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MAGNETIC PHASE DIAGRAM IN THE PERIODIC ANDERSON MODEL (PAM): AN EXACT DIAGONALIZATION APPROACH

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ABSTRACT: *A detailed and qualitative matrix representation of the one-dimensional periodic Anderson model (PAM) is presented giving the ground state as a function of band filling using the exact diagonalization technique.The simplest lattice system of two electrons on two sites is consider, in the study the results of the matrix element were compared and it was found that for the symmetric case where the energy of the f electrons E_f =-U/2 and the hybridization matrix element V switched off, the results are consistent with the Kondo model Hamiltonian matrix in the J =0 region.The results obtained in the study are also in agreement with the famous Hubbard (t – u) model if the Hybridization term V of the PAM and the energy of the localized f orbital E_f are switched off. The results of the ground state energies were used to determine the transition from antiferromagnetic (AFM) phase to a ferromagnetic (FM) phase and vice versa.*

KEYWORDS: Anderson model, transition point, Antiferromagnetism, Ferromagnetism

INTRODUCTION

The periodic Anderson Model (PAM)[1,2] describe the essential physics of many transition metals, rare earth and actinide compounds including the so-called heavy-fermion system. The model has also been proposed to describe the cuprate superconductors. It is one of the archetypical models of correlated fermions on a lattice, consisting of a band of "light" uncorrelated electrons [2].

The Anderson model (1961) is another model for a system of conduction electrons that interact with a local spin. The model has some terms that are similar to those of the Kondo and Hubbard models. Early workers thought that the Kondo and Anderson models made very similar predictions. Now it is known that the Anderson model has a variety of behaviour. It has a more interesting Physics. The Kondo model treats the local spin as a separate entity. The Anderson model treats the local spin as just another electron. It can undergo exchange and other processes with the conduction electrons. The Anderson model is more realistic [3].

The objective here is to explore the periodic Anderson model by numerical calculations in which exact solutions are obtained for clusters of one dimension. This kind of study has been very informative in applications to Hubbard, $t - J$, and the extended Hubbard models. The exact diagonalization technique is used in this context as a result of some of its advantages over other techniques. It allows us to study chains longer than what is achievable by other techniques. The ED technique also avoids the problem of Monte Carlo calculations where very low temperatures are difficult to attain. Another complication is: the Lanczos method which is commonly employed

to extract a few low lying eigenvalues of large matrices is inadequate in the case for many interesting values of the parameters; which can only be made available by exact diagonalization technique. This may occur if there is large difference in energy between *C* and *f* levels. The Lanczos method may not give accurate results over a large enough range of energies to describe all the interesting features. It main advantages are that there are no restrictions to infinite or large coulomb repulsion *U*, or to large degeneracy *N*. In addition, there is no finite size effects since the method offers an exact treatment of an impurity coupled with an infinite sea of conducting electrons. As a result, we have to employ a method which obtains all the eigenvalues. These considerations have limited our calculations so far to exact diagonalization technique in one dimension.

The scientific study of magnetism started in the 16th century, after people had come to some understanding of the principles of magnetic induction and magnetization [4]. Basically, magnetism is due to the motion of electric charges. The electrical basis for the magnetic properties of matter has been verified down to the atomic level. An electronic charge in motion gives rise to an tiny magnetic field, each electronic charge in motion always feel the presence of other neighbouring electrons because of the Coulomb and spin interactions between them. The resulting interaction of these charges in motion is what is usually referred to as *electron correlations* [5]. For a system of many electrons, the electrons are paired within energy levels, according to Pauli Exclusion Principle which states that no two electrons with the same spin can occupy the same site, this follows that for the two electrons to occupy the same site, and then their spins must be in opposite directions. Thus there are three possibilities of electronic pairing: The two electrons have opposite spin either at the same site or at two different sites, and in both cases we get a singlet state (i.e. a state with zero unit of spin); Each of the two electrons has a spin pointing up and each electrons has a spin pointing down. In the second and third possibilities, the electrons must necessary be on different sites yielding triplet states that is one unit of spin [6]. In the context of strongly correlated electron systems one is mainly interested in magnetic phase transition involving the conduction electrons [7]. As prototypes we will consider ferromagnetic (FM) and antiferromagnetic (AFM) phase transitions in this research.

