Solution of the Two-Channel Anderson Impurity Model
– Implications for the Heavy Fermion UBe$_{13}$ –

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We solve the two-channel Anderson impurity model using the Bethe-Ansatz. We determine the ground state and derive the thermodynamics, obtaining the impurity entropy and specific heat over the full range of temperature. We show that the low temperature physics is given by a line of fixed points describing a two-channel non-Fermi liquid behavior in the integral valence regime associated with moment formation as well as in the mixed valence regime where no moment forms. We discuss relevance for the theory of UBe$_{13}$.

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In recent years a large number of alloys have been observed to deviate from the Fermi liquid behavior, with the low temperature thermodynamics and transport properties described by logarithmic or fractional power laws. Among these are heavy fermion materials based on Ce$^{3+}$ or U$^{4+}$ ions containing inner shell $f$-electrons that do not delocalize. We shall concentrate henceforth on U-based materials, in particular UBe$_{13}$. Hund’s rules and spin-orbit coupling in the presence of a cubic crystalline electric field lead to modeling of the U ion by a $\Gamma_6$ Kramers doublet in a $5f^2$ configuration to be represented by the fermionic creation operator $f^\dagger_\alpha$ and a quadrupolar (non-magnetic) doublet $\Gamma_3$ in $5f^2$ configuration represented by the operator $b^\dagger_\alpha$. The doublets hybridize with conduction electrons in $\Gamma_8$ representation carrying both spin ($\sigma = \uparrow, \downarrow$) and quadrupolar ($\alpha = \pm 1$) quantum numbers. Strong Coulomb repulsion requires single occupancy of the localized levels, $f^\dagger_\alpha f_\alpha + b^\dagger_\alpha b_\alpha = 1$.

The resulting hamiltonian is the two channel Anderson impurity model, $H = H_{\text{bulk}} + H_{\text{imp}} + H_{\text{hybr}}$,

$$H_{\text{bulk}} = \int \psi^\dagger_{\alpha \sigma}(x) (-i\partial_x) \psi_{\alpha \sigma}(x) \, dx$$

$$H_{\text{imp}} = \varepsilon_s f^\dagger_\sigma f_\sigma + \varepsilon_q b^\dagger_\alpha b_\alpha$$

$$H_{\text{hybr}} = V \left[ \psi^\dagger_{\alpha \sigma}(0) b^\dagger_\alpha f_\sigma + \psi_{\alpha \sigma}(0) f^\dagger_\sigma b_\alpha \right]$$

The spectrum is linearized around the Fermi level and the Fermi velocity is set to one with the resulting density of states being $\rho = 1/(2\pi\varepsilon_F)$. We shall study the model in the grand canonical ensemble with the chemical potential $\mu$ coupled to the total number of electrons, $N = \int \psi^\dagger_{\alpha \sigma} \psi_{\alpha \sigma} \, dx + f^\dagger_\sigma f_\sigma$. The magnetic and quadrupolar impurity doublets are at energies $\varepsilon_s$ and $\varepsilon_q$ respectively. The last term gives the hybridization of the host with the impurity. The bar over $\alpha$ indicates that the index transforms according to the conjugate representation.

The model has been intensively studied recently via a new Monte Carlo method and by conserving slave boson theory. However, many open questions remain. In this letter we shall present the solution of the model via a Bethe-Ansatz construction, applicable in the past only to the single channel case. We shall give a complete determination of the energy spectrum and the thermodynamics, allowing us to follow the evolution of the impurity from its high temperature behavior with all four impurity states being equally populated down to the low energy dynamics characterized by a line of fixed point hamiltonians $H^\ast(\varepsilon, \Delta)$ where $\varepsilon = \varepsilon_+ - \varepsilon_-$ and $\Delta = \pi \rho V^2$ (we shall hold $\Delta$ fixed in what follows).

