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Mott Transition of Cerium Compound $CeCu_2Si_2$ in the Anderson Model.

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Abstract

The Exact-Diagonalization (ED) technique is applied to the Single Site Impurity Anderson Model (SIAM) and the Periodic Anderson Model (PAM) to elucidate the nature of the ground-state energy and the phase diagram of the two models.

The results obtained show a smooth phase transition from an antiferromagnetic (Metal) phase to a ferromagnetic (Insulator) phase at slightly away from half filling in the two electrons on three site lattice system (1-D) as the value of hopping matrix element, t increases in the SIAM and PAM. Experimental observation shows that increasing the Ce content in $CeCu_2Si_2$ leads to a phase transition from a Metallic to an Insulating phase.

Keywords: Antiferromagnetism, Ferromagnetism, Metal, Insulator, Transition point.

1.0 Introduction

The Mott transition is a metal-insulator transition caused by correlations between electrons. Materials which are predicted to be metals by band theory turn out to be insulators, and the cause is electrons blocking each others' motions. In a Mott insulator, however, the repulsive interaction *U* between electrons causes a gap of order *U* to form in the *middle* of a band, and materials which should be metals turn out to be insulators, for example NiO [1].

Although the Mott insulating state itself is well-understood, its relationship to the phases surrounding it remains controversial: how might the transition from a metal to an insulator take place, with changing doping levels or changing effective interaction strength?

The metal-insulator transition in strongly correlated materials remains a central problem of modern condensed matter physics [2].

The metal-insulator transition plays a central role in the study of quantum disordered systems. An insulator is associated with localized states of the system, while a metal generally displays diffusive transport associated with delocalized states. The Anderson model describes such a metal-insulator transition, due to quantum interference effects driven by the amount of disorder in the system. Starting from the "tight-binding" description of an electron in a crystal lattice, Anderson postulated in 1961 that the dominant effect of impurities in the lattice is to randomize the diagonal, on-site, term of the Hamiltonian, and showed that this generally leads to a localization of the wavefunction, in sharp contrast with the Bloch-wave solution for a perfect crystal. This model has progressively been extended from its original solid state physics scope to a whole class of systems in which waves propagate in a disordered medium, as for example quantum-chaotic systems and electromagnetic radiation [3]. Though the model is mathematically simple, the model predicts a wealth of interesting phenomena. In 1-D, the wavefunction is always localized as recently observed in experiments using atomic matter waves [4] in a disordered optical potential; in 3D it predicts a phase transition between a localized (insulator) and a delocalized (metal) phase at a well defined mobility edge, the density of impurities or the energy being the control parameter. Despite the wide interest on the Anderson transition, few experimental results are available. In a crystal, it is very difficult to obtain the conditions for a clean observation of the Anderson localization. Firstly, one has no direct access to the electronic wavefunction and must rely on modifications of bulk properties like conductivity. Secondly, it is difficult to reduce decoherence sources to a low enough level [4].

In the present work we shall test the validity of the Anderson model as the effective low energy Hamiltonian of the more realistic Single site Impurity Anderson Model (SIAM) and Periodic Anderson model (PAM). We shall do this within a well defined mathematical framework, namely, the Exact-Diagonalization technique (ED) that allows us to obtain essentially exact numerical (solutions). In particular we shall concentrate on the nature of the (antiferromagnetism) metal-insulator (ferromagnetism) transitions that occur in the SIAM and PAM with parameters that set it in the Mott- regime. In addition, our results should also be valuable for the interpretation of experimental spectroscopies of strongly correlated transition metal oxides, which experienced fantastic improvements in the last decade. In fact, the analysis of experimental data of systems

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which have a mixed orbital character is not always simple when strong correlations are present. Finally, our work addresses a very relevant issue in regard of the intense effort that is currently dedicated to the implementation of *ab initio* methods for strongly correlated materials which make heavy use of the ED methodology.