In this research work we followed the procedure employed where the spin and magnetic correlation of the I – D Hubbard model were investigated and the results show no clear transition from FM to AFM [8]. The ground state properties of interacting electrons in the Anderson Model were analyzed [9] where transitions were obtained using the Computaional ED Techniques.

Using the Density Functional theory and Inter – Atomic force constants [10,11,12], some of the authors here investigated theoretically the phonon phase diagrams in Aluminium(Al), Copper (Cu), Nickel (Ni), Platinium (Pt), Lead (Pb) and Palladium(Pd); the results shows that there are computational lattice error and underestimation of lattices in these metals.The rest of the paper is organized as follows: After introducing the periodic Anderson model (PAM) in section 2, the problem of two interacting electrons on two sites lattice systems under this Hamiltonian in one-dimension is solved in section 3. We present our results in section 4; and offer a summary and discussion in section 5.

The periodic Anderson Hamiltonian

We consider the standard periodic Anderson Hamiltonian in one-dimension:

$$H = -t\sum_{\langle ij\rangle}(C^{+}_{i\sigma}C_{i+1\sigma} + C^{+}_{i+1\sigma}C_{i\sigma}) + E_f\sum_{i\sigma} n^{f}_{i\sigma} + U\sum_{i} n^{f}_{i\uparrow}n^{f}_{i\downarrow} + V\sum_{i,\sigma}(C^{+}_{i\sigma}f_{i\sigma} + f^{+}_{i\sigma}C_{i\sigma}) \tag{2.1}$$

where $C^{+}_{i\sigma}$ and $C_{i\sigma}$ create and annihilate conduction electrons with spin $\sigma = \pm\frac{1}{2}$ at site 1, and $f^{+}_{i\sigma}$ and $f_{i\sigma}$ create and annihilate local *f* electrons. Here *t* is the hopping matrix element for conduction electrons between neighbouring sites and $\langle ij\rangle$ denotes a pair of nearest neighbours. E_f is the energy of the localized f orbital, U is the on-site coulomb repulsion of the f electrons, and V is the on-site hybridization matrix element between electrons in the f orbital and the conduction band *C*. In the limit of large *U*, the interaction term is the dominant term. We will assume that the conduction band is infinitely wide and structureless; therefore, *V*, is neither energy nor chemical dependent. The minus sign in the first term means that the lowest *C* level will have zero wavevector. Both direct hopping and direct exchange between *f* electrons are neglected here. In a situation of large *U* and negative E_f local moments of the *f* sites becomes well defined. Since there are two electronic orbital's on each site, the quarter filled case corresponds to $N_{el} = N$ and the half-filled case has $N_{el} = 2N$. Where N_{el} = number of electrons and N = number of sites in the lattice system.

It is useful to introduce a representation of the *f* electron operators in terms of auxiliary particles, which serves to linearize the coulomb interaction terms. Hence from (2.1)

$$n^{f}_{\uparrow} = f^{+}_{\uparrow}f_{\uparrow}, n^{f}_{\downarrow} = f^{+}_{\downarrow}f_{\downarrow} \; and, n^{f}_{i\sigma} = f^{+}_{\sigma}f_{\sigma} \tag{2.2}$$

A significant feature of this model is the hybridization term *V*, which allows the f electrons in heavy fermion systems to become mobile, despite the fact that they are separated by a great distance[1].

Two interacting electrons on a two-site lattice system (1-D)

Considering two interacting electrons on a two-site lattice system in one-dimension, these correspond to the quarter filled case ($N_{el} = N$). a maximum of four electrons can be accommodate in this lattice, but with only two electrons in each site (Quarter-filled band). Here we have six possible electronic states.

$$|1\rangle = |1\uparrow 1\downarrow\rangle, |2\rangle = |2\uparrow 2\downarrow\rangle, |3\rangle = |1\uparrow 2\downarrow\rangle, |4\rangle = |1\downarrow 2\uparrow\rangle, |5\rangle = |1\uparrow 2\uparrow\rangle and$$
$$|6\rangle = |1\downarrow 2\uparrow\rangle \tag{3.1}$$

