Renormalization Group Approach to Spectral Properties of the Two-Channel Anderson Impurity Model

Fritjof B. Anders

Department of Physics, Universität Bremen, P.O. Box 330 440, D-28334 Bremen, Germany

(Dated: 7-07-2004)

The impurity Green function and dynamical susceptibilities for the two-channel Anderson impurity model are calculated. An exact expression for the self-energy of the impurity Green function is derived. The imaginary part of the self-energy scales as $\sqrt{|\omega/T_K|}$ for $T \to 0$ serving as a hallmark for non-Fermi behavior. The many-body resonance is pinned to a universal value $1/(2\pi\Delta)$ at $\omega = 0$. Its shape becomes increasingly more symmetric for the Kondo-regimes of the model. The dynamical susceptibilities are governed by two energy scales $T_K$ and $T_0$ and approach a constant value for $\omega \to 0$, whereas relation $\chi''(\omega) \propto \omega$ holds for the single channel model.

PACS numbers: 71.10.Hf, 71.27.+a, 71.20.Eh

Introduction: In the last decade, the paradigm of a Fermi-liquid ground state in Heavy Fermion (HF) materials [1], which originally gave these mainly Ce and Uranium base compounds their name, has become strongly questioned. In addition to magnetic and superconducting phase transitions, many of these alloys show deviations from the Fermi-liquid behavior in the normal phase. Typically, logarithmic behavior and power laws with anomalous exponents have been reported in the low-temperature thermodynamic and transport properties [2]. These unusual properties are attributed to charge and spin fluctuations on the partially filled $f$-shells. Certain ballistic metallic point contacts, two-level systems [3] and coupled quantum-dot [4] have been argued to display similarly unusual properties.

While the $4f$-shell of Ce ions is usually occupied by one electron, the configuration of the $5f$-shell of U ions fluctuates between degenerate $5f^2$ and $5f^3$ crystal field states. Hund’s rules coupling and crystal field splitting in a cubic symmetry yield a Kramer’s degenerate $\Gamma_5$ ground state $|\sigma\rangle$ for the $5f^2$ and a quadrupolar $5f^2-\Gamma_3$ doublet $|\alpha\rangle$. On symmetry grounds, these states only hybridized with $\Gamma_5$ conduction electron labelled by a spin $\sigma$ and channel index $\alpha$ [5]. The Hamiltonian of this two-channel Anderson impurity model (TC-SIAM) is given by

$$H = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} (E_\sigma - E_0) X_{\sigma\sigma} + h_s S_z$$

$$+ h_c \tau_z + \sum_{k\sigma} V_\alpha \left(X_{\sigma\sigma\alpha} c_{k\sigma}^\dagger X_{-\sigma\sigma\alpha} + c_{k\alpha}^\dagger X_{\sigma\sigma\alpha} c_{k\sigma} X_{-\sigma\sigma\alpha}\right) \quad (1)$$

where the operator $c_{k\sigma}^\dagger$ creates an electron with energy $\epsilon_{k\sigma}$, momentum $k$, quadrupolar channel $\alpha = \pm$ and spin $\sigma$. $X_{m,m'} = |m\rangle \langle m'|$ is the usual Hubbard operator which destroys the ionic state $|m\rangle$ and creates the ionic state $|m\rangle$. The energy $E_\sigma$ is assigned to the magnetic doublet, the energy $E_0$ to the quadrupolar doublet containing one electron less than $|\sigma\rangle$. The last term describes the hybridization between the $f$-shell and the conduction electron host. The external magnetic and channel fields, $h_s$ and $h_c$, couple to the local spin or channel flavor operator, $S_z = \sum_\sigma \sigma X_{\sigma\sigma}/2$, and $\tau_z = \sum_\alpha \alpha X_{\alpha\alpha}/2$ and are used to calculate the local spin- or channel susceptibility $\chi_s = \langle s^\dagger s \rangle / h_s$ or $\chi_c = \langle \tau^\dagger \tau \rangle / h_c$, respectively, for $h_s, h_c \to 0$. This model was proposed in the context of UBe$_{13}$ by Cox [3,5] for a novel and unusual Kondo effect: the non-magnetic $5f^2-\Gamma_3$ ground state undergoes a quadrupolar charge rather than a magnetic Kondo-screening. Using a Monte-Carlo approach [6], it was shown that (i) the magnetic and quadrupolar moments are screened for $T \to 0$, (ii) the many-body resonance is pinned to a universal value $1/\omega$ for non-Fermi behavior. The spectral function would be given by

