Zero-temperature magnetism in the periodic Anderson model in the limit of large dimensions

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We study the magnetism in the periodic Anderson model in the limit of large dimensions by mapping the lattice problem into an equivalent local impurity self-consistent model. Through a recently introduced algorithm based on the exact diagonalization of an effective cluster hamiltonian, we obtain solutions with and without magnetic order in the half-filled case. We find the exact AFM-PM phase boundary which is shown to be of $2^{nd}$ order and obeys $V^2/U \approx \text{const}$. We calculate the local staggered moments and the density of states to gain insights on the behavior of the AFM state as it evolves from itinerant to a local-moment magnetic regime.

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I. INTRODUCTION

The periodic Anderson model (PAM) consists of a band of $d-$electrons that hybridizes with localized $f-$electron states at each lattice site. The double occupation of the $f-$sites is disfavored by a local term that corresponds to the repulsive Coulomb interaction.

This model Hamiltonian is widely considered to be relevant for the description of a large class of strongly correlated systems, most notably, the so called heavy fermions and Kondo insulators. Examples of these systems are, among others, $UPt_3$, $CeAl_3$, the insulators $Ce_3Bi_4Pt_3$, $CeNiSn$, and possibly $FeSi$ and $SmB_6$.

Despite much effort, our present theoretical knowledge about the variety of behaviors that solutions of this model may have, is still limited. Much of our current understanding of the model comes from approaches based in the consideration of a variational ansatz and also from its formulation in limiting cases where the problem becomes more tractable, as for instance, the large $N$ approach.

On the other hand, the steady increase of computational power, has recently made possible the numerical study of the model in 2-dimensional finite lattices by quantum Monte Carlo techniques. However, that numerical technique has some intrinsic limitations in regard of the parameter space that can be investigated, in particular the $T \to 0$ limit.

In this paper, we will consider the problem within the local impurity self-consistent approximation (LISA). This method was introduced in the present form by Georges and Kotliar in the context of the Hubbard model, and later generalized for other models (including the PAM) by Georges, Kotliar and Si. It can be thought of as a dynamical mean field theory for correlated electron systems. Its basic idea is to isolate a local site of the lattice model and embed it in an effective bath that contains the information of the response of the rest of the lattice.

The LISA method becomes exact in the limit of large number of spatial dimensions. Therefore, it also represents a limiting formulation of the model where simplifications occur (e.g. the self-energy becomes local), that allow us to obtain essentially exact results. This method has already been used in the periodic Anderson model for the investigation of the paramagnetic solution at finite temperature.

It should be emphasized here, that due to the local character of the approach, it should be most suitable for the study of electronic systems where the relevant orbitals are very localized. Also, since the interactions can be considered in a non perturbative manner, it is most appropriate when the correlations play a crucial role. These features are clearly a characteristic of experimental systems such as heavy fermions and Kondo insulators where the PAM is considered to be most relevant.

In this paper we focus on the study of solutions with magnetic order at $T = 0$. In particular, we will present the exact phase diagram. We will also study the nature of the different antiferromagnetic regimes that the solution displays. To this end we obtain the staggered magnetic moments and the densities of states in various regions of the model parameter space.

The question of the study of magnetically ordered solutions was previously considered by Doniach in the context of the Kondo lattice, and by Evans and , more recently, by Sun et al. in the PAM.
We conclude with a brief discussion on the relevance that our results may have for the interpretation of experimental results.

II. METHODOLOGY

The formulation of the LISA method has been already discussed in detail elsewhere[1], so here we shall limit ourselves to a brief presentation of the relevant expressions in particular we shall note how they are modified to consider solutions with magnetic order.

We begin by writing the action of the lattice model in its Function Integral form

$$ S = - \sum_{k,\sigma} \int_{0}^{\beta} d\tau d\tau' \psi_{k\sigma}^{\dagger}(\tau)G_{0\sigma}^{-1}(\tau - \tau')\psi_{k\sigma}(\tau') + U \sum_{i} \int_{0}^{\beta} d\tau (n_{i\uparrow}(\tau) - \frac{1}{2})(n_{i\downarrow}(\tau) - \frac{1}{2}) $$

(1)

where the annihilation operator is defined as $\psi_{k\sigma} \equiv \{f_{\sigma}, d_{k\sigma}\}$, $U$ is the local repulsion for double occupation of the $i^{th}$ $f$-site, and $k$ runs over the Brillouin zone. The inverse matrix propagator $G_{0\sigma}^{-1}$ is explicitly

$$ G_{0\sigma}^{-1}(k, i\omega) = \begin{pmatrix} i\omega + \mu + \epsilon^0_f & V_k \\ V_k & i\omega + \mu - \epsilon_k \end{pmatrix} $$

