Exact Critical Theory of the Two-Impurity Kondo Model

Ian Affleck[1],[2] and Andreas W. W. Ludwig[2],[3]

[1]*Canadian Institute for Advanced Research, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1*

[2]*Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z1*

[3]*Physics Department, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6*

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The two-impurity Kondo Hamiltonian is known to possess a multicritical point separating stable Fermi-liquid phases in which the two impurities either form a singlet or else are screened by the conduction electrons. We propose an exact critical theory for this non-Fermi-liquid multicritical point, using conformal field theory methods, which predicts all critical properties including the finite-size spectrum, specific heat, susceptibilities, renormalization-group behavior, residual entropy, scattering matrix, and local pair Green's function.

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The two-impurity Kondo problem has been studied as a step towards the Kondo lattice [1–5]. It exhibits two competing effects: a tendency for the two impurities to form a singlet when the interimpurity coupling K is large and antiferromagnetic, and a tendency for the conduction electrons to screen the impurities when K is large and ferromagnetic. In general, there need not be a phase transition between these two limiting situations. However, if particle-hole symmetry is maintained then a phase transition *must* occur, since the conduction electrons exhibit no phase shift in the interimpurity singlet phase and a $\pi/2$ phase shift in the Kondo-screened phase, and since the phase shift can only be 0 or $\pi/2$ by time-reversal and particle-hole symmetry [3]. Numerical renormalization-group methods have indicated [1] that the multicritical point separating these two phases is not of the Fermi-liquid type; in particular, the impurity specific heat vanishes less rapidly than linearly as the temperature $T \to 0$.

We have recently developed the powerful methods of conformal field theory to treat the single-impurity multichannel Kondo effect [6–10]. In this paper we demonstrate that essentially the same methods can be extended to treat the two-impurity Kondo problem. In fact, the methods are extremely general and should be applicable to essentially *any* problem involving local quantum-mechanical degrees of freedom interacting with a gapless continuum. Our approach is based on two lines of attack.

First of all, we use the techniques of two-dimensional boundary critical phenomena, developed primarily by Cardy [11]. At long wavelengths, the problem is equivalent to a $(1+1)$-dimensional field theory with both impurity degrees of freedom at the origin. Under renormalization we expect the impurity degrees of freedom to be absorbed by the continuum degrees of freedom leaving behind only an effective modified boundary condition. The boundary is the line $x=0$ in a two-dimensional space and (imaginary) time picture. At long wavelengths we expect this boundary condition to be conformally invariant. The existence of such a large symmetry group allows for a classification of conformally invariant fixed points and exact calculation of their critical properties.

Our second line of attack involves the separation of spin and charge degrees of freedom in a one-dimensional Fermi gas. More generally, when there are several channels of conduction electrons (even and odd parity for the two-impurity Kondo problem) there are several different ways of partitioning the degrees of freedom. These are known as conformal embeddings. Each conformal embedding corresponds to an equivalence between the Fermi gas (in the continuum limit) and a direct sum of commuting Hamiltonians for various Bose fields, each representing certain degrees of freedom of the electrons. Although the Hamiltonians are decoupled, certain selection rules (or "gluing conditions") govern the precise way that the various components are combined. In particular, the finite-size spectrum is obtained by taking a direct product of conformal towers from each sector with the gluing conditions determining which combinations of towers occur. Likewise, all operators are written as products of operators from the various sectors with the permissible products determined by the gluing conditions.

Bulk properties (such as the specific heat per unit length) are independent of the gluing conditions, which are determined by the boundary conditions. In fact, the various conformally invariant boundary conditions correspond exactly to the set of consistent gluing conditions. We find that absorption of the impurity degrees of freedom induces a particular modification of the gluing conditions. Depending on the resulting conditions the corresponding fixed point may or may not correspond to a local Fermi liquid. Generally, the existence of nontrivial conformal embeddings means that non-Fermi-liquid behavior is possible. Only very special gluing conditions "confine" the various degrees of freedom so as to reproduce trivial, Fermi-liquid behavior. In the single-impurity Kondo effect we found that the Kondo interaction only involved the electron-spin degrees of freedom. The modification of the gluing conditions was given by "fusion" of the spin degrees of freedom of the conduction electrons with the impurity. This is a particular mapping of each spin conformal tower into a set of other spin conformal towers governed by conformal field theory fusion rules. In the two-impurity case the Kondo interaction *cannot* be written in terms of electron-spin operators only

[6]. We find that the modification of the gluing conditions involves a rather different fusion process in this case which implies an analogy with boundary critical phenomena in the two-dimensional Ising model.

