

SINGLE AND MULTI – PHASE DYNAMICS OF THE (ANTI)FERROMAGNETIC CeCu_2Si_2 SYSTEMS.

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Abstract

We considered the single site impurity Anderson model with the aid of the application of Exact – diagonalization technique on an open boundary system of two interacting electrons on four sites with twenty eight basis electronic states.

The results obtained shows that Increasing Ce content experimentally in CeCu_2Si_2 is equivalent to increasing the hopping matrix element t in this study; and also increasing the values of the on-site hybridization element, V , the system which was originally AFM becomes FM. We also observed that the cost of performing these theoretical simulations is approximately the same as simulating 2 electrons on 4 sites (1-D) in the Anderson model and 4 electrons on 8 sites (1-D) in the one band Hubbard model.

KEYWORDS: CeCu_2Si_2 , ferromagnetism, antiferromagnetism, triplet state, ground state.

1.0 INTRODUCTION

The problem of two “magnetic” impurities in a non – magnetic metallic environment has attracted attention in the past decades (Zhong, 2022). The wealth of understanding gained in the past forty years on one – impurity has encouraged the attempt to clarify the rich behaviour of a system in which the Kondo effect (Itai and Fazekas 1996) (low-temperature suppression of the moment) competes against the tendency to magnetic behaviour induced by spin-spin Ruderman-Kittel-

Kasuya-Yosida (RKKY) or strong super – exchange interactions. Far from being yet understood, the interplay between Kondo effect and magnetism is indeed one of the key problems in the physics of heavy fermion systems (Irkhin and Streltsov, 2022). Theoretically, the simplest models which are believed to account for the essential physics of these systems are the single – site impurity Anderson model (Anderson, 1961; Fan et al, 2022) and the analogous version of the Kondo model (Amadon and Hirsch 1996). The challenges of the theorist are to explore the phase space of the parameters of these models in order to map the possible types of ground states that allow one to describe, and compare the theoretical findings with the rich variety of situation that nature provides (Enaroseha *et al*, 2021a).

In this respect, the study of a simple sigle site – impurity model can be seen as a preliminary step toward the understanding of the physics of metals with lattice of magnetic impurities.

2.0 MODEL AND METHODOLOGY

We consider the single site – impurity Anderson Hamiltonian (Anderson 1961; Zhu and Zhu, 2011; Enaroseha et al, 2021b, Enaroseha and Akpojotor, 2013) given by:

$$H = \sum_{k\sigma} \xi_k C_{k\sigma}^{\dagger} C_{k\sigma} + \sum_{i\sigma} E_d n_{i\sigma} + \sum_i U n_{i1} n_{i2} + \sum_{k\sigma} \sum_i V_k C_{k\sigma}^{\dagger} d_{i\sigma} + H.C. \quad (1)$$

here the $C_{k\sigma}^{\dagger}$'s are the creation operators associated with a set of itinerant state (conduction electrons) of energy ξ_k , hybridizing (V_k) with two localized orbitals ($d_{i\sigma}^{\dagger}$, associated with the magnetic impurities) of atomic energy E_d , located at the position R_1 and R_2 . U represents the impurity coulomb repulsion energy, and $n_{i\sigma} = d_{i\sigma}^{\dagger} d_{i\sigma}$. $H.C.$ is the Hermitian Conjugation.

We defined the Hilbert space for many-electron problems using the fermion operator formalism: the formalism is called “second quantization”. For each lattice site $x \in \mathbb{Z}$, and spin index $\sigma \in \uparrow, \downarrow$ we associate a fermion operator $C_{x,\sigma}$. One can freely take the conjugate, products, and linear combinations (with complex coefficients) of these operators (and the identity operator) to get new operators. We require that these operators satisfy the anticommutation relations

$$\{C_{x,\sigma}^\dagger, C_{y,\tau}\} = \delta_{x,y} \delta_{\sigma\tau}, \quad (2)$$

And

$$\{C_{x,\sigma}^\dagger, C_{y,\tau}^\dagger\} = \{C_{x,\sigma}, C_{y,\tau}\} = 0 \quad (3)$$

For any $x, y \in \mathbb{Z}$, and $\sigma, \tau = \uparrow, \downarrow$ where $\{A, B\} = AB + BA$. Note that equations (2) and (3) implies $(C_{x,\sigma})^2 = (C_{x,\sigma}^\dagger)^2 = 0$.

