Extended Dynamical Mean Field Theory Study of the Periodic Anderson Model

Ping Sun$^1$ and Gabriel Kotliar$^1$

$^1$Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019

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We investigate the competition of the Kondo and the RKKY interactions in heavy fermion systems. We solve a periodic Anderson model using Extended Dynamical Mean Field Theory (EDMFT) with QMC. We monitor simultaneously the evolution of the electronic and magnetic properties. As the RKKY coupling increases the heavy fermion quasiparticle unbinds and a local moment forms. At a critical RKKY coupling there is an onset of magnetic order. Within EDMFT the two transitions occur at different points and the disappearance of the magnetism is not described by a local quantum critical point.

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The interaction between local moments and conduction electrons is a long standing problem in condensed matter physics. As discussed early on [1,2], two competing interactions, the Kondo exchange between the conduction electrons and the moments, and the indirect exchange among the moments mediated by the RKKY interaction, are central to this problem.

The physics at high temperatures is well understood. Moments and conduction electrons retain their identities and interact weakly with each other. The central question in this field is to understand the characteristics of the state that develops as the temperature is lowered. When the RKKY interaction is much larger than the Kondo energy, the moments order magnetically and the conduction electrons follow their magnetization without undergoing a strong renormalizations. The spin entropy is mostly quenched by the ordering of the local moments. When the RKKY interaction is much weaker than the Kondo energy, the spin entropy is absorbed by the interaction of the moments and the conduction electrons. This results in the formation of a heavy Fermi liquid of quasiparticles which are composites of local moment spins bound to the conduction electrons. The description of the low temperature state, when both the RKKY and the Kondo interactions are of comparable magnitude, has been an important unresolved question. It has received renewed theoretical interest motivated by the intensive experimental investigation of two materials, YbRh$_2$Si$_2$ [4] and CeCu$_{6-x}$Au$_x$ [5], which can be driven continuously from the paramagnetic (PM) phase to the antiferromagnetic (AF) phase by application of pressure, alloying and magnetic field. Near the quantum critical point, RKKY and Kondo interactions are both essential and need to be treated on the same footing. It has not been possible [3,4] to describe the quantum phase transition in these materials within the standard Hertz-Millis-Moriya (HMM) framework [3,4,10] so far.

The interplay of Kondo and RKKY interactions has been addressed using slave boson mean field methods and large-N expansions [11]. This method can capture the Kondo effect and the Fermi liquid phase. The introduction of bond variables allows some description of the effects of magnetic correlations in the heavy Fermi liquid state. However the simultaneous description of the antiferromagnetism and heavy Fermi liquid behavior within this technique is still an open problem. Furthermore, mean field methods can not capture the incoherent part of the electron Green’s function which is important near the transition. This problem becomes more tractable near the PM metal to spin glass transition [12].

With the development of Dynamical Mean Field Theory (DMFT) [13], which can treat both the AF states and the Kondo effect, it has been possible to make further progress in this problem [14,15]. An extension of DMFT (EDMFT) [16], which allows a better treatment of the competition between the exchange interaction and kinetic energy, was first applied in the context of a one-band model by Parcollet and Georges [17] and more recently by Haule et al. [18] who established that the increasing exchange reduces the coherence temperature. The Kondo lattice with magnetic frustration in the large-N limit was recently studied by Burdin et al. [19] who found a paramagnet to spin liquid quantum phase transition. Si et al. [20] considered the $SU(2)$ Kondo lattice model in the view point that the model can be described in terms of the criticality of an impurity model in a self-consistent medium. They concluded that in 2D and within EDMFT this model a) has a quantum critical point, b) the quantum critical point has nonuniversal exponents, and c) a numerical calculation [21] of this exponent has remarkable similarity to some of the experimental observations in the CeCu$_{6-x}$Au$_x$ system. However, no study of the magnetism had been carried out and this is the subject of this paper.