The two-impurity Kondo interaction only involves electron operators ψ at the two impurity sites $\pm\mathbf{R}/2$. Assuming a rotationally invariant electron dispersion relation, it is convenient to perform averages over directions $\hat{\Omega}$ in k space: $\psi_{\pm,k}\equiv\int d^2\hat{\Omega}\,\psi_{k\hat{\Omega}}\exp(\mp ik\hat{\Omega}\cdot\mathbf{R}/2)$. We may define [1] normalized anticommuting linear combinations of these operators: $\psi_{e,k}\equiv[\psi_{+,k}+\psi_{-,k}]/N_e^{1/2}(k)$, $\psi_{o,k}\equiv[\psi_{+,k}-\psi_{-,k}]/N_o^{1/2}(k)$, with $N_{e,o}(k)=2\pi[1\pm(\sin kR)/kR]/k$. $\psi_{e,o}$ can be extended to form a complete orthonormal basis of eigenoperators of the kinetic energy. We may simply drop all operators but ψ_e and ψ_o from the Hamiltonian since the others do not participate in the interaction. This leaves an effective one-dimensional problem with two independent channels (e and o) of electrons. These are left movers on the entire real axis or, equivalently, left *and* right movers on the positive axis (see Ref. [8], Appendix A). The Kondo couplings in this one-dimensional problem are wave-vector dependent but we may simply evaluate them at the Fermi surface, up to irrelevant operators. Hence the two impurities effectively sit at the origin which makes the problem not fundamentally different than the one-impurity case. The only difference is that the impurity is two spins instead of one. We actually find it more convenient to work with the linear combinations $\psi_{1,2}\equiv(\psi_e\pm\psi_o)/\sqrt{2}$. The Kondo interaction may be written in terms of electron operators at the origin, $\psi_{i,\alpha}$, where α labels spin components and i labels the two linear combinations defined above:

$$H_{\text{Kondo}}=J_+[\psi_1^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_1+\psi_2^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_2]\cdot[\mathbf{S}_1+\mathbf{S}_2]+J_m[\psi_1^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_1-\psi_2^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_2]\cdot[\mathbf{S}_1-\mathbf{S}_2]$$
$$+J_-[\psi_1^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_2+\psi_2^\dagger\tfrac{1}{2}\boldsymbol{\sigma}\psi_1]\cdot[\mathbf{S}_1+\mathbf{S}_2]\,.$$

Here $\boldsymbol{\sigma}$ refers to the Pauli matrices and we use an implied summation over spin indices. $J_\pm\equiv(J_e\pm J_o)/2$, where $J_{e,o}$ are the Kondo couplings for even and odd channels defined in Ref. [1]; J_m, as defined in Ref. [1], mixes even and odd channels. We also include an impurity self-coupling, $H_{\text{self}}=K\mathbf{S}_1\cdot\mathbf{S}_2$.

It is quite easy to see that there are stable Fermi-liquid fixed points for large $|K|$ of either sign [1]. In these limits there is a large gap between the triplet and singlet sectors of the two impurities so we may "integrate out" one or the other. This leaves either no interaction for antiferromagnetic K or a single-impurity two-channel $s=1$ Kondo problem for ferromagnetic K. This problem is known to have a stable Fermi-liquid fixed point where the impurity is completely screened by the two channels. The process of integrating out the other impurity spin state produces only irrelevant operators [1]. The two Fermi-liquid fixed points are essentially the same except that the ferromagnetic one has a $\pi/2$ phase shift. Adopting the same linear dispersion relation for even and odd channels with a symmetric band cutoff, the problem has particle-hole symmetry (as well as time reversal). It then follows that the phase shift can only be 0 or $\pi/2$ [3]. Thus there must be some sort of phase transition between the two stable fixed points. Assuming that it is second order, the intermediate unstable critical point cannot be characterized by a simple phase shift; i.e., it must not be a local Fermi liquid.

It turns out to be useful to first consider the case $J_-=0$ because then the model has a higher symmetry; we will see below that J_- is irrelevant. (This was realized independently by Jones [5].) In this limit the Hamiltonian has, in addition to ordinary spin, two commuting "isospin" symmetries $\mathbf{I}_1$ and $\mathbf{I}_2$: $I_i^z=\frac{1}{2}\sum_k[\psi_{i,k}^\dagger\psi_{i,k}-1]$ and $I_i^-=\sum_k\psi_{i,\uparrow k}\psi_{i,\downarrow -k}$. ($k$ is measured from the Fermi level.) A nonzero J_- breaks this down to the diagonal SU(2) subgroup, $\mathbf{I}_1+\mathbf{I}_2\equiv\mathbf{I}$.

