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Analysis of Ground State Properties of Interacting Electrons in the Anderson Model

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ABSTRACT

The ground-state energy, wave-function, hybridization gap and magnetic phase diagram of the Single Site Impurity Anderson Model (SIAM) and the Periodic Anderson Model (PAM) were calculated using Exact-Diagonalization (ED) technique. The ED technique was applied to the SIAM and PAM in one dimension before speculating on Ce 4f being a test bed of the results, since it has 4f localized electrons in the Heavy fermion compound $CeCu_2Si_2$. Each of the results obtained describe the evolution of the electronic system in terms of a simple set of parameters. The parameter regimes studied suggest a smooth phase transition from an antiferromagnetic (AFM) phase to a ferromagnetic (FM) phase at quarter fillings in one dimension when t increases and a magnetic instability was observed as $U \rightarrow \infty$. The role of hybridization between the conduction electrons and the localized f orbital in the Anderson impurity in a semiconductor was also investigated as V increases in the SIAM and the PAM.

Keywords: transition point, hybridization gap, ferromagnetism, antiferromagnetism

INTRODUCTION

Ferromagnetism is a quantum mechanical many body phenomenon caused by electronic interactions. Since the direct spin-spin interaction is very weak,

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ferromagnetism in itinerant electronic system in transition metals must be due to the combination of the electrostatic coulomb interaction and the Pauli Principle. In spite of the basic understanding, it has not been possible till date to work out exact, detailed theoretical conditions for the occurrence of ferromagnetism in itinerant electronic systems. Such conditions must be derived from a microscopic band model of itinerant electrons (Enaibre and Idiodi, 2003)

The Anderson Model is the minimal model used in modeling the behavior of electrons in transition metals and in the rare earth and actinide metallic compound such as the 4f electrons in Ce (Anderson, 1961). The model is also used in supplying a valid explanation of the low temperature properties of many metals. It describes a simple electronic system in which a band of metal states interacts with a localized orbital, which can undergo a "Spin transition". However different magnetic phase behaviors arise in many interacting systems that exhibit a zero temperature magnetic phase transition. This paper is mainly concerned with such systems and it is therefore an investigation into the various phenomena seen in the phase diagram of interacting ferromagnetic systems. This paper concentrates on the wide range of novel states that appears and such exotic phases are magnetic in nature and investigate whether the onset of the ferromagnetic phase fluctuation can give rise to a certain class of such states. The extent of antiferromagnetism is determined and phases are considered.

Phase transitions are ubiquitous in Nature. It is a common observation that systems change their phase when subjected to certain changes in their environment. Usually this is due to a change in temperature. The transitions between ice, liquid water and water vapour and the associated enthalpy changes are important in regulating the earth's climate both globally and regionally. Within the condensed phases (liquids and solids) different phases are possible. In particular, structural transitions occur in many solids a function of an external parameter such as pressure, or temperature. Of particular interest are transitions that are driven by or directly affect the electronic degrees of freedom, e.g., transitions from a paramagnetic state to a magnetically ordered state or from a metallic state to an insulating state (Hilbert and Wolfle, 2008).

Since some of the interesting (and least understood) phase transitions occur in metals with strong electronic correlations. Of particular importance in the field of strongly correlated materials is the kondo effect, arising from the coupling between localized magnetic moments (generally arising from impurities) and conduction electrons. In the context of strongly correlated electron systems one is mainly interested in magnetic phase transition involving the conduction electrons. As prototype in this paper, ferromagnetic (FM) and antiferromagnetic (AFM) phase transitions will be consider.

The objectives of this paper are to investigate the parameter range giving rise to, the antiferromagnetic phase and ferromagnetic phase in the SIAM and PAM, elucidate the nature of the ground state and the magnetic properties of the SIAM and PAM,

determine the effect of the SIAM and PAM parameters on electrons interacting in 1 – D lattice, and demonstrate the role of hybridization gap Δ in semiconductors in SIAM and PAM.

