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"Exhaustion" physics in the periodic Anderson model from iterated perturbation theory

N. S. Vidhyadhiraja[1,2], A. N. Tahvildar-Zadeh[1], M. Jarrell[2] and H. R. Krishnamurthy[2]

[1] *Department of Physics, University of Cincinnati - Cincinnati, OH 45221, USA*
[2] *Department of Physics, IISc - Bangalore 560012, India*

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Abstract. – We discuss the "exhaustion" problem in the context of the periodic Anderson model using iterated perturbation theory (IPT) within the dynamical mean-field theory. We find that, despite its limitations, IPT captures the exhaustion physics, which manifests itself as a dramatic, strongly energy-dependent, suppression of the effective hybridization of the self-consistent Anderson impurity problem. As a consequence, low-energy scales in the lattice case are strongly suppressed compared to the "Kondo scale" in the single impurity picture. The IPT results are in qualitative agreement with recent Quantum Monte Carlo results for the same problem.

Introduction. – Metallic compounds containing rare-earth elements with partially filled f shells, such as $CeBe_{13}$ or UPt_3, belong to the general category of heavy-fermion materials [1]. They are characterized by large Pauli susceptibility and specific-heat coefficient as compared to ordinary metals, which indicate a huge effective electronic mass; and also by anomalous transport properties such as non-monotonic temperature-dependence of the resistivity. These anomalies are usually attributed to the formation of a narrow resonant state at the Fermi energy due to the admixture of strongly correlated local f orbitals with the metallic band of the host. Such materials are normally modelled in terms of an asymmetric periodic Anderson model (PAM). But many of the high-temperature properties of these materials are surprisingly similar to those of a single-impurity Anderson model (SIAM) [2]; so the formation of this resonance has also been sometimes interpreted in terms of the SIAM [3]. However, an impurity treatment clearly neglects the effects of correlations between the impurity sites and also of lattice coherence (*i.e.*, Bloch's theorem) which leads to what Nozières [4,5] termed as "exhaustion".

The "exhaustion" problem [4,5], originally posed by Nozières in the context of a *Kondo lattice*, occurs when a *few* mobile electrons, $N_{\rm scr}$, have to coherently screen *many* local moments, $N_{\rm f}$, in a metallic environment, *i.e.* $N_{\rm scr} \ll N_{\rm f}$. This situation is engendered by the fact that only the electrons roughly within $T_{\rm K}$ (the single-impurity Kondo temperature) of the Fermi surface can effectively participate in screening the local moments. Thus the number of

screening electrons can be estimated as $N_{\rm scr} = \rho_{\rm d}(\epsilon_{\rm F})T_{\rm K}$, where $\rho_{\rm d}(\epsilon)$ is the *conduction band* density of states (DOS) and $\epsilon_{\rm F}$ is the Fermi level. A measure of exhaustion is the dimensionless ratio [4]

$$p = \frac{N_{\rm f}}{N_{\rm scr}} = \frac{N_{\rm f}}{\rho_{\rm d}(\epsilon_{\rm F})T_{\rm K}}\,. \tag{1}$$

Nozières has argued that p is roughly the number of scattering events between a local moment and a mobile electron necessary for the mobile electron's spin to precess around a local moment by 2π [5]. In the case $p \gg 1$, when the number of screening electrons is much smaller than the number of local moments to screen, magnetic screening is necessarily collective and the single-impurity picture becomes invalid.

In a recent study [6] of the PAM using the dynamical mean-field theory (DMFT), which is exact in the ∞-dimensional limit [7], it was argued that exhaustion was responsible for the severe reduction of the Kondo scale of the PAM from that of the impurity problem with the same parameters. The issue was explored in detail [6] using the quantum Monte Carlo-maximum entropy method (QMC-MEM) for solving the self-consistent Anderson impurity problem of the DMFT. The reduction of the Kondo scale and the crossover between the two scales was interpreted in terms of Nozières exhaustion principle [4], and his mapping of the model which has exhausted all available conduction band screening states onto an effective Hubbard model. Using qualitative and semi-quantitative arguments, Nozières [5] has suggested that the temperature scale $T_{\rm c}$ associated with the onset of Fermi liquid coherence in this "exhaustion" limit is suppressed compared to the Kondo temperature of the single-impurity Anderson model (SIAM), $T_{\rm K}$, by the factor p,

$$T_{\rm c} \simeq T_{\rm K}/p = T_{\rm K}^2 \rho_{\rm d}(\epsilon_{\rm F})/N_{\rm f}\,. \tag{2}$$

