

Mean Field Studies of the 2D Kondo Lattice Model

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Abstract

We develop and study a model of the Kondo lattice system under the mean field approximation using a Hartree-Fock procedure as the spin polarization of the system is varied. The goal of this investigation is to provide a realistic model and a starting point for further investigations using more sophisticated techniques, as well as to provide information on mean field solutions calculated on larger lattice sizes. We compare energies for solutions of varied polarization and show that this model does generate known behavior of Kondo lattice systems.

I. INTRODUCTION

STRONGLY correlated electronic systems have been a forefront research area in materials physics since soon after the discovery of quantum mechanics, with early examples being the metal-insulator transitions introduced by Wigner (localization at low density) [1] and Verwey (known as charge ordering) [2] [3]. Electronic correlations within an open atomic shell have comprised most of the theoretical studies, with a strong, recent trend being to progress from the simplest, single-band platform to two, three, or occasionally five bands [4]. This generalization brings in an orbital degree of freedom in addition to the more thoroughly treated charge and spin correlations.

Another type of correlated system is that of a narrow band, with strong on-site repulsion, crossing a wide, weakly interacting band. This very localized regime constitutes the Kondo impurity system [5], in which a quantum spin is coupled to a "sea" of electrons in a Fermi liquid (conventional metal) state. The very strong scattering at low temperatures (i.e. low energies) ignited spirited theoretical work for nearly two decades, until the low energy behavior was solved by Wilson [6] using a renormalization group procedure. The lattice extension of this problem is the Kondo lattice system, which can display a

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variety of unusual phases, including heavy fermion behavior [7] and unconventional superconductivity [8], interspersed with several possible types of magnetic order and quantum criticality [9].

Many properties of the Kondo lattice require explicit treatment of inter-electronic correlations. Nevertheless, mean field methods have played an important role in this field. While the mean field approach, by construction, glosses over specific inter-particle correlations, it is non-perturbative (i.e. there is no expansion in a small parameter). Although we make approximations in the model, the benefit of this technique is that we can avoid dealing with approximations in the solutions.

In the lanthanides and actinides, a superconducting phase, as well as many magnetic phases, have been discovered [10], which has generated great interest in their study since, in conventional superconductors, the magnetism that arises from f-electrons tends to suppress superconductivity. The study of quantum critical points has provided great insight into these phases and, although there has been much experimental work done with these systems, a satisfying theoretical explanation for the superconducting phase has not yet been established.

In addition to the superconducting phase, experimentalists have shown interesting phenomena when these types of systems are placed under high pressure [11]. Dysprosium, gadolinium, and many other rare earth metals, when studied in a high pressure regime [12] [13], undergo volume collapse, which is often followed by a substantial increase in the magnetic ordering temperature—neither of which have been adequately explained.

II. MODEL

The Kondo lattice system is represented using a two-band Hubbard model which we treat primarily on a 24x24 lattice. The linearized mean field Hamiltonian for the model is:

$$H = \sum_{\alpha,\beta} -t_{\alpha,\beta} \sum_{j,\sigma} (\hat{c}_{j,\sigma,\alpha}^\dagger \hat{c}_{(j+1),\sigma,\beta} + \hat{c}_{j,\sigma,\alpha} \hat{c}_{(j+1),\sigma,\beta}^\dagger) + U_{\alpha,\beta} \sum_i \langle \hat{n}_{i,\alpha,\uparrow} \rangle \hat{n}_{i,\beta,\downarrow} + \hat{n}_{i,\alpha,\uparrow} \langle \hat{n}_{i,\beta,\downarrow} \rangle - \langle \hat{n}_{i,\alpha,\uparrow} \rangle \langle \hat{n}_{i,\beta,\downarrow} \rangle$$

The first term gives the kinetic energy of hopping between atoms, and the second gives the repulsive interaction between electrons on the same site. This model has several parameters which can be varied; below is a table documenting the possible parameters followed by a brief discussion.

Table 1: *Model Parameters*

Hopping	Band Center	Hubbard U
$t_{11} = -1$	$E_1 = 0$	$U_{11} = \frac{1}{10}$
$t_{22} = 0$	$E_2 = -1$	$U_{22} = 4$
$t_{12} = \frac{1}{8}$		$U_{12} = 0$

In the above table, subscripts refer first to the orbital on which the site is located, and second to the orbital with which it is interacting. The wide, weakly-interacting band is described by the parameters of the first row. The narrow band with strong on-site repulsion is represented by the parameters in the second row. Finally, the third row specifies how the orbitals are allowed to interact with one another. These parameters remain fixed throughout this investigation.