(2)

where $\epsilon^0_f$ is the atomic energy of the $f$-site, $\mu$ is the chemical potential, and $V_k$ is the hybridization matrix element between the $f$ and the $d$-sites. Here, for simplicity, we take $V_k = V$, and consider the particle-hole symmetric case setting $\epsilon^0_f = \mu = 0$. Since in the limit of $d \to \infty$ the self-energy becomes local, i.e. $k$-independent, we can write the inverse Green function as

$$ G_{\sigma}^{-1}(k, i\omega) = \begin{pmatrix} i\omega - \Sigma_\sigma(i\omega) & V \\ V & i\omega - \epsilon_k \end{pmatrix} $$

(3)

To proceed further we consider the model on two sublattices A and B as is usually the case when dealing with antiferromagnetically ordered states, and demand the self-consistency condition that follows from the fact that the local Green function obeys

$$ G(i\omega) = \frac{1}{N} \sum_{k} G(k, i\omega) = \int_{-\infty}^{\infty} \rho^{0}(\epsilon)G(\epsilon, i\omega) d\epsilon $$

(4)

We consider, for simplicity, the case of a Bethe lattice, which in the large dimensional limit has a semi-circular free density of states $\rho^{0}(\epsilon) = \frac{2}{\pi\beta}(1 - \frac{\epsilon^2}{\beta^2})^2$. The half-bandwidth $\beta$ corresponds to a hopping parameter $t$ between neighboring $d$-sites with $\beta = 2t$. We set $\beta$ equal to unity. This density of states has the further advantage that naturally incorporates the same band-edge behavior as a 3-dimensional model. For a discussion of the hypercubic lattice see Ref. [12].

As a result, we arrive at the following local effective action

$$ S_{\text{local}} = - \sum_{\sigma} \int_{0}^{\beta} d\tau d\tau' \psi_{\sigma}^{\dagger}(\tau)G_{\sigma}^{-1}(\tau - \tau')\psi_{\sigma}(\tau') + U \int_{0}^{\beta} d\tau (n_{\sigma\uparrow}(\tau) - \frac{1}{2})(n_{\sigma\downarrow}(\tau) - \frac{1}{2}) $$

(5)

where $\psi_{\sigma} \equiv \{f_{\sigma}, d_{\sigma}\}$ is the operator associated to a site that we call origin (of a given sublattice, say, A). The local inverse propagator $G_{\sigma}^{-1}$ has the explicit form

$$ G_{0\sigma A}^{-1}(i\omega) = \begin{pmatrix} i\omega & V \\ V & i\omega - \frac{\beta^2}{4}[G_{\sigma B}]_{dd}(i\omega) \end{pmatrix} $$

(6)

where $G$ is the “cavity” Green function which has the information of the response of the lattice. In the present case of a Bethe lattice it simply becomes $G = G$. The symmetry properties of the two sublattice representation imply

$$ G_{\sigma A} = G_{-\sigma B} $$

(7)

so the self-consistency condition can be more concisely rewritten as
\[ [G_{\sigma A}^{-1}]_{dd}(i\omega) = i\omega - \frac{D^2}{4} [G_{\sigma A}]_{dd}(i\omega) \] (8)

and the lattice index can be dropped.

At this point it is worth pointing out that \( G_0 \) should not be confused with \( G_0 \). While the latter is the free propagator of the lattice model, the former corresponds to the free propagator of the effective impurity model which is local. Furthermore, \( G_0 \) is a quantity that is unknown a priori, and that has to be solved for self-consistently from equations (4), (6).

We solve this system of equations numerically by a recently introduced exact diagonalization procedure. It basically consist in introducing a parametrization for the \( G_{dd} \) in terms of the parameters of two continued fraction expansions that describe the “particle” (\( \omega > 0 \)) and “hole” (\( \omega < 0 \)) excitations.

\[ G_{dd}(\omega) = G_{dd}^>(\omega) + G_{dd}^<\omega, \] (9)

with

\[ G_{dd}^>(\omega) = \frac{\langle gs|dd|gs\rangle}{\omega - a_0^\omega - \frac{b_1^\omega}{\omega - a_1^\omega - \frac{b_2^\omega}{\omega - a_2^\omega - \ldots}}}, \]

\[ G_{dd}^<\omega = \frac{\langle gs|dd|gs\rangle}{\omega - a_0^\omega - \frac{b_1^\omega}{\omega - a_1^\omega - \frac{b_2^\omega}{\omega - a_2^\omega - \ldots}}} \] (10)

The continued fractions can be then thought of as resulting from an effective electronic bath where the impurity site is embedded. This bath consists of two chains, one for each continued fraction. The hopping elements between sites of the chains are the parameters \( b_i^+/< \), and the atomic energies of the sites are the \( a_i^+/< \). In Fig. 4 we schematically show the resulting effective Hamiltonian model for the local impurity site plus the effective electron bath. It can be straightforwardly verified that it renders the self-consistency equation (6).