While the afore-mentioned suppression of $T_{\rm c}$ was clearly evident in the QMC simulations, no universal relation of $T_{\rm c}$ to $T_{\rm K}$ such as eq. (2) was found.

In this work, we explore the problem of exhaustion in the context of the asymmetric PAM once again within the DMFT, but using iterated perturbation theory (IPT) [8] for solving the self-consistent impurity problem. We calculate the spectral functions and as a check on the accuracy of IPT, compare them with earlier QMC-MEM results [6]. We find reasonable agreement between the two. The full width at half-maximum (FWHM) of the "Kondo Resonance" in the spectral functions calculated for the PAM and the SIAM provides *one measure* of the "coherence temperature" $T_{\rm c}$ and the "Kondo temperature" $T_{\rm K}$, respectively. We find that, consistent with the "protracted screening" picture of ref. [6] and the "collective Kondo screening" picture of Nozières [5], a key feature of exhaustion, namely the suppression of $T_{\rm c}$ as compared to $T_{\rm K}$, is recovered here as well. Furthermore, we find $T_{\rm c}$ and $T_{\rm K}$ to be related as

$$T_{\rm c} = \frac{T_{\rm K}}{\alpha(U,V)p_0}\,. \tag{3}$$

Here $\alpha(U,V)$ is the fitting parameter and p_0 is defined (similarly to eq. (1)) as $p_0 \equiv N_{\rm f}/(\rho(x)T_{\rm K})$, where $\rho(\epsilon)$ is the bare conduction DOS and x is determined by $n_{\rm d} = 2\int_{-\infty}^{x} {\rm d}\epsilon\, \rho(\epsilon)$.

Model and formalism. – The PAM Hamiltonian on a D-dimensional hypercubic lattice is

$$\begin{aligned} H \;=\; & \frac{-t^*}{2\sqrt{D}} \sum_{\langle ij\rangle\sigma} (d^\dagger_{i\sigma} d_{j\sigma} + {\rm H.c.}) + \sum_{i\sigma} (\epsilon_d d^\dagger_{i\sigma} d_{i\sigma} + \epsilon_f f^\dagger_{i\sigma} f_{i\sigma}) + \\ & + V \sum_{i\sigma} (d^\dagger_{i\sigma} f_{i\sigma} + {\rm H.c.}) + U \sum_i n_{fi\uparrow} n_{fi\downarrow}\,. \end{aligned} \tag{4}$$

In eq. (4), $d^{(\dagger)}_{i\sigma}(f^{(\dagger)}_{i\sigma})$ is a creation operator that creates a $d(f)$-electron with spin σ on site i; $d_{i\sigma}(f_{i\sigma})$ is the corresponding destruction operator. The hopping is restricted to the nearest neighbors and scaled as $t = t^*/2\sqrt{D}$. U is the on-site Coulomb repulsion for the localized f states, V is the hybridization between d and f states and ϵ_f, ϵ_d are the site energies for f and d electrons.

We work in the $D \to \infty$ limit where it was shown by Metzner and Vollhardt [7] that the irreducible self-energy and the vertex functions become purely local. As a consequence, the interacting lattice model can be mapped onto a local correlated impurity coupled to an effective bath that is self-consistently determined [9,10]. In this infinite-dimensional limit the non-interacting DOS has the Gaussian form [7] $\rho(\epsilon) = \frac{1}{\sqrt{\pi}\,t^*} \exp[-\frac{\epsilon^2}{t^{*2}}]$. We choose our energy scale such that $t^* = 1$.