MODEL AND METHODOLOGY

The SIAM Hamiltonian is given by

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

where $C^{+}_{i\sigma}$ and $C_{i\sigma}$ create and annihilate conduction electrons with spin $\sigma = \pm\frac{1}{2}$ at site i, 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 electron C. In the limit of large U, the interaction term is the dominant term. If it is assumed, as considered in this thesis, that the conduction band is infinitely wide and structureless; then, V, is neither energy nor chemical dependent. 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. In equation (1), $n^{f}_{\uparrow} = f^{+}_{\uparrow}f_{\uparrow}$, $n_{f\sigma} = f^{+}_{\sigma}f_{\sigma}$ and $n^{f}_{\downarrow} = f^{+}_{\downarrow}f_{\downarrow}$. 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.

Generalizing the single site impurity Anderson model (1) to a lattice of localized orbital, f, one obtains the so-called Periodic Anderson Model (PAM). The Hamiltonian, H, of the PAM is given by

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

(2) where all the symbols have their usual meaning. 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.

Illustration of The Anderson Model on a Two Site Systems.

Considering a system of two interacting electrons on two sites (1-D), the relevant electronic states of this system are:

$$|1\rangle = |1\uparrow 1\downarrow\rangle, |2\rangle = |2\uparrow 2\downarrow\rangle, |3\rangle = |1\uparrow 2\downarrow\rangle, |4\rangle = |1\downarrow 2\uparrow\rangle, |5\rangle = |1\uparrow 2\uparrow\rangle, |6\rangle = |1\downarrow 2\uparrow\rangle \quad (3)$$

With the six electronic states as basis states, the Hamiltonian matrix of site 1 and 2 of SIAM are given by (4) and (5) respectively

$$H_{ij} = \begin{Bmatrix} 2E_f + U + 4V & 0 & t & -t & 0 & 0 \\ 0 & o & t & -t & 0 & 0 \\ t & t & E_f + 2V & 0 & 0 & 0 \\ -t & -t & 0 & E_f + 2V & 0 & 0 \\ 0 & 0 & 0 & 0 & E_f + 2V & 0 \\ 0 & 0 & 0 & 0 & 0 & E_f + 2V \end{Bmatrix} \quad (4)$$

$$H_{ij} = \begin{Bmatrix} 0 & 0 & t & -t & 0 & 0 \\ 0 & 2E_f + U + 4V & t & -t & 0 & 0 \\ t & t & E_f + 2V & 0 & 0 & 0 \\ -t & -t & 0 & E_f + 2V & 0 & 0 \\ 0 & 0 & 0 & 0 & E_f + 2V & 0 \\ 0 & 0 & 0 & 0 & 0 & E_f + 2V \end{Bmatrix} \quad (5)$$

Considering a particular case where E_f =1, U=1, V=2 and t=1. The ground state energies for both the singlet (E_s) and triplet state (E_t) of sites 1 and 2 are given below

- Site 1 of SIAM E_s = -0.384001
- And the components of the corresponding Eigenvector are:
- X_1 = -0.384001, X_2 = 5.0, X_3 = 5.05873, X_4 =11.3253
- E_t = 5.0
- And the component corresponding to the Eigenvectors are X_5 = 1 and X_6 = 0
- Site 2 of SIAM , E_s = -0.384001
- And the components of the corresponding Eigenvector are:
- X_1 = -0.384001, X_2 = 5.0, X_3 = 5.05873, X_4 =11.3253
- E_t = 5.0
- And the component corresponding to the Eigenvectors are X_5 = 1 and X_6 = 0