Switching on the interaction \( U \), the cluster of \( N_S \) sites is then exactly diagonalized and the local Green functions are calculated as continued fractions. The parameters of this newly obtained continued fractions, are then feed back as new parameters for the effective bath chains. It should be noted that in the present case, where solutions with antiferromagnetic order are allowed, one should connect the spin \( \sigma \) chains to the spin \(-\sigma\) local \( d\) site as follows from equation (8).

The self-consistency is thus translated into the self-consistent determination of the parameters of a continued fraction representation of \( G_{dd} \). This numerical procedure represents an essentially exact solution of the model. The only approximation consists in the truncation of the length of the continued fractions, due to the finite size of the effective electron bath that can be dealt with. It has been demonstrated elsewhere that this approach is in excellent agreement with the solution obtained from a quantum Monte Carlo calculation. Moreover, it allows the investigation of regions of parameter space that are inaccessible for QMC, for instance, the \( T \to 0 \) and large \( U \) limit.

### III. MAGNETIC ORDER

#### A. Phase Diagram

We have performed extensive calculations for effective Hamiltonian clusters of \( N_S = 4, 6, \) and 8 sites in the \((U,V)\) parameter plane for fix \( D = 1 \). In Fig. 5 we show the exact magnetic phase diagram of the model. The parameter space is divided into two regions, one paramagnetic and the other with long range antiferromagnetic order. As is shown in the inset, the boundary line has the approximate form \( U_c \propto V_c^2 \). The interpretation of this result is simple. The onset of magnetic order is controlled by the crossing of two energy scales that depend on a single parameter \( J \) proportional to the exchange constant \( \frac{V^2}{U} \). If \( \frac{V}{D} >> 1 \), the magnetic moment on the \( f \)-site is Kondo-quenched by the band of \( d \)-electrons, rendering a paramagnetic state. On the other hand, for \( \frac{V}{D} << 1 \), the RKKY interaction \((\sim \langle F \rangle^\alpha, \alpha > 1)\) becomes dominant over the Kondo effect \((\sim e^{-\langle F \rangle})\). Therefore, the screening of the local moment becomes incomplete and the residual magnetic interaction along with the bipartite nature of the lattice drives the system to an antiferromagnetic state. We thus see that these energy scales cross at a critical value \( J_c \), and in consequence the \((U,V)\) parameter space is split into two phases with a boundary that obeys \( \frac{V^2}{U} \approx J_c \). We find from
the numerical solution that \( J_c \approx 0.075D \). This result is consistent with Doniach’s estimate for the critical value of \( J_c \). In the context of a one dimensional Kondo lattice, he found that at the mean field level \( \frac{J_c}{\Delta} \approx O(1) \) and argued that fluctuation effects should strongly reduce the ratio.

It is interesting to note that this result is qualitatively similar to the recently obtained by Vekić et al. for a 2-dimensional finite size lattice using quantum Monte Carlo. This lack of dimensional dependence represents a strong evidence for the applicability of the LISA method in the study of electronic systems where localized states and correlations play an essential role.

As it turns out, the transition is of 2\(^{nd}\) order along the whole critical line. This will be illustrated by the study of the magnetization below.

### B. Staggered Magnetization

We now consider the evaluation of the staggered magnetization. Since the present effective cluster hamiltonian method treats explicitly the \( f \) and \( d \)–sites, their local magnetization can be simply and efficiently evaluated as expectation values on the ground state.

\[
m_{Zf} = \langle gs|n_{f\uparrow} - n_{f\downarrow}|gs\rangle, \quad m_{Zd} = \langle gs|n_{d\uparrow} - n_{d\downarrow}|gs\rangle
\]

In Fig. 3, we show the magnetic moments as a function of the hybridization \( V \) for different values of the interaction \( U \). Both moments \( m_{Zd} \) and \( m_{Zf} \) vanish continuously at the transition for any value of \( U \) indicating that the transition is of 2\(^{nd}\) order along the whole critical line.

