HEAVY – FERMION SEMICONDUCTOR BEHAVIOUR AND PHASE TRANSITION OF $CECU_2SI_2$ IN THE SINGLE SITE IMPURITY ANDERSON MODEL

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ABSTRACT

We investigate the electronic properties of $CeCu_2Si_2$ in the low temperature regime using the Exact-Diagonalization technique. This technique allows the study of the physics of strongly correlated electron systems. We show that when the hybridization term in the Single Site Impurity Anderson Model (SIAM) is increased: (1) there is a smooth phase transition from an antiferromagnetic phase to a ferromagnetic phase and (2) there is a semiconductor gap Δ between the singlet state and triplet states energies as the lattice sites and dimensions are increasing. The basic features of this theory are in qualitative agreement with the experimentally observed heavy-fermion semiconductor of some rare-earth compounds.

Keywords: Transition point, hybridization gap, Antiferromagnetic phase, Ferromagnetic phase

INTRODUCTION

The discovery of carrier-induced ferromagnetism in diluted magnetic semiconductor (DMS) has attracted considerable attention from both theoreticians and experimentalists. The interest in these material is mainly stimulated by the possible technological applications e.g. semiconductor spin devices. For example by doping GaAs with magnetic impurities Mn^{2+}, T_c exceeding 100 K has been reached. The doping of a III-V semiconductor compound with Mn impurities introduces simultaneously local magnetic moments and itinerant valence-band carriers[1].

The Sigle Site Impurity Anderson model (SIAM), in which a single, locally correlated orbital couples to a non-interacting metallic band of electrons, is a longstanding paradigm of strongly-correlated electron physics [2]. Conceived originally[3] to explain the formation of localized magnetic moments on impurities in non-magnetic hosts, it has since formed the cornerstone of our understanding of the Kondo effect[4] and related many-body phenomena. Interest in the area is currently particularly strong, both experimentally and theoretically, after the Kondo effect was predicted and then directly confirmed to arise in mesoscopic quantum dot systems[5]. After some 50 years of intense theoretical work, the spin- 1/2 Kondo effect as manifest in Anderson's original model is naturally rather well understood. Below some characteristic Kondo temperature TK, a complex many-body state develops in which the impurity spin is completely screened by the host metal, leading at low energies to a 'local' Fermi-liquid and universal transport properties[2].

One of the hallmark of the Kondo effect[4] is the raise of a narrow resonance, at the Fermi level, in the spectral density function of the magnetic impurity embedded into a metallic host. The width of the resonance is proportional to the so-called Kondo temperature T_k, which is

the characteristic energy scale. Below the T_k the impurity spin is completely screened into a singlet by the host metal[6].

Subsequently, classes of rare-earth and actinide compounds, namely, the Heavy Fermion (HF) Systems, have been attracting much theoretical and experimental interest. These compounds present a variety of ground states, including superconductor, antiferromagnetic e.t.c. Recently a new class of such compounds was discovered, namely, that of HF semiconductors or Kondo insulators and a renewed interest has been attracted to these compounds. These compounds may be characterized as usual HF systems at moderately low temperatures; they behave as semiconductors with rather small energy gap [7].

$CeCu_2Si_2$ is the original HF compound with superconducting transition temperature T_c of about 0.6K [8,9]. The semiconductor behavior of $CeCu_2Si_2$ probably originates from interaction between the localized *Ce 4f* electrons and the conduction band. In the present work, we address a slightly different problem. That of a magnetic impurity in a degenerate semiconductor host which present a gap across the Fermi level in the conduction- electron spectrum and also try to investigate the role of the hybridization in the Single Impurity Anderson Model (SIAM) alongside that of *Ce* in the $CeCu_2Si_2$ HF compound. In removing the all-important low-lying states of the host, one would certainly expect the Kondo effect to be precluded for large enough gaps: the question is, can the effect still arise for sufficiently-small gaps, or is it destroyed as soon as a gap is opened? This question has indeed been the subject of a number of previous papers.

