Exact, Asymptotic, Three-Dimensional, Space- and Time-Dependent, Green's Functions in the Multichannel Kondo Effect

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Exact 3D *space- and time*-dependent Green's functions are computed for the k-channel Kondo effect in the universal large-distance, long-time regime, using conformal field theory. They exhibit crossover from Fermi-liquid form far away, to singular non-Fermi-liquid behavior near the impurity, where charge, spin, and "flavor" degrees of freedom become "deconfined." Explicit expressions are given for the resistivity, ρ, for all k and for the spin-density and pair-density Green's functions, for $k=2$. For $k=2$, $\rho(T)-\rho(0)\propto T^{1/2}$ and the pair susceptibility $\propto \ln T$.

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Consideration of the orbital structure of an impurity atom coupled to a (3D) electron gas led Nozières and Blandin [1] to study the multichannel Kondo problem. An infrared fixed point governs the low-temperature properties. When the number k of degenerate channels of electrons is not larger than $2s$, where s is the size of the quantum-mechanical impurity spin, this fixed point is a Fermi liquid. However, in the opposite case, $k>2s$, an interesting non-Fermi-liquid fixed point occurs. The two-channel case ($k=2$, $s=\frac{1}{2}$) has attracted particular attention recently in the form of the *quadrupolar Kondo effect* [2]. The latter was argued to account, under certain assumptions made in Ref. [2], for *marginal Fermi liquid* and *unusual superconductivity* properties of uranium-based heavy fermion systems and cuprate high-T_c superconductors. (Very recent experiments [3] seem to support this picture for the *dilute* compound $U_xY_{1-x}Pd_3$, but see below.)

Values for some thermodynamic exponents of the non-Fermi-liquid Kondo fixed points have been calculated using the Bethe ansatz [4]. Green's functions are not directly accessible by Bethe ansatz methods.

Recently [5,6], a complete, analytic solution of the low-temperature fixed points has been given, in terms of boundary critical phenomena of conformal field theory [7] (CFT) for all values of k and s. The exact non-Fermi-liquid exponents agree precisely with the Bethe ansatz values. New exact results, not known previously from Bethe ansatz studies, have been obtained in Refs. [5,6,8], such as, e.g., stability and new universal Wilson ratios for the non-Fermi liquids as well as their exact asymptotic finite-size excitation spectra. All results agree excellently with numerical values, whenever the latter are available [5,8,9].

In this Letter we show how to calculate the exact 3D, *time- and space*-dependent Green's functions at large length and time scales in the Kondo problem. It turns out that they are determined by the universal spectrum of excitations of the strongly coupled system. Explicit expressions will be given for the two-channel case ($k=2$, $s=\frac{1}{2}$). (For details and the explicit results obtained for arbitrary number k of channels and impurity spin s see the longer version in Ref. [10].) Interestingly, as our results show, only the p-wave pairing susceptibility diverges logarithmically as $T\to 0$ in the two-channel ($s=\frac{1}{2}$) case; however, for anisotropic Kondo coupling also the ($s^z=0$ component of the) s-wave pair susceptibility diverges. Possibly, this may provide a new mechanism for unusual superconductivity (Ref. [2]).

In the single-channel Kondo effect, all Green's functions exhibit Fermi-liquid behavior in the asymptotic regime; i.e., at length scales long compared to v_F/T_K and times long compared to $1/T_K$. The only effect of the impurity in this limit is the $\pi/2$ phase shift. However, in the multichannel Kondo effect, in the overscreened case, $k>2s$, the critical behavior is more interesting. Green's functions again exhibit universal behavior in the asymptotic regime of long lengths and times; however, it is *not* Fermi-liquid-like. We give explicit expressions for the Green's function of the spin or pair operator, at points $\mathbf{r}_1$ and $\mathbf{r}_2$ far from the impurity and with a large time separation τ_{12}. When the distances are large compared to the time separation, $r_1,r_2\gg v_F|\tau_{12}|$, we must obtain Fermi-liquid behavior. However, in the opposite limit where we take $|\tau_{12}|\to\infty$, keeping r_1,r_2 fixed, we obtain a non-Fermi-liquid scaling exponent, which leads to a diverging susceptibility. Remaining in the asymptotic regime, we may vary the ratios of r_1,r_2 and $v_F\tau_{12}$. The Green's functions then exhibit nontrivial *crossover* behavior between Fermi-liquid and non-Fermi-liquid exponents. This crossover is described by *universal* functions of the ratios, which we calculate exactly here, for the first time. (They are inaccessible to Bethe ansatz techniques.)