The material of this paper is structured as follows: In the next section we briefly introduce the model Hamiltonian, and describe the novel ED approach [5] that is applied to the SIAM and PAM and present our results in Sec. 3. Discussion, Concluding remark and comparison with experimental results and other theoretical techniques were offered in Sec. 4.

1.0 Model And Methodology

For decades the electronic and magnetic properties of metallic Ce and heavy Fermion cerium compounds were considered in the frameworks of the single impurity problem mainly using Anderson impurity model [6,7]:

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

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 paper, 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 $n^{f}_{\downarrow} = f^{+}_{\downarrow}f_{\downarrow}$.

While Anderson impurity model (1) has allowed to capture main energy scale in heavy-Fermion physics , it cannot describe coherence effects, hence 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

$$H = -t\sum_{\langle ij\rangle\sigma}(C^{+}_{i\sigma}C_{i+1\sigma} + C^{+}_{i+1\sigma}C_{i\sigma}) + E_f\sum_{i\sigma} n^{f}_{i\sigma} + U\sum_{i} n^{f}_{i\uparrow}n^{f}_{i\downarrow} + V\sum_{i,\sigma}(C^{+}_{i\sigma}f_{i\sigma} + f^{+}_{i\sigma}C_{i\sigma}) \qquad (2)$$

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.

Considering a system of two interacting electrons on three sites (1-D) yield 15 basis electronic states, the lattice structure were generated within the limit of the following three assumptions. 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.

(i) 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
(ii) Each of the two electrons has a spin pointing up
(iii) Each of the two electrons has a spin pointing down

In the second and third possibilities, the electrons must necessary be on different sites yielding triplet states i.e. one unit of spin [8].

Generating the 15 relevant electronic states we have the states $|1\rangle - |9\rangle$ as the singlet states and the states $|10\rangle - |15\rangle$ as the triplet states, i.e.

$$|1\rangle = |1\uparrow 1\downarrow\rangle, |2\rangle = |2\uparrow 2\downarrow\rangle, |3\rangle = |3\uparrow 3\downarrow\rangle, |4\rangle = |1\uparrow 2\downarrow\rangle, |5\rangle = |1\downarrow 2\uparrow\rangle, |6\rangle = |1\uparrow 3\downarrow\rangle,$$
$$|7\rangle = |1\downarrow 3\uparrow\rangle, |8\rangle = |2\uparrow 3\downarrow\rangle |9\rangle = |2\downarrow 3\uparrow\rangle |10\rangle = |1\uparrow 2\uparrow\rangle, |11\rangle = |1\downarrow 2\downarrow\rangle, |12\rangle = |1\uparrow 3\uparrow\rangle,$$
$$|13\rangle = |1\downarrow 3\downarrow\rangle, |14\rangle = |2\uparrow 3\uparrow\rangle, |15\rangle = |2\downarrow 3\downarrow\rangle \qquad (3)$$

The expanded SIAM Hamiltonian (1) for site 1 and 2 are given in equation (4), (5) and that of PAM (2) is given in equation (6)

$$H_{SIAM} = t(C^{+}_{1\uparrow}C_{2\uparrow} + C^{+}_{2\uparrow}C_{1\uparrow} + C^{+}_{1\downarrow}C_{2\downarrow} + C^{+}_{2\downarrow}C_{1\downarrow} + C^{+}_{2\uparrow}C_{3\uparrow} + C^{+}_{3\uparrow}C_{2\uparrow} + C^{+}_{2\downarrow}C_{3\downarrow} + C^{+}_{3\downarrow}C_{21\downarrow}) + E_f(f^{+}_{1\uparrow}f_{1\uparrow} + f^{+}_{1\downarrow}f_{1\downarrow}) + Uf^{+}_{1\uparrow}f_{1\uparrow}f^{+}_{1\downarrow}f_{1\downarrow} +$$