We shall find that the line of fixed points is characterized by a zero-temperature entropy $S_{\text{imp}}^0 = k_B \ln \sqrt{2}$ and a specific heat $C_{\text{imp}}^\ast \sim T \ln T$ typical of the 2-channel Kondo fixed point. However the physics along the line varies with $\varepsilon$. Consider $n_c = \langle f^\dagger_\sigma f_\sigma \rangle$, the amount of charge localized at the impurity. For $\varepsilon \lesssim \mu - \Delta$, we find $n_c \approx 1$ signaling the magnetic integral valence regime. At intermediate temperatures a magnetic moment forms which undergoes frustrated screening as the temperature is lowered, leading to zero-temperature anomalous entropy and anomalous specific heat. For $\varepsilon \gtrsim \mu + \Delta$ it is the quadrupolar integral regime and a quadrupolar moment forms. In the mixed valence regime, $|\varepsilon - \mu| \lesssim \Delta$, similar low temperature behavior is observed though without the intermediate regime of moment formation. In more detail, each point on the line of fixed points is characterized by two energy scales, $T_{K}(\varepsilon)$. These scales describe the quenching of the entropy as the temperature is lowered: the first stage taking place at the high temperature scale $T_h$, quenching the entropy from $k_B \ln 4$ to $k_B \ln 2$, the second stage at $T_l$, quenching it from $k_B \ln 2$ to $k_B \ln \sqrt{2}$. In the integral valence regime, $|\varepsilon - \mu| \gg \Delta$, the two scales are well separated and as long as the temperature falls between these values a moment is present, (magnetic or quadrupolar depending on the sign of $\varepsilon - \mu$), manifested by a finite temperature plateau $S_{\text{imp}}^0 = k_B \ln 2$ in the entropy. It is quenched when the temperature is lowered below $T_l$, with $T_l \rightarrow T_K$ in this regime. For $\varepsilon = \mu$ the scales are equal, $T_l(\mu) = T_K(\mu)$, and the quenching occurs in a single stage. In a subsequent paper we shall
present the line of boundary conformal field theories corresponding to our Bethe-Ansatz solution, and show that the two scales parameterize the approach to the fixed points.

The Bethe-Ansatz wave functions consist of plane waves with momenta \( \{ k_j \} \), and amplitudes that are connected by a set of scattering matrices (S-matrices) derived from the Hamiltonian and obeying Yang-Baxter consistency conditions. The electron-impurity scattering matrix is,

\[
S_{1,0} = I - \frac{i 2 \Delta}{(k_1 - \varepsilon)} + i 2 \Delta Q_{1;0}
\]

where the index zero denotes the impurity. The operator \( Q \) acts on quadrupolar (or flavor) space as an “annihilation-creation” operator, \( [Q]_{\alpha;\beta} = \delta_{\alpha\beta} \delta^{\alpha;\beta} \). This S-matrix is unitary and group invariant. To find the solution to an arbitrary number of electrons, the two scales parameterize the approach to the fixed points.

In the thermodynamic limit for which it is convenient to introduce \( \lambda = \frac{\pi}{\Delta} (k - \mu) \). These functions, \( \{ \eta_b(\lambda), \eta_n(\lambda), \eta'_b(\lambda), \eta'_n(\lambda) \} \), determine the distribution probabilities of the various excitations at temperature \( T \) (entering the equations as \( \tau = \frac{\pi}{2 \Delta} \)):

Identifying the ground state and the excitations, we sum over the latter to derive the free energy. It is expressed in terms of an infinite set of functions of the variable \( \lambda = \frac{\pi}{\Delta} (k - \mu) \). These functions, \( \{ \eta_b(\lambda), \eta_n(\lambda), \eta'_b(\lambda), \eta'_n(\lambda) \} \), determine the distribution probabilities of the various excitations at temperature \( T \) (entering the equations as \( \tau = \frac{\pi}{2 \Delta} \)).

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in terms of dilogarithms). Thus in the absence of external fields, the ground state is built out of a sea of charge-spin strings filled up to \( \lambda = 0 \) (i.e. \( k = \mu \)) and a completely filled sea of 2-flavor-strings. The zero-temperature impurity level occupancy (and therefore also the charge susceptibility) can be deduced in a closed form: \( n_0^0 = \int_{-\infty}^{\infty} \frac{d\lambda}{4(\lambda^2 - J^2)} \). The occupancy is integral: \( n_0^0 \approx 1,0 \) for \( |\varepsilon - \mu| \gg \Delta \), and non-integral elsewhere.