Now the normalized wave-functions for the singlet states $|\psi\rangle_s$ can be written as

$$|\psi\rangle_s = \left[-0.384001|1\uparrow 1\downarrow\rangle + 5.0|2\uparrow 2\downarrow\rangle + 5.05873|1\uparrow 2\downarrow\rangle + 11.3253|1\downarrow 2\uparrow\rangle\right] \quad (6)$$

and the normalized wave-functions for the triplet states $|\psi\rangle_t$ can be written as

$$|\psi\rangle_t = |1\uparrow 2\uparrow\rangle \quad (7)$$

Considering (2), the Hamiltonian matrix of PAM is given below

$$H_{ij} = \begin{Bmatrix} 2E_f + U + 4V & 0 & -t & t & 0 & 0 \\ 0 & 2E_f + U + 4V & -t & t & 0 & 0 \\ -t & -t & 2E_f + 4V & 0 & 0 & 0 \\ t & t & 0 & 2E_f + 4V & 0 & 0 \\ 0 & 0 & 0 & 0 & 2E_f + 4V & 0 \\ 0 & 0 & 0 & 0 & 0 & 2E_f + 4V \end{Bmatrix} \quad (8)$$

and the generalized ground state energy is given

$$E_s = \frac{1}{2}\left[4E_f + U - \sqrt{16t^2 + U^2} + 8V\right]$$

(9)

While the ground state energies for both singlet (E_s) and triplet (E_t) are given by (10) and (11) respectively

$$Es = \frac{1}{2}[\ 4E_f + U - \sqrt{16t^2 + U^2} - 8V\ ] \quad (10)$$

$$Et = 2E_f + 4V \quad (11)$$

Also the components of the corresponding Eigenvalues are:

$$\left.\begin{aligned} X_1 &= -\frac{4t}{U + \sqrt{16t^2 + U^2}} \\ X_2 &= -1 \\ X_3 &= 0 \\ X_4 &= 1 \end{aligned}\right\} \quad (12)$$

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

$$|\psi\rangle_s = \left[-\frac{4t}{U + \sqrt{16t^2 + U^2}}|1\uparrow 1\downarrow\rangle - |2\uparrow 2\downarrow\rangle + |1\downarrow 2\uparrow\rangle\right] \quad (13)$$

and the normalized wave-functions for the triplet states $|\Psi\rangle_t$ can be written as

$$|\psi\rangle_t = |1\uparrow 2\uparrow\rangle \quad (14)$$

NUMERICAL RESULTS

The numerical analysis carried out to obtain the series coefficients for the ground state energies in order to determine the magnetic phase transition from AFM to FM and the Hybridization gap are given by table 1, 2, 3 for the SIAM and table 4, 5, 6 for the PAM with their corresponding graphs.

Table 1: Singlet (E_s) and Triplet (E_t) State Energies as U Varies and Other Parameters Remaining Constant

t	V	$E_f=-^u/_2$	U	E_s	E_t
0.50	0.375	5.00	-10.00	-0.09	5.75
0.50	0.375	2.50	-5.00	-0.16	3.25
0.50	0.375	0.00	0.00	-0.5	0.75
0.50	0.375	-2.50	5.00	-2.12	-1.75
0.50	0.375	-5.00	10.00	-4.45	-4.25
0.50	0.375	-7.50	15.00	-6.89	-6.75
0.50	0.375	-10.00	20.00	-9.35	-9.25
0.50	0.375	-12.50	25.00	-11.82	-11.75
0.50	0.375	-15.00	30.00	-14.31	-14.25
0.50	0.375	-17.50	35.00	-16.81	-16.75
0.50	0.375	-20.00	40.00	-19.29	-19.25

