Kinks in the Kondo Problem

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(Received 3 May 1993)

We find the exact quasiparticle spectrum, elastic S matrix, and free energy for the continuum Kondo problem of k species of electrons coupled to an impurity of spin S. Here, the impurity becomes an immobile quasiparticle sitting on the boundary. The particles are "kinks," which can be thought of as field configurations interpolating between adjacent wells of a potential with $k+1$ degenerate minima. For the overscreened case $k>2S$, the impurity in the continuum is a kink as well, which explains the noninteger number of boundary states.

PACS numbers: 75.20.Hr, 11.20.Dj

It is possible to solve integrable models directly in the continuum, without recourse to a lattice Bethe ansatz. First, one finds the spectrum by using simple symmetry arguments extracted from conformal field theory, the underlying lattice model, exact solutions of related models, etc. The strict requirements of an integrable theory allow these guesses to be made precise, and exact quantities can then be derived. This continuum approach is more than just convenient: There are cases where it leads to results previously unsuspected. The classic example is the critical Ising model in a magnetic field, which is solvable only in the continuum [1].

The purpose of this paper is show how to apply these methods to the Kondo problem and other integrable models with impurities. The idea is simple: One starts with the quasiparticle description in the bulk, and then finds a variety of ways of coupling the impurity while keeping the model integrable. The only complication is in identifying what model has just been solved.

Here we find the exact quasiparticle spectrum in the general Kondo problem and see that these excitations are in fact kinks. This gives a simple qualitative picture and allows us to rederive the exact Bethe ansatz solution. A nice feature is that everything is always finite: There is no Fermi sea to fill because we study directly the excitations above the sea. Moreover, we give a simple explanation and derivation of the noninteger number of ground states on the boundary. Here it follows from the restrictions on placing kinks next to each other: With q one-particle states, there are not necessarily q^N N-particle states.

The general Kondo problem is a three-dimensional nonrelativistic problem, consisting of k species of massless free electrons antiferromagnetically coupled to a single fixed impurity of spin S by a term $\lambda\delta(x)\sum_{i=1}^{k}\mathbf{S}_j\psi_i^\dagger\sigma^j\psi_i$ in the Hamiltonian (fermion spin indices are suppressed). By looking at s waves, we restrict to the radial coordinate and this becomes a $(1+1)$-dimensional problem where fermions move on the half line with the impurity at the boundary. Through a variety of methods [2–4], it was found that there are two critical points. At $\lambda=0$, there is a (high-temperature or UV) unstable one where the impurity is decoupled. When this is perturbed, the model flows to a (low-temperature or IR) strongly coupled one where the electrons bond to the impurity and "screen" its spin. The Kondo temperature T_K is the scale at which the model crosses over from the region of one fixed point to the other. Numerous properties can be calculated exactly by using the Bethe ansatz [5–8] or by perturbed conformal field theory [9,10].

We must first understand the "bulk" properties of the model, which are independent of the impurity coupling. Since the Kondo problem is integrable, we can find the exact quasiparticles and their exact S matrix in the bulk. (This is obviously true since the Bethe ansatz solution exists. In cases when such a solution is not known, one can use perturbed conformal field theory to find the nontrivial conserved currents required for integrability [1].) The quasiparticles are the "physical" left- and right-moving excitations on the half line. They are massless (i.e., they have no gap, $p=\pm E$) because without the impurity there is no scale in the problem. Because left-right scattering is trivial here, we can work on the full line with only left movers: The particles with $x>0$ ($x<0$) are the original left (right) movers and the impurity is at the "boundary" $x=0$. We define the rapidity θ_i of a left mover by $E=-p\equiv\exp(-\theta_i)$. Since the bulk problem is scale invariant the two-particle S matrix can only depend on the ratio of the two momenta, so we write this as $S_{LL}(\theta)$, where $\theta\equiv\theta_1-\theta_2$. Because the model is integrable, the individual momenta of the particles do not change in a collision (complete elasticity) and the n-particle S matrix is the product of these two-body ones (factorizability) [11].