Using the Hamiltonian (2.1) to act on the basis electronic states (3.1), the Hamiltonian matrix form is:

$$H_{ij} = \begin{Bmatrix} 2E_f + u + 4v & 0 & -t & t & 0 & 0 \\ 0 & 2E_f + u + 4v & -t & t & 0 & 0 \\ -t & -t & 2E_f + 4v & 0 & 0 & 0 \\ t & t & 0 & 2E_f + 4v & 0 & 0 \\ 0 & 0 & 0 & 0 & 2E_f + 4v & 0 \\ 0 & 0 & 0 & 0 & 0 & 2E_f + 4v \end{Bmatrix} \tag{3.2}$$

The ground state energy E_g is:

$$E_g = \frac{u - \sqrt{16t^2 + u^2} + 8v + 4E_f}{2} \tag{3.3}$$

From (3.2) the eigenvalues corresponding to the singlet states energy (E_s) and triplet state energy (E_t) are given by (3.4) and (3.5) respectively.

$$E_s = \frac{u - \sqrt{16t^2 + u^2} + 8v + 4E_f}{2} \tag{3.4}$$

$$E_t = 2E_f + 4v \tag{3.5}$$

And component of the corresponding eigenvector are given in (3.6)

$$X_1 = \frac{-4t}{u + \sqrt{16t^2 + u^2}}, X_2 = -1, X_3 = 0 \text{ and } X_4 = 1 \tag{3.6}$$

Now the normalized wave-functions for the singlet states $|\Psi\rangle_s$ can be written as (3.7):

$$|\psi\rangle_s = \left[\frac{-4t}{u + \sqrt{16t^2 + u^2}} |1\uparrow 1\downarrow\rangle - |2\uparrow 2\downarrow\rangle + |1\downarrow 2\uparrow\rangle \right] \tag{3.7}$$

And the normalized wave-function for the triplet state $|\Psi\rangle_t$ can also be written as (3.8)

$$|\psi\rangle_t = |1\uparrow 2\uparrow\rangle \tag{3.8}$$

RESULTS

For simplicity, we shall concentrate here on two particular cases of the Anderson Hamiltonian: The symmetric case in which $E_f = -U/2$ with V term switched off and, the case of where $E_f = -U/2$ with V term switched on.

CASE ONE: $E_f = -U/2$ with V term switched off.

The table obtained is given below, where we varies t and keep U constant (i.e. U = 10)

Table 4.1

u	t	Es	Et
10	-0.08	-10.0026	-10
10	-0.07	-10.002	-10
10	-0.06	-10.0014	-10
10	-0.05	-10.001	-10
10	-0.04	-10.0006	-10
10	-0.03	-10.0004	-10
10	-0.02	-10.0002	-10
10	-0.01	-10	-10
10	0	-10	-10
10	0.01	-10	-10
10	0.02	-10.0002	-10
10	0.03	-10.0004	-10
10	0.04	-10.0006	-10
10	0.05	-10.001	-10