The local f- and d-propagators for the PAM are given by

$$G_{d,\mathrm{loc}}(\omega) = \tilde{D}\left(\omega^+ - \epsilon_d - \frac{V^2}{\alpha(\omega)}\right), \tag{5}$$

and

$$G_{f,\mathrm{loc}}(\omega) = \frac{1}{\alpha(\omega)}\left[1 + \frac{V^2}{\alpha(\omega)} G_{d,\mathrm{loc}}(\omega)\right], \tag{6}$$

where $\tilde{D}(z) \equiv \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{\rho(\epsilon)}{z-\epsilon}$ is the Hilbert transform of $\rho(\epsilon)$ and $\alpha(\omega) \equiv \omega^+ - \epsilon_f - \Sigma(\omega^+)$, where $\omega^+ = \omega + i0$.

The self-consistent host is determined by the bare local propagator of the effective single site problem as

$$\mathcal{G}^{-1} = G^{-1}_{f,\mathrm{loc}} + \Sigma\,. \tag{7}$$

and self-consistency is achieved through the use of eqs. (5), (6) and the result for the self-energy for the single-site, or the impurity problem $\Sigma \equiv \Sigma(\mathcal{G})$.

Given a starting self-energy, we use eqs. (5), (6) and (7) to compute $\mathcal{G}$, and then a prescription for the effective single-impurity problem to calculate the new self-energy. This procedure is repeated until self-consistency is achieved. We use Iterated Perturbation Theory (IPT) [8] as the prescription to calculate the self-energy for the effective impurity problem. The motivation for using this scheme is that it is semi-analytical and much easier to implement than Quantum Monte Carlo (QMC). While it has the disadvantage that it is perturbative, its advantages are that we obtain real-frequency data directly at zero temperature and can study a wide range of parameters with much less effort compared to the QMC method. We now briefly review this scheme.

The IPT ansatz [8] for the total self-energy is given by

$$\Sigma_{\mathrm{int}}(\omega) = \frac{U\langle n_f\rangle}{2} + \frac{A\Sigma_2(\omega)}{[1 - B\Sigma_2(\omega)]}\,, \tag{8}$$

where $\Sigma_2(\omega)$ is the second-order self-energy defined in terms of a modified bare local propagator $\tilde{\mathcal{G}}^{-1} = \mathcal{G}^{-1} + \epsilon_f + \mu_0$. The parameter μ_0 is adjusted so as to satisfy Luttinger's theorem [11], $\mathrm{Im}\int_{-\infty}^{0} \frac{\partial\Sigma(\omega)}{\partial\omega} G_f(\omega)\mathrm{d}\omega = 0$. A and B are chosen so as to reproduce the atomic limit and the high-frequency behavior of the self-energy at any filling, which yields [8]

$$A \equiv \frac{n_f(2-n_f)}{n_0(2-n_0)};\; B \equiv \frac{4((1-n_f/2)U + \epsilon_f + \mu_0)}{n_0(2-n_0)U^2}\,. \tag{9}$$

Here $n_f \equiv 2\int_{-\infty}^{0} \rho_f(\omega)\mathrm{d}\omega$ is the f-band filling and n_0 is defined by $n_0 \equiv 2\int_{-\infty}^{0} \rho_{\tilde{\mathcal{G}}}(\omega)\mathrm{d}\omega$, where ρ_f and $\rho_{\tilde{\mathcal{G}}}$ are the spectral functions of G_f and $\tilde{\mathcal{G}}$, respectively: $\rho_f \equiv -\frac{1}{\pi}\mathrm{Im}G_f(\omega^+)$, and $\rho_{\tilde{\mathcal{G}}} \equiv -\frac{1}{\pi}\mathrm{Im}\tilde{\mathcal{G}}(\omega^+)$.