To study this critical point we adopt a convenient conformal embedding that makes explicit all three SU(2) symmetries. Essentially we introduce three independent bosonic fields $g_\alpha,(h_i)_A$ for ordinary spin and the two isospins. α is an ordinary spin index and A is an isospin index. i labels the two different isospins. These fields can be thought of as being the left-moving parts of SU(2) Wess-Zumino-Witten fields [12]. The Kac-Moody central charges are determined by the free-fermion current algebras to be $k=2$ for spin and $k=1$ for isospin. It turns out that these fields alone are not equivalent to the four species of free fermions (two spins, even and odd). We must also include an Ising-model sector [13]. The Virasoro central charges then add up correctly to four: $c=\frac{3}{2}+1+1+\frac{1}{2}$. The conformal embedding corresponds to "bosonization formulas" of the form $\psi_{i,\alpha}=g_\alpha(h_i)_1\sigma$, $\psi_i^{\alpha\dagger}=g^{\alpha\dagger}(h_i)^{1\dagger}\sigma$. Here σ is the Ising order parameter, $g^{1\dagger}\equiv g_2$, $g^{2\dagger}\equiv -g_1$, $(h_i)^{1\dagger}=(h_i)_2$, $(h_i)^{2\dagger}=-(h_i)_1$. For the SU(2) sectors the conformal towers are labeled by isospin and spin quantum numbers I_i,j. For the Ising sector the three conformal towers are $\mathbf{1}$ (identity), σ (order parameter), and ϵ (energy operator). The free-fermion gluing conditions give the combinations of conformal towers (I_1,I_2,j,Ising): (0,0,0,1) (ground state); $(\frac{1}{2},0,\frac{1}{2},\sigma)$ and $(0,\frac{1}{2},\frac{1}{2},\sigma)$ (single particle or hole); (0,0,1,ϵ), $(\frac{1}{2},\frac{1}{2},1,\mathbf{1})$, and $(\frac{1}{2},\frac{1}{2},0,\epsilon)$ (two particles, two holes, or particle-hole). Parity, which switches ψ_1 and ψ_2, interchanges the two SU(2)'s. A consistent embedding also requires that we associate an intrinsic parity of -1 with the $j=1$ conformal tower and $+1$ with all other spin and Ising towers.

The Kondo interactions (for $J_-=0$) take the form

$J_+\mathbf{J}\cdot[\mathbf{S}_1+\mathbf{S}_2]+J_m\phi\epsilon\cdot[\mathbf{S}_1-\mathbf{S}_2]$. (Here $\mathbf{J}$ is the spin current operator and ϕ is the $j=1$ primary field.) It is far from obvious what the gluing conditions are at the multicritical point. However, we found a simple hypothesis which gives excellent agreement with numerical renormalization-group (NRG) results and physically reasonable conclusions. The modified gluing conditions are obtained by fusion in the Ising sector with the order parameter σ. The Ising fusion rules give $\sigma\cdot 1\sim\sigma$, $\sigma\cdot\sigma\sim 1+\epsilon$, and $\sigma\cdot\epsilon\sim\sigma$. It should be emphasized that this fusion hypothesis gives a fully consistent boundary theory. With this very simple hypothesis all critical properties of the multicritical point can now be calculated exactly, using established methods.

The finite-size spectrum implied by the above fusion is given by the conformal towers in Table I. To compare with the NRG results of Ref. [4], primary states have been resolved (in the first column) into multiplets of diagonal isospin (I) using ordinary angular momentum addition rules and the total parity deduced by multiplying the intrinsic parity (shown in the sixth column) by the symmetry of the wave function under the interchange of $\mathbf{I}_1$ and $\mathbf{I}_2$. Agreement with Fig. 3 in Ref. [4] is excellent. Good agreement is also obtained with a much more extensive set of energy levels calculated by Jones [5]. The same spectrum is also obtained if we begin with a degenerate ground state, i.e., start with a $\pi/2$ phase shift in the zero coupling limit. This means that the multicritical point is, in some sense, symmetric with respect to interchanging the two equivalent stable (ferromagnetic or antiferromagnetic) Fermi-liquid fixed points. [The three SU(2) factors in the conformal embedding are equivalent to an SO(7), $k=1$ model. This SO(7) symmetry of the free theory is preserved by the Ising fusion and hence appears at the multicritical point.]