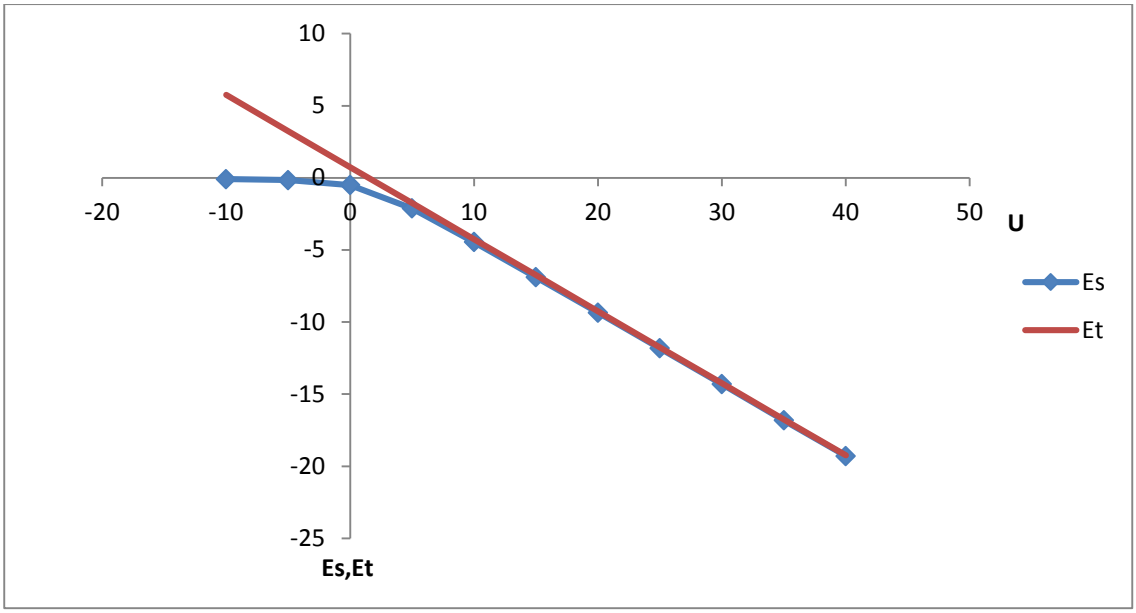

Figure 1: Lowest Energies of the Singlet (E_s) and Triplet States (E_t) Against U, for a System of 2 Electrons on 2-Sites at Sites 1 and 2, Using SIAM (1-D)

Table 2: Singlet (E_s) and Triplet (E_t) State Energies as T Varies and Other Parameters Remaining Constant

$E_f=-^u/_2$	U	V	t	E_s	E_t
-1.00	2.00	0.375	-20.00	-39.76	-0.25
-1.00	2.00	0.375	-15.00	-29.76	-0.25
-1.00	2.00	0.375	-10.00	-19.77	-0.25
-1.00	2.00	0.375	-5.00	-9.89	-0.25
-1.00	2.00	0.375	0.00	-0.25	-0.25
-1.00	2.00	0.375	5.00	9.39	-0.25
-1.00	2.00	0.375	10.00	19.03	-0.25
-1.00	2.00	0.375	15.00	28.67	-0.25
-1.00	2.00	0.375	20.00	38.31	-0.25

