# DMFT/MPT STUDIES OF THE THERMODYNAMIC AND TRANSPORT PROPERTIES OF HEAVY FERMION SYSTEMS*

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The periodic Anderson model (PAM) is mapped on an effective single-impurity model (SIAM) within the dynamical mean-field theory (DMFT). The SIAM is treated in modified perturbation theory (MPT), which is exact up to second order in the Coulomb correlation and reproduces the atomic limit and the lowest moments. We present results for the specific heat, the magnetic susceptibility, the resistivity, the thermopower and the frequency dependent (dynamical) conductivity.

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## 1. Model and approximations

The most characteristic unusual properties of metallic heavy fermion systems (HFS) are experimentally obtained in measurements of the temperature ($T$) dependence of the specific heat $c_V(T)$, of the magnetic susceptibility $\chi(T)$, the electrical resistivity $R(T)$, the thermoelectric power $S(T)$ and the dynamical (frequency dependent) conductivity $\sigma(\omega, T)$.

In this paper we show that these features can qualitatively be reproduced within a DMFT/MPT treatment of the periodic Anderson model (PAM). Its standard form with only a two-fold degeneracy of the $f$-levels is given by ($n^c_{\boldsymbol{k}\sigma} := c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$ and $n^f_{\boldsymbol{R}\sigma} := f^\dagger_{\boldsymbol{R}\sigma} f_{\boldsymbol{R}\sigma}$ as usual):

$$H = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}} n^c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{R}\sigma} \left[ E_f n^f_{\boldsymbol{R}\sigma} + \frac{U}{2} n^f_{\boldsymbol{R}\sigma} n^f_{\boldsymbol{R}-\sigma} + V(c^\dagger_{\boldsymbol{R}\sigma} f_{\boldsymbol{R}\sigma} + \text{c.c.}) \right]. \quad (1)$$

Here $\epsilon_{\boldsymbol{k}}$ is the band electron dispersion, $E_f$ is the bare $f$-level energy, $U$ is the Coulomb correlation between two $f$-electrons and $V$ the hybridization

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between $f$- and conduction electrons at the same lattice site. For the actual calculations we assume a semielliptical model density of states for the unperturbed conduction band corresponding to the assumption

$$\frac{1}{N}\sum_{\boldsymbol{k}}\frac{1}{z-\epsilon_{\boldsymbol{k}}} = 8z\left(1-\sqrt{1-(4z)^{-2}}\right), \tag{2}$$

which becomes exact for a Bethe lattice in the limit of infinite coordination number. The chosen band width 1 sets the unit of energy (temperature and frequency) in the reminder of the paper.

We solve the PAM within the DMFT [1], which becomes exact for an infinite dimensional lattice [2]. Then the self-energy is $\boldsymbol{k}$-independent (as the local approximation becomes exact in infinite dimensions), and the PAM can be mapped onto an effective SIAM, for which an effective hybridization function $\Delta(E)$ has to be determined selfconsistently so that the $f$-electron Green function of the SIAM equals the site-diagonal $f$-Green function of the PAM for the same self-energy $\Sigma(E)$:

$$G^f(E) = \frac{1}{E-E_f-\Delta(E)-\Sigma(E)} \stackrel{!}{=} \frac{1}{N}\sum_{\boldsymbol{k}}\frac{1}{E-E_f-\Sigma(E)-\frac{V^2}{E-\epsilon_{\boldsymbol{k}}}}\,. \tag{3}$$

The MPT is an approximation for calculating the self-energy of the SIAM starting from the following ansatz for the self-energy:

$$\Sigma(E) = U\langle n_f\rangle + \frac{\alpha\ \Sigma^{(2)}(E)}{1-\beta\ \Sigma^{(2)}(E)}. \tag{4}$$

It is based on ordinary second order perturbation theory [3] relative to Hartree–Fock with $U$ as expansion parameter, where the self-energy reads: $U\langle n_f\rangle+\Sigma^{(2)}$. The parameters $\alpha$ and $\beta$ are constructed such that the exactly solvable atomic limit (as first suggested by Martín-Rodero *et al.* [4]) and the first four spectral moments are correctly reproduced, for details see Ref. [5].

All quantities to be calculated can be obtained from the one-particle (band and $f$-electron) Green functions and thus from the self-energy. The specific heat follows from the total energy being related to occupation numbers and the static magnetic susceptibility from differences of spin-up and -down occupation numbers in a magnetic field. We also get the transport quantities directly from one-particle Green functions because vertex corrections vanish within DMFT [1,3]. Then the frequency dependent conductivity and the thermopower are given by the expressions [3]:

$$\sigma(\omega) \;=\; \frac{1}{R_0}\int dE\,\frac{f(E)-f(E+\omega)}{\omega}\,L(E,E+\omega), \tag{5}$$

$$S = \frac{\int dE \left(-\frac{df}{dE}\right) (E-\mu)\, L(E,E)}{eT \int dE \left(-\frac{df}{dE}\right) L(E,E)}, \tag{6}$$

here $R_0 \approx 10^3\,\mu\Omega$cm is some constant, $f$ is the Fermi function, and $L$ is abbreviation for:

$$L(E_1,E_2) = \frac{2}{N}\sum_{\boldsymbol{k}\sigma}\Big(\operatorname{Im} G^c_{\boldsymbol{k}\sigma}(E_1+i0)\operatorname{Im} G^c_{\boldsymbol{k}\sigma}(E_2+i0)\Big) \tag{7}$$

with the band electron Green function $G^c_{\boldsymbol{k}\sigma}(z) = \left(z - \frac{V^2}{z-E_f-\Sigma(z)} - \varepsilon_{\boldsymbol{k}}\right)^{-1}$.