Physically, $C_{x,\sigma}$ and $C_{x,\sigma}^\dagger$ are interpreted as the operators which respectively annihilate and create an electron at site x and spin σ .

3.0 THEORETICAL CALCALATIONS

3.1 CALCULATION FOR A SYSTEM OF 2-ELECTRONS ON A 4-SITE (1-D) USING THE SINGLE-SITE IMPURITY ANDERSON HAMILTONIAN AT SITE 1

Consider a system of two interacting electrons on four-sites with open boundary conditions using the single site impurity Anderson model (1), shown in Fig. 3.1 .

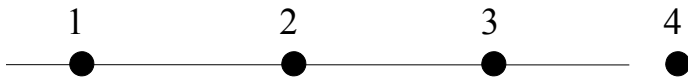


Fig 3.1: Four interacting electrons on sites 1, 2, 3 and 4 in 1-D (SIAM).

[illegible]
$$\begin{aligned}
H = & \mathfrak{h}_{\square} \mathfrak{t} \mathfrak{t} \mathfrak{t} \mathfrak{t} \\
& C_{3\downarrow}^{+\mathfrak{t} C_{211}} + \mathfrak{t} \mathfrak{t} C_{3\uparrow}^{+\mathfrak{t} C_{41}} + C_{4\uparrow}^{+\mathfrak{t} C_{31} + C_{31}^{+\mathfrak{t} C_{41}} + C_{31}^{+\mathfrak{t} C_{31}} + \mathfrak{t} \mathfrak{t}} \mathfrak{t} \\
& E_f \mathfrak{t} \mathfrak{t} \mathfrak{t} \mathfrak{t} \mathfrak{t} \mathfrak{t} + \mathfrak{t} f_{1\uparrow} + f_{1\downarrow}^{+\mathfrak{t} f_{1\uparrow} + \mathfrak{t} \mathfrak{t}} \mathfrak{t} \quad V \mathfrak{t} \mathfrak{t}
\end{aligned} \tag{5}$$

For simplicity, a 16 x 16 matrix was formed representing the singlet states matrix for the net spin 0 states (the antiferromagnetic states), see equation (6) and a 12 x 12 matrix was also formed representing the triplet states matrix for the net spin ± 1 (the ferromagnetic states), see (9). Because of the complex nature of the matrices, the eigenvalues, eigenvectors and the wave function for a particular case was considered. Consider the case where $E_f=1$, $u = 1$, $v = 2$ and $t=1$.

4

$$\begin{pmatrix}
2E_f & u & 4v & 0 & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & t & -t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & -t & 0 & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & -t \\
t & -t & 0 & 0 & E_f & 2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & t & 0 & 0 & 0 & E_f & 2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t & 0 & E_f & 2v & 0 & t & 0 & 0 & t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & t & 0 & E_f & 2v & 0 & t & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f & 2v & 0 & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f & 2v & 0 & 0 & 0 & t & 0 & 0 \\
0 & t & t & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & E_f & 2v & 0 & 0 & 0 & 0 \\
0 & -t & -t & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & E_f & 2v & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & t & -t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & t \\
0 & 0 & t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 \\
0 & 0 & -t & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0
\end{pmatrix} \quad (6)$$