Our result for the spin-density Green's function, in the limit $r_1,r_2\ll v_F|\tau_{12}|$, agrees with that conjectured in Ref. [11]. However, we disagree on the form of the one-particle Green's function conjectured in Ref. [11], where charge and flavor degrees of freedom are completely ignored, as well as on the discussion of superconductivity properties.

The Kondo interaction only affects the s-wave part $\Psi(r)$ of the electron operator, $\Psi(\mathbf{r})$, which we write

$$\Psi(\mathbf{r}) = (1/i\pi r 2\sqrt{2})\Psi(r) + \text{higher partial waves}, \quad (1)$$

where

$$\Psi(r) = [e^{ik_F r}\psi_L(r) - e^{-ik_F r}\psi_R(r)]. \quad (2)$$

ψ_L and ψ_R are incoming and outgoing waves, or left and right movers in the effective one-dimensional field theory description, satisfying the boundary condition $\psi_L(r=0) = \psi_R(r=0)$. (See Ref. [5], Appendix A.)

The k-channel Kondo Hamiltonian reads, when expressed in terms of excitations near the Fermi surface,

$$H(\lambda_K) = \frac{v_F}{2\pi}\left\{\int_0^\infty dr\left[i\psi_L^{\dagger,aj}(r)\frac{d}{dr}\psi_{L,aj}(r) - i\psi_R^{\dagger,aj}(r)\frac{d}{dr}\psi_{R,aj}(r)\right] + 2\pi\lambda_K \mathbf{J}_L(r=0)\cdot\mathbf{S}\right\}, \quad (3)$$

where

$$\mathbf{J}_L(r) = \psi_L^{\dagger,\bar{a}i}(r)\,\tfrac{1}{2}\sigma_{\bar{a}}^{a}\psi_{L,ai}(r) \quad (4)$$

is the spin current and $\mathbf{S}$ is the impurity-spin operator [labels $\alpha = 1,2$ of the two spin states, and $j = 1,\ldots,k$ of the channels ("flavors") are summed over; σ are Pauli matrices].

The Kondo coupling constant λ_K is asymptotically free and flows to a strong-coupling fixed point, governing the low-temperature properties. In a space- (imaginary) time ($\tau = -it$) picture the physical region is the upper half complex plane $\{z = v_F\tau + ir;\ r \geq 0\}$ (the imaginary axis being space). The Kondo interaction occurs only at the boundary, the real axis $\{r \equiv 0\}$. The free bulk Hamiltonian is conformally invariant due to the linear dispersion relation. At the fixed point the Kondo impurity spin has completely disappeared, leaving behind a particular conformally invariant boundary condition (see Refs. [5,6, 12]), characterized by a "Kondo" *boundary state* $|K\rangle$.

For the non-Fermi-liquid fixed points this state cannot be expressed in terms of properties of free fermions. Free fermions can also be described in bosonized form by a direct product of Wess-Zumino-Witten (WZW) models [13] associated with charge (Q), spin (j), and flavor (ρ) degrees of freedom, supplemented by a constraint on combining [5,14] them. It turns out that the Kondo boundary state *can* be expressed in terms of charge, spin, and flavor degrees of freedom. It is in fact given [12], using a modular transformation, by the exact excitation spectrum of the non-Fermi-liquid. For the Kondo problem this can be obtained [5] using the *fusion rules* of the WZW models. By means of the *Verlinde formula* we obtain [6] simple closed form expressions for $|K\rangle$ in terms of the *modular S matrix* [see Eq. (10)]. The boundary state $|K\rangle$ determines [15] the correlation functions exactly.

In bulk CFT a Green's function is a sum of products of left and right factors

$$\langle\Phi^{(1)}(r_1,\tau_1)\Phi^{(2)}(r_2,\tau_2)\cdots\rangle = \sum_{(a),(b)}\langle\phi_L^{(1)}(z_1)\phi_L^{(2)}(z_2)\cdots\rangle_{(a)}\langle\bar{\phi}_R^{(1)}(z_1^*)\bar{\phi}_R^{(2)}(z_2^*)\cdots\rangle_{(b)}\cdot M_{(a),(b)} \quad (5)$$

[in this sense one can speak of a factorization $\Phi(r,\tau) \to \phi_L(z)\bar{\phi}_R(z^*)$]. Here $(a),(b)$ label different "conformal blocks" [16]. In the presence of a conformally invariant boundary [7]

$$\langle\Phi^{(1)}(r_1,\tau_1)\Phi^{(2)}(r_2,\tau_2)\cdots\rangle_{\text{bound}} = \sum_{(a)}\langle\phi_L^{(1)}(z_1)\bar{\phi}_L^{(1)}(z_1^*)\phi_L^{(2)}(z_2)\bar{\phi}_L^{(2)}(z_2^*)\cdots\rangle_{(a)}\cdot D_{(a)} \quad (6)$$

