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Physica B 281&282 (2000) 47–49

PHYSICA B

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Oral Presentation

Exhaustion physics in heavy fermion systems: A $T = 0$ NRG study

Th. Pruschke[a,*], R. Bulla[b], M. Jarrell[c]

[a]*Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany*
[b]*Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany*
[c]*Department of Physics, University of Cincinnati, Cincinnati, OH 45221, USA*

Abstract

The theoretical description of heavy fermion physics, in particular the formation and energy scale of the heavy electron liquid, is still an open issue. One of the competing points of view is based on Nozières' exhaustion scenario that predicts a strongly reduced Kondo scale in concentrated systems. We study the properties of the paramagnetic phase of the periodic Anderson model within the dynamical mean-field theory at $T = 0$ using Wilson's numerical renormalization group. Special emphasis is laid on the relation between lattice and impurity energy scales.

Keywords: Periodic Anderson model; Exhaustion physics

Heavy fermion compounds [1] can be viewed as paradigm for strong correlation effects in solids. The physics of these systems can in several cases, like e.g. $CeAl_3$,CeB_6 or $CeCu_6$ [1], be at least qualitatively understood by a picture of independent, but coherent Kondo scatterers, with the low-energy scale set by the impurity Kondo temperature. However, for UPt_3,URu_2Si_2 or Yb_4As_3 [2,3] there seem to exist two distinct energy scales; one high-temperature scale, T_K, describing conventional incoherent Kondo scattering, and a much smaller scale, T_0, marking the onset of Fermi liquid formation.

One possibility to understand this discrepancy is based on Noziéres' exhaustion scenario that predicts a reduced scale for the Fermi liquid formation in concentrated systems due to the small number of screening states available [4–9]. Evidence for such behaviour has recently been observed in studies of the periodic Anderson model (PAM)

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \varepsilon_f \sum_k f^\dagger_{k\sigma} f_{k\sigma} + V \sum_{k\sigma} (c^\dagger_{k\sigma} f_{k\sigma} + \text{h.c.}) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow}, \quad (1)$$

within the dynamical mean-field theory (DMFT) [10] for $\langle n^f \rangle = 1$ and a value of $U/V^2 \approx 4$ [6–9]. Except for the work by Vidhyadhiraja et al. [9], which is based on second-order perturbation theory in U (IPT), the results were obtained by quantum Monte-Carlo. However, for large U/V^2, the identification of exponentially small energy scales with QMC is problematic due to its restriction to finite temperatures. The IPT as a perturbational approach in U, on the other hand, certainly cannot produce exponentially small energy scales. Thus, for a quantitative description of the low-temperature phase and especially a reliable calculation of the low-energy scale T_0, a non-perturbative technique at $T = 0$ is necessary.

Such a method has become available recently by the application of Wilson's NRG [11,12] to the DMFT [13–15], which we use to study the paramagnetic phase of the PAM within the DMFT at $T = 0$. The conduction band is described by a Gaussian density of states, the position of its center of mass ε_c controls the filling. As

* Corresponding author. Tel.: +49-941-9432030/2046; fax: +49-941-943-4382.
E-mail address: thomas.pruschke@physik.uni-regensburg.de (T. Pruschke)

0921-4526/00/$ - see front matter
PII: S0921-4526(99)00782-6

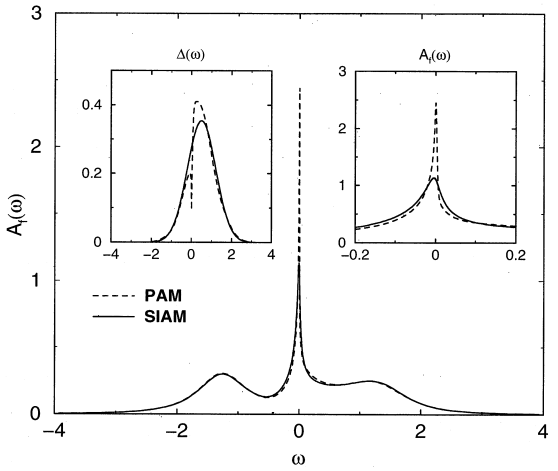

Fig. 1. f-density of states $A_f(\omega)$ for PAM (dashed line) and SIAM (full line) for $U = -2\varepsilon_f = 2, V^2 = 0.2$ and $\varepsilon_c = 0.5$.

a typical result we show in Fig. 1 the local density of f-states $A_f(\omega)$ for $U/V^2 = 10$, $\langle n^f \rangle \approx 1$ and $\varepsilon_c = 0.5$ ($\langle n^c \rangle \approx 0.6$) for the PAM (dashed line) and the single impurity Anderson model (SIAM, full line). One sees the characteristic structures, namely the charge–excitation peaks at $\omega \approx \pm U/2$ and the Kondo resonance at the Fermi level. The height of the Kondo peak in the PAM is strongly enhanced as compared to the SIAM, while its width is narrowed (right inset to Fig. 1) [6–9]. The enhancement in the Kondo peak is connected with a depletion of the effective hybridization function $\Delta(\omega)$ (left inset of Fig. 1) at the Fermi level. This depletion has been coined as hallmark of exhaustion physics in the PAM and related models [6–9], since according to Nozières phenomenological picture [4,5] due to screening at other sites the effective density of conduction states available at a given site should be reduced. The reduced effective hybridization at the Fermi level gives also rise to a reduced low-energy scale, characterised by an effective mass $m^*/m \approx 17$ in the PAM, whereas the corresponding quantity for the SIAM is $m^*/m \approx 8$.