Poor man's scaling, the 1/N expansion and the non-crossing approximation predict that the Kondo effect always arises whenever the gap is less than the Kondo temperature in the absence of the gap, while for larger gaps the system undergoes a quantum phase transition to an 'local moment' (LM) phase where the impurity spin remains unscreened as $T \rightarrow 0$. In addition the problem has been studied numerically by the density-matrix renormalization group and quantum Monte Carlo but with no general consensus reached regarding the nature of the quantum phase transition. The numerical renormalization group (NRG)[6] on the other hand has been used to argue that the Fermi liquid regime associated with the Kondo effect exists only away from particle–hole-symmetry, and then only below a certain critical gap. In the particle-hole–symmetric limit it is found that the Kondo effect never arises and the ground state is the doubly-degenerate LM phase for arbitrarily small gaps.

We apply the Exact Diagonalization (ED) technique and consider the notionally simple problem of an Anderson impurity in a gapped host, where the density of states vanishes over a finite range about the chemical potential, a model not only of relevance to Anderson impurities in semiconductors but also to the topical issue of impurities in BCS superconductors[10]. The rest of the paper will be organized as follows. In section 2, we presented the theoretical model for the Cerium-based HF compound, and then the results of the ground state properties are presented in section 3. Discussion and concluding remark were offered in section 4.

MODEL AND METHODOLOGY

To describe a local, quantum impurity state, coupled to a conduction band, we use the standard notation generic Anderson Hamiltonian [2,3,9]

$$\hat{H} = \sum_{k,\sigma} \in_k \hat{n}_{k\sigma} + \sum \in_i \hat{n}_{i\sigma} + U\ \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{k,\sigma} (V_i C^{+}_{k\sigma} C_{i\sigma} + H.C.) \quad (1)$$

where $\hat{n}_{j\sigma} = C^{+}_{j\sigma} C_{j\sigma}$ is the number operator for σ-spin electrons on 'site' j (with j = i referring to the impurity site and j ≡ k to the host band states). The first term in eqn. (1) thus describes the non-interacting host band, the second and third terms describe the impurity with onsite Coulomb interaction U, and the fourth term hybridizes the two. For a symmetric host band, the particle-hole symmetric limit corresponds to the $\in_i = -\frac{u}{2}$. H. C. is the

Hermitian conjugation

The region of relevance corresponds to transition from an antiferromagnetic phase to a ferromagnetic phase and the gap values, of the order of Kondo temperature. We consider only quarter fillings of the SIAM, and this corresponds to when the number of interacting electrons N_e are equal to the number of lattice sites N_s ($N_e = N_s$) in one and two dimensions.

A much more rigorous analysis of the problem is possible by using the ED technique [11,12] which is a reliable approach to study a variety of quantum impurity models. The ED technique is based upon the representation of the effective action by an impurity model with a *finite* number of sites. The approximate Hamiltonian can only produce limited forms of the Hamiltonian *H*, but it can be diagonalized exactly if there are not too many sites: the Hamiltonian is rewritten as a matrix connecting different many particle states, and all the eigenvalues and eigenvectors found. To obtain the eigensystem, the matrix elements were evaluated with the help of an analytical diagonalization routine provided by Wolfram Mathematica software. Having obtained the results of the eigensystem, the lowest of the eigenvalues provides the ground-state energy of the system. This technique has proved to be surprisingly successful, and does not suffer from some of the problems of Quantum Monte Carlo: zero temperature is easy, and there is no problem with calculating densities of states and can be analytically continued.

RESULTS

We consider a qualitative description of the ED flow diagrams of SIAM in the open boundary conditions, and use the symmetrical model where $\in_i = -\frac{u}{2}$, U = 2.00, t = 0.50 and varies the value of V from -2.00 to +2.00. The flow diagrams below describe the behavior of the hybridization matrix element in the SIAM. However, due to edge effects, the lattice sites at the edge of the open system will produce the same result. For example in the 2 electrons on 2 lattice sites, both site 1 and 2 will have the same results while in the case of 3 electrons on 3 lattice sites; site 1 and 3 will yield same result and 2 will produce a different result.