A notable feature of the results is that the size of the magnetic moments of the \( f \) and \( d \)–sites are very different, except close to the critical point. We also point out that while the magnetization of the \( f \)–site becomes always rapidly saturated at \( m_{Zf} \approx 1 \), independently of the strength of the interaction, the same does not occur on the \( d \)–sites. As \( U \) is increased, the maximum of \( m_{Zd} \) is enhanced. This suggests that it would be interesting to consider a limiting case of the model with both \( V, U \rightarrow \infty \) (or equivalently \( D \rightarrow 0 \)) and \( \frac{J_c}{\Delta} \) kept constant (i.e., \( \frac{J_c}{\Delta} \rightarrow \infty \)). This model may present an almost compensated total magnetic moment.

An important remark is that the deep Kondo regime, with an exponentially small gap in the paramagnetic density of states, is actually hindered by the onset of the magnetic instability. This is relevant for the understanding of the very small gaps observed in the Kondo insulators. This situation could, in principle, be modified by introducing frustration in the model, as for instance through \( n.n.n. \) hopping, or by the consideration of degeneracy in the \( f \)–orbital.

Let us now consider in more detail the behavior of these quantities in the case where the critical line is approached and also when \( J \rightarrow 0 \) \( (\frac{V^2}{J} \rightarrow 0) \).

In Fig. 4, we show the magnetic moments as a function of the hybridization \( V \) for a fixed value of the interaction \( U = 2 \) in clusters of various sizes. A similar result was obtained by Sun et al., using a variational Gutzwiller approximation.

As was already pointed out in that paper, the behavior of the magnetization as \( V \rightarrow 0 \) and as \( V \rightarrow V_c \), near the phase transition, is quite different. In the latter case, both \( m_{Zf} \) and \( m_{Zd} \) vanish when the Kondo effect becomes relevant close to the transition line. In the former case, however, we see that while the magnetic moment of the \( f \)–site becomes saturated and fully developed \( m_{Zf} = 1 \), the local moment of the \( d \)–electron band goes to zero. This result is demonstrated by the data shown in the inset, where we plot the magnetization at small \( V \) as 0.01 as a function of the size of the cluster.

It is also important to note from the comparison of the results from clusters of size \( N_g = 4, 6 \) and 8 shown in the main part of the figure, that although the value of the magnetization is notably affected by the system size, the critical point for the ordering transition remains basically size independent. This feature makes the phase diagram presented in the previous section an essentially exact result for this model. Also, a scaling \( \propto \sqrt{1 - \frac{V}{V_c}} \) for the moments \( m_{Zd} \) and \( m_{Zf} \) is found near the critical line. Moreover, we note that the results for \( m_{Zf} \), which are essentially independent of the system size, can be very well fit in the whole interval \( 0 < V < V_c \) with the function \( \sqrt{1 - (\frac{V}{V_c})^3} \) with only \( V_c \) as fitting parameter.

We now investigate the behavior of the moment along the other direction in the \((U,V)\) plane. In Fig. 5, we show the results for the magnetization as a function of \( U \) with fixed \( V = 0.5 \). A notable feature is that a relatively large magnetization on the \( d \)–sites seems to persist for extremely high values of the interaction \( U \sim 100 \) (which are easily accessible within the present numerical technique), despite the fact that the RKKY coupling should be very small. However, as the inset demonstrates, when the data are plotted against the relevant energy scale of the model, i.e.
\[ J \sim \frac{V^2}{U}, \] the behavior turns out to be qualitatively similar as in the previous case (which is also an indication that finite size effects are important in this parameter region).

To fully elucidate the behavior of the magnetization in the limit \( \frac{V^2}{U} \ll D < U \) (\( J/D \to 0 \)), we obtain the Hartree-Fock solution of the model (c.f. Appendix). The approximation becomes essentially an exact result in this limit, where correlation effects are less important. We find that the staggered magnetization of the \( d \)-sites behaves as

\[ m_{zd} \approx \frac{8}{\pi} \frac{J}{D} \ln \left( \frac{2D}{J} \right), \quad J << D \]  

where \( J \equiv \frac{V^2}{U} \). This result is plotted for comparison with the corresponding data from exact diagonalization in Fig. \( \text{Fig. 4} \) (dotted line).