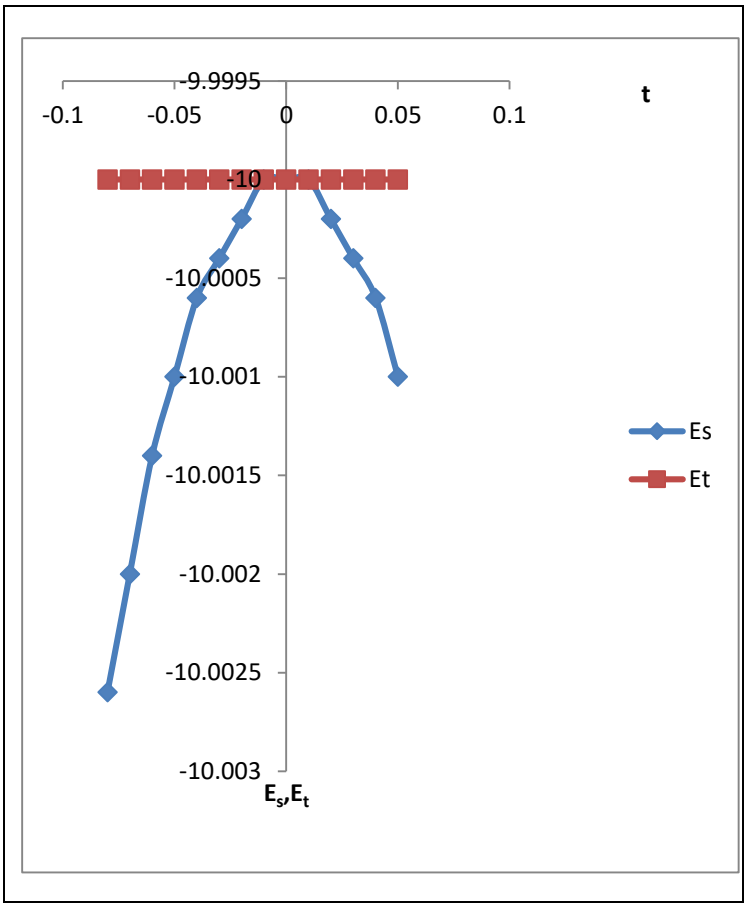

Fig 4.1 Graph of E_s,E_t against t (Colour on-line)

Now let's consider the case where we varies u and keep t constant (i.e. t = 0.5)

Table 4.2

t	U	E_s	E_t
0.5	0	-1	0
0.5	1	-1.61803	-1
0.5	2	-2.41421	-2
0.5	3	-3.30278	-3
0.5	4	-4.23607	-4
0.5	5	-5.19258	-5
0.5	6	-6.16228	-6
0.5	7	-7.14005	-7
0.5	8	-8.12311	-8
0.5	9	-9.10977	-9
0.5	10	-10.099	-10
0.5	11	-11.0902	-11
0.5	12	-12.0828	-12
0.5	13	-13.0765	-13

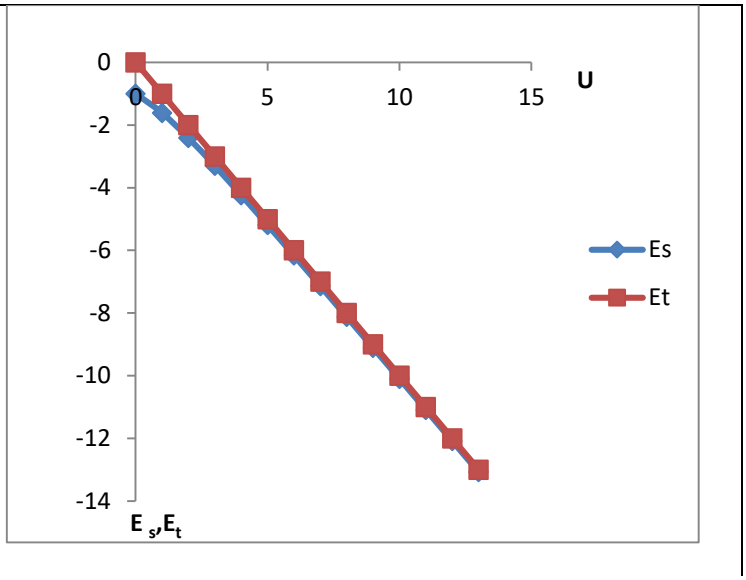

Fig. 4.2 Graph of E_s, E_t against u

CASE TWO: E_f = -U/2 with V term switched on.

Keeping the values of the hybridization term constant (i.e. V = 10) and the Hopping matrix element t (t =1)

Table 4.3

V	t	U	E_s	E_t
10	1	49	-11.4689	-9
10	1	49.2	-11.3627	-9.2
10	1	49.4	-11.2565	-9.4
10	1	49.6	-11.1503	-9.6
10	1	49.8	-11.0441	-9.8
10	1	50	-10.938	-10
10	1	50.2	-10.8318	-10.2
10	1	50.4	-10.7257	-10.4
10	1	50.6	-10.6196	-10.6
10	1	50.8	-10.5134	-10.8
10	1	51	-10.4073	-11
10	1	51.2	-10.3012	-11.2
10	1	51.4	-10.1951	-11.4
10	1	51.6	-10.089	-11.6