We turn next to study the low temperature physics, \( \tau \ll 1 \). In the integral valence regimes, \( |\varepsilon - \mu| \gg \Delta \), \( |J| \gg 1 \) and the main contribution to the free energy comes from \( |\lambda| \approx \pi/|J| \gg 1 \). It is convenient to rewrite some equations in the TBA. Using the exact relation: \( \ln \eta_{\mu} - \ln \eta_{\mu+1} = \lambda/\tau \), we can eliminate \( f_k \) from the equations for \( \eta_\mu \) and \( \eta_\mu \) and write them as: \( \ln \eta_\mu = -E_\pm^d/\tau + G^* [f_{\lambda^1} + f_{\lambda^2}] \) and \( \ln \eta_{\mu+1} = -E_\pm^d/\tau + G^* [f_{\lambda^1} + f_{\lambda^2}] \) with \( E_\pm^d/\tau = G \ln \left( 1 + e^{\pm(\lambda - \tau \ln \eta_{\lambda})} \right) \). The terms \( E_\pm^d \) become driving (inhomogeneous) terms at low temperatures as \( \tau \ln \eta_{\lambda} \) tends to zero (with \( \tau^2 \) corrections). We can further approximate them as follows:

\[
E_\pm^d/\tau \rightarrow G \left| \lambda/\tau \right|^\pm \rightarrow \begin{cases} e^{\pm \lambda/\pi \tau} & \tau \ll 1 \\
\alpha \lambda \leq 1 \rightarrow \lambda/2 \tau & \tau \gg 1 \end{cases}
\]

Changing variables, \( \zeta = \lambda - \frac{\pi}{2} \), the driving terms become, in the integral valence regime: \( E_\pm^d/\tau = e^{\pm \zeta - \ln T/T_\pm} \) where \( T_\pm = \frac{2\pi}{\lambda} e^{\mp \pi/2} \). The relation of \( T_\pm \) to \( T_{l,h} \) depends on the sign of \( \varepsilon - \mu \) and is discussed below.

We analyze separately the magnetic and quadrupolar moment regimes. Consider first the magnetic case where \( \varepsilon \ll \mu - \Delta \), and therefore \( \lambda \ll -1 \). In the limit of small \( \tau \), the driving term \( E_\pm^d \) diverges faster than \( E_\pm^d \) that is compensated by a decaying exponential in the numerator; thus \( \eta_{\mu} \) tends to zero exponentially fast cutting away the equations for the higher q-flavor \( \eta^q \). After the identifications \( \eta_{\lambda_{1}} \rightarrow \eta_{1}^{*}, \eta_{\mu_{n}} \rightarrow \eta_{n_{2}}^{*} \) and \( \eta_{\mu_{n+1}} \rightarrow \eta_{n_{2}}^{*} \), we recover the TBA equations of the 2-channel Kondo problem. The Kondo temperature is \( T_K = T_l = T_\mp \). \( T_\mp \) is large, outside the low temperature approximation range. The identification of the resulting TBA equations in this limit with those of the 2-channel Kondo model indicates that at low temperatures, when \( E_\pm^d/\tau \) becomes very large, the system has a localized magnetic moment. When temperature goes below \( T_K \), overscreening will take place and in particular an entropy \( S_{\text{imp}} = k_B \ln \sqrt{2} \) will arise. This will also be found numerically (see below).

On the other hand, when \( \varepsilon \gg \mu + \Delta \), the limit of vanishing \( \tau \) drives \( \eta_{\lambda} \) to zero exponentially fast and cuts away the spin \( \eta^q \)'s. No remapping is required, and we recover again the TBA equations of the 2-channel Kondo model but this time for the quadrupolar degrees of freedom. The relative minus sign in the driving term reverses the ‘direction of lowering temperatures’ with respect to the previous case and has no further consequences. The Kondo temperature is \( T_K = T_l = T_\mp \), below which the two spin channels will overscreen a localized quadrupolar moment.

Now we study the mixed valence regime, \( |\varepsilon - \mu| \lesssim \Delta \), where \( n_{\pm} \approx 1/2 \). As \( |J| \gg 1 \), we need the solutions around \( \lambda \approx 0 \). Then both driving terms are approximately \( E_\pm^d/\tau = e^{\pm \zeta - \ln T/T_\pm} \) and both diverge simultaneously in the low temperature limit. We repeat the standard procedure of shifting variables with \( \pm \ln T/T_K \). Depending on the choice of sign, one of the driving terms diverges as \( 1/\tau^2 \) and the temperature ‘disappears’ from the other one. We recover one of the two cases outlined above but this time the equations are valid only at temperatures below \( T_l \) and there is no localized moment regime. However, a residual entropy \( S_{\text{imp}} = k_B \ln \sqrt{2} \) arises also in this regime.