Our goal is to address these issues within the periodic Anderson model (PAM), focusing more on the evolution of the electronic structure at finite temperatures and not too close to the phase transition. We solve the model using EDMFT and a continuous field Hubbard-Stratonovich QMC method as an impurity solver [22,23].

The PAM Hamiltonian is given by:

$$H = \sum_{k\sigma} \epsilon_k n_{k\sigma} + V \sum_{i\sigma} (c_{i\sigma}^f f_{i\sigma} + f_{i\sigma}^f c_{i\sigma}) + E_f \sum_{i\sigma} n_{i\sigma}^f$$
where \(c_{i\sigma} (f_{i\sigma})\) annihilates a conduction (localized \(f\)) electron of spin \(\sigma\) at site \(i\). \(\eta_0 = a_{i\sigma}^\dagger a_{i\sigma}\), with \(a = c, f\), and \(S_{f\sigma}^f = n_{f\sigma}^f - n_{f\sigma}^f\). We introduce an independent RKKY interaction which can be induced by hybridization of the \(f\)-electron with either the \(c\)-electrons or the electrons in the other orbitals which are not included explicitly \[24\]. There is experimental evidence that the spin fluctuations \[25, 26\] near the critical doping are of quasi-2D nature in \(\text{CeCu}_{6-x}\text{Au}_x\). For technical convenience, we take a short range Ising AF RKKY exchange of the form \(J_{\text{RKKY}}(\cos q_x + \cos q_y)/2\). For the \(c\)-band we take the dispersion, \(\epsilon_{k} = (\cos k_x + \cos k_y + \cos k_z)/3\).

We then make the EDMFT approximation \[16, 22, 23\]. To describe the AF phase \[13\] we introduce formally two effective impurity models and use the symmetry that electrons at one impurity site is equivalent to the electrons on the other with opposite spins. The self-consistent condition involves the self-energies of both spins. The EDMFT equations in the PM phase are obtained when the self-energies do not depend on spin. The local Green’s functions and the self-energies are obtained from the quantum impurity model:

\[
S_{0} = -\int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{\sigma} f_{0,\sigma}^\dagger(\tau)G_{0,\sigma}^{-1}(\tau - \tau')f_{0,\sigma}(\tau')
\]

\[
\frac{1}{2} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \phi_0(\tau)D_{0}^{-1}(\tau - \tau')\phi_0(\tau')
\]

\[
+ U \int_{0}^{\beta} d\tau \left[ n_{0,\uparrow}^f(\tau) - 1/2 \right] \left[ n_{0,\downarrow}^f(\tau) - 1/2 \right]
\]

\[- \int_{0}^{\beta} d\tau \phi_0(\tau) \left[ n_{0,\uparrow}^f(\tau) - n_{0,\downarrow}^f(\tau) \right]. \tag{2}\]

\(G_0\) and \(D_0\) play a role of the dynamical Weiss functions and describe the effect of the environment on the \(f\) electron and its spin. Their behavior is obtained from a self-consistent solution of the EDMFT equations:

\[
G_{ff,\sigma}^{\text{imp}}(ip_n) = \sum_{k} \frac{\xi_{\sigma}(k, ip_n)}{[\xi_{\sigma}(k, ip_n)][\xi_{-\sigma}(k, ip_n)] - \eta(k, ip_n)^2}.
\tag{3}\]

\[
D_{\sigma}^{\text{imp}}(i\omega_n) = \sum_{q} J_{q}/[1 - J_q(\Pi(i\omega_n))]. \tag{4}\]