(reminiscent of the "method of images"). If the left-hand side of Eq. (6) is a two-point function, (a) labels conformal towers (Fig. 1). At $|z_1 - z_2| \ll |z_1|$, the bulk operator-product expansion (OPE) has the form $\Phi^{(1)}\Phi^{(2)} \sim \sum_a C_{(a)}^{(1),(2)}\Phi^{(a)}$. This identifies [7] $D^{(a)}$ as the product of the bulk OPE coefficient multiplied by the amplitude [17] $A^{(a)} = \langle a;0|B\rangle/\langle 0;0|B\rangle$ of the one-point function $\langle\Phi^{(a)}(r,\tau)\rangle_{\text{bound}}$. Here $|B\rangle$ is the boundary state. In the case of invariance (of bulk and boundary) under a direct product of conformal algebras, the conformal blocks factorize. This is the case in the Kondo problem when the boundary condition cannot be expressed in terms of fermions, and bosonization becomes essential: The fermion can be decomposed into charge, spin, and flavor parts:

$$\psi_{L,ai}(z) \to e^{i\phi_L(z)/\sqrt{2k}}\mathbf{g}_{L,a}(z)\mathbf{h}_{L,i}(z),$$
$$\psi_{R,ai}(z^*) \to e^{i\phi_R(z^*)/\sqrt{2k}}\mathbf{g}_{R,a}(z^*)\mathbf{h}_{R,i}(z^*), \quad (7)$$

where ϕ is a U(1) boson, while $\mathbf{g}_L$ and $\mathbf{h}_L$ are the left-handed parts of matrix fields in the fundamental representation of the SU(2)-level-k and SU(k)-level-2 WZW

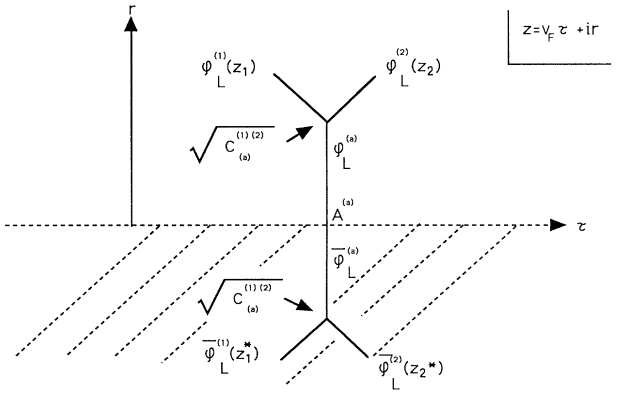

FIG. 1. Conformal block describing a two-point function in the presence of the boundary.

model [13], respectively. Thus, for example,

$$\langle \psi_{L,ai}(z_1)\psi_R^{\dagger,\bar{a}\bar{i}}(z_1^*)\psi_L^{\dagger,\bar{\beta}\bar{j}}(z_2)\psi_{R,\beta i}(z_2^*)\rangle_{\text{bound}} = \langle e^{i[\phi_L(z_1)-\phi_L(z_1^*)]/\sqrt{2k}} e^{-i[\phi_L(z_2)-\phi_L(z_2^*)]/\sqrt{2k}}\rangle \sum_{(j),(\rho)} \mathcal{G}_{(j)}\mathcal{H}_{(\rho)}\cdot D_{j,\rho}\,, \tag{8}$$

where

$$\mathcal{G}_{(j)}(z_1,z_1^*,z_2,z_2^*) = \langle \mathbf{g}_{L,a}(z_1)\mathbf{g}_L^{\dagger,\bar{a}}(z_1^*)\mathbf{g}_L^{\dagger,\bar{\beta}}(z_2)\mathbf{g}_{L,\beta}(z_2^*)\rangle_{(j)} \tag{9}$$

is a WZW conformal block [13] (and a similar block $\mathcal{H}_{(\rho)}$ for $\mathbf{h}$). The coefficients $D_{j,\rho}^{(0)}$ for the noninteracting theory, characterized by a fermionic boundary state $|F\rangle$, are easily determined by the requirement that Eq. (8) be expressible in terms of free fermions. The ratio of amplitudes

$$\frac{A^{(Q,j,\rho)}}{A^{(0),(Q,j,\rho)}} = \frac{\langle 0,0,0;0|F\rangle\langle Q,j,\rho;0|K\rangle}{\langle 0,0,0;0|K\rangle\langle Q,j,\rho;0|F\rangle} = (S_s^j/S_0^j)(S_0^0/S_s^0)\,, \tag{10}$$

which, for the Kondo problem, can be derived using the Verlinde formula [6,12] from the exact spectrum (given by the fusion rules), determines $D_{j,\rho}$, hence the exact strong-coupling Green's functions. [Here S_j^j represents [18] a modular transformation on the WZW characters.] Finite-temperature Green's functions are obtained by conformal mapping [5].