The crucial observation is that in this continuum quasiparticle description, the effect of the impurity is that of a single immobile particle sitting at $x=0$. We can derive the S matrix for a left mover to scatter off of this, because the integrability implies that this S-matrix element must satisfy the same constraints as S_{LL}. The only dimensionless quantity is the ratio of the particle's momentum to the Kondo temperature T_K; defining $T_K\equiv\exp(-\theta_K)$, the S matrix can thus be written as $S_{BL}(\theta)$ where here $\theta\equiv\theta_i-\theta_K$. To understand what the "boundary particle" actually is (i.e., what states it can have), we will look at the qualitative behavior at the IR fixed point,

0031-9007/93/71(15)/2485(4)$06.00

but the exact solution extends all the way up to the UV fixed point where the impurity decouples.

To find the quasiparticles in the bulk, we investigate the symmetries. Along with the spin symmetry [which in the $(1+1)$-dimensional reduction is an internal, not a space-time, symmetry], we have a "flavor" symmetry interchanging the k species of electrons, as well as a U(1) charge symmetry. These three symmetries can be decoupled into the current algebras [9,12]

$$\mathrm{SU}(2)_k \otimes \mathrm{SU}(k)_2 \otimes \mathrm{U}(1)\,, \tag{1}$$

where the subscript is the level of the affine Lie algebra. The technique of non-Abelian bosonization [13] means that a model with a G_k current algebra is equivalent to a sigma model where the fields take values in the group G and the Wess-Zumino-Witten (WZW) term is proportional to k. Thus our model in the bulk can be described by the sum of three sigma models, one for each term in (1).

Once the Kondo bulk piece is described in this manner, there is an important simplification: the impurity [an SU(2) spin] couples only to the $\mathrm{SU}(2)_k$ sigma model [9]. The other parts contribute only to bulk properties. Thus all we need is the quasiparticles of the $\mathrm{SU}(2)_k$ sigma model, and these are already known [14–16]. They are massless, and form doublets under the global SU(2) symmetry. However, there is additional structure: Each particle is also a kink. Kinks occur in models with multiple ground states. Classically, a kink K_{ab} in one space dimension is a field configuration which takes the value a at spatial negative infinity and b at positive infinity. In the quantum theory, this restricts multiparticle configurations to be of the form $K_{ab}K_{bc}K_{cd}\cdots$. In our case, the vacua a run from 1 to $k+1$, and allowed kinks interpolate between adjacent vacua. This is pictorially described for $k=3$ in Fig. 1. We label the left-moving particle doublets by $(u_{a,a\pm 1}, d_{a,a\pm 1})$. The SU(2) symmetry rotates $u \leftrightarrow d$ without changing the vacuum indices.

In the simplest case $k=1$, the only nontrivial structure is that of a (u,d) doublet; all the kinks do is go back and forth between the two wells. The $\mathrm{SU}(2)_1$ model is the continuum description of the spin $\frac{1}{2}$ XXX spin chain, so this statement is equivalent to saying that its spin waves have spin $\frac{1}{2}$ [5,17].

We can now find the "boundary particles." They follow from the qualitative behavior at the infrared fixed point, which depends crucially on the screening. In the underscreened case ($k<2S$), one electron from each species binds to the impurity, effectively reducing the impurity spin to $q \equiv S-(k/2)$. In this case, the boundary particle can be any member of a $(2q+1)$-dimensional SU(2) multiplet. For example, for $q=\frac{1}{2}$ the boundary is a (u,d) doublet under the SU(2), just like the bulk particles. In the exactly screened case ($k=2S$), the electrons completely screen the impurity. Thus the boundary should not transform under the SU(2) and so it is a single particle. In neither of these cases is there any reason to expect that the boundary has any kink structure.

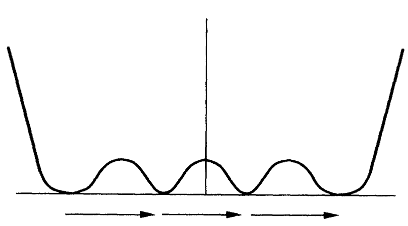

FIG. 1. The kink structure for $k=3$. Each arrow represents a (u,d) doublet.