The ground state energy is given by

$$E_s = -2.91137 \quad (7)$$

The corresponding ground state amplitudes are

$$\begin{aligned}
\phi_s = & \{ -0.00632628 \phi_{1\uparrow 1\downarrow} - 0.28448 \phi_{2\uparrow 2\downarrow} \\
& - 0.481464 \phi_{3\uparrow 3\downarrow} - 0.227213 \phi_{4\uparrow 4\downarrow} \\
& + 0.0440036 \phi_{1\uparrow 2\downarrow} - 0.0440036 \phi_{1\downarrow 2\uparrow} \\
& - 0.0573223 \phi_{1\uparrow 3\downarrow} + 0.0573223 \phi_{1\downarrow 3\uparrow} \\
& + 0.0393841 \phi_{1\uparrow 4\downarrow} - 0.0393841 \phi_{1\downarrow 4\uparrow} \\
& + 0.37011 \phi_{2\uparrow 3\downarrow} - 0.37011 \phi_{2\downarrow 3\uparrow} \\
& - 0.25426 \phi_{2\uparrow 4\downarrow} + 0.25426 \phi_{2\downarrow 4\uparrow} \\
& + 0.330751 \phi_{3\uparrow 4\downarrow} - 0.330751 \phi_{3\downarrow 4\uparrow} \}
\end{aligned} \quad (8)$$

The matrix of the Hamiltonian for the triplet states is given by equation (9)

$$\begin{pmatrix}
E_{f,2,v} & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & E_{f,2,v} & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
t & 0 & E_{f,2,v} & 0 & t & 0 & t & 0 & 0 & 0 & 0 & 0 \\
0 & t & 0 & E_{f,2,v} & 0 & t & 0 & t & 0 & 0 & 0 & 0 \\
0 & 0 & t & 0 & E_{f,2,v} & 0 & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & E_{f,2,v} & 0 & 0 & 0 & t & 0 & 0 \\
0 & 0 & t & 0 & 0 & 0 & E_{f,2,v} & 0 & 0 & t & 0 & 0 \\
0 & 0 & 0 & t & 0 & 0 & 0 & E_{f,2,v} & 0 & 0 & t & 0 \\
0 & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 & t & 0 \\
0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & 0
\end{pmatrix} \quad (9)$$

The ground state energy of the triplet states is given by:

$$E_t = -1.55332$$

The corresponding ground state amplitude is

$$\begin{aligned}
|\phi\rangle_t = & \{ -0.0150754 |1\uparrow 2\uparrow\rangle + 0.00266558 |1\downarrow 2\downarrow\rangle \\
& + 0.0987942 |1\uparrow 3\uparrow\rangle - 0.0174684 |1\downarrow 3\downarrow\rangle \\
& - 0.121166 |1\uparrow 4\uparrow\rangle + 0.0214241 |1\downarrow 4\downarrow\rangle \\
& - 0.511189 |2\uparrow 3\uparrow\rangle + 0.0903863 |2\downarrow 3\downarrow\rangle \\
& + 0.695246 |2\uparrow 4\uparrow\rangle - 0.122931 |2\downarrow 4\downarrow\rangle \\
& - 0.447587 |3\uparrow 4\uparrow\rangle + 0.0791404 |3\downarrow 4\downarrow\rangle \}
\end{aligned} \quad (10)$$

3.3b CALCULATION FOR A SYSTEM OF 2-ELECTRONS ON A 4-SITE (1-D) USING THE SINGLE-SITE IMPURITY ANDERSON HAMILTONIAN AT SITE 2

[illegible][illegible]

The Hamiltonian matrix for the singlet states is given by (13):

$$\mathbf{H} = \begin{pmatrix}
0 & 0 & 0 & 0 & t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2E_f & u & 4v & 0 & 0 & t & t & 0 & 0 & 0 & 0 & t & t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & t \\
t & t & 0 & 0 & E_f & 2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
t & t & 0 & 0 & 0 & E_f & 2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & t & 0 & 0 \\
0 & t & t & 0 & 0 & 0 & t & 0 & 0 & 0 & E_f & 2v & 0 & t & 0 \\
0 & t & t & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & E_f & 2v & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & E_f & 2v & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & E_f & 2v \\
0 & 0 & t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 \\
0 & 0 & t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0
\end{pmatrix} \quad (13)$$

