead, nonuniversal behavior as a function of Δ/T_K is obtained, as expected from a line of fixed points joining the two stable fixed end-points corresponding to $\Delta \to \pm\infty$. Our results reproduce all relevant limits correctly. The method can be extended to more complex systems, e.g., impurities with a Γ_8 ground state.

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