$$\rho(\omega) = \frac{\rho_0}{|\omega|^{1-\alpha_s-\alpha_\alpha}} B(1 - \alpha_s, 1 - \alpha_\alpha) \propto \rho_0 |\omega|^{-2/3(1-c_n^(-1))}$$

for $|\omega| \to 0$ using the exact threshold exponents [7]; $B$ is the beta function. Hence, the spectral function should diverge for $n_c \neq 0, 1$, indicating that vertex corrections are as important as the exact exponents $\alpha_M$ for obtaining the correct spectral function from $I_M(z)$ [8].

In this Letter, the first accurate solution for the dynamical properties of the model using Wilson’s numerical renormalization-group method (NRG [8]) is presented. It is shown that (i) the scaling behavior of $\rho_0\omega$ is given by $\rho_0 \omega \propto \sqrt{|\omega|/T_K}$ with a very weak $n_c$ dependence of the constants $a_{\pm}$, (ii) the many-body resonance becomes increasingly more symmetric in the Kondo regime in contrast to the NCA result, (iii) the total self-energy consists of a resonant level term and a local non-Fermi
liquid self-energy with vanishing imaginary part at \( \omega = 0 \), (iv) the dynamical spin and channel susceptibility \( \chi''(\omega) \) approach a constant for \( |\omega| < T_K \) and \( T \ll T_K \), corresponding to logarithmically divergent \( \chi(T) \) for \( T \to 0 \).

The Hamiltonian (1) is solved using the NRG [13]. The core of the NRG approach is a logarithmic energy discretization of the conduction band around the Fermi energy, \( \omega^{\pm}_n = \pm D\lambda^{n-\mu} \) and \( \Lambda > 1 \), and a unitary transformation of the base \( \psi_{\alpha\sigma}^{\pm} \) onto a basis such that the Hamiltonian becomes triagonal. The first operator \( f_{\alpha\sigma} \) is defined as \( f_{\alpha\sigma} = \frac{1}{\Lambda} \sum_n (c_{\alpha\sigma+n} + c_{\alpha\sigma-n}) \) [13]. Only \( f_{\alpha\sigma} \) couples directly to the impurity degrees of freedom. Eqn. (1) is recasted as a double limit of a sequence of dimensionless NRG Hamiltonians:

\[
\mathcal{H} = \lim_{\Lambda \to 1^+} \lim_{N \to \infty} \left\{ D\Lambda^{-(N-1)/2} \mathcal{H}_N \right\}, \tag{2}
\]

with \( D\Lambda \) equal to \( D(1+\Lambda^{-1})/2 \), and

\[
\mathcal{H}_N = \frac{\Lambda^{N-1}}{2} \left[ \sum_{\sigma} \frac{E_{\alpha\sigma}}{D\Lambda} \sum_{\sigma} X_{\alpha\sigma} + \sum_{\alpha\sigma} \left\{ \tilde{V}_\alpha f_{\alpha\sigma+1}^\dagger f_{\alpha\sigma} + H.c. \right\} \right] + \sum_{n=0}^{N-1} \sum_{\alpha\sigma} -\frac{\Lambda^2}{2} \xi_{\alpha\sigma} \left\{ f_{\alpha\sigma+1}^\dagger f_{\alpha\sigma} + H.c. \right\}.
\]