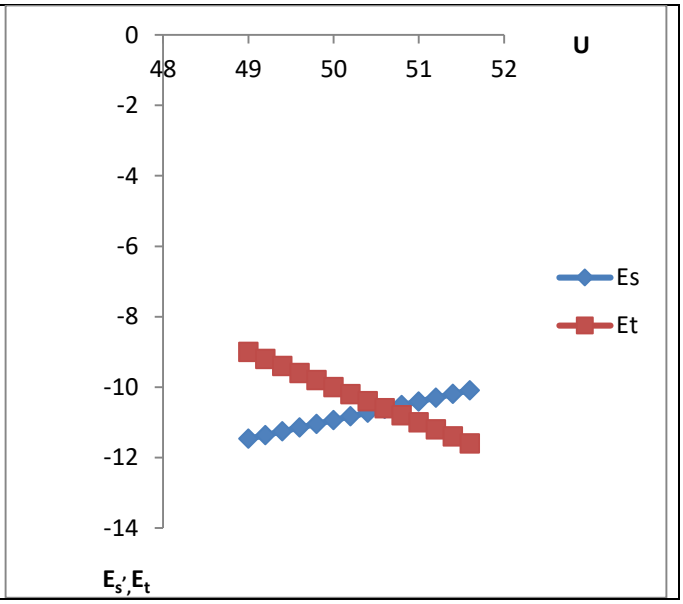

Fig 4.3 Graph of E_s, E_t against U

SUMMARY AND CONCLUSION

Summary

Usually, the eigenvalue solution of the matrix form of the Hamiltonian will yield the total energy which is the energy spectrum of the system and the lowest of them is the ground state energy of the system.

The condition to produce a ferromagnetic phase is that the lowest state energy of the triplet state, E_t must be smaller than that of the singlet state, E_s, i.e $E_t<E_s$ [13]. If the singlet states provides the lowest energy, then the system will be Antiferromagnetic (i.e. zero spin polarization), while it will be ferromagnetic (i.e. full polarization) if the triplet state provides the ground state energy.

The value at which $E_t = E_s$ gives rise to a transition from antiferromagnetic phase to the ferromagnetic phase or vice-versa. This point is called the transition point, T_p.

We first consider two electrons on two sites system using the symmetric case $E_f = -u/2$ and V =0. In this strong coupling case, the Anderson Model Hamiltonian matrix is consistent with the Kondo Model Hamiltonian Matrix giving the same ground State Energy in the small J or J = 0 region. The Hubbard Hamiltonian matrix was also recovered if the hybridization term V and Energy of the localized *f* orbital E_f are switched off.

In the context of the Kondo lattice Model, table 4.1 and Fig. 4.1 the *f* electrons will interact mainly with the single unpaired electron and will tend to align ferromagnetically. The physical meaning of this nature of graph is not completely antiferromagnetic or ferromagnetic, which indicates that it is unstable; hence it shows no transition. We note that, for an *f* electron to interact with one electron of the doubly occupied conduction band and produce a spin flip , one conduction electron needs to hop to a higher energy level. When the effective Kondo coupling J, is zero, the effect becomes more important, as there is no finite separation between the conduction energy level. From table 4.2 and fig. 4.2, it was observed that U, the on-site coulomb repulsion energy of the *f* electron, suppresses ferromagnetism tendencies in the lattices considered. It was discovered from computations, that in table 4.3 and fig. 4.3 , as the values of U increases, from 49 to 50.5, the lattice is still antiferromagnetic. At U =-10.6 which is the transition point, T_p a cross-over from antiferromagnetic phase to ferromagnetic was observed. Within this section, the relationship becomes $E_s \rangle E_t$, which is condition for ferromagnetism.

While the technique gives energy that is in principle exact, it has proven to give quite accurate results for One-Dimensional (1-D) quantum lattice system.

The method provides a controlled way of numerically diagonalizing a finite system. One can increase the accuracy by increasing the number of states.

Within the Exact method we fixed the number of electrons N_{el} to be equal to number of sites N (quarter filled band), and find the ground state energy.

In conclusion, we constructed the matrix of the one –dimensional Anderson Lattice using the Exact diagonalization technique, as we consider the symmetric cases, $E_f = -u/2$, where we either switch

on or off the hybridization term V. When this is done, the results are consistent with Hubbard (t-U) Model and Kondo Model Hamiltonian Matrix. Hence the Anderson Model is in qualitative agreement with these two famous models.

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NOTE: Technically speaking the symmetric case corresponding to E_f -U = -u/2, where u is the chemical potential of the non interacting conduction electrons which varies as a function of the filling. The E_f = -u/2 corresponds to the symmetric case at half filling for which u = 0.