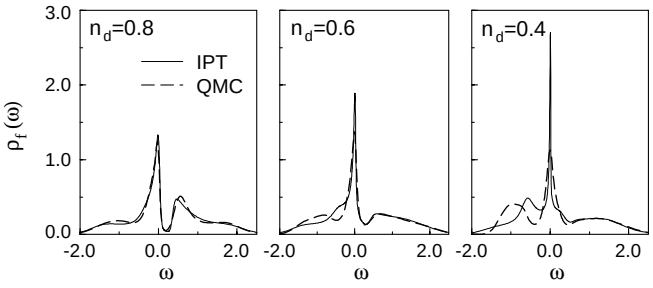


Fig. 1 – Comparison of the f density of states obtained from IPT and QMC for three fillings of the conduction band, $n_d = 0.4, 0.6, 0.8$, with $n_f \simeq 1$, for $U = 1.5$, $V = 0.6$. $T = 0$ for IPT and $T = 0.025$ for QMC. The agreement is quite good for d-fillings close to one.

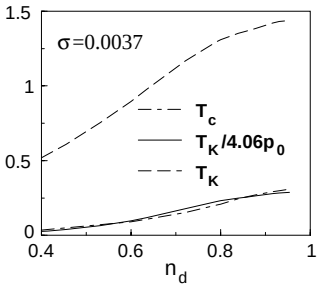
The conduction band filling is varied by varying ϵ_d. We maintain an f-band filling close to one, *i.e.* $n_f \simeq 1$ by adjusting ϵ_f. The actual value used for n_f was 0.99, and the accuracy achieved in fixing this value was ~ 1 in 10^5. For reasons of numerical convenience, we calculate the second-order self-energy directly for real frequencies in two steps. We first calculate the imaginary part of Σ_2 using convolution integrals on a Lorentzian frequency grid; then use Kramer's-Kronig relations to find its real part. Typically we achieve self-consistency of the Green functions within 3 to 4 iterations and the solution for ϵ_f and μ_0 is found within 10 (outer loop) iterations using a non-linear equation solving routine.

Results. – We have performed the calculations described above for various values of U and V and we present and discuss some representative results. Since IPT is a perturbative technique, we have checked its accuracy by comparing it with the earlier QMC-MEM [6] results for $U = 1.5$ and $V = 0.6$.

Figure 1 shows the f-spectral function for IPT at zero temperature and QMC-MEM at $T = 0.025$ for three conduction band fillings, namely $n_d = 0.4, 0.6$ and 0.8. Both the QMC-MEM and IPT results share some common features. For small n_d a single narrow Kondo peak is centered at the Fermi energy $\omega = 0$; however as $n_d \to 1$, the peak broadens and splits into two, with both peaks shifted from the Fermi energy. Apparently, the latter is a remnant of the insulating gap found when $n_f + n_d = 2$. We see that the IPT results match rather well with QMC-MEM for $n_d = 0.8$, but as n_d is decreased the deviation increases. The difference in the width of the Kondo resonance between IPT and QMC in the low n_d or the exhaustion limit could be due to two factors: 1) the calculations for the latter were carried out at higher temperatures which would lead to temperature broadening, 2) IPT is perturbative in U while the impurity Kondo energy scale, $T_{\rm K}$ is exponential in U. Thus, IPT could become less accurate for very small n_d since the effective $\Gamma(0)$ is decreasing as n_d decreases (see below).

In the QMC-MEM work [6], the SIAM Kondo scales and the PAM coherence scales were identified from the $T \to 0$ limit of the inverse of the appropriate impurity spin susceptibility, $\chi^{-1}_{\rm imp}(T \to 0)$. Since the IPT is not a conserving approximation, it does not provide a unique prescription for calculating $\chi_{\rm imp}$. Hence, *as an alternate measure of the Kondo and coherence scales*, we calculate the Full Width at Half-Maximum (FWHM) of the Kondo resonance in the f-spectral function for the SIAM and PAM and identify these with $T_{\rm K}$ and $T_{\rm c}$, respectively ([1]). We present our results for these in fig. 2(a) for $U = 1.5$ and $V = 0.6$. $T_{\rm c}$ is seen to be much

([1]) For the SIAM, it is well known [12] that both $\chi^{-1}_{\rm imp}(T \to 0)$ and the FWHM are proportional to the same $T_{\rm K}$.



