Fermi Liquid Properties of the Anderson Impurity Model within a Conserving Pseudoparticle Approach

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Abstract

The spin-1/2 Anderson impurity model in the limit of infinite Coulomb repulsion is considered in pseudoparticle representation. We extend the Conserving T-Matrix Approximation (CTMA) to the calculation of thermodynamic and spectral properties. In the Kondo regime the CTMA reproduces the exact screening of the local moment below the Kondo temperature T_K and down to the lowest temperatures of at least $T \simeq 0.01 T_K$, indicative of Fermi liquid behavior. The impurity selfenergy is quadratic in ω and T for T well below T_K.

Key words: Kondo effect, Fermi liquid properties, slave particle technique, DMFT

1. Model and Conserving Technique

The physics of strong on-site Coulomb repulsion is at the heart of strongly correlated electron systems. In order to tackle these problems, it is highly desirable to develop flexible, but well-controlled methods for quantum impurity systems to be used as "impurity solvers" within the Dynamical Mean Field Theory (DMFT) [1] approach. As a standard model we consider the single impurity Anderson model (SIAM) in the limit of infinite Coulomb repulsion between electrons on the impurity site, where consequently the impurity or d-level, will be at most singly occupied. It is well known, that in the Kondo regime the SIAM displays a crossover from the weak coupling behavior at high energies to strong coupling behavior below the Kondo temperature T_K. The low-energy properties are controlled by a Fermi liquid fixed point with a $\pi/2$-scattering phase shift of the conduction electrons [2]. The correct description of the Fermi liquid behavior is crucial for applications within DMFT. Perhaps the most flexible correlated electron method is the conserving auxiliary particle technique which is generalizable to arbitrary density of states (DOS) in the conduction band, to multiorbital-, and nonequilibrium problems alike. In this approach, the singly occupied (empty) level is created by fermionic (bosonic) operators $f^\dagger_\sigma$ ($b^\dagger$), which exactly satisfy the constraint $Q = \sum_\sigma f^\dagger_\sigma f_\sigma + b^\dagger b = 1$. The SIAM Hamiltonian is given by

$$H = H_0 + \sum_\sigma \varepsilon_{d,\sigma} f^\dagger_\sigma f_\sigma + V \sum_{\vec{k},\sigma} (c^\dagger_{k\sigma} b^\dagger f_\sigma + h.c.)\,, \quad (1)$$

where $H_0 = \sum_{\vec{k}\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$ is the conduction band Hamiltonian. $c^\dagger_{k\sigma}$ creates a conduction electron with wave vector $\vec{k}$ and $\varepsilon_{d,\sigma} = \varepsilon_d + \sigma g \mu_B B$ is the d-level in a magnetic field B, with μ_B and g the Bohr magneton and the Landé factor. Bare perturbation theory breaks down at energies of the order of the Kondo temperature, $T_K = \sqrt{2\mathcal{N}(0) D V^2}\, \exp\{-|\epsilon_d|/2\mathcal{N}(0)V^2\}$, where $2D$ is the bandwidth and $\mathcal{N}(0)$ is the density of states at the Fermi energy. A conserving approximation scheme, the CTMA, has been put forward in [3] to describe the high and low energy region of Eq.(1) in a unified manner and has been evaluated in [4], [5]. The CTMA can be seen as a selfconsistent expansion

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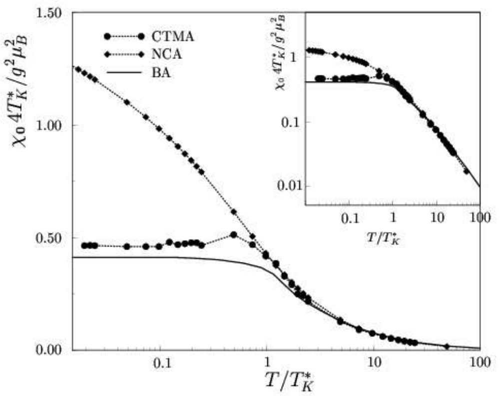

Fig. 1. Static local susceptibility: CTMA captures correctly the (asymptotically) free moment susceptibility at high energies and the Pauli susceptibility of the spin-screened regime, where the NCA susceptibility diverges. The Bethe ansatz result was taken from [6]. $T_K^\star$ is the Kondo temperature obtained from Wilson's original definition, so that $4\chi_0(T=0)T_K^\star/g^2\mu_B^2$ coincides with the Wilson number.

of the local irreducible two-particle vertex in terms of V. It incorporates in a conserving scheme the full the two-particle vertex functions in the spin and charge channels by summing up all diagrams with a maximum number of spin and charge fluctuations at any given order in V. For details see [4,5].