To end this section we would like to briefly consider the behavior of the double occupation \( \langle D \rangle \). This quantity is simply related to the square of the magnetization by \( \langle m^2 \rangle = 1 - 2\langle D \rangle \). The results for fixed \( V \) and as a function of \( U \) from exact diagonalization are presented in Fig. \( \text{Fig. 5} \). For comparison, we also plot similar results for the two-site local model which corresponds to the limit where the band-width \( D \to 0 \) and can be solved analytically. When \( U = 0 \), we have \( \langle D \rangle = 1/4 \) for both the \( d \) and \( f \)-sites since, in the non-interacting case, the four spin configurations at each site appear with equal probability. As \( U \) is increased, the singlet state becomes energetically favorable and the double occupation decreases. This behavior is qualitatively well captured by the two-site model, however, as it does not contain the lattice feedback, it underestimates the value of \( \langle D_f \rangle \) and overestimates \( \langle D_d \rangle \). This difference can be understood from the following arguments: For the \( f \)-electrons the lattice contains the RKKY interaction (that the two-site model lacks) which favors the development of the local magnetic moment to minimize the energy. On the other hand, for the \( d \)-electrons, the enhancement of the double occupation respect to the two-site model is simply due to their band-like character which is brought in through the self-consistency condition.

When the interaction \( U \) is further increased the transition into the antiferromagnetic state takes place, as shown by the results for the staggered magnetization \( m_{zd} \) that we reproduce in the figure for comparison. The most notable feature is that \( \langle D_d \rangle \) has non-monotonic behavior. It experiences an upturn and returns to the non-interacting limit value when \( U \to \infty \). This behavior merely reflects the fact that as \( U \) increases, the effective magnetic exchange interaction \( J \) between the sites becomes small. More precisely, one may perform a Schrieffer-Wolff transformation and realize that \( d \) and \( f \)-sites become gradually decoupled with the \( d \)-electrons approaching the non-interacting band limit, as \( J \sim \frac{V^2}{U} \to 0 \), i.e., when \( U \to \infty \). On the other hand, for the case of the \( f \)-electrons, where the local repulsion is the dominant interaction, the simple two-site model can still capture the correct qualitative behavior.

**IV. ITINERANT AND LOCALIZED MAGNETIC BEHAVIOR**

In this section we consider the behavior of the \( f \)-electrons as they evolve from the itinerant to the localized magnetic regime. Different aspects of this question were first discussed by Doniach \( ^{14} \) and Evans \( ^{15} \), and later by Sun \( ^{16} \) et al. \( ^{17} \).

The existence of two qualitatively different regimes was already suggested by the two routes in which the system looses its magnetic order: (i) when \( V \to 0 \) or \( U \to \infty \) (\( J \to 0 \)), the \( f \)-moments became free local spins with \( m_{zf} \to 1 \) and the \( d \)-electrons, having \( m_{zd} \to 0 \), approach a non-interacting band; and (ii) at the \( 2^{nd} \) order critical line, as both \( m_{zd} \) and \( m_{zf} \to 0 \).

In what follows, we shall gain new insights on these two distinct regimes by studying the redistribution of spectral weight of the electronic density of states.

At \( T = 0 \), the Green functions of the problem can be obtained as two continued fraction \( G_{c \sigma}(\omega) = G_{c \sigma}^{>}(\omega) + G_{c \sigma}^{<}(\omega) \), with \( G_{c \sigma}^{>}(\omega) \) and \( G_{c \sigma}^{<}(\omega) \) corresponding to “particle” and “hole” excitations respectively. \( ^{13} \)

\[ G_{c \sigma}^{>}(z) = \frac{1}{z - (H_{eff} - E_{gs})c_\sigma^\dagger g_\sigma} \]
\[ G_{c \sigma}^{<}(z) = \frac{1}{z + (H_{eff} - E_{gs})c_\sigma g_\sigma} \]  

where the anihilation (creation) operator \( c (c^\dagger) \) generically stands for \( d (d^\dagger) \) and \( f (f^\dagger) \), and \( H_{eff} \) is the effective cluster hamiltonian introduced before. The \(-\sigma\) Green function is by symmetry \( G_{c \sigma}(-\omega) = -G_{c \sigma}(\omega) \).