Calculating m^*/m for fixed U/V^2 and $\langle n^f \rangle \approx 1$ as function of $\langle n^c \rangle$, one can compare this quantity for the SIAM and the PAM. To allow a convenient distinction between the scale of the lattice and the impurity model we denote the former as T_0 and the latter as T_K hereafter. An example for $U/V^2 = 8$ is shown in Fig. 2, where we plotted $m/m^* \propto T_0$ as function of $\langle n^c \rangle$. Note that for $\langle n^c \rangle \approx 1$ the value T_0 for the PAM is enhanced over the impurity scale [16,17], with an enhancement $\ln(T_K)/\ln(T_0) \approx 3/2$. Below $\langle n^c \rangle \approx 0.8$ the energy scale of the PAM decreases rapidly below T_K, being almost two orders of magnitude smaller for $\langle n^c \rangle \approx 0.25$.

Nozières' phenomenological arguments also lead to an estimate of T_0 as function of $\langle n^c \rangle$, namely $T_0 \propto$

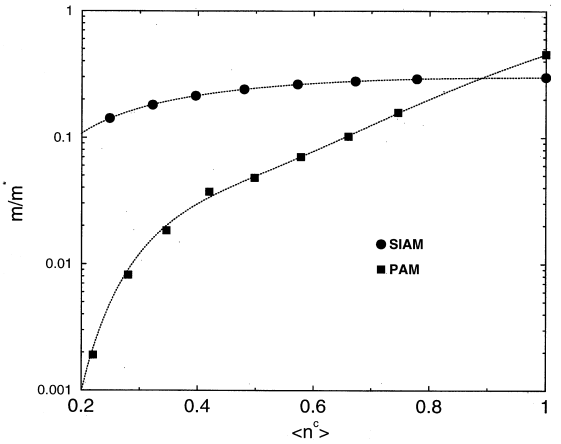

Fig. 2. $m/m^* \propto T_0$ versus $\langle n^c \rangle$ for $U/V^2 = 8$.

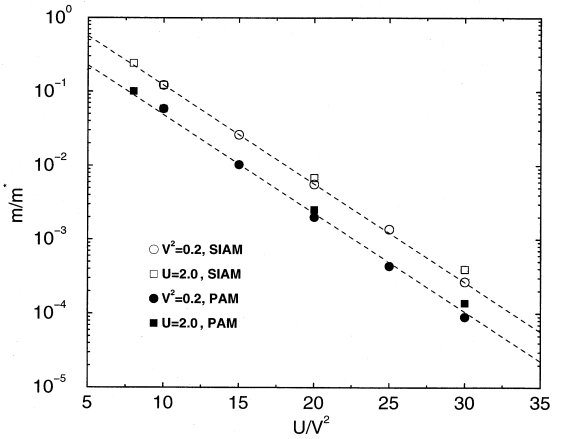

Fig. 3. m/m^* as function of U/V^2 for $\langle n^c \rangle \approx 0.6$. The circles (squares) denote varying $U(V^2)$ for fixed $V^2 = 0.2$ ($U = 2$).

$(T_K)^2/A_c^{(0)}(0)$ [5], where $A_c^{(0)}(0)$ is the free band-electron DOS at the Fermi energy. This relation has recently been tested with IPT [6–9] and found to be fulfilled at least for $U/V^2 \approx 4$ between $0.4 \leqslant \langle n^c \rangle \leqslant 0.8$. A much more sensitive check is a comparison of T_0 and T_K as function of U/V^2 for fixed $\langle n^c \rangle$, since $A_c^{(0)}(0)$ is constant in this case and the estimate reads $T_0 \propto (T_K)^2$. The result for $\langle n^c \rangle \approx 0.6$ as function of U/V^2 for both varying U at constant $V^2 = 0.2$ (circles) and varying V^2 at constant $U = 2$ (squares) is shown in Fig. 3 on a semi-logarithmic scale. Evidently T_K and T_0 follow an exponential law $T_0, T_K \propto \exp(-aU/V^2)$. However, both curves are parallel in the semi-logarithmic plot in Fig. 3, i.e. the coefficients of U/V^2 in the exponents of both quantities are identical. This of course means $T_0 \propto T_K$ rather than $T_0 \propto (T_K)^2$, as predicted by Nozières.

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