The operator content is obtained by applying fusion twice (see Ref. [8]), i.e., $\sigma\rightarrow\sigma$; $1,\epsilon\rightarrow 1+\epsilon$. In particular, there are now two operators with dimension less than 1: $(0,0,0,\epsilon)=\epsilon$ and $(\frac{1}{2},\frac{1}{2},0,1)=(h_1)_A(h_2)_B$, both of dimension $\frac{1}{2}$. The second operator is forbidden in the Hamiltonian by the isospin symmetry but the first is not. Thus ϵ is the relevant operator which destabilizes the multicritical point; i.e., if we move the impurity self-coupling K slightly away from its critical value K_c, we produce a term in the fixed-point Hamiltonian proportional to $(K-K_c)\epsilon$. This is precisely what happens in a pure Ising system when a magnetic field is applied to a free boundary. The two stable Fermi-liquid fixed points correspond to the spin-up and spin-down boundary conditions in the Ising model. A standard scaling argument then determines the divergence of the impurity specific-heat coefficient $\gamma\equiv\lim_{T\rightarrow 0}C(T)/T\propto(K-K_c)^{-2}$, in perfect agreement with the NRG result [4]. The behavior of $C(T)$ right at the multicritical point is determined by the leading irrelevant operator, the first descendent $L_{-1}\epsilon$ of dimension $\frac{3}{2}$. This has the same dimension as the leading irrelevant operator in the two-channel $s=\frac{1}{2}$ one-impurity Kondo problem and the same reasoning [8] leads to $C(T)\propto(T/T_K)\ln(T_K/T)$, where T_K is the Kondo temperature.

The impurity susceptibility (induced by a uniform field) is nonsingular at the multicritical point, in agreement with the NRG result. This is different than in the two-channel, $s=\frac{1}{2}$ one-impurity case [8]. The crucial difference is that the dimension-$\frac{3}{2}$ irrelevant operator $\mathbf{J}_{-1}\cdot\phi$, where ϕ is the (0,0,1,1) primary field, occurs in the Hamiltonian in that case but not in this one since it is odd under parity. This operator is necessary to obtain a singular susceptibility [8]. By contrast, the staggered susceptibility χ^s, i.e., the zero-frequency response to a field coupling to $S_1^z-S_2^z$, *is* singular since this field breaks parity and hence can couple to ϕ^z, of dimension $\frac{1}{2}$. This leads to a logarithmic divergence of the staggered susceptibility, with T, at the multicritical point. The weakness of this divergence (i.e., logarithmic) may account for the nonsingular behavior observed in quantum Monte Carlo studies [2].

We now consider the effect of other, symmetry-breaking interactions. Apart from ϵ, the only other two relevant charge-conserving rotationally invariant operators at the multicritical point are $(h_1)^{A\dagger}(h_2)_A$ and $(h_1)^{A\dagger}(\tau^3)^B_A(h_2)_B$, where τ^3 is the Pauli matrix in isospin space. Both of these operators break isospin down to diagonal subgroups, $\mathbf{I}$ in the first case and I^3 in the second. The first operator is odd under parity and even under particle-hole conjugation while the second operator is the reverse. [The usual particle-hole transformation, $\psi_{i,\alpha}\rightarrow\epsilon_{\alpha\beta}\psi_i^{\beta\dagger}$, where $\epsilon_{\alpha\beta}$ is the antisymmetric tensor, interchanges $(h_i)_1$ and $(h_i)^{1\dagger}$.] Considering only parity-invariant interactions, we see that they will only be relevant if they break isospin down to I^3 *and* are odd under particle-hole conjugation. A nonzero Kondo interaction, J_-, fails on both counts and so is irrelevant. Since there is only one relevant operator we generally expect to pass through the multicritical point by varying a single

TABLE I. Conformal towers giving the spectrum at the multicritical point. All states with $lE/v_F\pi<1$ are contained in the table (i.e., are primaries). In the first column, I is the total isospin and P the total parity of the primary states.