The ground state energy is given below:

$$E_s = -2.20148 \quad (14)$$

The corresponding ground state amplitude is

$$\begin{aligned}
|\phi\rangle_s = & \{ 0.0159005 |1\uparrow 1\downarrow\rangle + 0.0180259 |2\uparrow 2\downarrow\rangle \\
& + 0.52829 |3\uparrow 3\downarrow\rangle + 0.436096 |4\uparrow 4\downarrow\rangle \\
& - 0.0175024 |1\uparrow 2\downarrow\rangle + 0.0175024 |1\downarrow 2\uparrow\rangle \\
& - 0.0921165 |1\uparrow 3\downarrow\rangle + 0.0921165 |1\downarrow 3\uparrow\rangle \\
& - 0.0838086 |1\uparrow 4\downarrow\rangle + 0.0838086 |1\downarrow 4\uparrow\rangle \\
& - 0.101482 |2\uparrow 3\downarrow\rangle + 0.101482 |2\downarrow 3\uparrow\rangle \\
& + 0.0923863 |2\uparrow 4\downarrow\rangle - 0.0923863 |2\downarrow 4\uparrow\rangle \\
& - 0.480028 |3\uparrow 4\downarrow\rangle + 0.480028 |3\downarrow 4\uparrow\rangle \}
\end{aligned} \quad (15)$$

The matrix of the Hamiltonian for the triplet state is given by (16)

$$\begin{pmatrix}
E_{f, 2, v} & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & E_{f, 2, v} & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
t & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 & 0 & 0 \\
0 & t & 0 & 0 & 0 & t & 0 & t & 0 & 0 & 0 & 0 \\
0 & 0 & t & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 \\
0 & 0 & t & 0 & 0 & 0 & E_{f, 2, v} & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & 0 & 0 & E_{f, 2, v} & 0 & t & 0 & 0 \\
0 & 0 & 0 & 0 & t & 0 & t & 0 & E_{f, 2, v} & 0 & t & 0 \\
0 & 0 & 0 & 0 & 0 & t & 0 & t & 0 & E_{f, 2, v} & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_{f, 2, v} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_{f, 2, v}
\end{pmatrix} \quad (16)$$

The ground state energy of the triplet states is given by:

$$E_t = -1.28684 \quad (17)$$

The corresponding ground state amplitude is

$$\begin{aligned}
|\phi\rangle_t = & \{ 0.112253|1\uparrow 2\uparrow\rangle + 0.00377247|1\downarrow 2\downarrow\rangle \\
& - 0.705719|1\uparrow 3\uparrow\rangle - 0.0237169|1\downarrow 3\downarrow\rangle \\
& + 0.660665|1\uparrow 4\uparrow\rangle + 0.0222028|1\downarrow 4\downarrow\rangle \\
& + 0.13523|2\uparrow 3\uparrow\rangle + 0.00454464|2\downarrow 3\downarrow\rangle \\
& - 0.144452|2\uparrow 4\uparrow\rangle - 0.00485457|2\downarrow 4\downarrow\rangle \\
& + 0.112253|3\uparrow 4\uparrow\rangle + 0.00377247|3\downarrow 4\downarrow\rangle \}
\end{aligned} \quad (18)$$

4.0 RESULTS AND DISCUSSION.

4.1 RESULTS FOR A SYSTEM OF 2 ELECTRONS ON A 4 SITES (1-D) USING THE SIAM HAMILTONIAN AT SITE 1 AND 4.

The Hamiltonian matrix form is given by (6) for the singlet state energy and (9) for the triplet states energy respectively at site 1 and 4. Due to edge effect in the interactions, site 1 and 4 are treated together, as open boundary condition is considered here. Hence sites 1 and 4, shown in Fig. 3.1 are having the same ground

state energies for both the singlet states and triplet states. Numerical analyses carried out to obtain the series coefficients for the ground state energies in order to determine the single and multi – phase dynamics are given in Fig. 4.1, 4.2 and 4.3 respectively.