Finally, we turn to the finite temperature thermodynamics. We obtain it by solving numerically the TBA equations. In Fig. 1 we show the behavior of the impurity entropy as a function of temperature for different values of \( \varepsilon \). At high temperatures the entropy is \( k_B \ln 4 \) in agreement with the size of the impurity Hilbert space. For \( |\varepsilon - \mu| \gg \Delta \) the impurity entropy is quenched in two stages. The degrees of freedom corresponding to the higher energy doublet are frozen first. The entropy becomes \( k_B \ln 2 \) and the system is in a localized magnetic or quadrupolar moment regime depending on the sign of \( \varepsilon - \mu \). As the temperature is further decreased, the remaining degrees of freedom undergo frustrated screening leading to entropy \( k_B \ln \sqrt{2} \). On the other hand, for values of \( |\varepsilon - \mu| \ll \Delta \), the quenching process takes place in a single stage. As \( \varepsilon - \mu \) is varied the behavior interpolates continuously between the magnetic and the quadrupolar scenarios. The zero temperature entropy is found to be independent of \( \varepsilon \) in accordance with the analytic study of the TBA equations. Note also the presence of a crossing point, a temperature \( T_{cross} \approx 0.1 \Delta \) where all
entropy takes the value \( S_{\text{imp}} = k_B \ln 2 \) independently of \( \varepsilon \) (cf. Ref. [1]).

In Fig. 2 we show the impurity contribution to the specific heat. The two stage quenching process gives rise to two distinct peaks. The lower temperature peak is the Kondo contribution centered around \( T_1 \) whereas the higher temperature peak is the Schottky contribution centered around \( T_1 \). Approximate expressions for \( T_{\text{Kondo}} \) can be read off from the curves: \( T_{\text{Kondo}}(\varepsilon) \approx \frac{\pi^2 k_B}{6} \ln(1 + 2a e^{2\pi(\varepsilon - \mu) / h}) \) with \( 1 < a < 4 \) (this expression goes over to \( T_{\pm} \) defined before in the appropriate limits). For large \( |\varepsilon - \mu| \) the two peaks are clearly separated and the area under the Kondo peak is \( k_B \ln \sqrt{2} \) while that under the Schottky peak is \( k_B \ln 2 \).

As mentioned earlier, the model was proposed as a description for the U ion physics of UBe\(_{13}\). It is expected to describe the lattice above some coherence temperature. We provide in the inset of Fig. 2 the experimental data for the 5\( f \)-derived specific heat of UBe\(_{13}\).

Concentrating on the temperature range containing the Kondo and Schottky peaks we conclude that no values of \( \varepsilon \) and \( \Delta \) yield a good fit. Further, the entropy obtained by integrating the weight under the experimental curve falls between \( k_B \ln 4 \) and \( k_B \ln 6 \). This suggests that a full description of the impurity may involve an other high energy multiplet (possibly a triplet cf. Ref. [3]), almost degenerate with the \( \Gamma_3 \) to yield a single peak for the Schottky anomaly. The nature of the multiplet could be deduced from further specific heat measurements. For an n-plet degenerate with the \( \Gamma_3 \), one has an \( SU(2) \times SU(n + 2) \) Anderson model and the area under \( C_{\text{imp}} / T \) is then given by \( k_B \ln [2 + \sec(\pi/2)] \) while if the n-plet is slightly split off the doublet, the area is given by \( k_B \ln [2 + \sec(\pi/2)] \). In order to be certain of having eliminated lattice effects it would be better to carry out the measurements on U\(_{1-x}\)Th\(_x\)Be\(_{13}\) for \( x > 0.1 \) the compound has no longer a superconducting transition and the lattice coherence effects are largely suppressed.

In subsequent work we shall present the solution of the general \( SU(N) \times SU(M) \) model and study the effects of magnetic and quadrupolar fields. These will help identify what particular impurity model is best fit for describing U\(_{1-x}\)Th\(_x\)Be\(_{13}\).

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