$$V(C^{+}_{1\uparrow} f_{1\uparrow} + f^{+}_{1\uparrow} C_{1\uparrow} + C^{+}_{1\downarrow} f_{1\downarrow} + f^{+}_{1\downarrow} C_{1\downarrow}) \quad (4)$$

$$H_{SIAM} = t(C^{+}_{1\uparrow} C_{2\uparrow} + C^{+}_{2\uparrow} C_{1\uparrow} + C^{+}_{1\downarrow} C_{2\downarrow} + C^{+}_{2\downarrow} C_{1\downarrow} + C^{+}_{2\uparrow} C_{3\uparrow} + C^{+}_{3\uparrow} C_{2\uparrow} + C^{+}_{2\downarrow} C_{3\downarrow} + C^{+}_{3\downarrow} C_{2\downarrow}) + E_f(f^{+}_{2\uparrow} f_{2\uparrow} + f^{+}_{2\downarrow} f_{2\downarrow}) + U f^{+}_{2\uparrow} f_{2\uparrow} f^{+}_{2\downarrow} f_{2\downarrow} + V(C^{+}_{2\uparrow} f_{2\uparrow} + f^{+}_{2\uparrow} C_{2\uparrow} + C^{+}_{2\downarrow} f_{2\downarrow} + f^{+}_{2\downarrow} C_{2\downarrow}) \quad (5)$$

$$H_{PAM} = t(C^{+}_{1\uparrow} C_{2\uparrow} + C^{+}_{2\uparrow} C_{1\uparrow} + C^{+}_{1\downarrow} C_{2\downarrow} + C^{+}_{2\downarrow} C_{1\downarrow} + C^{+}_{2\uparrow} C_{3\uparrow} + C^{+}_{3\uparrow} C_{2\uparrow} + C^{+}_{2\downarrow} C_{3\downarrow} + C^{+}_{3\downarrow} C_{2\downarrow}) + E_f(f^{+}_{1\uparrow} f_{1\uparrow} + f^{+}_{1\downarrow} f_{1\downarrow} + f^{+}_{2\uparrow} f_{2\uparrow} + f^{+}_{2\downarrow} f_{2\downarrow} + f^{+}_{3\uparrow} f_{3\uparrow} + f^{+}_{3\downarrow} f_{3\downarrow}) + U(f^{+}_{1\uparrow} f_{1\uparrow} f^{+}_{1\downarrow} f_{1\downarrow} + f^{+}_{2\uparrow} f_{2\uparrow} f^{+}_{2\downarrow} f_{2\downarrow} + f^{+}_{3\uparrow} f_{3\uparrow} f^{+}_{3\downarrow} f_{3\downarrow}) + V(C^{+}_{1\uparrow} f_{1\uparrow} + f^{+}_{1\uparrow} C_{1\uparrow} + C^{+}_{1\downarrow} f_{1\downarrow} + f^{+}_{1\downarrow} C_{1\downarrow} + C^{+}_{2\uparrow} f_{2\uparrow} + f^{+}_{2\uparrow} C_{2\uparrow} + C^{+}_{2\downarrow} f_{2\downarrow} + f^{+}_{2\downarrow} C_{2\downarrow} + C^{+}_{3\uparrow} f_{3\uparrow} + f^{+}_{3\uparrow} C_{3\uparrow} + C^{+}_{3\downarrow} f_{3\downarrow} + f^{+}_{3\downarrow} C_{3\downarrow}) \quad (6)$$

2.0 Results

The results of the interaction on using the Hamiltonian (4), (5) and (6) to act on the 15 basis electronic states (3), the results obtained are summarized in the Hamiltonian matrix (7), (8) and (9) respectively. Sites 1 and 3 provide the same result due to side effects. Because of the complex nature of the matrices, the eigenvalues, for a particular case was considered. These complex matrices were solved using Wolfram Mathematica 6.0 [9]. Considering a case where E_f =1, u = 1, v = 2 and t =1. The Hamiltonian matrix of equation (4) becomes

$$H = \begin{bmatrix}
2E_f+u+4v & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & t & -t & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
t & t & 0 & E_f+2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -t & 0 & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & E_f+2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -t & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & t & t & 0 & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -t & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & t & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f+2v & 0 & t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f+2v & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0
\end{bmatrix} \quad (7)$$