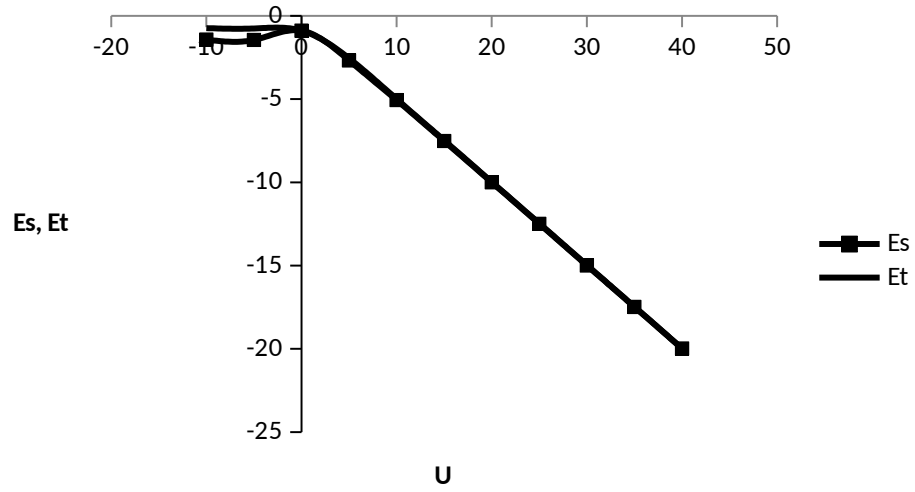


Fig. 4.1: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U for a system of 2 electrons on 4 lattice sites at sites 1 and 4 Using the SIAM (1-D).

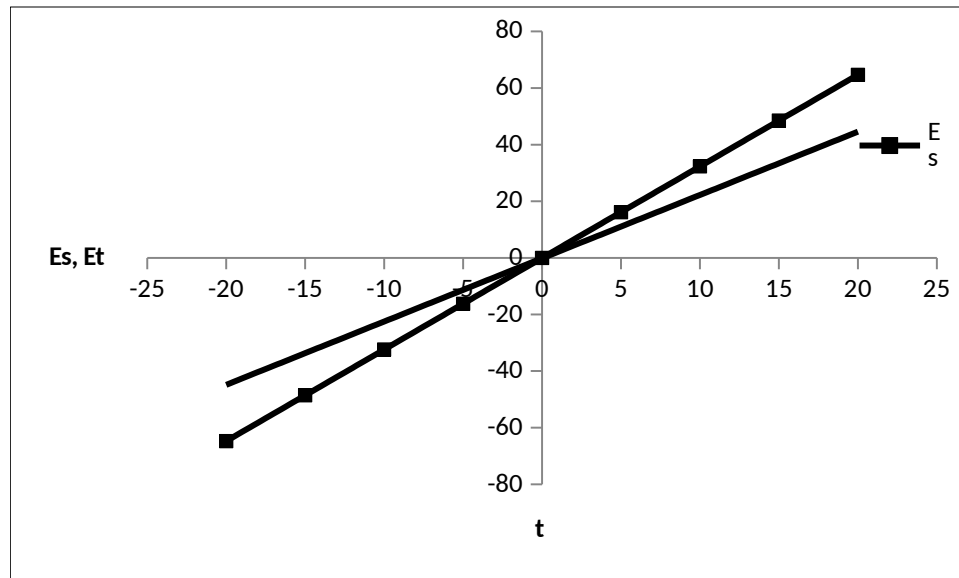


Fig 4.2: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t for a system of 2 electrons on 4 lattice sites at site 1 and 4 using SIAM (1-D).