In Fig. \( \text{Fig. 6} \) we display the density of states for the \( f \) and \( d \)-electrons. They are obtained from the imaginary part of the local Green functions of clusters with 8 sites. Note that, unlike the quantum Monte Carlo technique that has also been applied to this problem, our results are directly obtained on the real axis with no need for analytic continuation. However, the price we pay is a discrete number of poles that we broaden in the figures for easier visualization.
The figure illustrates the changes that take place in the density of states as we move through the different regimes on the phase diagram. The three sets of curves correspond to the antiferromagnetic phase, as we move away from the 2nd order critical line towards the small $J$ regime ($V^2 \ll UD$). The two curves on the top of the figure correspond to $U = 3$ and $V = 0.5$ that places the system close to the critical point. Both spectra are slightly asymmetric which correspond to the simultaneous vanishing of the magnetic moments that we discussed before. A notable aspect is that a central feature can be clearly observed in the $f$–electron spectral function. This corresponds to the Kondo coherent quasiparticle excitations that are characteristic in the paramagnetic solution of the model. In this case it is interesting to observe that the quasiparticle excitations can survive the onset of magnetic order. In Fig. 8 we display the behavior of the $f$–electron density of states in greater detail. The symmetric curve (grey line) is obtained in the paramagnetic region very close to phase boundary. This solution corresponds to the well known scenario of a hybridization band insulating state with the hybridization amplitude being renormalized by the effect of the correlations. The low energy features are originated in the splitting of the Kondo resonance due to the lattice effect. This scenario is borne out from many different approaches, as for instance the Gutzwiller variational wavefunction. We now proceed to slowly move into the antiferromagnetic phase. The comparison of the paramagnetic solution to the curves obtained close to phase boundary, but in the antiferromagnetic regime, provides us new insights as we realize that the transfer of weight actually occurs at all energy scales. Both, the high energy features and the low energy excitations associated with the quasiparticles on the left side of the spectrum, are loosing their weight at a similar rate. This interesting behavior actually makes difficult the task of reducing the the problem to simpler effective model that could be more tractable. It also does not allow for a simple interpretation of which aspect, the itinerant quasiparticles or the localized moments, is the driving force behind the transition.

We now come back to Fig. 7 as we decrease the coupling between sites, setting $U = 3$ and $V = 0.3$ (central curves). We, thus, move away from the 2nd order line well into the antiferromagnetic regime. The quasiparticles features have gradually disappeared as the weight is transferred to the high energy part of the spectrum. This corresponds to the rapid increase in the size of the $f$–magnetic moment as $V^2$ becomes much greater than $UD$ and the $f$–electrons localize.

As we finally enter the small $J$ regime, setting $V = 0.1$ (lower curves), we clearly observe how the electron become decoupled. The $f$–electron spectrum corresponds to a fully saturated and polarized moment with the totality of the spectral weight at high energies. The lack of any low frequency feature indicates that these electron have essentially localized. On the other hand, the $d$–electron density of states seems to have closely approached that of a non-interacting band. However, we shall see next, this is not exactly the case.

Once more we can gain further insights in this limit by using the Hartree-Fock approximation, which is very accurate as $J \ll D$ ($V^2 \ll UD$). We focus on the $d$–electrons which have a more interesting behavior. In this case, we can obtain an analytic expression for the density of states (c.f. Appendix),

$$\rho_d(\omega) = \frac{2}{\pi D^2} \sqrt{\left[\left(\omega - \frac{V^2}{\omega + \frac{U}{2}}\right)\left(\omega - \frac{V^2}{\omega - \frac{U}{2}}\right)\right]^2 - \left[\left(\omega - \frac{V^2}{\omega + \frac{U}{2}}\right)\left(\omega - \frac{V^2}{\omega - \frac{U}{2}}\right)\right]}$$

We plot this density of states, along with the results from an 8 site cluster, is Fig. 8. It is remarkable to observe the effort that the few poles from the exact diagonalization method do to best approximate the essentially exact continuum result. Even details as the small weight at $\omega \approx 1.5$ that originates from the hybridization with the high energy feature of $\rho_f$ (c.f. Fig. 5) are well captured. As expected, the $d$–electron density of states is insulating with a small gap of size of the order of $J$. However, it is surprisingly far from regularly approaching the non-interacting limit. A very sharp peak develops on the low frequency edge of the gap. When the $J \to 0$ limit is approached the peak becomes narrower and gradually looses its spectral weight. This feature could, in principle, be observed in infrared photoemission spectroscopy. Also, in transport measurements it may be possible to observe a strong pressure dependence at temperatures of the size of the gap.

V. CONCLUSIONS

In this work we have considered solutions with magnetic order in the periodic Anderson model in the limit of large dimensionality using the LISA method. Our results validate and expand on that of Sun et al. who obtained approximate solutions based on a variational procedure.

The $T = 0$ exact magnetic phase diagram of the model is obtained in detail by a recently introduced numerical algorithm that is based on the exact diagonalization of an effective cluster hamiltonian. We find a paramagnetic-antiferromagnetic 2nd order phase boundary that splits the $(U, V)$ parameter space in two regions. The critical line
obeys $U_c \propto V_c^2$ as $U$ becomes large. This is a concrete realization of earlier ideas of Doniach in the context of the Kondo lattice, and is consistent with recent numerical results on 2-dimensional finite lattices.

The consistent picture that emerges from this work, very similar to the two dimensional lattice results, represents further evidence of the applicability of the LISA method to investigate the physical behavior of systems that are characterized by the simultaneous presence of localized orbitals and strong correlations.