We choose parameters that will generate the system while keeping the level of complexity low. Given the correct parameters, our model has the ability to generate a more realistic case in which orbital interactions are allowed, Our investigation neglects this in favor of simplicity. In contrast with orbital interactions turned off, we have a simpler model which allows a more direct view of the physics involved in the f-electron interactions in real Kondo lattice materials. We compare the energy and types of solutions generated by our model and point out any results that show known behavior of Kondo lattice systems.

A final parameter of the system is the number of electrons in the system and how this number is distributed between up-spins and down-spins. In our investigations the system contains ($24 \times 24 \times 2 = 1152$) electrons; however, the polarization of the system is varied, which will be discussed in a later section.

$$P = \frac{N_{\uparrow} - N_{\downarrow}}{N_{total}}$$

One final note about the parameters should be addressed: U_{11} is set equal to 0.1 (in units of $|t_{11}|$) to avoid an instability that occurs in the density of states as the band center moves closer to the Fermi level. This number is purposely made small to allow for weak on-site repulsion in band 1, and to stabilize the calculation without drastically changing the physics. Both the on-site repulsion of $U_{22} \gg U_{11}$ and the model depend heavily on orbital 2 being able to easily repel electrons on the same site.

A. NOTE ON METHODOLOGY

The self-consistent iteration (SCI) procedure frequently converges to local minima, which requires several tweaks to the methodology in order to allow the SCI to converge to the ground state. The details of this are described below.

To alleviate the abundance of local minima, the initial charge densities are set to one of two highly-symmetric, low-energy configurations. The two densities are extremely different in character, which is done to ensure that the starting density does not exclude solutions. The most simplistic case is that of polarization $P = 0$, which we refer to as the antiferromagnetic (AF) start. In this case, band 1 and band 2 both start with AF order, hence the polarization value of zero. The second, more complicated, case corresponding to $P = 0.5$, is referred to as the ferromagnetic (FM) start. In this configuration, the density in the narrow band (band 2) is completely ferromagnetic, with all sites occupied by up-spin electrons. The wide band (band 1) maintains the AF order of the original configuration. Our treatment varies the polarization around $P = 0$ and $P = 0.5$.

Aside from the two special cases which are used as reference, all other values of P have the magnitude of the starting densities in band 1 randomized in such a way that the underlying AF configuration is still intact. This is done so that the starting points for each case are different, allowing the simulation to be run one hundred times with the same parameters. This tactic increases the probability that at least one simulation will bypass any local minima and converge to the ground state. These tweaks work with a large degree of success when applied to our simulation, the results of which will be discussed in the next section.

III. RESULTS

Because calculations on this lattice size are already computationally costly, these are made using single precision to lower the computation time needed. For this project it was necessary to develop several visual tools for analyzing the data, each of which will be briefly described.

The colormaps throughout the paper are maps of the spin density on an orbital. Each pixels references a specific site on a 24x24 grid, and its color indicates the value of the spin on that site. The next type are graphs plotting the energy of a solution versus iteration. The purpose of this graph is to illustrate the spread of energy values for a particular case (i.e. out of 100 simulations, x converge to the ground state). The final graphic is a standard density of states plot, where we superimpose the densities

of both orbital 1 and 2 onto the total density of states. Below are the results of our calculations.

For each polarization, the energy of the ground state solution is calculated and compared. (Fig.1)