Using Eq. (2), the s-wave *one-particle Green's function* is a sum of four terms involving LL, RR, LR, and RL products of fields. A general feature of boundary conformal field theory is that any (bulk) Green's function involving purely left-moving (or purely right-moving) fields is completely unaffected by the boundary. Thus the LL and RR terms have exactly the same asymptotic behavior as at $\lambda_K=0$, i.e., $\langle \psi_L^\dagger(z_1)\psi_L(z_2)\rangle = 1/(z_1-z_2)$ and $\langle \psi_R^\dagger(z_1)\psi_R(z_2)\rangle = 1/(z_1^*-z_2^*)$. The LR and RL terms have the values $S/(z_1-z_1^*)$ and $S/(z_1^*-z_2)$, respectively, i.e., S times their zero-coupling values, where S is a universal constant:

$$S = \frac{\cos[\pi(2s+1)/(2+k)]}{\cos[\pi/(2+k)]}\,.$$

S is the (scattering) S matrix restricted to the one-particle sector. While $S=-1$ (corresponding to a $\pi/2$ phase shift) at the Fermi-liquid Kondo fixed point, $|S|<1$ at the nontrivial fixed points indicating scattering processes in which one electron goes into one electron plus one or more electron-hole pairs. From the Friedel sum rule, the excess electron number in the vicinity of the impurity is $\delta N = k(1-S)/2$. In the dilute impurity limit [19], the retarded self-energy is given by $\Sigma = (in_i/2\pi\nu)(1-S)$, where ν is the density of states per spin per channel and n_i is the impurity density. The residual resistivity is $\rho(0) = 3n_i(1-S)/2k\pi(ev_F\nu)^2$, i.e., $(1-S)/2$ times the unitary limit [in agreement with the perturbative result in the large-k limit, s=fixed]. The leading low-frequency, ω, correction to Σ is $\propto i(i\omega/T_K)^{2/(2+k)}$ and the leading temperature dependence of the dc resistivity is $\rho(T)/\rho(0)-1 \propto (T/T_K)^{2/(2+k)}$. Note that in the case $k=2$, $\rho(0)$ takes on half the unitary-limit value and the temperature exponent is $\frac{1}{2}$, unlike the value near 1 (heuristic argument by Cox [20]) observed in experiments on $Y_{1-x}U_xPd_3$ [3] and unlike Ref. [11].

Green's functions of *two-particle operators* involve double-s-wave terms, which show nontrivial behavior and then various other terms involving higher partial waves, including cross terms with the s-wave part, which all factor into products of one-particle Green's functions. Using Eq. (2) the 1D fermion bilinears consist of four terms: LL, RR, LR, and RL, involving different k_F-dependent prefactors. Thus the double-s-wave two-particle Green's function contains sixteen terms, with k_F-dependent prefactors of the form: $\exp[ik_F(n_1r_1+n_2r_2)]$, with $n_i=0,\pm1$. All terms involving purely left-moving (or purely right-moving) fields have the same values as at $\lambda_K=0$.

We give explicit expressions for the two-channel case ($k=2$, $s=\frac{1}{2}$). In the limit $v_F|\tau_{12}| \gg r_1,r_2$, Green's functions exhibit boundary scaling dimensions, Δ, decaying as $|\tau_{12}|^{-2\Delta}$. The minimum possible value of Δ for an operator of charge Q, spin j, and flavor "pseudospin" [from the second flavor SU($k=2$) group] j_f is [5] $\frac{1}{8}Q^2+\frac{1}{4}j(j+1)+\frac{1}{4}j_f(j_f+1)$. Thus a logarithmically divergent susceptibility, corresponding to $\Delta=\frac{1}{2}$, is only possible for a two-particle operator with (Q,j,j_f) equal to $(\pm2,0,0)$ or $(0,1,0)$ or $(0,0,1)$. These correspond to the spin-singlet, flavor-singlet pair operator, the spin density, and the pseudospin density, respectively. The spin-triplet pair (i.e., $Q=\pm2$) susceptibility is nondivergent.