The overscreened ($k>2S$) case is a little stranger. The impurity is still completely screened and does not transform under the SU(2), but there are now "leftover" electrons. Since there is the flavor symmetry among the electrons, the impurity must still couple to all of them. Therefore, if the boundary is to have nontrivial structure, it must be a kink. We have the nice qualitative picture that in the underscreened case, the impurity couples to the spin structure, while in the overscreened case it couples to the kinks. First look at when there is one leftover electron ($k=2S+1$). Here we expect that the boundary is a kink interpolating between adjacent vacua, just like the bulk particles. The boundary, however, is not a (u,d) doublet because spin has been screened out. In the general case with p leftover electrons ($k=2S+p$), we expect that the boundary is a "multiple" kink, which can interpolate farther than just adjacent vacua. To make this precise while keeping the model solvable, one uses a procedure called "fusion" [18]. This is the kink version of what we did for the underscreened case. There, to get a spin 1 boundary particle, we multiplied two spin $\frac{1}{2}$ representations and projected out the singlet. Here one defines the boundary "incidence" matrix I_p, whose rows and columns correspond to the vacua; $(I_p)_a^b=1$ if the vacua a and b are connected by a boundary kink and is 0 otherwise. The kinks in the bulk always have incidence matrix I_1, no matter what p is. The I_p follow from the analog of angular-momentum multiplication:

$$I_1 I_p = I_{p-1} + I_{p+1}\,, \tag{2}$$

where I_0 is the identity matrix. Thus for the $k=3$ case of Fig. 1,

$$I_1=\begin{pmatrix}0&1&0&0\\1&0&1&0\\0&1&0&1\\0&0&1&0\end{pmatrix},\quad I_2=\begin{pmatrix}0&0&1&0\\0&1&0&1\\1&0&1&0\\0&1&0&0\end{pmatrix}.$$

Thus for $k=3$ and $s=\frac{1}{2}$, the boundary spectrum consists of kink doublets 13, 31, 24, 42, 22, and 33.

Knowing the spectrum on the boundary provides a simple way to understand the ground-state degeneracy (i.e., the number of boundary states) at the critical points [7,8,10]. This number is not necessarily an integer when the volume of space is infinite. In the overscreened case it is not, a fact which the boundary kinks explain nicely. At the UV critical point, the impurity is decoupled from the bulk, so the degeneracy is simply the number of states of the impurity, which is $2S+1$. For the underscreened and exactly screened IR cases, the answer is equally simple: It is $2S-k+1$. The overscreened case presents an interesting problem: How many states is a boundary kink? The question is easy to answer. We represent the jth vacuum by the vector $v_j=(0,0,\ldots,0,1,0,\ldots)$ where the 1 is in the jth place. Multiplying this vector by the incidence matrix tells you what vacua are allowed to be adjacent to it. Thus the kth entry of the vector $I_pI_1^Nv_j$ is the number of N-kink configurations with vacuum j on one end and k on the other; the I_p takes care of the fact that the boundary can change the vacuum. The number of N-particle configurations with periodic boundary conditions and N large is simply $\lambda_p\lambda_1^N$, where λ_p is the largest eigenvalue of I_p. (Since the bulk particles are massless, in infinite volume there can be an arbitrary number of them even as the temperature goes to zero; thus generically N is large.) The contribution to the zero-temperature entropy coming from the boundary is thus just $\log\lambda_p$; it is easy to show using (2) that

$$\lambda_p=\frac{\sin[\pi(p+1)/(k+2)]}{\sin[\pi/(k+2)]}\,. \tag{3}$$

This number is the largest eigenvalue of the structure-constant matrix n^p_{ab} [10], a fact which follows from a deep result in conformal field theory [19,20]. The matrix n^p is related to the boundary states in any conformal field theory [20], which hints that kinks appear in any conformal field theory, with n^p taking the role of I_p; a similar program has been proposed in [21].