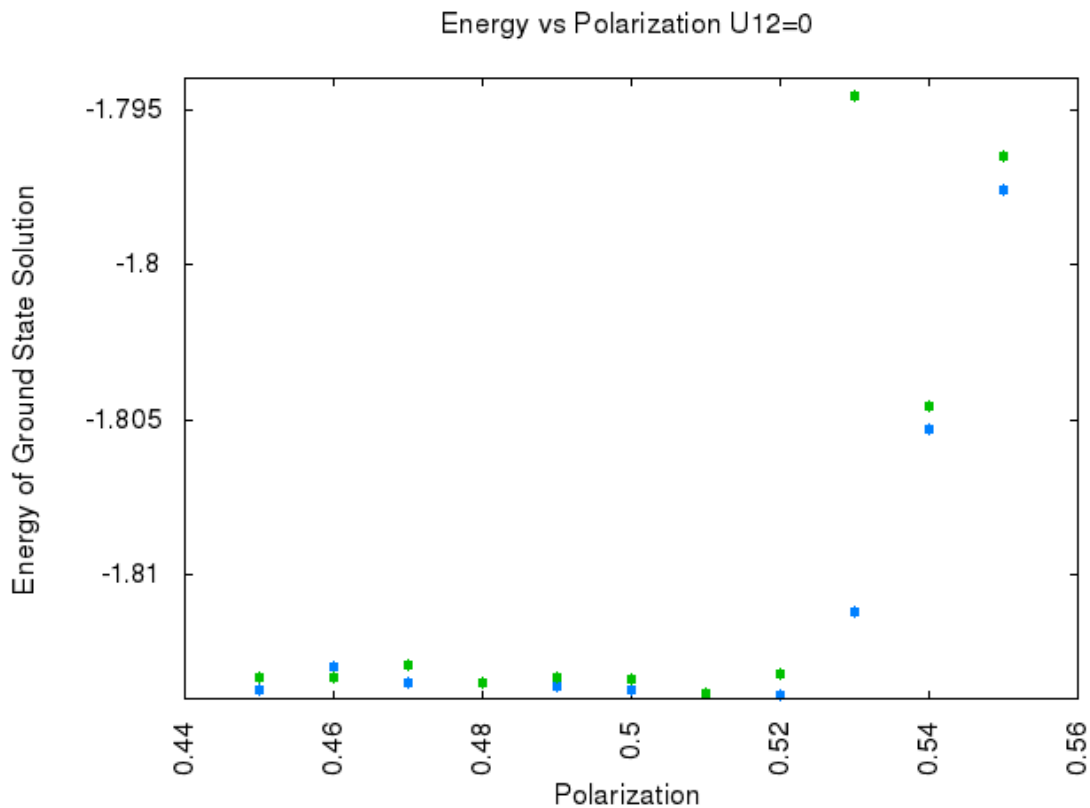


Figure 1: Energy vs. Polarization for FM start (blue) and AF start (green) at $U_{12} = 0$

The solutions have very similar energies and seem to follow the same trend. In general, the FM start has lower energy, but the ΔE is very small and could be close to machine precision. The point at 0.53 which does not follow this trend is anomalous and requires further investigation, however the most likely cause is non-convergence of the solution. In Fig. 2 the wide-banded orbital is shown for several values in order to illustrate how the types of solutions are changing with polarization. For the polarization values on the extremes, more unique solutions are found (Fig. 3), while the center values seem to be similar to each other.

At the highest values of polarization, the solutions seem to become saturated and are completely ferromagnetic.