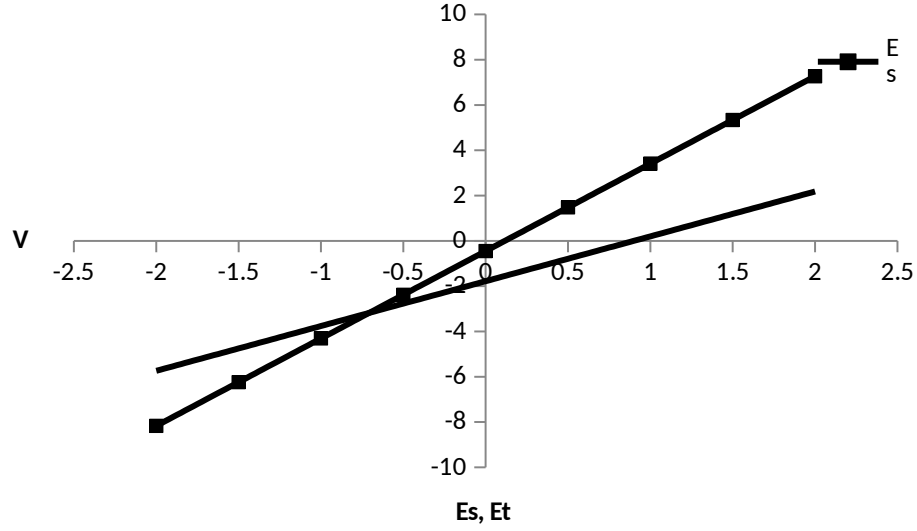


Fig 4.3: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V for a system of 2 electrons on 4 lattice sites at site 1 and 4 using the SIAM (1-D).

4.3b RESULTS FOR A SYSTEM OF 2 ELECTRONS ON A 4 SITE (1-D) USING THE SIAM HAMILTONIAN AT SITES 2 AND 3.

The Hamiltonian matrix form for the SIAM is given by (13) for the singlet state energies at site 2 and site 3 while (16) provides the Hamiltonian matrix for the triplet states energies at site 2 and 3. There is edge effect in the interactions, as open boundary condition is used here. Hence site 2 will interact with both sites 1 and 3, while site 3 will interact with sites 2 and 4, as shown in Fig 3.1. As a result of the edge effects, sites 2 and 3 will provide the same ground state energies for the singlet and triplet states.

Numerical analyses carried out to obtain the series coefficients for the ground state energies in order to determine the magnetic phase diagram are given in Fig 4.4, 4.5 and 4.6 respectively.

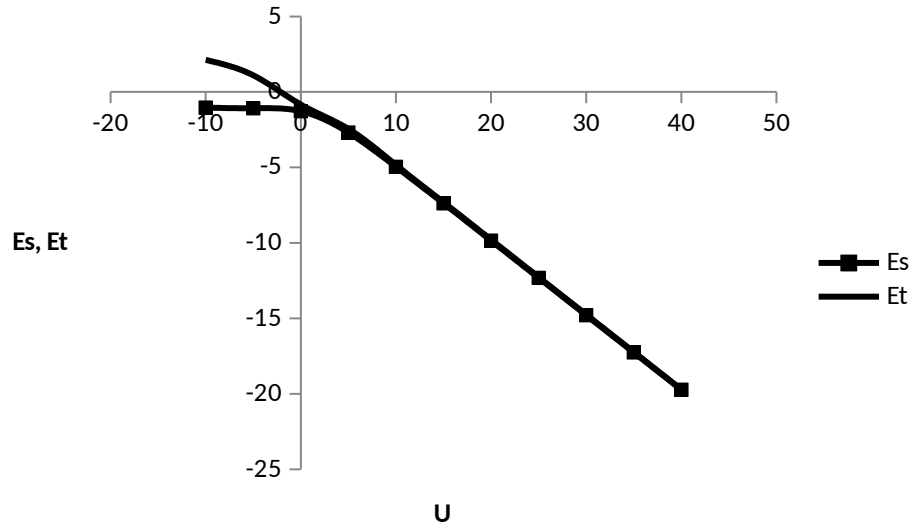


Fig 4.4: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U for a system of 2 electrons on 4 lattice sites at site 2 and 3 Using the SIAM (1-D).