In Eq\(3\) we used

\[
\xi_{\sigma}(k, ip_n) = ip_n + \mu - [J_{q=0} + D_{0}(i0)]S_z
\]

\[-E_f - \Sigma_{-\sigma}(ip_n) - V^2 \frac{ip_n + \mu}{(ip_n + \mu)^2 - e_k^2} \eta(k, ip_n) = V^2 \epsilon_k/[(ip_n + \mu)^2 - e_k^2], \text{ and } S_z = G_{ff,\uparrow}^{\text{imp}}(0^-) - G_{ff,\downarrow}^{\text{imp}}(0^-).\] The \(f\)-electron and the boson self-energies are obtained by the local Dyson equations. \(p_n\) and \(\omega_n\) are the fermion and boson Matsubara frequencies, respectively. The boson self-energy and the experimentally relevant spin susceptibility are related by \[23\]:

\[
[\chi(q, i\omega_n)]^{-1} = -J_q + [\Pi(i\omega_n)]^{-1}. \tag{5}\]

We use QMC \[23\] to solve the impurity problem described by Eq\.(2). Eqs\.(3) and \(4\) are then applied. This forms one iteration loop from which the new dynamical Weiss functions are obtained for the next iteration until convergence. We use \(U = 3.0, V = 0.6, E_f = -0.5, \mu = 0.0\). The number of time slices in QMC is \(L = 16\) for \(\beta \leq 8.0, L = 32\) for \(8.0 \leq \beta \leq 20.0\), and \(L = 64\) for \(16.0 \leq \beta \leq 32.0\). The number of QMC sweeps is typically \(10^6\). We measure the energies in terms of the Kondo temperature at zero \(J_{\text{RKKY}}\) coupling, \(T_k^x = 1/\beta\). \(S_z \equiv 1/8.0\), which is determined from the position of the peak in the local susceptibility vs temperature plot (see Fig\. 3 below).

![FIG. 1: The EDMFT phase diagram of the PAM. The diamonds and circles are the EDMFT results of the phase boundaries. In between the two solid lines connecting the symbols, \(J_{c1}\) and \(J_{c2}\), we find both the PM and the AF solutions.](attachment:figure1.png)
tends to be more strongly first order at low temperatures. As we increase $J_{RKKY}$ at fixed $T$, the $f$-electron becomes more localized (Im$\chi^{-1}_n(\omega_n)$ becomes smaller at low frequencies) while the local spin fluctuations are strongly enhanced in the neighborhood of the $J_{c2}$ line ($D_0(\omega_n)$ becomes bigger at low frequencies) [27]. EDMFT self-consistency is crucial in obtaining the results, which are absent in the simple impurity model.

An important question is the effect of the RKKY interaction on the quasiparticle mass. The RKKY interaction partially locks the spins and thus reduces the effective mass and the spin entropy. But it also serves as an additional interaction among the quasiparticles which increases the effective mass. To address this question, we plot at $T/T^0_k = 1.0$ the inverse quasiparticle residue $Z^{-1}$ as a function of $J_{RKKY}$ in Fig. 2 $Z^{-1}$, which is proportional to the effective electron mass, gets enhanced as the transition is approached from both sides. This mass enhancement is not included in the HMM. We predict that the mass enhancement of the majority carriers is larger than that of the minority carriers in the AF phase. In the inset to Fig. 2 we display the extrapolation of the self-energy to zero Matsubara frequency. The bigger this value, the shorter the lifetime of the excitations.

We now turn to the evolution of the magnetic properties as a function of temperature and $J_{RKKY}$. In Fig. 4 we plot the local susceptibility. Following the PM solution we sweep the phase diagram from $J_{RKKY} = 0$ up to the line $J_{c2}$ in Fig. 1. In this procedure, the position of the Kondo peak moves towards lower temperature and its height has an increment of about 37%. If we solve the EDMFT equations without forcing any magnetic order, either the PM or AF solution can appear. For $J_{RKKY}/T^0_k \geq 2.00$, we see the Neel cusp first occurs below the Kondo peak which disappears as $J_{RKKY}$ increases further. This happens before the Kondo temperature goes to zero, consistent with the HMM.