The ground state energies of the singlet states (E_s) and triple states (E_t) of equation (7) are given by
E_s = -2.17087 and E_t = -0.199705

Similarly equation (5) becomes

$$H = \begin{bmatrix}
0 & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2E_f+u+4v & 0 & t & -t & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & t & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
t & t & 0 & E_f+2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -t & 0 & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & t & 0 & 0 & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & t & t & 0 & 0 & t & 0 & E_f+2v & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -t & -t & 0 & 0 & 0 & -t & 0 & E_f+2v & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & t & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & 0 & 0 & t \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f+2v & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & t & 0 & E_f+2v
\end{bmatrix} \quad (8)$$

with E_s = -1.00016 and E_t =.-0.372281
Finally equation (6) becomes

$$H=\begin{bmatrix}
2E_f+u+4v & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2E_f+u+4v & 0 & -t & t & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2E_f+u+4v & 0 & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -t & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
t & t & 0 & 0 & E_f+2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -t & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & t & 0 & E_f+2v & 0 & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -t & -t & 0 & 0 & -t & 0 & E_f+2v & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & t & t & 0 & 0 & 0 & t & 0 & E_f+2v & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v & 0 & -t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & E_f+2v & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & E_f+2v & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E_f+2v
\end{bmatrix} \quad (9)$$

with E_s = 7.4921 and E_t = 8.58579
A numerical analysis carried out, in order to determine the magnetic phase diagram are given by Tables 1, 2 and 3 with the corresponding graphs given by Fig. 1, 2 and 3 respectively.

Table 1: Singlet (E_s) and Triplet (E_t) state energies as t varies and other parameters remaining constant.

E_f=-$^u/_2$ (Energy of the localized *f* orbital)	**U** (On-site Coulomb repulsion of the *f* electrons)	**V** (On-site hybridization element between the *f* orbitals and the *C* band)	**t** (Hopping matrix element of the conduction electron)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
-1.00	2.00	0.375	-20.00	-56.57	-28.47
-1.00	2.00	0.375	-15.00	-42.43	-21.4
-1.00	2.00	0.375	-10.00	-28.29	-14.33
-1.00	2.00	0.375	-5.00	-14.15	-7.26
-1.00	2.00	0.375	0.00	-0.01	-0.19
-1.00	2.00	0.375	5.00	14.13	6.88
-1.00	2.00	0.375	10.00	28.27	13.95
-1.00	2.00	0.375	15.00	42.41	21.02
-1.00	2.00	0.375	20.00	56.55	28.09