For $k=2$, $s=\frac{1}{2}$, we find that all the terms involving three left-moving operators and one right-moving one vanish at the strong-coupling fixed point (unlike the zero coupling case), up to corrections dropping off more rapidly than $1/z^2$. Thus we only need to specify terms with two left-moving operators and two-right-moving operators. The singular part of the *Green's function* of the *spin-density* comes from the double-s-wave part, $\mathbf{S}(\mathbf{r}) = (1/4\pi r^2)\mathcal{S}(r)+\cdots$, where $\mathcal{S}(r) = (1/4\pi)\Psi(r)^{\dagger,\bar{a}i}\sigma_{\bar{a}}^{a}\times\Psi(r)_{ai}$, with

$$\langle \mathcal{S}^a(z_1)\mathcal{S}^b(z_2)\rangle_{\text{sing}} = \frac{\delta^{ab}}{2\pi^2(z_1-z_2^*)(z_1^*-z_2)}\eta^{-1/2}\{2\cos[2k_F(r_1+r_2)]+\cos[2k_Fr_{12}][2+\eta/(1-\eta)]\}\,, \tag{11}$$

where η is the cross ratio:

$$\eta = \frac{(z_1^*-z_1)(z_2-z_2^*)}{(z_1-z_2^*)(z_1^*-z_2)} = \frac{4r_1r_2}{v_F^2\tau_{12}^2+(r_1+r_2)^2}\,. \tag{12}$$

This expression illustrates the universal crossover from Fermi-liquid form, in the "bulk" limit where $r_1, r_2 \gg v_F|\tau_{12}|$ and hence $\eta \to 1$, to non-Fermi-liquid behavior, in the "boundary" limit, i.e., as $\eta \to 0$. Note that the spin-density Green's function approaches

$$2\delta^{ab}\cos[2k_F r_{12}]/(r_{12}^2 + v_F^2\tau_{12}^2) \tag{13}$$

for $r_1, r_2 \gg |z_1 - z_2|$, but approaches

$$4\delta^{ab}\cos[2k_F r_1]\cos[2k_F r_2]/[v_F(\tau_{12}^2)^{1/2}(r_1 r_2)^{1/2}] \tag{14}$$

for $v_F|\tau_{12}| \gg r_1, r_2$, exhibiting the non-Fermi-liquid exponent, 1, and consequently a logarithmically divergent local susceptibility.

Of particular interest [2] is the *correlation function of the pairing field.* The nontrivial piece of the pair two-point function is

$$\langle(\psi_{L,ai}(z_1)\psi_{R,\beta j}(z_1^*))(\psi_L^{\dagger\bar{\alpha}i}(z_2)\psi_R^{\dagger,\bar{\beta}j}(z_2^*))\rangle_{\text{bound}}$$
$$= \frac{\eta^{-1/2}}{(v_F\tau_{12})^2 + (r_1 + r_2)^2}\left\{R_0\tilde{R}_0\frac{1}{2}\left[\frac{1}{1-\eta} + 3\right] + (R_0\tilde{R}_1 + R_1\tilde{R}_0 + R_1\tilde{R}_1)\frac{1}{2}\frac{\eta}{1-\eta}\right\}, \tag{15}$$

where $R_{1,0} = (1/\sqrt{2})(\delta_\alpha^{\bar{\alpha}}\delta_\beta^{\bar{\beta}} \pm \delta_\beta^{\bar{\alpha}}\delta_\alpha^{\bar{\beta}})$ are projectors onto triplet and singlet channels, respectively (and a similar expression for $\tilde{R}$ for the flavor part). We see that only the spin-singlet flavor-singlet channel has a divergent susceptibility, as mentioned above. Therefore, by Fermi statistics, the susceptibility of the pairing field $\Psi_{ai}(\mathbf{r})\Psi_{\beta j}(\mathbf{r})$ itself does *not* diverge. However, the most divergent part of the p-wave pairing field is

$$\Psi_{ai}(\mathbf{r})\frac{\partial}{\partial r^a}\Psi_{\beta j}(\mathbf{r}) = \frac{ik_F r^a}{8\pi^2 r^3}[\psi_{L,ai}\psi_{R,\beta j} + \psi_{L,\beta j}\psi_{R,ai}] + \cdots \tag{16}$$

which *does* lead to a logarithmically divergent susceptibility as $T \to 0$. If the Kondo interaction is made anisotropic (in spin space) then the $S^z = 0$ component of the triplet pair operator can mix with the singlet pair operator and hence also has a singular susceptibility. The $S^z = \pm 1$ components remain nonsingular.

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