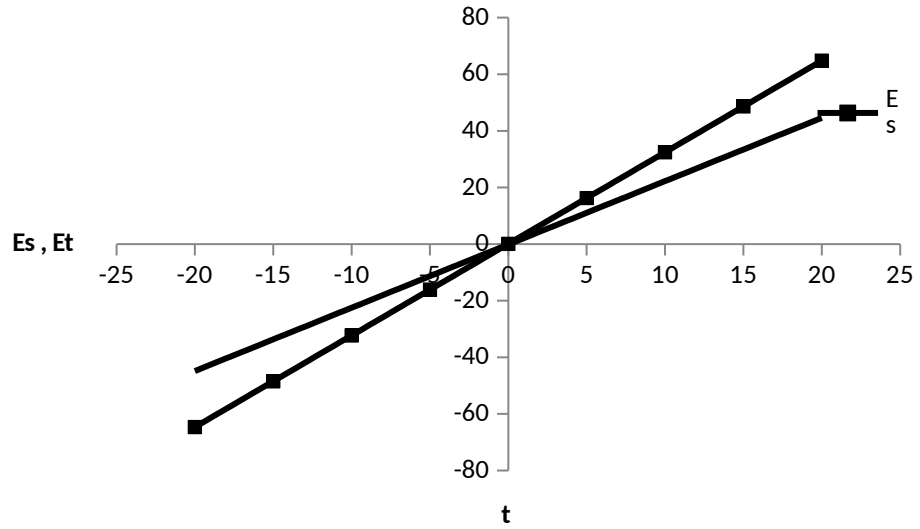


Fig. 4.5: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t for a system of 2 electrons on 4 lattice sites at site 2 and 3 using SIAM (1-D).

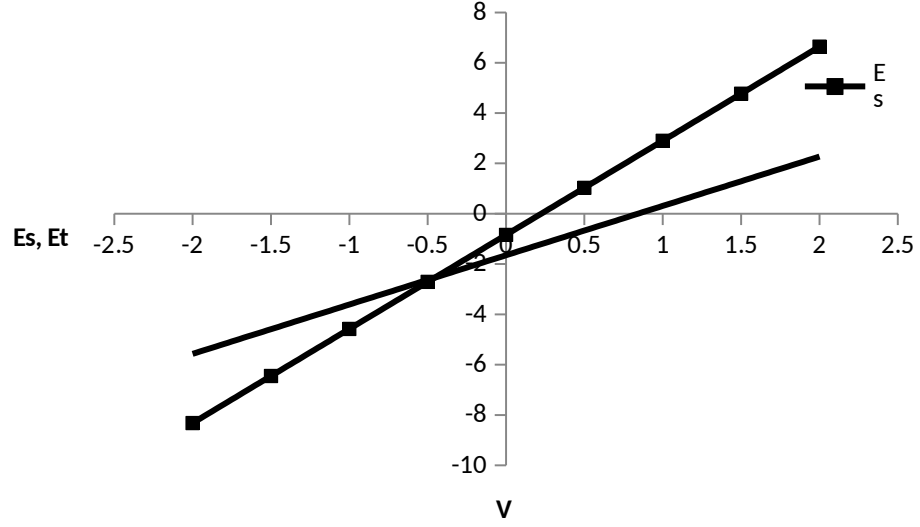


Fig 4.6: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V for a system of 2 electrons on 4 lattice sites at sites 2 and 3 using the SIAM (1-D).