From the determination of the phase diagram we found that the paramagnetic Kondo regime with an exponentially small gap, which is relevant for the description of Kondo insulator compounds, is inaccessible in all parameter space due to the onset of the antiferromagnetic instability.

The calculation of the magnetic moments in the phase with long range order, revealed that the possibility of a nearly perfect magnetic spin compensation that would be relevant for the problem of the “small moments”, is not a general feature of the solutions of the model.

An almost perfect compensation of the moments is only obtained near the 2$^{nd}$ order boundary line, where the total site magnetization starts to become non-zero as the Kondo screening ceases to be complete. Therefore, a small moment regime would require a fine tuning of the parameters of the model, which is not a priori a feature that one expects to find in real systems. The question whether this situation would persist in the non particle-hole symmetric case and how the introduction of frustration may modify the present picture is currently under investigation.

Finally, the method allows to obtain reliable information on the distribution of the spectral weight in the density of states which provided interesting new insights on the nature of the phase transition and that of the different antiferromagnetic regimes.

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APPENDIX A: THE HARTREE-FOCK SOLUTION

We present in this appendix the solution of the self-consistent equations (5,6,8) in the limit $V^2 << D < U$. It is a useful exercise that would allow the interested reader to better grasp some details of the method. Performing the Hartree-Fock decoupling to interaction term of the effective local action (5), and using that $\langle n_f^+ - n_f^- \rangle = \langle m_Z \rangle$ and $\langle n_f^- + n_f^- \rangle = 1$, the action becomes quadratic and we can immediately obtain the local Green function for the $f_\sigma$-electrons.

$$G_{Af \pm \sigma}(\omega) = \frac{1}{\omega \mp m_Z U^2 - V^2 G_{Bd \pm \sigma}(\omega)} \quad (A1)$$

where $A$ and $B$ denote the sublattice. We now combine this expression with the symmetry relation between the sublattices Green functions (7), to obtain

$$G_{Af \pm \sigma}(\omega) = \frac{1}{\omega \mp m_Z U^2 - V^2 G_{Ad \pm \sigma}(\omega)} \quad (A2)$$

since the expression involves only quantities on the same sublattice, the index may be dropped. We now need to find an expression for the $d$-electron Green function. Once more, from the local action we obtain,

$$G_{Ad \pm \sigma}(\omega) = \frac{1}{\omega \mp V^2 U - t^2 G_{Bd \pm \sigma}(\omega)} \quad (A3)$$

where from the same symmetry considerations we have,

$$G_{d \pm \sigma}(\omega) = \frac{1}{\omega \mp V^2 U - t^2 G_{d \pm \sigma}(\omega)} \quad (A4)$$

This equation is actually two coupled equations for $G_{d_\uparrow}$ and $G_{d_\downarrow}$. We then replace $G_{d_\sigma}$ into its same expression, in order to decouple them. We obtain,
\[ G_{d_{\pm,\sigma}}(\omega) = \frac{1}{\omega - \frac{V^2}{2} - t^2 - \frac{1}{\omega - \frac{V^2}{2} - t^2} G_{d_{\pm,\sigma}}(\omega)} \]  

(A5)

We are left now with two quadratic equations, each with a single unknown, which we can solve to obtain the explicit result,

\[ G_{d_{\sigma}}(\omega) = \frac{\left(\omega - m_{Zf} \frac{U}{2}\right) \pm \sqrt{\left(\omega - m_{Zf} \frac{U}{2}\right)^2 - 4t^2 \left(\frac{\omega - m_{Zf} \frac{U}{2}}{\omega + m_{Zf} \frac{U}{2}}\right)}}{2t^2} \]  

(A6)

from which follows the \( d \)-electron density of states that we express in terms of the half-bandwidth \( D = 2t \)

\[ \rho_{d_{\sigma}}(\omega) = \frac{2}{\pi D^2} \sqrt{\left[ \left(\omega - \frac{V^2}{2} \right) \left(\omega - \frac{V^2}{2} + m_{Zf} \frac{U}{2}\right) \right]^2 - D^2 \left[ \left(\omega - \frac{V^2}{2} \right) \left(\omega - \frac{V^2}{2} - m_{Zf} \frac{U}{2}\right) \right]^2} \]  

(A7)

We still need an equation for \( m_{Zf} \). It is simply obtained from its definition,

\[ m_{Zf} = -\frac{1}{\pi} \int_{-\infty}^{0} Im \left( G_{f\uparrow}(\omega) - G_{f\downarrow}(\omega) \right) d\omega \]  

(A8)

Thus, (A2,A6,A8) form a system of equations that have to be self-consistently solved for.