U	1.5	1.5	2.0	2.0
V	0.5	0.6	0.5	0.6
α	1.4	4.06	0.75	2.55
σ	0.0041	0.0037	0.0050	0.0033

Fig. 2 – (a) The full width at half-maximum for the Kondo resonance in the f-spectral function (which is taken as a measure of "$T_{\rm K}$" for the SIAM and "$T_{\rm c}$" for the PAM) for $U = 1.5$ and $V = 0.6$ as a function of the conduction band filling. The solid line shows $T_{\rm K}/\alpha(U,V)p_0$. σ is the standard deviation for fitting the above relation to $T_{\rm c}$ with α as the adjustable parameter. (b) Table showing the values of α and σ for four sets of U and V.

suppressed as compared to $T_{\rm K}$, consistent with Nozières' arguments [4,5] and the QMC-MEM results [6]. As mentioned earlier, we find that $T_{\rm c}$ and $T_{\rm K}$ are related according to eq. (3). We have checked this for four sets of parameters and we show the values of α and σ (standard deviation of the fit in eq. (3)) in fig. 2(b) for each of these sets.

The PAM, even at zero temperature, clearly has many other scales, *e.g.* $\kappa^{-1} = [\partial^2\Sigma_{\rm Im}/\partial\omega^2|_{\omega=0}]^{-1}$, although they are also related to one another. In the exhaustion limit, they are all typically suppressed compared to $T_{\rm K}$, though to different degrees. We have studied all of them, and hope to discuss them elsewhere.

But the important point is that, given that the PAM is being treated using DMFT, all the energy scales in the problem are clearly determined by U and by the effective hybridization of the self-consistent Anderson-impurity problem $\Gamma_{\rm PAM}(\omega) \equiv \ {\rm Im}\mathcal{G}^{-1} = {\rm Im}(G^{-1}_{f,{\rm loc}} + \Sigma)$.

$\Gamma_{\rm PAM}$ is shown in fig. 3 as calculated within QMC-MEM [6] and IPT, and again the agreement is reasonable over a fairly wide frequency scale. In as much as $\mathcal{G}$, the (self-consistent) host propagator, has built into it the self-energy (and hence the "Kondo" screening) processes at all other sites of the lattice except the one under consideration, $\Gamma_{\rm PAM}(\omega)$ *necessarily encapsulates the essential constraints of lattice coherence and collective screening that leads to "exhaustion".* In fig. 4(a), we compare $\Gamma_{\rm PAM}(\omega)$ with the bare hybridization $\Gamma_{\rm SIAM}(\omega) \equiv \pi V^2\rho(\omega+x)$ (where ρ and x are defined below eq. (3)). Note that $\Gamma_{\rm PAM}$ is overall strongly suppressed compared

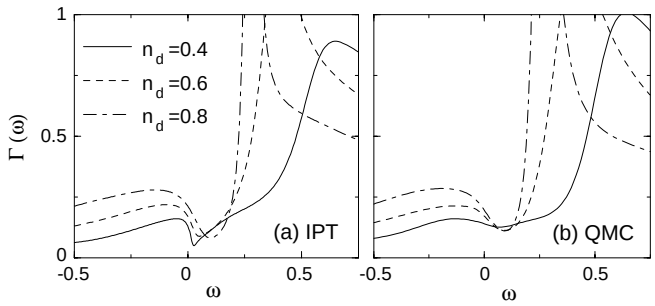


Fig. 3 – The effective hybridization within (a) IPT and (b) QMC-MEM for the same parameters as fig. 1 showing the decrease in the number of states available for Kondo screening near the Fermi level.