## 2. Results

We use the parameters $V = 0.2$, $U = 1$, $E_f = -0.5$ and $n_{\text{total}} = 1.5$ (*i.e.* the Coulomb correlation $U$ is of the same magnitude as the band width).

The $f$-DOS (Fig. 1) shows the expected behaviour with one-particle peaks at $E_f$ and $E_f + U$ and a $T$-dependent resonance at the chemical potential.

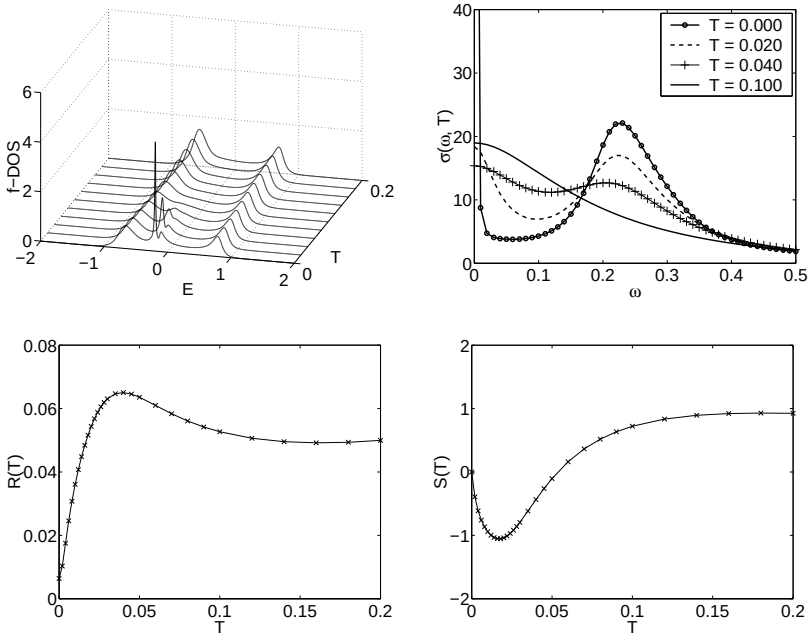


Fig. 1. $f$-DOS (on the top left; as function of band energy $E$), dynamical conductivity (on the top right; as function of frequency $\omega$), static resistivity (on the bottom left; as function of $T$, in units of $R_0 \approx 10^3\,\mu\Omega$cm) and thermoelectric power (on the bottom right; as function of $T$, in units of $(k_{\mathrm{B}}/e) \approx -86\,\mu$V/K)

For the resistivity (Fig. 1) we obtain a small residual resistance at $T = 0$, a rapid increase $\sim T^2$ for very small $T$, and then a maximum at a characteristic temperature $T^* \approx 0.04$. The thermopower is absolutely very large and shows a sign change in the low-$T$ regime (typical for systems of heavy fermions). The frequency dependent conductivity has a Drude peak at zero frequency at low $T$ and, in addition, a (mid-infrared) peak at some finite frequency; with increasing $T$ the Drude peak quickly disappears and only the resonance peak at finite frequency survives.

The specific heat (Fig. 2) shows the linear $T$-dependence $c_V(T) = \gamma T$ characteristic for metals, but with a large value of $\gamma(T) = c_V(T)/T$ which decreases from its strongly enhanced low temperature value at $T \ll T^*$ to a small value typical for conventional metals at $T \gg T^*$. The magnetic susceptibility shows a crossover from a Curie behaviour $\chi(T) \sim T^{-1}$ at high $T \gg T^*$ to a constant Pauli behaviour (with again strongly enhanced absolute value) at low $T \ll T^*$.

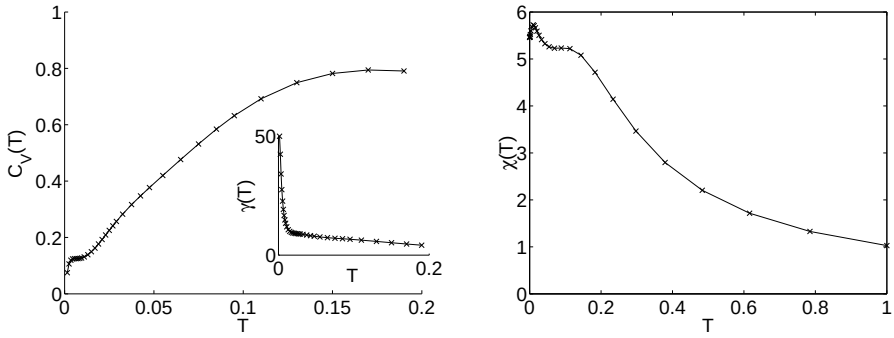


Fig. 2. Specific heat (on the left) and its $\gamma$-coefficient (in the inset) and magnetic susceptibility (on the right) as functions of $T$

In conclusion the typical experimental results for HFS are qualitatively well reproduced within the DMFT/MPT.

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