I^P	I_1	I_2	j	Ising	Intrinsic parity	$\frac{lE}{v_F\pi}$
0^+	0	0	0	σ	+	0
$(\frac{1}{2})^\pm$	$\frac{1}{2}$	0	$\frac{1}{2}$	1	+	$\frac{3}{8}$
	0	$\frac{1}{2}$	$\frac{1}{2}$	1	+	$\frac{3}{8}$
0^-	0	0	1	σ	−	$\frac{1}{2}$
$0^-,1^+$	$\frac{1}{2}$	$\frac{1}{2}$	0	σ	+	$\frac{1}{2}$
$(\frac{1}{2})^\pm$	$\frac{1}{2}$	0	$\frac{1}{2}$	ϵ	+	$\frac{7}{8}$
	0	$\frac{1}{2}$	$\frac{1}{2}$	ϵ	+	$\frac{7}{8}$
$0^+,1^-$	$\frac{1}{2}$	$\frac{1}{2}$	1	σ	−	1

coupling constant (i.e., J_+, J_-, J_m, or K). Next we consider the effect of potential scattering, which breaks particle-hole symmetry. Equal potential scattering in even and odd channels corresponds to the operator $\psi_1^{a\dagger}\psi_{a,1}+\psi_2^{a\dagger}\psi_{a,2}\propto I^3$. This breaks isospin down to a $U(1)\times U(1)$ subgroup I_1^3, I_2^3, and hence does not produce any relevant operators when $J_-=0$. The current operators themselves are expected to produce a critical line joining smoothly with the multicritical point. The additional symmetry that must be broken corresponds to interchanging ψ_e and ψ_o. This can be achieved either with a nonzero J_- or else with unequal potential scattering for even and odd channels. Hence even-odd symmetric potential scattering is relevant iff $J_e\neq J_o$, a conclusion also found from the numerical renormalization group [5]. In the case where even-odd and particle-hole symmetry are both broken, and the relevant operator $(h_1)^{A\dagger}(\tau^3)^B_A(h_2)_B$ is generated, we expect the system to cross over to Fermi-liquid behavior. Since the relevant operator has dimension $\frac{1}{2}$, the specific-heat coefficient γ diverges as V^{-2}, where V is the strength of the potential scattering, for $J_e\neq J_0$, or as $(V_e-V_o)^{-2}$ if $J_e=J_o$. (V_e and V_o are the scattering potentials in the even and odd channels.)

The residual entropy is another universal feature of boundary fixed points [9]. It equals zero at the Fermi-liquid fixed points but has a value $\ln g$ at the multicritical point determined by the Ising-model modular S matrix: $g=S^1_\sigma/S^1_1=\sqrt{2}$. Another property of interest is the scattering matrix projected onto the one-electron subspace, $S_{(1)}$, which is determined by the one-particle Green's function. This has the values $+1$ and -1 at the antiferromagnetic and ferromagnetic Fermi-liquid fixed points, respectively, corresponding to phase shifts of 0 and $\pi/2$. At a non-Fermi-liquid fixed point it generally has a value of magnitude less than 1 [10], corresponding to inelastic scattering in the electron basis at zero energy (i.e., energy-conserving processes in which one electron goes into several electrons and holes). In this case the scattering matrix can be expressed in terms of the Ising modular S matrix [10] as $S_{(1)}=(S^\sigma_\sigma/S^\sigma_1)/(S^1_\sigma/S^1_1)=0$; i.e., the scattering is *purely inelastic* in the electron basis at zero energy. The same result was found for the two-channel $s=\frac{1}{2}$ single-impurity Kondo problem. In both cases it seems to be connected with the fact that the non-Fermi-liquid fixed point is symmetric with respect to two Fermi-liquid fixed points at which $S_{(1)}=\pm 1$.

We can also calculate exact space- and time-dependent Green's functions in the critical region. We find, for example, that the singlet electron pair operator, $\psi_{1,\alpha}\psi_{2,\beta}\epsilon^{\alpha\beta}+\psi_{2,\alpha}\psi_{1,\beta}\epsilon^{\alpha\beta}$, exhibits a logarithmically divergent local susceptibility near the impurities, as in the two-channel single-impurity case [10].

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[13] The free theory has two SU(2) spin symmetries, with currents $\mathbf{J}_1,\mathbf{J}_2$, as well as two SU(2) isospin symmetries, one for each species, ψ_1 and ψ_2. There is a well-known bosonization [see, for example, I. Affleck, A. W. W. Ludwig, H.-B. Pang, and D. L. Cox, Phys. Rev. B (to be published)] respecting all of this symmetry, in terms of these four sets of SU(2) currents, each of Kac-Moody central charge $k=1$. The interactions break the spin symmetry down to the diagonal SU(2) subgroup; the corresponding spin currents, $\mathbf{J}=\mathbf{J}_1+\mathbf{J}_2$, have Kac-Moody algebra central charge $k=2$. The well-known Goddard-Kent-Olive construction [P. Goddard, A. Kent, and D. Olive, Commun. Math. Phys. **103**, 105 (1986)] proves the equivalence of the sum of the two $k=1$ (spin) Hamiltonians with a single $k=2$ Hamiltonian together with an Ising Hamiltonian.