4.2 DISCUSSION OF RESULTS FOR THE 2 ELECTRONS ON 4-SITES (1-D).

Inspection of Fig. 4.1 and 4.4, shows that, as the values of the on-site Coulomb repulsion of the f electrons, U increases, the lattice system that was originally AFM becomes unstable as $U \rightarrow \infty$, the instability is in agreement with the result obtained by Batista *et al* (2001).

Batista *et al* (2001) applied constrained-path QMC method to the SIAM at half fillings and obtained magnetic instability as $U \rightarrow \infty$, and the system has antiferromagnetic groundstate. Increasing U slightly, produces a FM groundstate. The behaviour with doping of one and two electrons is reminiscent of Nagaoka FM and its instability as $U \rightarrow \infty$ in the nearest-neighbour hopping hubbard model. While our model (Anderson and Hubbard) are not the same, the proposed mechanism for FM is very similar: An electron lower its kinetic energy by moving through a FM groundstate which agrees qualitatively with results obtained by Zhong (2022). In this study the electron lowers the system's kinetic energy by inter band processes

enabling its hopping between two occupied f -state anti-aligned with its spin. The need for inter band processes differentiate our mechanism from Nagaoka's. The cost of performing these simulations is approximately the same as simulating 2 electrons on 4 sites (1-D) in the Anderson model and 4 electrons on 8 sites (1-D) one band Hubbard model.

Observations from Fig. 4.2 and 4.5 shows that, as the values of the hopping matrix element, t is increased, the system which was originally AFM (metal) becomes FM (Insulator), in agreement with theoretical and experimental results obtained by Streltsov *et al* (2011).

Streltsov *et al* (2011) applied Green's function technique with the use of Linear Muffin-Tin Orbital (LMTO) and the local density approximately methods to show the $4f$ for Ce- α , Ce- β , Ce- γ and CeCu₂Si₂ can produce a metal to insulator transition which they confirmed on experimentally increasing the Cerium content of CeCu₂Si₂ using different types of spectra (Photoemission Bremsstrahlung isochromatic and Electron Energy Loss) experiments. Increasing Ce contents in CeCu₂Si₂ is equivalent to increasing t in this study.

Inspection of Fig. 4.3 and 4.6 shows that, as the values of the on-site hybridization element, V is increased, the system which was originally AFM becomes FM.

5.0 CONCLUSION

In this research work, the Exact-Diagonalization technique has been employed to provide information on the behavior of two interacting electrons in quarter filled band on 1-D lattices. The lattices considered are small in size. It is not obvious that the results obtained for larger lattices in the literature are applicable here. In 1-D, the lattice systems considered are 2 electrons on 4 sites with open boundary condition. Finite sized lattices with open boundary condition

were specifically considered and the dynamics of the interacting electrons were described by the single site – impurity Anderson Hamiltonians used.

The good agreement of the results in this work with the results of workers like Streltsov *et al* (2011) who applied Green's function technique with the use of Linear Muffin-Tin Orbital (LMTO) and the local density approximately methods to show the $4f$ for Ce- α , Ce- β , Ce- γ and CeCu₂Si₂ can produce a metal to insulator transition which they confirmed on experimentally increasing the Cerium content of CeCu₂Si₂ using different types of spectra (Photoemission Bremsstrahlung isochromatic and Electron Energy Loss) experiments. Increasing Ce contents in CeCu₂Si₂ is equivalent to increasing t in this study.

The theoretical treatment covers the SIAM at quarter fillings in 1-D. The maximum number of electrons encountered in this work are two, keeping up to twenty eight basis electronic states.

In all these systems, even though the underlying solid state chemistry are rather different, the resulting phase diagrams are strikingly similar and robust. This similarity suggests that the overall feature of these phase diagrams is controlled by a single energy scale.

The results obtained reveal that the ED technique represents a suitable approach for a deeper understanding of the rich single and multi - phase dynamics of CeCu₂Si₂.

The results obtained here should also be of relevance for actual Heavy Fermion systems like CeCu₂Si₂ or related compounds.

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