\( \tilde{V}_\alpha \) is related to the hybridization width \( D\Lambda \tilde{V}_\alpha = \tilde{V}_\alpha \), \( \Delta E = E_{\alpha\sigma} = E_\alpha - \epsilon_\alpha \), while the pre-factor \( \Lambda^{(N-1)/2} \) guarantees that the low-lying excitations of \( \mathcal{H}_N \) are of order one for all \( N \) [13]. In the absence of a symmetry breaking channel or magnetic field, the Hamiltonian has three fixed points: the free orbital fixed point \( \mathcal{H}_{\text{FO}}^* \) with \( \Delta E = 0 \), \( V = 0 \), and the two local moment fixed points \( \mathcal{H}_{\text{LM}}^* \) and \( \mathcal{H}_{\text{LM}}^\perp \) with \( \Delta E = \frac{1}{2} \sum_n (c_{\alpha\sigma+n} + c_{\alpha\sigma-n}) \) [13]. For large values of \( \Delta E/\Delta \) \( \gg 1 \), the Hamiltonian crosses over to the local moment fixed point \( (S_{\text{LM}} = \log(2)) \) first, before reaching the line of two channel fixed-points \( \mathcal{H}_{\text{LM}}^* \). \( T_K \) associated with the quenching of the lower doublet is shown in the inset. Parameters: \( D = 10 \), \( N = 3000 \), \( \Lambda = 3.5 \).

The logarithmically divergent susceptibilities to the low temperature form \( \chi(T) = \frac{1}{\Delta E} \log(T) + b \) was fitted to extract \( T_K \). \( T_K \) can also be defined as the temperature at which the effective moment of the lower doublet, \( \mu_{\alpha\beta}^2(T) = T\chi(T) \), is reduced to \( \mu_{\alpha\beta}^2(T_K) = 0.07 \) [14]. These two temperatures coincide within the numerical error. The local spin susceptibility \( \chi_s \) for \( \Delta E \leq 0 \), or channel susceptibility \( \chi_\alpha \) for \( \Delta E \geq 0 \) is plotted in the lower graph of Fig. 4 for five different values of \( \Delta E \) as a function of \( T/T_K \), to illustrate the scaling. The inset shows the exponential behavior of \( T_K(NRG) \) and the excellent agreement with the Bethe ansatz wide band limit \( T_K = \frac{\Delta E}{\lambda} \exp[-\frac{\Lambda\lambda^2(\Delta E)}{2\lambda^2}] \), taking into account the dis-
cretization correction \( A_\Lambda = \frac{1}{2} \log \Lambda \) for the Kondo coupling \( J \rightarrow J_{\text{eff}} = J/A_\Lambda \).

**Dynamical properties:** Using the equation of motion for Fermionic Green functions, \( z \ll A/B \gg \langle \{A, B\} \rangle + \ll [A, H]B \gg \), the commutators of the operators \( X_{\alpha, \sigma} \) and \( c_{k, \alpha, \sigma} \) with the Hamiltonian, \([X_{\alpha, \sigma}, H]\) and \([c_{k, \alpha, \sigma}, H]\) respectively, and the local completeness \( \sum_\sigma X_{\sigma, \sigma} + \sum_\alpha X_{\alpha, \sigma} = 1 \), it is straightforward to derive

\[
[z - E_{\alpha, \sigma} - \Gamma_{\alpha, \sigma}] \ll X_{\alpha, \sigma}X_{\sigma, \alpha} \gg = P_{\alpha, \sigma} + \ll \hat{O}_{\alpha, \sigma}X_{\alpha, \sigma} \gg . \tag{3}
\]

The expectation value of anti-commutator \( P_{\alpha, \sigma} = \langle X_{\alpha, \sigma} \rangle + \langle X_{\sigma, \alpha} \rangle \) is always 1/2 in the absence of a symmetry breaking field. The local composite operator \( \hat{O}_{\alpha, \sigma} \)

\[
\hat{O}_{\alpha, \sigma} = \sum_k V_{\alpha, \sigma} (X_{-\sigma, -\alpha} c_{k, -\alpha, -\sigma} - X_{-\sigma, -\alpha} c_{k, -\alpha, -\sigma})
+ \sum_k (V_{\alpha, \sigma} X_{\alpha, -\sigma + \alpha} X_{-\alpha, -\sigma} c_{k, -\alpha, -\sigma})(4)
\]