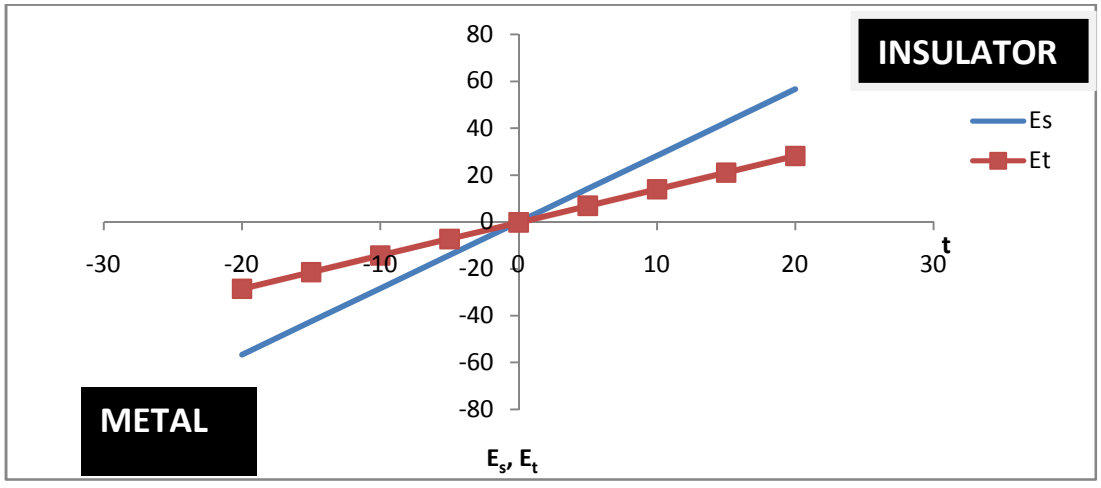

Fig 1: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t for a system of 2 electrons on 3 lattice sites at site 1 and 3 using the SIAM (1-D).

Table 2: Singlet (E_s) and Triplet (E_t) state energies as t varies and other parameters remaining constant.

E_f=-U/2 (Energy of the localized *f* orbital)	**U** (On-site Coulomb repulsion of the *f* electrons)	**V** (On-site hybridization element between the *f* orbitals and the *C* band)	**t** (Hopping matrix element of the conduction electron)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
-1.00	2.00	0.375	-20.00	-56.33	-28.41
-1.00	2.00	0.375	-10.00	-42.19	-21.34
-1.00	2.00	0.375	0.00	-28.05	-14.27
-1.00	2.00	0.375	10.00	-13.91	-7.20
-1.00	2.00	0.375	20.00	0.23	-0.13
-1.00	2.00	0.375	30.00	14.37	6.94
-1.00	2.00	0.375	40.00	28.51	14.01

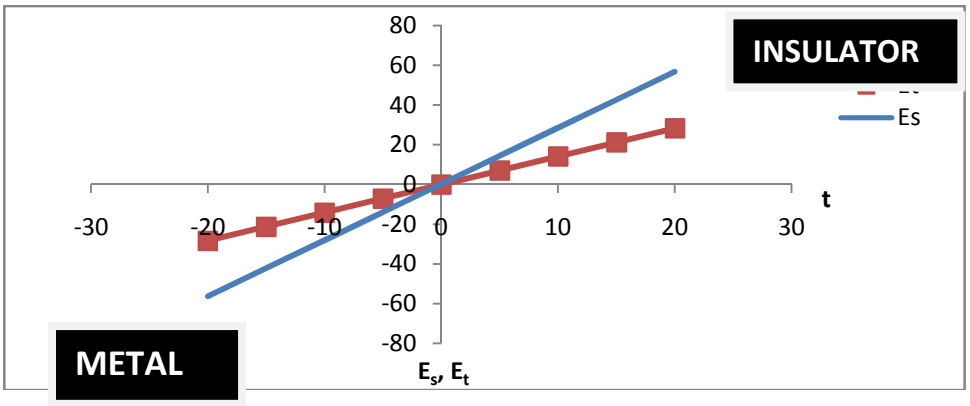

Fig 2: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t for a system of 2 electrons on 3 lattice sites at site 2 using the SIAM(1-D).

Table 3: Singlet (E_s) and Triplet (E_t) state energies as t varies and other parameters remaining constant.

E_f=-U/2 (Energy of the localized *f* orbital)	**U** (On-site Coulomb repulsion of the *f* electrons)	**V** (On-site hybridization element between the *f* orbitals and the *C* band)	**t** (Hopping matrix element of the conduction electron)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
-1.00	2.00	0.375	-20.00	-56.33	-28.78
-1.00	2.00	0.375	-10.00	-28.06	-14.64
-1.00	2.00	0.375	0.00	0.21	-0.50
-1.00	2.00	0.375	10.00	28.48	13.64
-1.00	2.00	0.375	20.00	56.75	27.78
-1.00	2.00	0.375	30.00	85.02	41.92
-1.00	2.00	0.375	40.00	113.29	56.06

