Exact Perturbative Solution of the Kondo Problem

P. Fendley and H. Saleur
Department of Physics, University of Southern California, Los Angeles, California 90089-0484
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We explicitly evaluate the infinite series of integrals that appear in the "Anderson-Yuval" reformulation of the anisotropic Kondo model in terms of a one-dimensional Coulomb gas. We do this by developing a general approach relating the anisotropic Kondo model of arbitrary spin with the boundary sine-Gordon model, which describes an impurity in a Luttinger liquid and tunneling in the fractional quantum Hall effect. The Kondo solution then follows from the exact perturbative solution of the latter model in terms of Jack polynomials.

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It was shown some 25 years ago that the partition function of the anisotropic Kondo model could be expressed as a power series in the impurity coupling [1,2]. Even though the coefficients were given only as formal multidimensional integrals, this led to progress in the understanding of the Kondo problem. For example, this enabled renormalization-group calculations to be done and the phase structure determined [3]. In subsequent years, various additional aspects of the problem were further understood by methods like the numerical renormalization group [4], expansions around the low-temperature fixed point [5], and by the Bethe ansatz [6,7]. Despite all this progress, the problem is still not completely solved. For example, the finite-temperature resistivity (which motivated Kondo's analysis [8]) has yet to be calculated exactly. Moreover, the coefficients of the perturbative expansion still could not be evaluated explicitly.

This latter aspect highlights a general puzzle of the Bethe ansatz approach. Its results are nonperturbative and can determine physical quantities to arbitrary accuracy by numerical solution of the nonlinear integral equations. However, no technique is known for solving them systematically around the noninteracting fixed point, so the small-coupling perturbative expansion cannot be found analytically (except when $T = 0$). One can find the coefficients only by fitting the full result numerically by a power series, and this gives accurate results only for the first few coefficients. Moreover, the thermodynamic Bethe ansatz equations are not continuous in the anisotropy parameter g (even though the results are) and are quite complicated for generic values of g. Therefore, knowing the perturbative expansion explicitly would be an easier way of doing calculations in many situations. In this paper, we solve this problem and "do" the Anderson-Yuval integrals at general g, by expressing them in terms of infinite sums of ratios of gamma functions [9], which can be easily evaluated numerically.

We derive a simple relation between the partition functions of the Kondo model and another one-dimensional quantum system, the boundary sine-Gordon (BSG) model. These two models are each of considerable interest, and it is remarkable that they are simply related. Treating them in the same framework requires the use of a quantum group, which is a topic of current mathematical interest. We show that the BSG model can be considered as a particular anisotropic Kondo model where the boundary spin is in a "cyclic" representation of the quantum group $SU(2)_q$. The perturbative coefficients of both of these partition functions can be expressed as the partition function of a one-dimensional classical "log-sine" gas with positive and negative charges which have logarithmic interactions. In the Kondo problem the charges must alternate in sign in space, while in the BSG model they may occur in any order. With unrestricted ordering, the partition function can be evaluated [9] by utilizing various properties of Jack polynomials [10]. Since the functional relation gives the appropriate Kondo coefficients simply in terms of the BSG ones, it therefore allows their determination as well.

We first review the BSG and Kondo perturbative expansions, and show how the BSG model can be expressed as a Kondo model. Utilizing some results of [11], we then derive the (nonperturbative) relation between these partition functions, which gives one set of perturbative coefficients in terms of the other. Both models have physical applications. The Kondo model is realized in various impurity compounds, and is also equivalent (in the anisotropic case) to the dissipative quantum mechanics of a particle in a double well [12]. The BSG model describes tunneling through an impurity in a Luttinger liquid (with application to fractional quantum Hall edges) [13,14], while in dissipative quantum mechanics it corresponds to an infinite number of wells [15].