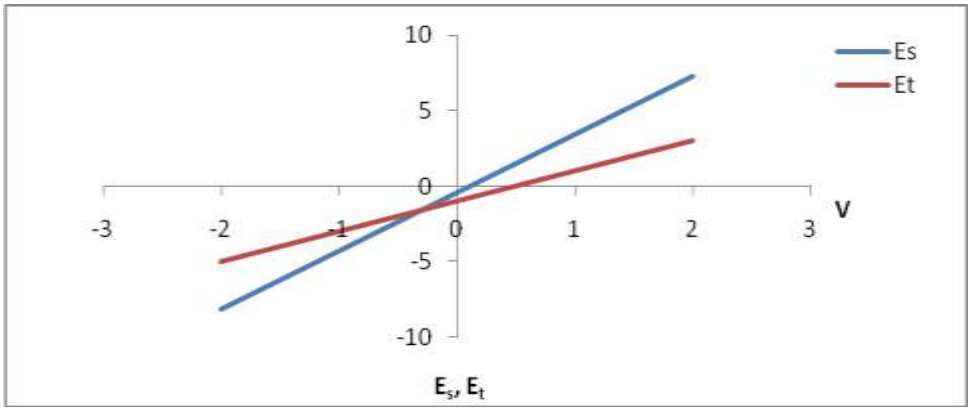

Fig 1: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V, showing the transition between E_s and E_t in the 2 electrons on 2-sites system at site 1 and 2 (SIAM). Energy units are in eV.

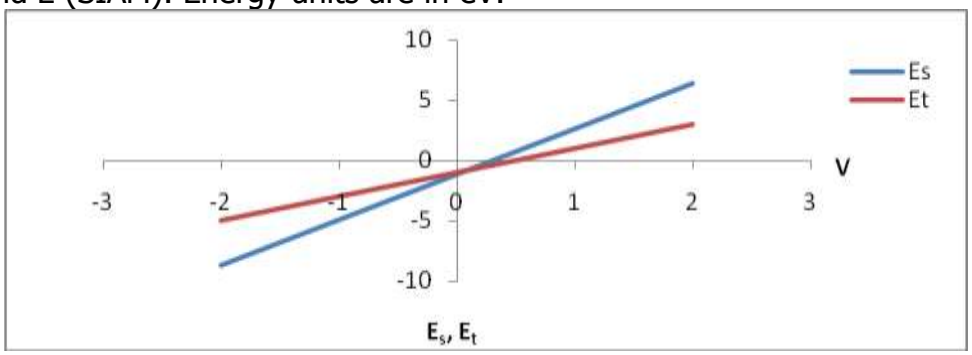

Fig 2: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V in the 3 electrons on 3-sites lattice system at sites 1 and 3, using the SIAM (1-D).

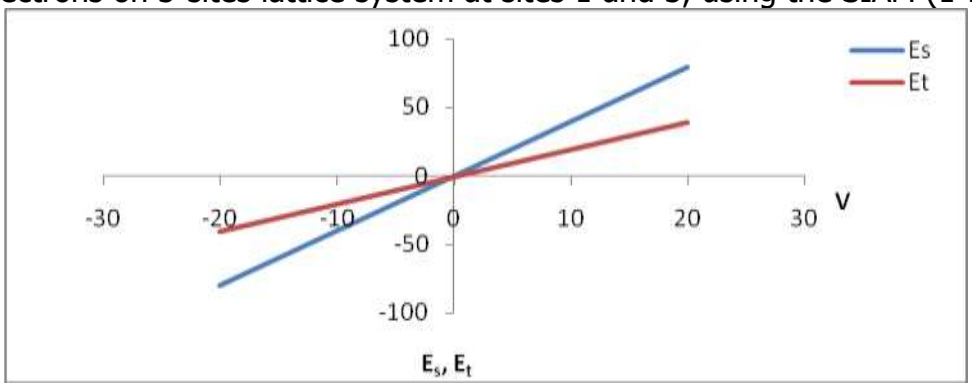

Fig 3: Graph of lowest energies of the Singlet (E_s) and Triplet (E_t) states plotted against V, in the 3 electrons on 3-sites lattice system at site 2, using the SIAM (1-D).