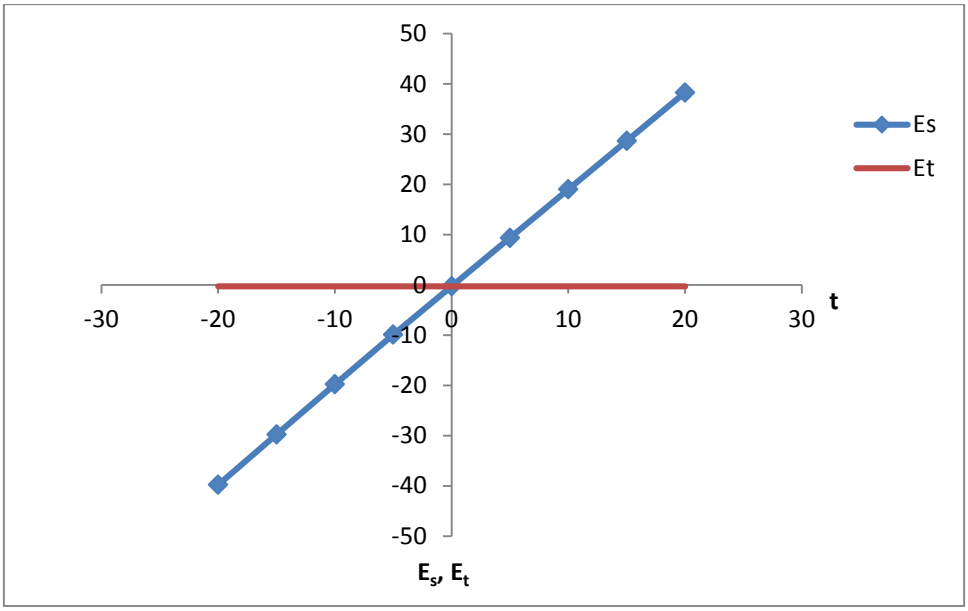

Figure 2: Lowest Energies of the Singlet (E_s) and Triplet States (E_t) Against t.

Table 3: Singlet (E_s) and Triplet (E_t) State Energies as V Varies and other Parameters Remaining Constant

$E_f=-^u/_2$	U	t	V	E_s	E_t
-1.00	2.00	0.50	-2.00	-8.16	-5.00
-1.00	2.00	0.50	-1.50	-6.23	-4.00
-1.00	2.00	0.50	-1.00	-4.30	-3.00
-1.00	2.00	0.50	-0.50	-2.37	-2.00
-1.00	2.00	0.50	0.00	-0.44	-1.00
-1.00	2.00	0.50	0.50	1.49	0.00
-1.00	2.00	0.50	1.00	3.42	1.00
-1.00	2.00	0.50	1.50	5.35	2.00
-1.00	2.00	0.50	2.00	7.28	3.00

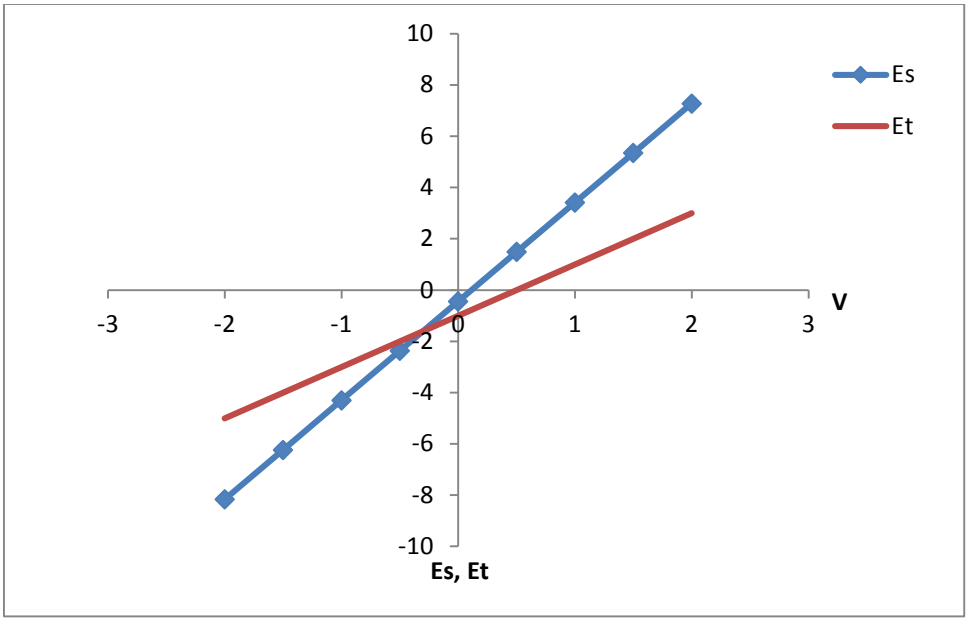

Figure 3: Lowest Energies of the Singlet (E_s) and Triplet (E_t) State Against V.