The boundary sine-Gordon model describes a free boson $\phi(\sigma, t)$ on the half-line $\sigma \geq 0$ with an interaction at the boundary $\sigma = 0$. We study the problem at nonzero temperature T; in the path integral this corresponds to a system where Euclidean time (denoted by τ) is a circle of periodicity $1/T$. The bulk action is

$$S = -\frac{1}{4\pi g} \int_0^\infty d\sigma \int_0^{1/T} d\tau [(\partial_\tau \phi)^2 + (\partial_\sigma \phi)^2], \quad (1)$$

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while the boundary action is

$$S_B = 2\lambda \int_0^{1/T} d\tau \cos[\phi(\sigma = 0, \tau)]. \qquad (2)$$

The coupling λ is not scale invariant and interpolates between Neumann ($\lambda = 0$) and Dirichlet ($\lambda \to \infty$) boundary conditions on the boson.

Defining as usual the partition function via the path integral as $Z = \int[d\phi]e^{S+S_B}$ we introduce $Z \equiv Z(\lambda)/Z(\lambda = 0)$. We can rewrite this as a series by expanding out $\exp(S_B)$ in powers of λ. The coefficients of this series are then integrals of correlators in the free-boson theory. Using the bosonic propagator on the edge of a half-cylinder with Neumann boundary conditions,

$$\langle\phi(0,\tau)\phi(0,\tau')\rangle = -2g \ln \left| \frac{\kappa}{\pi T} \sin\pi T(\tau - \tau') \right|$$

(κ is the cutoff), one finds, for example,

$$\langle e^{i\phi(0,\tau)} e^{\pm i\phi(0,\tau')}\rangle = \left| \frac{\kappa}{\pi T} \sin\pi T(\tau - \tau') \right|^{\pm 2g}.$$

Using Wick's theorem one finds the general correlators as ratios of various $C(\tau, \tau') \equiv [2\sin\pi T(\tau - \tau')]^{2g}$. The partition function is the series

$$Z = \sum_{n=0}^{\infty} x^{2n} Z_{2n}, \qquad x \equiv \frac{\lambda}{T}\left(\frac{2\pi T}{\kappa}\right)^g, \qquad (3)$$

$$Z_{2n} = \frac{T^{2n}}{(n!)^2} \int_0^{1/T} \prod_i [d\tau_i d\tau_i'] \times \frac{\prod_{j<l}[C(\tau_j, \tau_l)C(\tau_j', \tau_l')]}{\prod_{i,k} C(\tau_i, \tau_k')}, \qquad (4)$$

where all indices run from 1 to $2n$, and all integrals run from 0 to $1/T$ independently. This expression requires regularization for $g \geq 1/2$, but is well defined otherwise. The sum (3) is the grand canonical partition function for a classical two-dimensional Coulomb gas of charged particles restricted to lie on a (one-dimensional) circle of circumference $1/T$. The charges are $\pm\sqrt{2g}$, and the whole gas is electrically neutral; x is the fugacity.

Series expressions were found for the Z_{2n} [9] by expanding the denominator of (4) in terms of Jack polynomials [10], and using orthogonality relations of these polynomials. Jack polynomials are indexed by a partition of an integer, so we define $\mathbf{m} \equiv (m_1, m_2, \ldots, m_{(\mathbf{m})})$, where the m_i are integers with $m_1 \geq m_2 \cdots \geq m_{(\mathbf{m})} \geq 0$. One finds [9]

$$Z_{2n} = \left(\frac{1}{\Gamma(g)}\right)^{2n} \sum_{\mathbf{m}} \prod_{i=1}^{n} \left\{\frac{\Gamma(g(n+1-i) + m_i)}{\Gamma(g(n-i) + 1 + m_i)}\right\}^2, \qquad (5)$$

where the sum is over all $\mathbf{m}$ with $l(\mathbf{m}) \leq n$. The sum converges only for $g < 1/2$, which is where the integrals in (4) are well defined.

For $n = 1$, the sum can be done (or the integral can be done without Jack functions) giving $Z_2 = \Gamma(1 - 2g)/\Gamma^2(1 - g)$. Notice that the divergence at $g = 1/2$ (the well-known "free-fermion point") is just a simple pole, so we can analytically continue around it to study behavior for $g > 1/2$. In fact, it turns out that at the free-fermion point only the first coefficient f_2 in the expansion of the free energy ($\sum f_{2n}x^{2n} \equiv -T \ln Z$) diverges, making it possible to analytically continue all the Z_{2n} to $g > 1/2$ [16]. It also turns out that there is a simple pole in f_{2n} at $g = 1 - 1/(2n)$ whose residue we can calculate. These poles are a signal that there are logarithmic terms in the perturbative expansion at $g = 1 - 1/(2n)$, which can in fact be computed exactly [16]. Thus at these values of g (including the free-fermion point, which corresponds to the Toulouse limit of the Kondo problem) the model is pathological in some respects.