Knowing the particle spectrum, the S matrix is essentially fixed uniquely by the constraints of factorizability, unitarity, and crossing symmetry [11,15]. For $k=1$, the S matrix has already been derived from the Bethe ansatz [5,17]: The only massless two-particle S matrix for a doublet (u,d) consistent with factorizability and SU(2) symmetry is [11,15]

$$\begin{aligned}
&S(u(\theta_1)u(\theta_2)\to u(\theta_2)u(\theta_1))=Z(\theta)(\theta-i\pi)\,,\\
&S(u(\theta_1)d(\theta_2)\to d(\theta_2)u(\theta_1))=Z(\theta)\theta\,,\\
&S(u(\theta_1)d(\theta_2)\to u(\theta_2)d(\theta_1))=Z(\theta)i\pi\,,
\end{aligned} \tag{4}$$

with a symmetry under $u\leftrightarrow d$. Unitarity and crossing fix Z to be

$$Z(\theta)=\frac{1}{\theta-i\pi}\exp\frac{i}{2}\int_{-\infty}^{\infty}\frac{dt}{t}\sin t\theta\frac{e^{-\pi|t|/2}}{\cosh(t\pi/2)}\,. \tag{5}$$

For general k, the simplest possibility (and the correct answer) is that the scattering in the SU(2) (u,d) labels is independent of the kink labels:

$$S_{LL}=S_{u,d}\otimes S_{\rm kink}\,.$$

A two-kink configuration can be labeled by three vacua; a two-particle S-matrix element can be labeled by four because only the middle vacuum can change in a collision. The resulting massless kink S matrix [16,22] is the restricted solid on solid solution of [23],

$$\begin{aligned}
&\begin{array}{c|c} m\pm1 & m \\ \hline m & m\mp1\end{array}(\theta)=\tilde Z(\theta)\left(\frac{\beta_m}{\beta_{m+1}^{1/2}\beta_{m-1}^{1/2}}\right)^{i\theta/\pi}\sinh\gamma(i\pi-\theta)\,,\\
&\begin{array}{c|c} m & m\mp1 \\ \hline m\pm1 & m\end{array}(\theta)=\tilde Z(\theta)\left(\frac{\beta_{m+1}^{1/2}\beta_{m-1}^{1/2}}{\beta_m}\right)^{1+i\theta/\pi}-\sinh\gamma\theta\,,\\
&\begin{array}{c|c} m & m\pm1 \\ \hline m\pm1 & m\end{array}(\theta)=\tilde Z(\theta)\left(\frac{\beta_{m\pm1}}{\beta_m}\right)^{i\theta/\pi}\frac{\beta_1}{\beta_m}\sinh\gamma(im\pi\pm\theta)\,,
\end{aligned} \tag{6}$$

where $\beta_m=\sinh(im\gamma\pi)$ and $\gamma=1/(k+2)$. The horizontal line denotes a kink with rapidity θ_1 and the vertical with θ_2; m and $m\pm1$ denote the vacua they interpolate between. The first element, for example, describes the process

$$K_{m,m\mp1}(\theta_1)K_{m\mp1,m}(\theta_2)\to K_{m,m\pm1}(\theta_2)K_{m\pm1,m}(\theta_1)\,.$$

Remember that the allowed vacua run from 1 to $k+1$, and adjacent vacua must differ by ±1. Unitarity and crossing restrict $\tilde Z(\theta)$ to be

$$\tilde Z(\theta)=\frac{1}{\sinh\gamma(\theta-i\pi)}\exp\frac{i}{2}\int_{-\infty}^{\infty}\frac{dt}{t}\sin t\theta\frac{\sinh[(k+1)\pi t/2]}{\sinh[(k+2)\pi t/2]\cosh(t\pi/2)}\,. \tag{7}$$

This S matrix was effectively confirmed by calculating the correct bulk central charge [14].