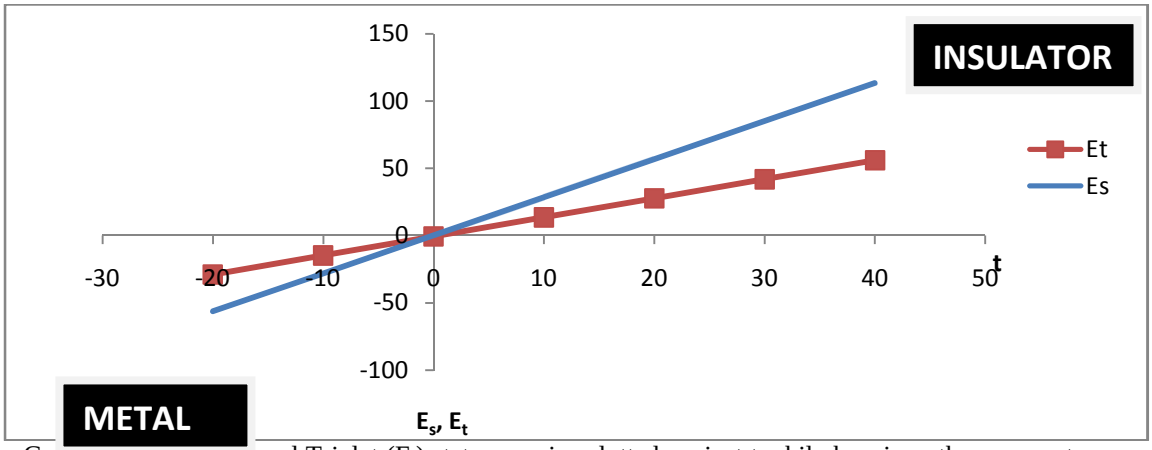

Fig. 3: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t while keeping other parameters constant of the 2 electrons on 3-sites, using PAM.

3.0 DISCUSSION AND CONCLUSION

Observation from Table 1, 2 of SIAM and 3 of PAM and their corresponding graphs Fig. 1, 2 and 3 show that, as the value of the hopping matrix element of the conduction electrons, t increases, the ground-state continues to increase until it reaches a transition point, where $E_s=E_t$ and as the valuesof the hopping matrix element, t are further increased, where $E_s > E_t$ the system becomes Ferromagnetic (FM). If t is increasing, it will be costly to provide enough energy for the hopping, hence the hopping is suppressed. Relatively, increasing t is like increasing the band gap which is related to the insulating state of the system. The physical implication is that the electronic correlations favouring antiferromagnetism (AFM) gets weaker while that of FM gets stronger as the values of the hopping matrix element, t increases. This continues until the electronic correlation favouring FM begins to dominate (i.e. there is cross-over to ferromagnetism) and this domination is enhanced as t is increased. The experimental implication is that the electronic correlations favouring Metallic state gets weaker while those favoring Insulators get stronger as the content of Cerium (Ce) in the Heavy Fermion compound Cerium Copper Silicate ($CeCu_2Si_2$) is increased [4]. Hence, this direct exchange interaction provides a natural way for stabilizing ferromagnetic states [2,10,11,12,13] rather than a sudden jump [14].

In conclusion Finite sized lattices with open boundary condition and periodic or cyclic boundary conditions were specifically considered in the SIAM and PAM respectively, and the dynamics of the interacting electrons were described by the two Hamiltonians used. The results obtained reveal that the ground state energy is a spin singlet and the ED technique represents a suited approach for a deeper understanding of the rich phase diagram of $\mathbf{CeCu_2Si_2}$. Therefore, the results obtained in this paper with the application of ED technique to the SIAM and PAM confirm the rich phase diagram experimentally observed in $CeCu_2Si_2$. The results obtained here should also be of relevance for actual HF systems like $\mathbf{CeCu_2Si_2}$ or related compounds.

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