The perturbative expansion for the Kondo problem found in [1,2] is closely related. The Kondo problem is a three-dimensional nonrelativistic problem, with free electrons antiferromagnetically coupled to a single fixed impurity. By looking at s waves only, we restrict to the radial coordinate and this becomes a one-dimensional quantum problem where massless fermions $\psi_i(\sigma, t)$ ($i = 1, 2$ are the spin indices) move on the half-line $\sigma \geq 0$ with a quantum-mechanical spin S_a at $\sigma = 0$. The interaction parameters are $I_z, I_+ = I_-$; in the isotropic case $I_z = I_+$. The impurity action is

$$S_B = \sum_{i,j,a} I_a \int_0^{1/T} d\tau\, \psi_i^\dagger(0, \tau) S_a \sigma_{ij}^a \psi_j(0, \tau), \qquad (6)$$

where the σ^a are the Pauli matrices. By a well-known bosonization procedure [2], this can be rewritten in terms of a free boson $\phi(x, t)$ with bulk action (1) and

$$S_B = I_+ \int_0^{1/T} d\tau (S_+ e^{i\phi(0,\tau)} + \text{H.c.}),$$

where I_z has been absorbed into the definition of g. The anisotropy is thus parametrized by g, with $g = 1$ the isotropic case and $g = 1/2$ the Toulouse limit.

In the perturbative expansion, we get correlators of $\exp(\pm i\phi)$ like before. The crucial difference arises from the $S_\pm$. When the impurity has spin 1/2, we have $S_+^2 = S_-^2 = 0$, and only terms of the form $S_+S_-S_+S_- \ldots$ survive in the perturbative expansion. In the one-dimensional gas, this is the requirement that charges alternate in sign. We define the partition function of the spin-1/2 Kondo problem as $Z_K = 2Z_K(I_+)/Z_K(0)$, where the factor of 2 ensures that the entropy is ln2 in the noninteracting limit $I_+ = 0$. Thus

$$Z_K(x_K) = 2 + \sum_{n=1}^{\infty} (x_K)^{2n} Q_{2n}, \qquad x_K \equiv \frac{I_+}{T}\left(\frac{2\pi T}{\kappa}\right)^g.$$

The Q_{2n} are the integrals in (4) times $2(n!)^2$, but where the region of integration is restricted to be $0 \leq \tau_1 \leq \tau_1' \leq \tau_2 \leq \cdots \tau_n' \leq 1/T$. The periodicity of the integrand means that $Z_2 = Q_2$, but the others are different.

Our central result relates the partition functions of the Kondo and BSG models. Defining $q = \exp(i\pi g)$, we find that

$$Z_K[(q - q^{-1})x]Z(x) = Z(qx) + Z(q^{-1}x). \quad (7)$$

One simple check is that the equation is consistent with the fact that $Z(x) = 1$ in the isotropic case $q = -1$. Plugging in the perturbative expansions gives the Kondo coefficients Q_{2n} in terms of the BSG coefficients Z_{2n}. For example,

$$4\sin^2(\pi g)Q_4 = -4\cos^2(\pi g)Z_4 + (Z_2)^2, \quad (8)$$

$$16\sin^6(\pi g)Q_6 = \sin^2(3\pi g)Z_6 + (Z_2)^3\sin^2(\pi g) - [\sin^2(2\pi g) + \sin^2(\pi g)]Z_2Z_4. \quad (9)$$

Using the series (5), we can easily find values for the Z_{2n} and hence the Q_{2n} for $g < 1/2$ by truncating the series and summing it numerically. For example, we have $Q_2 = Z_2 = \Gamma(1 - 2g)/[\Gamma(1 - g)]^2$. We give some numerically determined values for the higher coefficients in Table I.