2. Results

In the following we present results for the impurity susceptibility $\chi_i(T)$ and the local selfenergy $\Sigma_{d\sigma}(\omega)$ for the typical parameter set $\epsilon_d/D = -0.81$, $\Gamma/D = 0.2$, yielding a low-temperature impurity occupation number per spin of $n_{d\sigma} \simeq 0.47$ and $T_K = 4.16 \cdot 10^{-4} D$. $\chi_i(T)$ is of prime interest, since it is sensitive to the spin-screened state in the Kondo regime. We calculated the static susceptibility via $\chi_i(T) = \frac{dM}{dB}\big|_{B=0}$, where the magnetization is obtained from $M = g\mu_B \sum_\sigma \sigma n_{d\sigma}$. Fig. 1 shows that the CTMA indeed captures the absence of local moments at temperatures below T_K. Another fundamental quantity is the impurity electron Green function,

$$G_{d\sigma}(\omega \pm i0) = \frac{1}{\omega - \varepsilon_d \pm i\pi\mathcal{N}(0)V^2 - \Sigma_{d\sigma}(\omega \pm i0)}. \quad (2)$$

It follows from the nature of the strong-coupling fixed point, that

$$\mathrm{Im}\Sigma_{d\sigma}(\omega - i0) \,=\, a\,\Gamma\,\frac{\omega^2 + (\pi T)^2}{T_K^2}, \quad \omega, T \lesssim T_K, \quad (3)$$

and the (exact) prefactor for our data set is given by $a = 0.1195$ [2,5]. In Fig. 2 we show the CTMA selfenergy around its minimal value at ω_0 at frequencies below T_K in a log-log representation. Within the numerical evaluation, this minimum is in general shifted away from the Fermi energy, $\omega = 0$, by an amount of $O(T_K)$. This is likely caused by an inaccurate treatment of high energy potential scattering contributions. An easily tractable correction scheme has been put forward in [5]. The behavior of $\mathrm{Im}\,\Sigma_{d\sigma}(\omega) - \mathrm{Im}\,\Sigma_{d\sigma}(\omega_0)$ is clearly quadratic, and from the slope of the dashed line we obtain a value for the prefactor a in Eq. (3), $\tilde{a} = 0.122$, in excellent agreement with the exact result. The inset of Fig. 2 shows the behavior of $\mathrm{Im}\Sigma_{d\sigma}$ as a function of T, which is as well in agreement with Eq. (3), deduced from Fermi liquid properties.

In conclusion, the CTMA correctly describes the low-lying many-particle excitations of the SIAM and the crossover to a local moment regime above the Kondo temperature, which makes it suitable for DMFT applications.

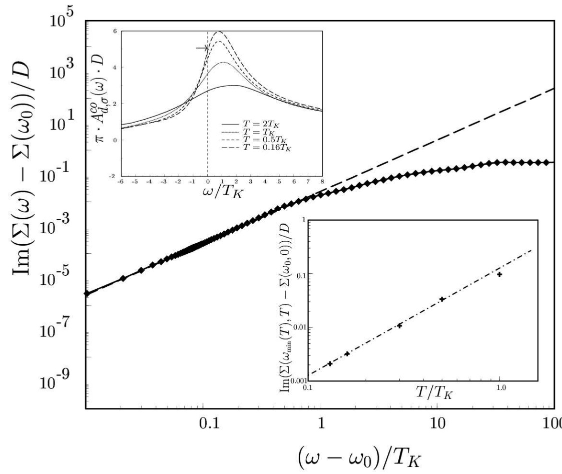

Fig. 2. Log-log plot of $\mathrm{Im}\,\Sigma_{d\sigma}(\omega - i0) - \mathrm{Im}\,\Sigma_{d\sigma}(\omega_0 - i0)$ versus frequency, $(\omega - \omega_0)/T_K$, for $T = 0.16\ T_K$. ω_0 is the position of the minimum of $\mathrm{Im}\,\Sigma_{d\sigma}(\omega - i0)$. The dashed line is the fit to the low-frequency quadratic behavior of $\mathrm{Im}\,\Sigma_{d\sigma}(\omega - i0)$ and represents the function $y = 0.02440(\omega - \omega_0)^2/T_K^2$. The lower inset shows the minimum value of the imaginary part of the selfenergy versus T/T_K in a log-log representation. The dashed line is given by $y = 0.013\, D \cdot (\pi\, T/T_K)^2$. The upper inset shows the spectral function at various temperatures and the arrow marks the $(T = 0)$ value predicted by Friedel's sum rule.

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