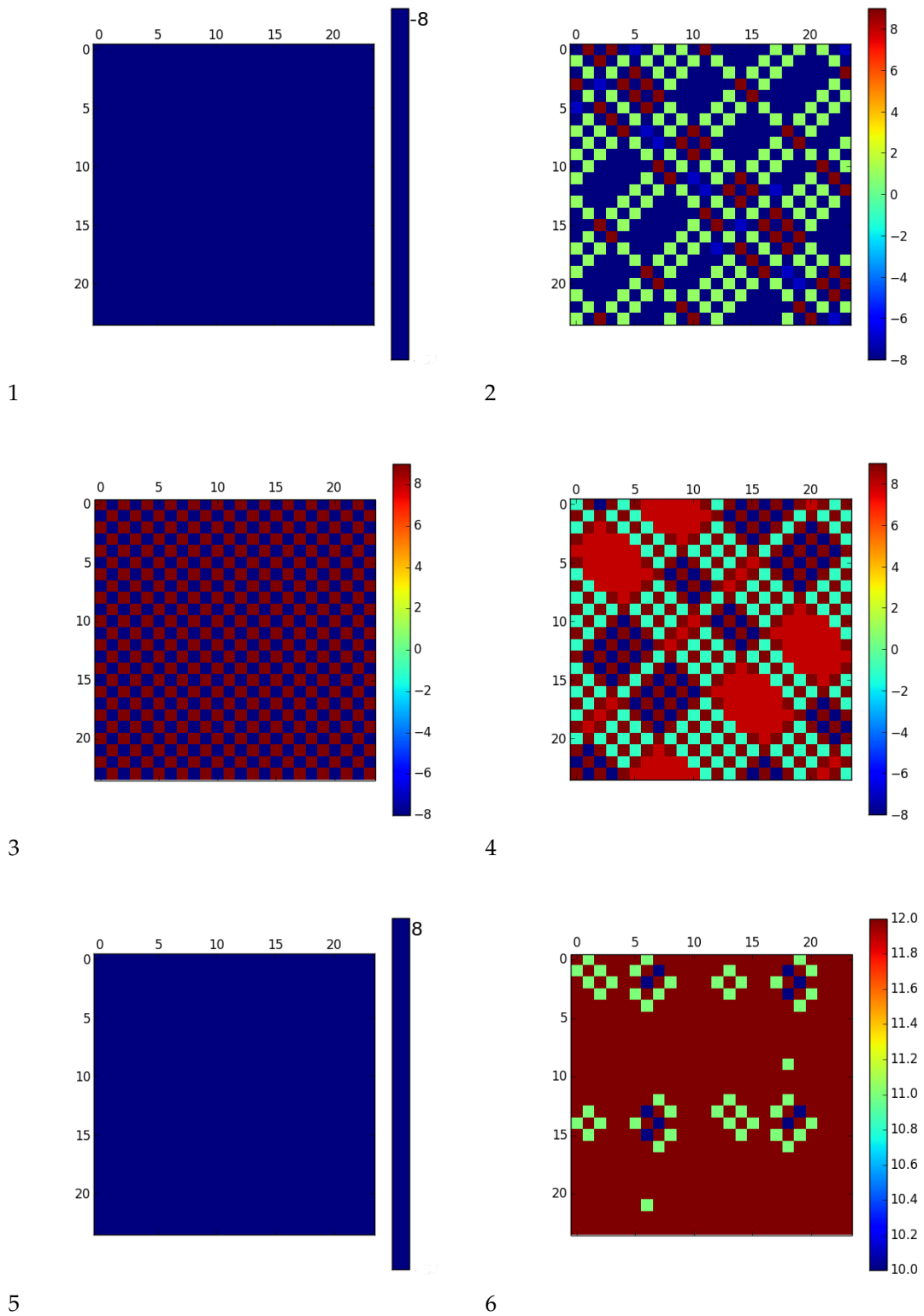


Figure 2: Solutions for wide band (FM start) with values of polarization (P) ranging from 0.48 (1) - 0.53 (6).

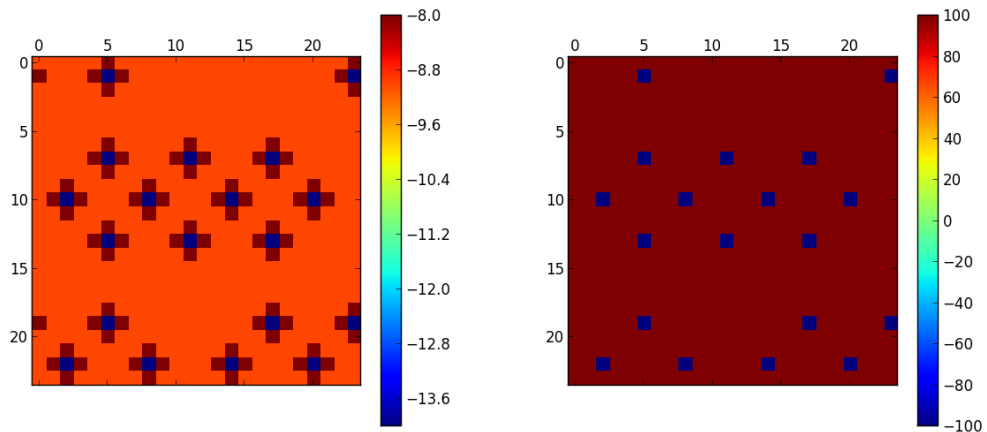


Figure 3: Results for $P = 0.45$. Wide band (left), narrow band (right).

The solutions have a type of symmetry around $P = 0.50$, more unique solutions on the extremes, and similar solutions at the central values. This can also be seen in the ability of the SCI to converge to these solutions (Fig. 4).