As a check, some of the integrals were explicitly evaluated using Monte Carlo methods; the agreement is good. As discussed in [9], for g rational there are relations between the numbers beyond those in (7); for example, for $g = 1/4$, $Q_{2n} = Z_{2n}/2^{n-1}$. Knowledge of the first few coefficients Q_{2n} provides a very good numerical solution of the problem. The series can be extrapolated using Padé approximants and for instance the flow of the boundary entropy is reproduced fairly accurately [9].

The proof of (7) uses the "quantum-group" algebra $SU(2)_q$, which is a one-parameter deformation of the SU(2) algebra [17]. The three generators S_+, S_-, and S_z have commutation relations

$$q^{S_z}S_+q^{-S_z} = qS_+, \qquad q^{-S_z}S_-q^{S_z} = qS_-,$$

$$[S_+, S_-] = \frac{q^{2S_z} - q^{-2S_z}}{q - q^{-1}}.$$

Like SU(2), the quantum-group algebra has representations of any spin. A careful analysis shows that the general anisotropic Kondo problem of arbitrary spin is integrable only if the spins in (6) obey the $SU(2)_q$ algebra. For the isotropic problem $q = -1$, the distinction is irrelevant because $SU(2)_{-1}$ is identical to SU(2). The distinction is also irrelevant for any q for spin 1/2 or 1, because the two-dimensional representation of $SU(2)_q$ is given by the Pauli matrices as for SU(2), and the spin-1 representation is also the same up to a rescaling of S_+ and S_-. Other representations differ, however, so one must be careful when discussing the anisotropic Kondo problem at higher spin.

TABLE I. Numerical values for the perturbative coefficients Q_{2n} and Z_{2n} for $g = 2/5$, 1/3, and 1/4.

	Values of coefficients		
	$g = 2/5$	$g = 1/3$	$g = 1/4$
Z_4	1.910750624	0.837804224	0.4644013099
Z_6	1.088518710	0.276783311	0.0968299150
Z_8	0.439166887	0.061847648	0.0129159832
Z_{10}	0.135465650	0.010210054	0.0012208002
Q_4	0.982706435	0.432237451	0.2322006549
Q_6	0.291860092	0.074496009	0.0242074788
Q_8	0.061852434	0.008729195	0.0016144979
Q_{10}	0.010067801	0.000757798	0.0000763000

Following [11], we introduce the "quantum monodromy operator" $L_j(x)$, which is defined as

$$L_j(x) = \mathcal{T}\exp\left[I_+q^{-1}\int_0^{1/T}d\tau(e^{2i\phi_L(0,\tau)}q^{S_z}S_+ + e^{-2i\phi_L(0,\tau)}q^{-S_z}S_-)\right], \quad (10)$$

where the $SU(2)_q$ generators are in the spin-j representation and $\mathcal{T}$ indicates time ordering. The field ϕ_L is the left-moving component of ϕ; with Neumann boundary conditions we have $2\phi_L(0,\tau) = \phi(0,\tau)$. The "quantum transfer matrix" $T_j \equiv \mathrm{Tr}L_j$ is a fundamental part of the Kondo problem: $\langle T_j(x)\rangle$ is identical to the spin-j anisotropic Kondo perturbative expansion, e.g., $Z_K(x) = \langle T_{1/2}(x)\rangle$. This follows from expanding (10) in powers of x (the factors $q^{\pm S_z}$ cancel), and using the fact that the vacuum is an eigenstate of T_j.

As shown in [11], the L_j satisfy the Yang-Baxter equation. This results in a number of remarkable properties. In particular, one finds that all of the T_j can be generated from spin 1/2 via the relation [11]

$$T_j(q^{1/2}x)T_j(q^{-1/2}x) = 1 + T_{j-1/2}(x)T_{j+1/2}(x). \quad (12)$$

Using induction, it follows that

$$T_{1/2}(q^{j+1/2}x)T_j(x) = T_{j+1/2}(q^{1/2}x) + T_{j-1/2}(q^{-1/2}x).$$

This gives enough information to relate the two partition functions Z and Z_K (and do much more). When one expands $T_j(x)$ for higher j in powers of x, one obtains integrals with all sorts of charge orderings, with weights depending on q (because S_+ and S_- depend on q for representations other than spin 1/2, and because of the monodromy of the chiral fields). For example, $S_\pm^3 = 0$ for spin 1, so $+ + - - + -$ appears at order x^6 in T_1, but $+ + + - - -$ does not. Therefore, the unordered integrals Z_{2n} in (4) can be constructed by summing over appropriate combinations of terms from the $T_j(x)$. Since the relations (11) or (12) give all of the higher $T_j(x)$ in terms of $T_{1/2}$, this means that any Z_{2n} can in principle be expressed in terms of the Q_{2n}. The perturbative results (8) and (9) follow directly from (11).