Table 4: Singlet (E_s) and Triplet (E_t) State Energies as U Varies and Other Parameters Remaining Constant, Using the PAM.

t	V	E_f	U	E_s	E_t
0.50	0.375	5.00	-10.00	1.40	11.50
0.50	0.375	2.50	-5.00	1.30	6.50
0.50	0.375	0.00	0.00	0.50	1.50
0.50	0.375	-2.50	5.00	-3.69	-3.50
0.50	0.375	-5.00	10.00	-8.60	-8.50
0.50	0.375	-7.50	15.00	-13.56	-13.50
0.50	0.375	-10.00	20.00	-18.55	-18.50
0.50	0.375	-12.50	25.00	-23.54	-23.50
0.50	0.375	-15.00	30.00	-28.53	-28.50
0.50	0.375	-17.50	35.00	-33.52	-33.50
0.50	0.375	-20.00	40.00	-38.53	-38.50

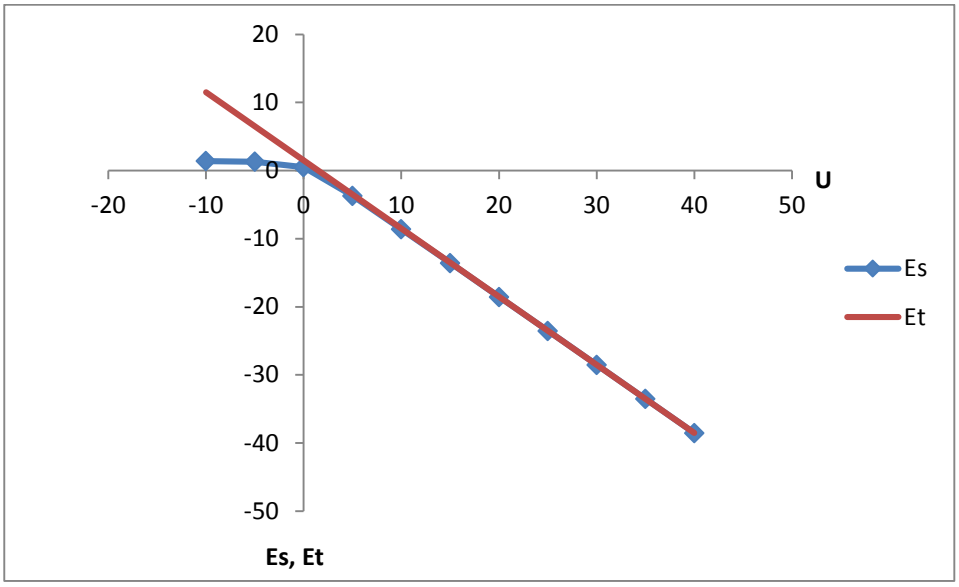

Figure 4: Lowest Energies of the Singlet (E_s) and Triplet (E_t) States Against U. Energy Units are in Ev.

Table 5: Singlet (E_s) and Triplet (E_t) State Energies as t Varies and Other Parameters Remaining Constant (PAM).

$E_f = -u/2$	U	V	t	E_s	E_t
-1.00	2.00	0.375	-20.00	-39.51	-0.50
-1.00	2.00	0.375	-10.00	-19.53	-0.50
-1.00	2.00	0.375	0.00	0.45	-0.50
-1.00	2.00	0.375	10.00	20.43	-0.50
-1.00	2.00	0.375	20.00	40.41	-0.50
-1.00	2.00	0.375	30.00	60.39	-0.50
-1.00	2.00	0.375	40.00	80.37	-0.50