The boundary S matrix $S_{BL}(\theta)$ follows from the same constraints of integrability. For the overscreened case $p=1$, the boundary kink structure is the same as the bulk, so $S_{BL}=S_{\rm kink}$ as defined in (6). The fusion procedure then gives the S matrix for arbitrary p up to an overall prefactor [18]. For $p=2$,

$$\begin{array}{c|c} b & c \\ \hline a & d\end{array}(\theta)\propto\sum_f\begin{array}{c|c} b & g \\ \hline a & f\end{array}\left(\theta-\frac{i\pi}{2}\right)\begin{array}{c|c} g & c \\ \hline f & d\end{array}\left(\theta+\frac{i\pi}{2}\right)\,, \tag{8}$$

where the thick line denotes the boundary kink, and the S-matrix elements on the right are those given in (6). The construction ensures that the result is independent of the choice of g. One builds up the elements for arbitrary p by products of the form

$$\prod_{n=0}^{p-1}S\left(\theta+\frac{i\pi}{2}(2n+1-p)\right)\,.$$

The prefactor $Z^{(p)}(\theta)$ is

$$Z^{(p)}\equiv\begin{array}{c|c} m+p+1 & m+1 \\ \hline m+p & m\end{array}=\exp\frac{i}{2}\int_{-\infty}^{\infty}\frac{dt}{t}\sin t\theta\frac{\sinh[(k+2-p)\pi t/2]}{\sinh[(k+2)\pi t/2]\cosh(t\pi/2)}\,, \tag{9}$$

where we suppressed the β_m.

The underscreened case proceeds in the same manner. When $k=2S-1$, the boundary particle is an SU(2) doublet like the bulk ones, so $S_{BL}=S_{u,d}$ as defined in (4). For general underscreening with $q \equiv S-k/2$, we use the spin analog of (8). The analog of (9) is that the S-matrix element for scattering a u bulk particle with the highest member ($S_z=q$) of the boundary multiplet is given by $Z^{(2q)}(\theta)$ from (9) with $k \rightarrow \infty$.

For the exactly screened case, the answer is not as obvious because the boundary particle is neither a kink nor does it have any SU(2) structure. The simplest nontrivial solution of the consistency requirements is

$$S_{BL}=\tanh(\theta/2-i\pi/4)\,. \tag{10}$$

This result also has some simple analogs. Because of the lack of structure of the boundary in the IR the irrelevant operator by which one perturbs is simply the left-moving energy-momentum tensor T_L [9]. In the similar flows from the tricritical Ising model to the Ising model [24] and from the $SU(2)_1$ principal chiral model into the WZW model [15], the irrelevant perturbing operator is $T_L T_R$. Both of these cases have a LR S matrix of (10), so it is not surprising this is true here as well.

With the exact S matrices, we can calculate the exact free energy by finding the allowed momenta for the particles on a circle of circumference l, and then using this constraint to minimize and hence derive the free energy [24]. This is similar to ordinary Bethe ansatz thermodynamics [25], but here we work with the "physical" quasiparticles instead of the "bare" electrons previously used [7,8]. In this approach there are no infinities. We quantize a momentum p_i by demanding periodicity of the wave function when the particle is "brought around the world":

$$e^{ip_i l}\Lambda(\theta_i|\theta_K;\theta_1,\theta_2,\ldots,\theta_N)=1\,, \tag{11}$$

where Λ is the eigenvalue for scattering one particle through an ensemble of all the others and the impurity. When the S matrix is diagonal, $\Lambda=\prod_j S(\theta_i-\theta_j)$; in our nondiagonal case one must use some of the formal tools of the Bethe ansatz to find it. For both parts of our tensor-product S matrix this has already been done [15,16,24]; we only need to add the effect of the boundary particle. We find, of course, the same result as in the bare calculation displayed in [7,8].

It is reasonable to expect that some of the many generalizations of the Kondo problem (e.g., the two-impurity Kondo problem and defects in spin chains) can be exactly solved by these methods, even if such problems are not solvable in their bare versions. Determining the spectrum is generally the most difficult part of such a calculation, but the methods described in this paper provide the simplest application of such a program. In particular, it is clear that finding the ground-state degeneracy from conformal field theory provides an important clue to this structure. We have seen that kinks appear in the Kondo problem; it would not be surprising for them to appear in many other impurity problems.

I would like to thank Mark Goulian, Ken Intriligator, and Hubert Saleur for useful conversations. This work was supported in part by DOE Grant No. DEAC02-89ER-40509.

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