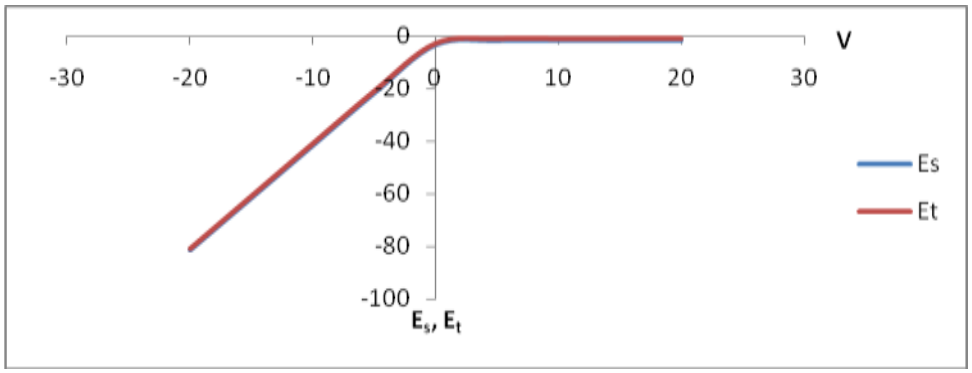

Fig 4: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V, showing the ferromagnetic alignment caused by the hybridization gap between E_s and E_t in the 4 electrons on 4-sites at sites 1 and 4, using the SIAM (1-D).

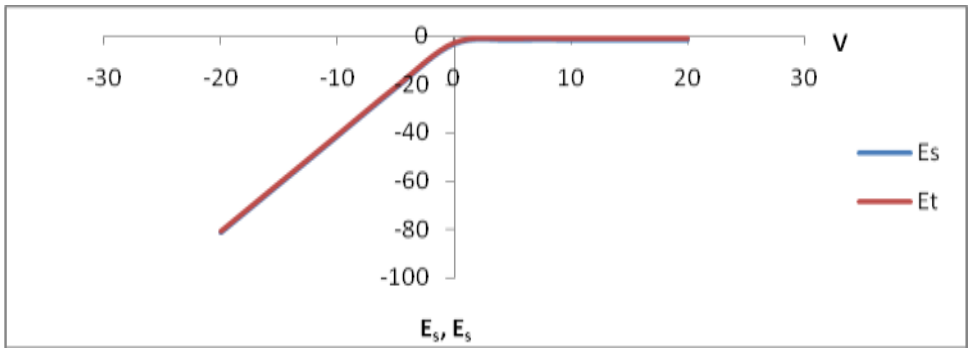

Fig. 5: Graph of Singlet (E_s) and Triplet (c) state energies plotted against V in the 4 electrons on 4-sites lattice system at site 2 and 3, using the SIAM (1-D).

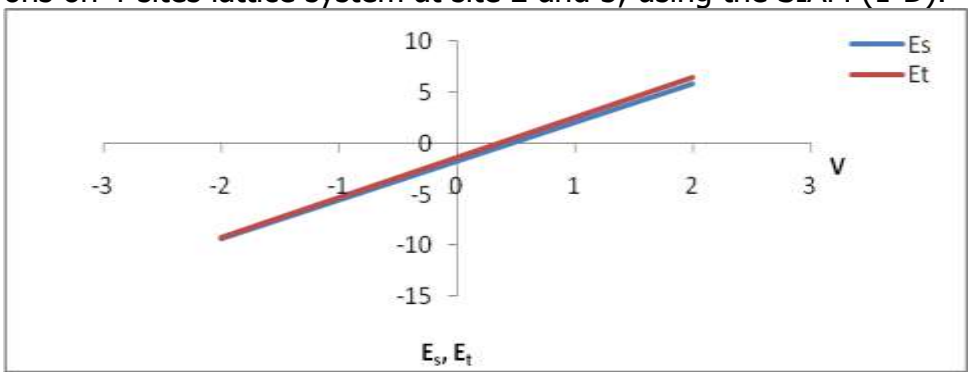

Fig. 6: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V in the 4 electrons on 2 x 2 square lattice sites system at sites 1 and 4, using the SIAM (2-D).