To further test the local critical scenario [21] we follow the evolution of the PM solution as a function of temperature and frequency. In Fig. 4 we plot $-1/\chi_{AF}(\omega_n)$, which is defined as $-1/\chi(\tilde{q}, \omega_n)$ at $\tilde{q} = (\pi, \pi)$, as $J_{RKKY}$ is changed. One can see from the inset that, as the transition is approached, the zero frequency value $1/\chi_{AF}(i0)$ vanishes. From the curvature of the lines one can see that the frequency dependences of $1/\chi_{AF}(\omega_n)$ does not seem to be consistent with a sublinear behavior required by the local quantum critical scenario. In stead, it is compatible with the standard HMM picture and a recent large-N study [28].

In summary we have studied the PAM within EDMFT.

FIG. 2: The evolution of the inverse quasiparticle residue $Z^{-1}$ at a fixed temperature $T/T^0_k = 1.0$ as a function $J_{RKKY}$. In our calculation, the majority spin is spin-up. The majority spin band in the AF phase is more strongly renormalized. In the inset, we plot the extrapolation of the $f$-electron self-energy to zero Matsubara frequency. The bigger this value, the shorter the lifetime of the excitations.

FIG. 3: The evolution of Kondo peak into the Neel cusp as $J_{RKKY}$ is increased. In the cases where the symbols are connected by the solid lines, we solve the EDMFT equations by forcing the PM order. The results with dashed lines are obtained without such a constraint. The inset shows the behavior around the Kondo peak with the same symbol scheme.

FIG. 4: The inverse static spin susceptibility at the AF ordering wave vector $\tilde{k} = (\pi, \pi)$ at $T/T^0_k = 0.25$. We plot the frequencies $\omega_n \leq 2\pi/\beta^0_k$. The inset is the susceptibility at zero Matsubara frequency vs the RKKY exchange.
In the parameter regime studied, we found that the heavy quasiparticles first form, and then undergo a magnetic phase transition. This would indicate that the HMM description of the quantum phase transition would apply to this model. On the other hand, we also find a large enhancement of the effective mass and reduction of the quasiparticle lifetime, which are beyond the standard model.

This paper raises a large number of questions that require further investigations. The first one is the connection between our results and those reported in EDMFT studies of the Kondo lattice models by Si et al. [20, 21, 22]. Our model is in the mixed valence region where the charge fluctuations can not be neglected. To reconcile the difference in the results one could study the Anderson model in a regime of parameters that is closer to the Kondo lattice model. This probably will require the use of a different impurity solver, to test if the PM-AF transition becomes more weakly first order as the Kondo limit (larger $U$ and more negative $E_F$) is approached. The second question is the relevance of the EDMFT results to real materials and how the mean field theory should be interpreted. EDMFT is a mean field treatment of the spatial degrees of freedom and breaks down in the immediate vicinity of the transition. Clearly in the coexistence region of the upper part of the phase diagram (region I), EDMFT is unreliable [30]. In finite dimensions the system has a non-trivial anomalous dimension and the transition is second order. There is a region in the vicinity of the transition where non-Gaussian thermal fluctuations are important in reality and they are absent in the EDMFT theory. But outside the vicinity of this transition we expect the predictions of the theory such as the weak enhancement of the effective mass to be observable. Indeed, while EDMFT induces a spurious first order transition, in the high temperature regime where the semiclassical evaluation of the free energy is valid, EDMFT gives a very accurate determination of the location of the first order phase transition [24, 30].

The EDMFT solution existed between $J_1(T)$ and $J_2(T)$ lines at low temperatures (region II) suggests a crossover to a different regime where non-local effects become important. This has been recently observed in the YbRh$_2$Si$_2$ system [31]. Here again EDMFT is not reliable in the vicinity of the transition and some element of non-locality becomes important. To improve the description of this region and to reduce the strength of the first order phase transitions and other deficiencies of EDMFT, in particular the fact that the spins in the bath are treated classically rather than quantum mechanically, a different extension of DMFT to treat a cluster of spins in a self-consistent medium is needed. This line of work will lead to a two impurity Kondo or Anderson model [32, 33] in a self-consistently determined bath which is known to have a different critical point than the spin model in a random magnetic field.

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