also transforms as \( X_{\alpha, \sigma} \). If the Green function \( G_{\alpha, \sigma}(z) \) is parameterized by the self-energy \( \Sigma_{\alpha, \sigma}(z) \), \( G_{\alpha, \sigma}(z) = P_{\alpha, \sigma}[z - E_{\alpha, \sigma} - \Gamma_{\alpha, \sigma} - \Sigma_{\alpha, \sigma}(z)]^{-1} \), this self-energy is given by the exact relation

\[
\Sigma_{\alpha, \sigma}(z) = M_{\alpha, \sigma}(z)/G_{\alpha, \sigma}(z) , \tag{5}
\]

defining \( M_{\alpha, \sigma}(z) = \ll \hat{O}_{\alpha, \sigma}X_{\alpha, \sigma} \gg \). In contrary to the single channel model \([17]\), there exists no non-interacting limit, and the spectral weight is reduced to \( P_{\alpha, \sigma} = 1/2 \).

It is straightforward to calculate the matrix elements of operator \( \hat{O}_{\alpha, \sigma} \) within the NRG. The spectral functions for \( M_{\alpha, \sigma} \) and \( G_{\alpha, \sigma} \) are obtained from their Lehmann representation by broadening the \( \delta \)-function of the discrete spectrum on a logarithmic scale, i.e. \( \delta(\omega - E) \rightarrow e^{-b^2/4E - (\log\omega/E)/b^2}/(\sqrt{\pi}bE) \). The broadening parameter is usually chosen as \( 0.5 < b < 1 \), and we used \( b = 0.8 \). The self-energy \( \Sigma(\omega) \) is then calculated through \([15]\). Fig. 2 shows the spectral function \( \rho_{\alpha, \sigma}(\omega) \) in comparison with the results obtain by the NCA \([5]\). The overall agreement between the NRG and NCA curves for the same parameter is reasonably good in spite of the incorrect threshold exponents of the NCA. The NRG tends to overestimate the broadening of the high energy peaks at \( \omega \approx \Delta E \), but produces highly accurate results for small frequencies \( |\omega| < T_K \). The inset of Fig. 2 depicts the many-body resonance in the region for \( |\omega|/T_K < 10 \) on a rescaled axis \( |\omega|/T_K^{1/2} \). It highlights three major aspects of spectral function: (i) \( \rho(\omega) \propto 1 - a_{\sigma} |\omega|/T_K^{1/2} \) for \( |\omega| < T_K \), (ii) for increasing \( |\Delta E| \), the spectral function becomes more symmetric around \( \omega = 0 \) and should approach a universal curve, (iii) the peak value is pinned to \( 1/(2\pi \Delta) \) at \( \omega = 0 \) independent of \( \Delta E \). Even though the vertex correction to the NCA spectra vanishes only in the limit of large spin and channel degeneracy \( N \) and \( M \), the scaling behavior of the NCA spectra is apparently correct. The NCA peak, however, saturates at \( \pi/(16\Delta) \) for \( T \rightarrow 0 \) and remains asymmetric for \( \Delta E \gg \Delta \).

Fig. 3 shows the corresponding imaginary part of the NRG self-energy \( \Sigma(\omega - i\delta) \): it vanishes at \( \omega = 0 \), independent of \( \Delta E \), which is a necessary condition for the pinning of the spectral function for all values of \( \Delta E \). In addition, \( \Re \Sigma(0) + \Delta + E_{\alpha, \sigma} = 0 \), leading to the pinning of the resonance to \( \omega = 0 \), depicted in Fig. 2. In the scaling regime \( |\omega|/T_K < T_h \), \( 3m\Sigma(\omega - i\delta) \propto |\omega|/T_K^{1/2} \). This region extends to multiples of \( |\omega|/T_K \) for \( T_h \gg T_K \).