The quickest way to derive (7) is to introduce cyclic representations of $SU(2)_q$. These occur when q is any root of unity $q^t = \pm 1$ and have no analog in ordinary SU(2). They are labeled by an arbitrary complex parameter δ and have t states $|m\rangle$, $m = 0, \ldots, t-1$ with generators acting as

$$S_\pm |m\rangle = \frac{q^{\delta \mp m} - q^{-\delta \pm m}}{q - q^{-1}} |m \pm 1\rangle, \qquad S_z|m\rangle = m|m\rangle,$$

where states $|m\rangle$ and $|m+t\rangle$ are identified. Notice that in this representation arbitrary powers of the generators do not vanish [18]. Referring to cyclic representations as spin δ, one finds that relation (12) holds with $j \to \delta$. In the formal limit where $\delta = -i\Delta$ with $\Delta \gg 1$ we have $S_\pm \approx e^{\pi g \Delta} q^{\mp m}/(q - q^{-1})$. In this limit the commutator $[S_+, S_-]$ becomes negligible, so the traces of all monomials with n generators S_+ and n generators S_- become identical, e.g.,

$$\mathrm{Tr}\,(S_+S_-)^n = t\left(\frac{q^{1/2}e^{\pi g \Delta}}{q - q^{-1}}\right)^{2n}.$$

Hence one way of expressing Z is

$$Z(x) = t^{-1}\left\langle T_{-i\Delta}\left[(q - q^{-1})q^{-1/2}e^{-\pi g \Delta}x\right]\right\rangle_{\Delta \gg 1}. \quad (13)$$

We substitute $j \to \delta = -i\Delta$ and $x \to (q - q^{-1})q^{-\delta - 1/2}x$ into (12). Letting $\Delta \gg 1$ proves (7) for q any root of unity (rational g). The result follows for any $|q| = 1$ (real g) by continuity. The renormalization of the Kondo coupling in (7) can be checked through the identity $Z_2 = Q_2$. This renormalization ensures that (7) makes sense in the isotropic limit $q \to -1$, where the Kondo partition function is a nontrivial object but $Z(x) = 1$.

Having obtained the fundamental relation (7), higher-spin Kondo partition functions follow from fusion, using the relations (11) or (12). For instance, one has

$$\begin{aligned}\langle T_1[(q - q^{-1})x]\rangle Z(q^{1/2}x)Z(q^{-1/2}x) \\ = Z(q^{3/2}x)Z(q^{1/2}x) + \text{H.c.} + Z(q^{3/2}x)Z(q^{-3/2}x).\end{aligned} \quad (14)$$

Other such relations give integrals of the form (4) with any charge ordering. Slightly more complicated ordered integrals arise in many places, and we hope our results can be extended. One possibility is in the Keldysh calculation of the non-zero-frequency noise in the BSG model [19]. Another is the quantity $P(t,T)$ in the double-well problem of dissipative quantum mechanics, which is the probability that a particle at temperature T is in one well at time t given that it is localized in that well when $t \le 0$ [12]. We have found the curious result that $P(iT, T) = T_1/2 - 1/2$, but its significance is not clear.

We have therefore succeeded in computing explicitly the Coulomb-gas integrals for the anisotropic Kondo problem. Our approach suggests a very deep structure, where the integral equations of the Bethe ansatz can be solved in terms of Jack symmetric functions and quantum-group combinatorics. For example, one can see how the quantum-group structure is responsible for the truncation of the thermodynamic Bethe ansatz equations at rational g [16]. We hope that further studies will uncover more features of these relations.

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