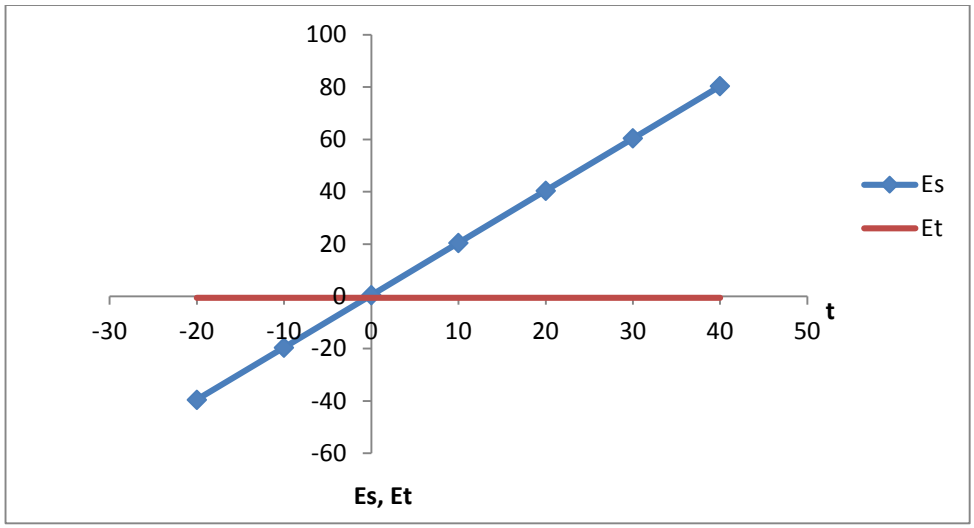

Figure 5: Lowest Energies of the Singlet (E_s) and Triplet (E_t) States Against t. Energy Units are in Ev.

Table 6: Singlet (E_s) and Triplet (E_t) State Energies as V Varies and Other Parameters Remaining Constant.

$E_f = -U/2$	U	t	V	E_s	E_t
-1.00	2.00	0.50	-2.00	-10.41	-10.00
-1.00	2.00	0.50	-1.50	-8.41	-8.00
-1.00	2.00	0.50	-1.00	-6.41	-6.00
-1.00	2.00	0.50	-0.50	-4.41	-4.00
-1.00	2.00	0.50	0.00	-2.41	-2.00
-1.00	2.00	0.50	0.50	-0.41	0.00
-1.00	2.00	0.50	1.00	1.59	2.00
-1.00	2.00	0.50	1.50	3.59	4.00
-1.00	2.00	0.50	2.00	5.59	6.00

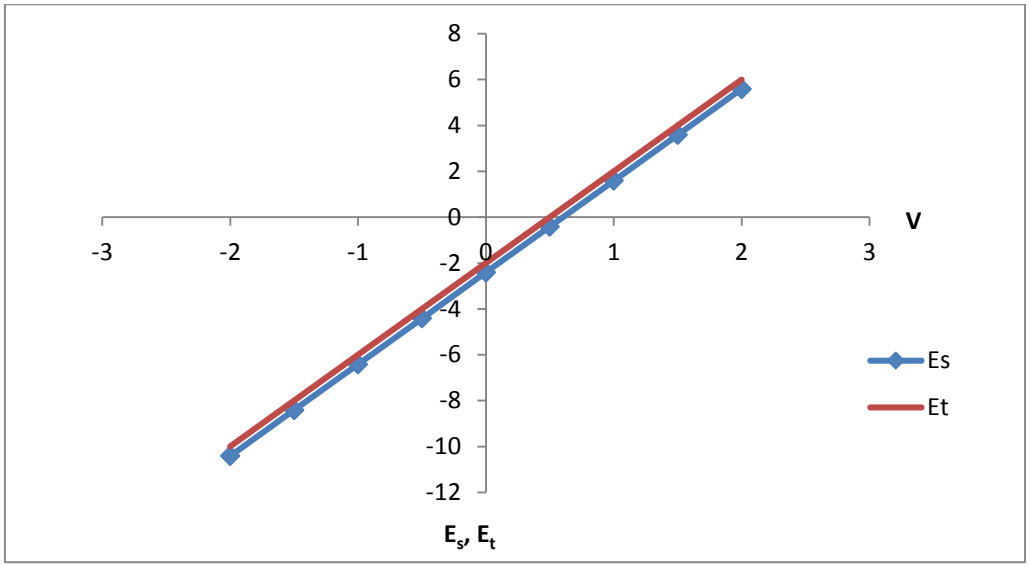

Figure 6: Lowest Energies of the Singlet (E_s) and Triplet (E_t) States Against V.