The definition of the self-energy via the parameterization of \( G_{\alpha, \sigma}(z) \) turns out to be very useful for the understanding of its properties. The conformal field theory result for the \( T \)-matrix of two-channel Kondo model \([17]\)
The imaginary parts of the dynamical impurity spin and quadrupolar or charge susceptibility, hallmark of a local non-Fermi liquid. The scaling holds for $\chi''(\omega)$ as displayed in the inset; the values of $\omega_{\text{max}}$ are $0.0126, 0.0046, 0.00235$ for $\Delta E = 2, 4, 6$. The scaling curve (b) for $\chi''(\omega)$ vs $\omega/T_K$ at $T = 0$ for $\Delta E \geq 0$. Parameters as Fig. 2

conveys to the TC-SIAM. The self-energy $\Sigma(z)$ exhibits similar features as the correlation self-energy $\Sigma^U(z) = \Sigma(z) - \Gamma(z)$ of the single-channel model: its imaginary part also vanishes for $\omega \rightarrow 0$ and its scaling behavior reflects the nature of the local electronic excitation. While $\Sigma(z)$ is characterized by a power law behavior: $\Sigma(z) \propto (\omega/T_K)^{1/2}$ in the single channel model, the scaling as $\Sigma(z) \propto \sqrt{\omega/T_K}$ represents the hallmark of a local non-Fermi liquid.

The imaginary parts of the dynamical impurity spin and quadrupolar or charge susceptibility, $\chi''(\omega)$, $\chi'_{s/q}(\omega)$ respectively, are plotted in Fig. 4 for $T = 0$ and positive $\Delta E \geq 0$. Since the Hamiltonian is symmetric with respect to a particle-hole transformation, and simultaneous $\Delta E \rightarrow -\Delta E$ and interchanging the spin and quadrupolar indices, Fig. 4 also contains the information for $\Delta E < 0$. Both $\chi''$ show two frequency regimes. In contrast to the single channel model where the relation $\chi'' \propto \omega$ holds, $\chi''_{s/q}(\omega)$ approaches a constant at low frequencies, $|\omega| < T_K$. This corresponds to the logarithmic divergence of both $\chi(T)$ for $T < T_K$, and the slope of the logarithm is given by this constant. A scaling curve is found for the charge susceptibility (or spin susceptibility for $\Delta E < 0$) when plotted in dimensionless units of the low temperature scale $T_K$, as shown in Fig. 4 (b). The scaling holds for $\omega/T_K < 1$ above which non-universal band edge effects govern the physics. The intermediate frequency range $T_K < |\omega| < T_h$ is characterized by a power law behavior: $\chi''(\omega) \propto (\omega/T_K)^{-1.2}$. The peak position in $\chi''(\omega)$ scales with $T_h$ and corresponds to $\Delta E$ for large $\Delta E$. The values of $\chi''(\omega_{\text{max}})$ become increasing smaller with reduction of the occupation of the spin-doublet.

**Discussion and Conclusion:** The dynamical properties of the two-channel Anderson model were accurately calculated for $T = 0$ using the NRG approach. The analytical form of the spectral function is given by $1/(2\pi\Delta)(1 - a_+ i\omega/T_K)$ for $|\omega| < T_K$. Its peak is pinned to a universal value, and the self-energy scales as $\sqrt{\omega/T_K}$ independent of $n_c$. Since the self-energy $\Sigma(z)$ does not contain the resonant level part $\Delta_\alpha$, and $\Im\Sigma(\omega - i\delta) \rightarrow 0$ for $\omega \rightarrow 0$, its anomalous scaling serves as a hallmark for local non-Fermi liquid behaviour. The NCA result for the spectral function agrees remarkably well with the accurate NRG result. The two energy scales characterising the screening of the moments of upper and lower doublets also appear as charge excitation energy and as effective width of the many-body resonance at $\omega = 0$ in the spectral function. At finite temperatures - not shown here - the many-body resonance decreases for increasing temperature and vanishes for $T \gg T_K$. The dynamical susceptibility of the lower doublet maps to a universal scaling curve for $\omega < \min\{D, T_h\}$ and $T = 0$, while a peak at $\omega_{\text{max}} \approx T_h$ is found in the dynamical susceptibility of the upper doublet.

We have benefited greatly from fruitful discussions with N. Andrei, C. Bolech and A. Schiller and would like to acknowledge the funding of the NIC, Forschungszentrum Jülich, under project no. HHB00.