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Exact results on the two-channel Anderson impurity model: single-electron Green's function and resistivity

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Abstract

We exploit our recent boundary conformal field theory description (Johannesson et al., Phys. Rev. B 68 (2003) 075112) of the two-channel Anderson impurity model to construct its exact space- and time-dependent single-electron Green's function. The universal zero-temperature resistivity and leading temperature-dependent term are derived. We discuss possible implications for a quadrupolar-magnetic mixed-valent scenario for the UBe₁₃ compound. \bigcirc 2005 Elsevier B.V. All rights reserved.

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The possibility of non-Fermi liquid (NFL) behavior in certain cerium- and uranium-based alloys has been a topic of intense discussion and research ever since the first discovery of the anomalous transport and thermodynamics in these materials [1]. Recently, the two-channel Anderson impurity model was proposed to account for the NFL physics of UBe₁₃ [2]. In this model, a lowlying quadrupolar $5f^2$ doublet mixes with a magnetic $5f^3$ doublet via the hybridization between the local f orbital and the conduction band:

$$H = H_0 + \varepsilon_{\mathfrak{A}} f^{\dagger}_{\sigma} f_{\sigma} + \varepsilon_q b^{\dagger}_{\mathfrak{A}} b_{\mathfrak{A}} + V(\psi^{\dagger}_{\alpha\sigma}(0) b^{\dagger}_{\tilde{\mathfrak{A}}} f_{\sigma} + f^{\dagger}_{\sigma} b_{\tilde{\mathfrak{A}}} \psi_{\alpha\sigma}(0)).$$
(1)

The free electron Hamiltonian is denoted here by H_0 , with the conduction electrons represented by radial (1D) fields $\psi^{\dagger}_{\alpha\sigma}$ carrying spin ($\sigma = \uparrow, \downarrow$) and quadrupolar ($\alpha = \pm$) quantum numbers. The electrons hybridize with the local f levels via the matrix element V. The quadrupolar [magnetic]

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doublet of energy ε_q [ε_s] is created by a boson [fermion] operator b_{α}^{\dagger} [f_{σ}^{\dagger}]. Strong Coulomb repulsion implies single occupancy of the localized levels: $f_{\alpha}^{\dagger}f_{\sigma} + b_{\alpha}^{\dagger}b_{\alpha} = 1$. For more details, see Ref. [3].

We have applied our recent boundary conformal field theory (BCFT) description of the model [3] to construct its exact space- and time-dependent single-electron Green's function in the limit of low temperatures. Within the BCFT formalism, a quantum impurity gets replaced by a scaleinvariant boundary condition on the free electron fields, inserted at the location of the impurity [4]. The specific boundary condition that emulates the presence of the f levels in Eq. (1) was identified in Ref. [3]. The single-electron Green's function picks up a dependence on this boundary condition (alias the impurity) via the one-particle *S*-matrix.

$$S_{(1)}(\omega_{\rm F}) = {\rm e}^{2{\rm i}\delta_{\rm F}} C_{(1)}(\omega_{\rm F}).$$
 (2)

Here $C_{(1)}(\omega_{\rm F})$ is the amplitude for a single electron to scatter elastically off the impurity at the Fermi level $\omega_{\rm F}$, and $\delta_{\rm F} = \pi n_{\rm c}/4$ is the corresponding single-electron scattering phase shift, with $n_{\rm c}$ the impurity charge valence. Carrying out the same kind of analysis as in Ref. [5] for the two-channel Kondo model (integer valence limit, $n_{\rm c} = 1$, of the present model), we find that $C_{(1)}(\omega_{\rm F}) = 0$, independent of the value of $n_{\rm c}$. In other words, the outgoing scattering state has no remaining singleelectron component after interaction with the impurity. This extreme non-Fermi liquid behavior is the same as for the two-channel Kondo model and *is not modified as one moves into the mixed valence regime where* $n_{\rm c} \neq 0, 1$.

Using the BCFT machinery to extract the effective scaling Hamiltonian at low temperatures, a perturbative analysis combined with the result for the one-particle S-matrix, produces an exact analytic expression for the leading terms of the single-electron Green's function. For a dilute distribution of uncorrelated impurities we obtain the standard form

$$G(\omega_n, k) = \frac{1}{i\omega_n - \varepsilon_k - \Sigma(\omega_n)},$$
(3)

where the Matsubara self-energy $\Sigma(\omega_n)$ splits into a universal zero-temperature part which is independent of frequency ω_n and impurity valence n_c , and a finite-*T* part which contains two n_c dependent "scaling fields" λ_q and λ_s which measure the participation of the quadrupolar and spin degrees of freedom in the scattering of the conduction electrons off the impurity [6].

Having obtained the self-energy $\Sigma(\omega_n)$ in Eq. (3) we can calculate the resistivity ρ of the model by analytically continuing $\Sigma(\omega_n) \rightarrow \Sigma^R(\varepsilon_k)$, with Σ^R the self-energy of the retarded Green's function. As follows from the analysis in Ref. [7] for this class of problems, vertex corrections to the resistivity involve s-wave correlations which vanish identically. The resistivity is thus determined by the quasi-particle life time

$$\tau(\varepsilon_k) = -\frac{1}{2} (\operatorname{Im} \Sigma^R(\varepsilon_k))^{-1}, \qquad (4)$$

via the simple Kubo formula

$$\rho^{-1}(T) = \frac{4e^2}{3m_e} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \left[-\frac{\mathrm{d}n_{\mathrm{F}}(\varepsilon_k)}{\mathrm{d}\varepsilon_k} \right] k^2 \tau(\varepsilon_k).$$
(5)

Here *e* and m_e are the electron charge and mass, respectively, with $n_F(\varepsilon_k)$ the Fermi distribution function. From Eqs. (4) and (5) we obtain

$$\rho(T) = \frac{3n_i}{4\pi (eg_F v_F)^2} (1 - A(n_c)\sqrt{T} + \ldots),$$
(6)

with "..." denoting subleading temperature corrections. The T = 0 resistivity is universal and is the same as for the two-channel Kondo model [5]. The leading finite-T term also exhibits the same \sqrt{T} scaling as the two-channel Kondo model, but now with an amplitude $A(n_c)$ which depends on the impurity valence n_c . This amplitude can be determined numerically by fitting the BCFT scaling fields $\lambda_{q,s}$ to the impurity-free energy obtained from the exact *Bethe Ansatz* solution of the model [8]. This work is currently underway [6].

As we mentioned in the introduction, the twochannel single-impurity Anderson model has been proposed as a description of the NFL physics of the UBe₁₃ alloy [2]. However, our exact result for the resistivity does not support this conjecture: The experimentally observed $T^{\frac{1}{2}}$ -behavior of the low-temperature resistivity for this material [9] is in conflict with the $T^{\frac{1}{2}}$ -scaling in Eq. (6). This may not come as a surprise: The thermodynamics of the model found in Ref. [8] also does not seem to agree with available experimental data on UBe₁₃. Moreover, experimental results for the third-order susceptibility are difficult to explain with the present model [11]. Taken together, these results suggest that additional effects (near-degenerate impurity multiplets [8], excited crystalline electric field states [10], etc.) may have to be taken into account in order to explain the anomalous behavior of this compound.

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