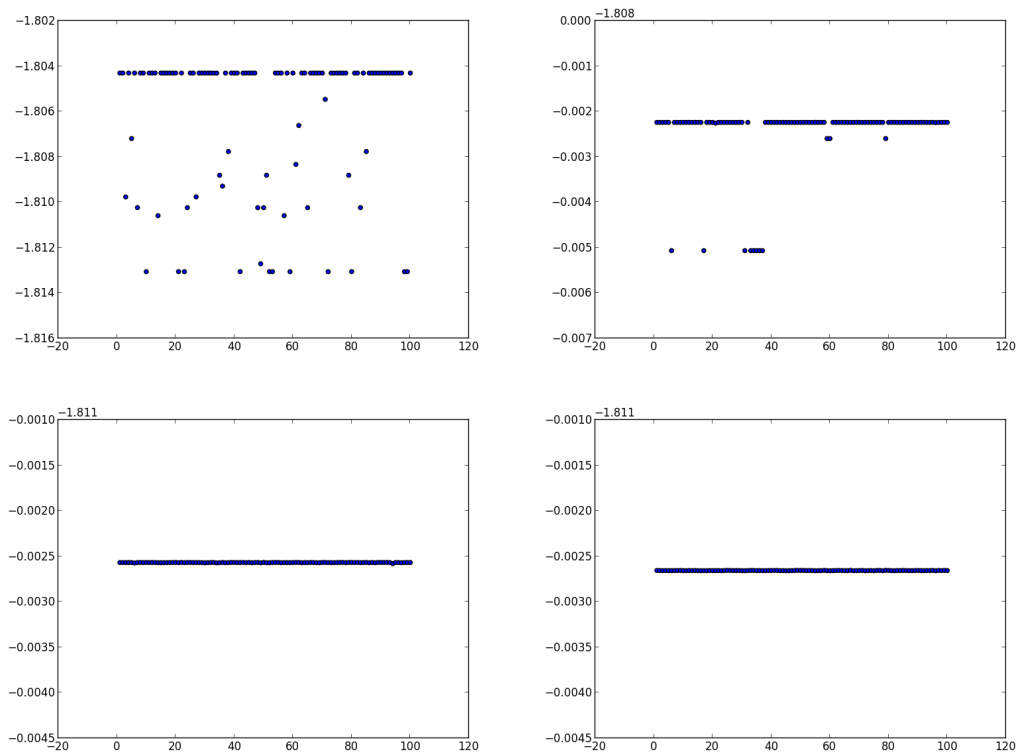


Figure 4: Left to right: energy of solution for 100 runs for $P = 0.45$ to $P = 0.49$. Final graph is representative of the remaining values of P .

Through all of the calculations, every FM start converges to a ferromagnetic solution, which is commonly displayed in real Kondo lattice systems. The density of states plots for $P = 0.49$ and $P = 0.51$ (Fig. 5), which show the most order in their spin densities, are distorted and look similar to density of states plots for heavy fermion systems, in which a split peak shows strong coupling to f-electrons. It is also interesting to note that peaks are symmetric but mirrored on each side of $P = 0.50$.

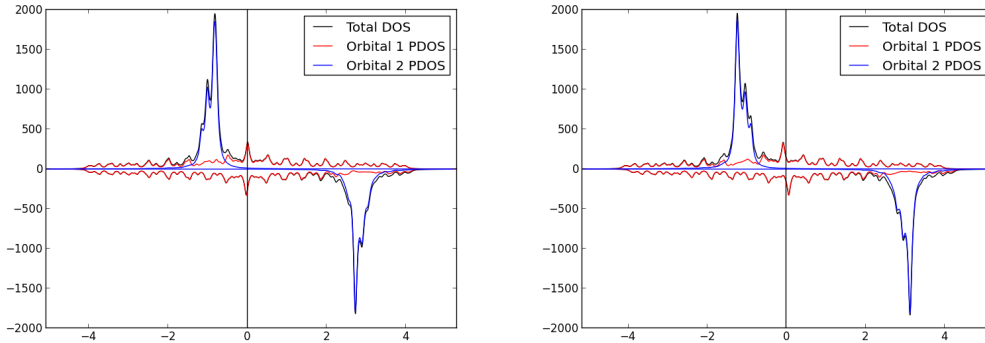


Figure 5: Density of state plots for $P = 0.49$ and $P = 0.51$ showing heavy fermion behavior

The AF starts are not shown because they produce solutions similar to those of the FM starts. Numerically, their solutions are very close in energy, though slightly higher. The wide band solutions are all ferromagnetic, but the density of states shows AF characteristics. This is likely caused by the starting density of the narrow band being AF and staying that way throughout the calculations.

IV. CONCLUSIONS

The goal of this study was to provide computational physicists with information on mean field solutions done on larger lattice sizes. We chose the Kondo lattice model because very little work has been done on this system with more than one band, and because this model is one of few which can be realistically scaled to larger lattice sizes. It is evident that this model can be used to accurately model some of the physics of real Kondo lattice systems [14] and will be a useful starting point for further investigations into these systems. Our model, while simple, shows many known behaviors of Kondo lattice systems, including strong spin-coupling heavy fermion behavior, and it produces ferromagnetic results. This study was intended as a large overview of the system and further studies focusing perhaps on a specific value of doping or polarization could indeed provide interesting and exciting results.

A few things that could be done to further investigate this model are listed below.

- Investigate the results produced by the model in more detail and with different techniques to verify that the model is producing accurate results.
- Allow for orbital interactions, although this may require a more sophisticated method.
- Study at certain level of doping known to occur in these types of systems
- Compare results on increasing lattice sizes (e.g. 8x8, 12x12, 16x16, 24x24, and 36x36).

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