DISCUSSION OF RESULTS

From the computations, it was observed from Table1 and Figure1 that as the value of the on-site coulomb repulsion, U is increase from -10, the lattice system which was originally Antiferromagnetic (AFM) becomes unstable just immediately after the point U=15.0; this magnetic instability of the system is in agreement with results obtained by Rice and Ueda (1986).

Observation from Table 2 and 3 and their corresponding graphs Figure 2 and 3 shows that, as the value of the hopping matrix element of the conduction electrons, t and the on-site hybridization element between the f orbital and the conduction electron, V are increased respectively, the ground-state continue to increase to a transition point T_p, where $E_s=E_t$ and as their values are further increased beyond T_p, where $E_s > E_t$ the system becomes Ferromagnetic (FM). The physical implication is that the electronic correlations favouring AFM gets weaker while that of FM gets stronger as the values

of the hopping matrix element, t and on-site hybridization element, V are increased. This continue on till the electronic correlation favouring ferromagnetism begins to dominate (i.e. there is cross-over to ferromagnetism) and this domination is enhanced as t and V are increased. Hence, this direct exchange interaction provides a natural way for stabilizing ferromagnetic states, Kollar *et al*., (1995).

From computations, it was observed from Table 4 and Figure 4 that as the energy of the localized orbital, E_f or on-site coulomb repulsion, U of the f electrons are increased the system which was AFM becomes unstable. The instability of the system is in agreement with Rice and Ueda (1986); using the Gutzwiller approach, they found that the Energy of the localized orbital, E_f is well below the Fermi surface, there is always a ferromagnetic instability (assuming there is no orbital degeneracy).

From the computations in Table 5 and Figure 5 shows that, as the values of t increases, there is a smooth transition from an AFM phase to a FM phase at half fillings as indicated by Paolo *et al*., (1993). Table 6 and Figure 6 shows that, as the values of the on-site hybridization element, V is increased, the hybridization gap or semiconducting gap Δ was observed between E_s and E_t. The gap observed in this system is constant (i.e. $\Delta \sim 0.14$) for the 2-site chain. This result is in agreement with the results obtained by Clare and Guerrero (1996), and Mitsumoto and Ono (2010) that studied Anderson impurity in a semiconductor using DMRG technique. The importance of hybridization gap is well known in semiconductors. After all, it is the hybridization that allows ordinary donor and acceptor impurities to contribute carriers to a semiconductor.

CONCLUSION

In this paper the power of ED technique is applied to SIAM and PAM to study the effect of two interacting electrons on parameters E_f, U, V and t on the tendency to ferromagnetism. Attention was focused on the parameter region where a transition from AFM to FM and Hybridization or semiconducting gap occurs.

In the lattice systems studied, the results obtained for sites 1 and 2 of SIAM are the same, as this may be as a result of edge effects since open boundary condition was use for the SIAM and periodic boundary condition applied to PAM. The ground state was always a spin singlet and the first excited state was always a singlet for both the SIAM and the PAM and, there is always a magnetic instability as the value of U increases for the SIAM and PAM. The results obtained also shows a smooth transition from an AFM phase to a FM phase when the value of t increases as indicated by Paolo *et al*., (1993) who studied the PAM in 1-D using a different technique. It is also seen that the hybridization gap or semiconducting gap Δ has a strong dependence on the values of E_f and V. The smaller E_f or the larger V is, i. e. the stronger the hybridization between the on-site f and the conduction electrons, the wider the gap in the PAM. This

may account for the role of hybridization in a semiconductor and the Heavy fermion semiconductor behavior for $CeCu_2Si_2$.

On the whole, this is the first time the SIAM and PAM are combine in 1-D. In this paper, only nearest neighbor (NN) interaction were considered; consideration of the next nearest neighbor (NNN) is highly desirable which hopefully will become possible in the near future.

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