In general, these equations can be solved numerically. However, from the results of section II we learn that in the limit \( \frac{V^2}{2U} \ll D < U \), which we are currently concerned with, we can take \( m_{Zf} = 1 \) to an excellent approximation (c.f. Fig. 4). Thus, equation (A7) immediately leads to the expression for the density of states (14) in section IV. We can finally obtain the behavior of the magnetization \( m_{Zd} \) by replacing into

\[ m_{Zd} = -\frac{1}{\pi} \int_{-\infty}^{0} Im \left( G_{d\uparrow}(\omega) - G_{d\downarrow}(\omega) \right) d\omega \]  

(A9)

an extracting the leading contribution in this limit (c.f. Eq. (13) in section III).

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FIG. 1. Effective cluster hamiltonian. It consists of a central impurity site with a $d$ and $f$-electron site connected to an effective electron bath. $U$ is the on site repulsion of the $f$-site, $V$ is the $d-f$ hybridization matrix element, and $t$ is the $d-d$ hopping amplitude.

FIG. 2. Phase diagram of the PAM. The inset shows in a log-log plot that the 2nd order critical line obeys $U_c \approx V_c^2$ as $U$ becomes large. $N_S = 6$.

FIG. 3. The staggered magnetic moments $m_{Zd}$ and $m_{Zf}$ as a function of the hybridization $V$ for different values of the interaction $U = 1, 5, 10$. $N_S = 6$.

FIG. 4. The staggered magnetic moments $m_{Zd}$ and $m_{Zf}$ a function of the hybridization $V$ for a fix value of the interaction $U = 2$. For comparison we plot similar results for $N_S = 6$ (bold lines) and $N_S = 4$ (thin lines). Note that while the magnitude of $m_Z$ depends on the size of the cluster, the position of the critical point does not. The dotted line in the top part of the figure indicates the Hartree-Fock results, while the one in the bottom is the fit $\sqrt{1 - \left(\frac{V}{V_c}\right)^3}$. The inset shows $m_{Zd}$ and $m_{Zf}$ (top and bottom) for a small value of $V = 0.01$ as a function of the inverse of the cluster size $1/N_S$. $m_{Zd}$ becomes small while $m_{Zf}$ remains saturated at $m_{Zf} = 1$.

FIG. 5. The staggered magnetic moments $m_{Zd}$ and $m_{Zf}$ as a function of the interaction $U$ for a fixed value of the hybridization $V = 0.5$. $N_S = 6$. The inset contains the same quantities plotted as a function of $V^2$ (for fixed $U = 5$), and of $1/U$ (for fixed $V = 0.5$). As the relevant energy scale of the problem is $J \sim V^2/U$, the behavior of the magnetic moments is qualitatively similar in both cases.

FIG. 6. Double occupation $\langle D \rangle$ as a function of $U$ for $V = 0.5$ from exact diagonalization of a 6 sites cluster (bold lines). $\langle D_d \rangle$ is the upper curve and $\langle D_f \rangle$ the lower one. For comparison we include in dotted line similar results for a 2 sites cluster ($\langle D_d \rangle = \langle D_f \rangle$). The thin line corresponds to $m_{Zd}$ that indicates the magnetic regimes.

FIG. 7. The local density of states $\rho_{f,\sigma}$, $\rho_{d,\sigma}$ (left and right) in different magnetic regimes. The top spectra correspond to $V = 0.5$ and $U = 3$ close to the 2nd order critical line. The low energy features of the $\rho_{f,\uparrow}$ correspond to quasiparticle AFM. The bottom spectra correspond to $V = 0.1$ and $U = 3$. The single peak at a frequency $\approx \frac{U}{3}$ and the absence of quasiparticles indicate local moment magnetism. The middle spectra correspond to $V = 0.3$ and $U = 3$ in the crossover region. $N_S = 8$.

FIG. 8. The local density of states $\rho_{f,\sigma}$ for $U = 2$ and $V = 0.45$ in the paramagnetic phase (grey line) and $V = 0.40, 0.35$ in the antiferromagnetic phase (dotted and full lines).

FIG. 9. The local density of states $\rho_{d,\sigma}$ for $U = 3$ and $V = 0.2$. The bold line corresponds to the Hartree-Fock solution and the thin line to the exact diagonalization of an 8 sites cluster.
The graph shows the dependence of $m_{Zd}$ and $m_{Zf}$ on $V$ with $1/N_s$ as the inset. The curves indicate a non-linear relationship with $V$, highlighting the sensitivity of the variables to changes in $V$. The inset graph provides additional data points for $1/N_s$.