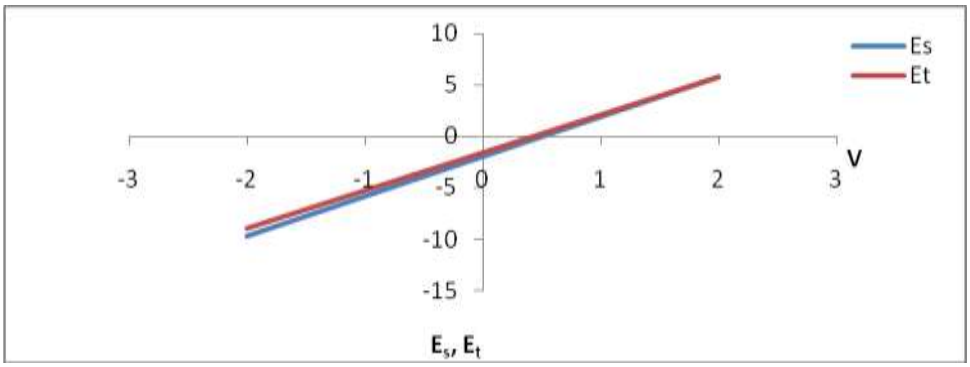

Fig. 7: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V in the 4 electrons on 2 x 2 square lattice sites system at sites 2 and 3, using the SIAM (2-D).

DISCUSSION OF RESULTS

Identifying the origin of itinerant ferromagnetism in metals and specifying simple models inhibiting it are two of the most intriguing and long-standing problems in theoretical Physics.

Using the eigenvalue solution of the matrix form of the Hamiltonian will yield the total energy which is the energy spectrum of that system and the lowest of them is the ground state energy of the system. This follows that 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 state 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 states provides the ground state energy.The value at which $E_t = E_s$ give rise to a transition from antiferromagnetic phase to a ferromagnetic phase or vice-versa. This point is called the transition point, T_p[14].

Observation from Fig. 1 shows that, as the value of the on-site hybridization element between the *f* orbital and the conduction electron, *V* are increased, the ground-state continue to increase to transition point T_p, where $E_s=E_t$ and as the values are further increased beyond T_p, where $E_s > E_t$ the system becomes ferromagnetic. The physical implication is that the electronic correlations favouring antiferromagnetism gets weaker while that of ferromagnetism gets stronger as the values of the 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 the values of *V* increases. Hence, this direct exchange interaction provides a natural way for stabilizing ferromagnetic states,[15] .

Observations from Fig 2 and 3 shows that, as the values of the on-site hybridization element between the *f* orbital and the *C* band, *V* are increased, there was transition from an antiferromagnetic phase to a ferromagnetic phase.

Results from Fig. 4 and 5 shows that, as the values of the on-site hybridization element between the *f* orbital and the conduction band, *V* is increased there is a ferromagnetic

alignment between the singlet and triplet state energies giving a hybridization gap or semiconducting gap Δ in the lattice system. At site 1 and 4, in Fig 4, the semiconducting gap Δ is uniform and does not increase or decrease irregularly, hence the gap is about 0.7; but at site 2 and 3, in Fig. 5, the gap increases as the values of V continue to increase.

Computation from Fig. 6 and 7 shows that, as the V term is increased, the hybridization gap continue to increase at site 1 and 4 and decreases at site 2 and 3. This is as a result of edge and finite size effects. The lattice sizes considered in this paper are two to four and keeping up to seventy basis electronic states. In 1-D, the lattice systems considered are 2 electrons on 2 sites, 3 electrons on 3 sites, and 4 electrons on 4 sites. In 2-D, the system studied is 4 electrons on a 2 X 2 square lattice sites. Finite sized lattices with open boundary condition are specifically considered, and the dynamics of the interacting electrons was described by the Hamiltonians used.

In conclusion, evaluations are performed with approximate scheme that become exact in high dimensions. Comparison with results in the literature for 1-D, shows that the results are remarkably accurate for all the values of the coupling. Hence the results for D = 2, can be expected to be even more accurate and may serve as a benchmark for future numerical work for D›1.

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