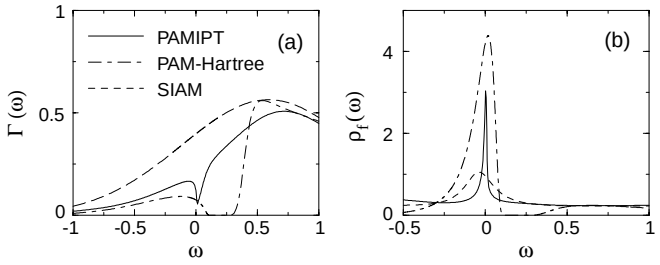


Fig. 4 – (a) The PAM-IPT, the PAM-Hartree and the SIAM hybridization showing the effects of lattice coherence and exhaustion for $U = 1.5$, $V = 0.5$, and $n_d = 0.4$. Near the Fermi level, the PAM-IPT Γ has a dip reflecting a strong energy dependence. Both the PAM-IPT and Hartree Γ are seen to be much suppressed compared to the SIAM Γ. (b) The corresponding f-spectral functions are shown for the same parameters as (a). The Kondo peak broadens for the three cases progressively.

to $\Gamma_{\rm SIAM}$, and in addition has a sharp dip near $\omega = 0$. The suppression of $T_{\rm c}$ (and of other scales) compared to $T_{\rm K}$ is directly related to the suppression of $\Gamma_{\rm PAM}$ compared to $\Gamma_{\rm SIAM}$, as dramatically brought out by the direct comparison of their spectral functions in fig. 4(b).

In fig. 4(a), we also compare $\Gamma_{\rm PAM}$ with the Hartree hybridization $\Gamma_{\rm Hartree}(\omega)(\equiv {\rm Im}(G^{-1}_{f,{\rm loc}})$ where the latter is computed within the Hartree approximation). $\Gamma_{\rm Hartree}$ can be interpreted as an effective hybridization that arises when the self-consistent impurity problem is treated within the Hartree approximation. Note that it is also strongly suppressed compared to $\Gamma_{\rm SIAM}$, which can be thought of as being due to exhaustion in the context of "resonant level screening". However, it is rather flat near the fermi level and misses the strong energy dependence contained in the dip in $\Gamma_{\rm PAM}(\omega)$. As shown in fig. 4(b), the FWHM of the Kondo resonance is of course much smaller than that of the Hartree spectral function, since the latter has only the resonant-level scales arising from $\Gamma_{\rm Hartree}$, while the former includes (at least some of the) non-trivial correlation effects which lead to local moment formation and *Kondo screening* and the associated narrowing of scales. This suggests that the strong *energy-dependent* suppression of $\Gamma_{\rm PAM}$ is the signature of exhaustion in the context of lattice coherent, collective, Kondo screening.

From the arguments we have presented, one would expect that there should be no such exhaustion effects if $N_{\rm scr} \gg N_{\rm f}$. We have studied such cases as well, and that is indeed what we find. As we decrease $N_{\rm f}$ keeping n_d fixed, we find an increase in the FWHM of the resonance at the Fermi level, the dip in the effective hybridization near the Fermi level gradually disappears. $\Gamma_{\rm Hartree}$ and $\Gamma_{\rm PAM}$, although still somewhat suppressed compared to $\Gamma_{\rm SIAM}$, become almost identical and have a weak energy dependence near the Fermi level, indicating that the screening processes in this limit are predominantly "resonant level screening".

Conclusions. – We have studied the "exhaustion" problem arising from lattice coherent, collective, Kondo screening in the context of the asymmetric PAM in the limit of infinite dimensions within IPT. The IPT calculations, despite their limitations, capture (qualitatively and in some regimes, even quantitatively) many of the features shown by the QMC calculations [6], including the "exhaustion" physics, which manifests itself as a strongly energy-dependent suppression of the effective hybridization $\Gamma(\omega)$. *As a consequence*, all the (low) energy scales of the PAM are strongly suppressed compared to the corresponding SIAM scales. We have presented detailed results for *one of them, namely the FWHM of the Kondo resonance*, and find that *its* suppression ratio is roughly as proposed by Nozières (except for

a (U, V)-dependent scale factor). Together, these results also suggest that IPT would be a useful method for incorporating moderate correlation effects into *ab initio* calculations of heavy-fermion materials [13].

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