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Superconductivity driven by magnetic instability in $CeCu_2Si_2$

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Abstract

The coexistent of superconductivity (SC) with antiferromagnetism (AFM) and ferromagnetism (FM) as $U \rightarrow \infty$ is studied in $CeCu_2Si_2$ on application of the Exact Diagonalization technique to the Single site Impurity Anderson Model and the Periodic Anderson Model. The results obtained show that magnetic instability is the key to understanding superconductivity in Heavy Fermion compounds as increasing the onsite coulomb repulsion, U, suppresses all ferromagnetic tendencies and enhances superconductivity. The results obtained here is in qualitative agreement with the inelastic neutron scattering experimental results obtained by Stockert et al (2011) on increasing the copper content in $CeCu_2Si_2$. U in this theoretical study behaves as Cu in the inelastic neutron scattering experiment.

Keywords: Heavy fermion, antiferromagnetism, superconductivity, ferromagnetism, singlet state energy, triplet state energy.

1. Introduction

A resurgence of interest in heavy fermion (HF) superconductivity (SC) in the last few years has been strongly driven by the discovery of a large number of new *Ce* and *U* based intermetallic superconductors. Most analyses of their behaviour have focused on the relationship between superconductivity and magnetism, specifically on the idea that the SC in these systems is mediated by low energy magnetic fluctuations around a so-called magnetic quantum critical point (QCP), where a magnetic ordering temperature is driven to zero by an external parameter such as pressure or chemical substitution (Holmes et al., *2007*). The celebrated BCS theory of SC by Bardeen *et al* (1957) provides a basic theoretical framework to understand this remarkable phenomenon in terms of the pairing of electrons with opposite spin and momenta to form a collective condensate state (Demler*et al*, 2004). However, the failure of the BCS to account for SC beyond the conventional superconducting materials has led to a diverse search for other theories (Hirsch, 2009, Schmalian, 2011, Akpojotor, 2011: 2012). One of these theories is the spin fluctuations due to superexchange interaction which was used to account for superconductivity in the cuprates (Akpojotor, 2008). The starting point is that superconductivity is the mixed states of singlet and triplet orderings described as the resonating valence bond states (Lewenstein et al., 2007). Here the electrons are localized to individual atoms and the fluctuations in the charge (density) degree of freedom are strongly suppressed. Therefore the physics is dictated by the remaining spin degree of freedom which interact via superexchange and this can result to the superposition of states in which random pairs of neighbouring pairs of atoms attains zero total spin (Nascimbene et al. 2012, Akpojotor, 2012).

The discovery of a superconducting state formed by heavy quasi-particles in $CeCu_2Si_2$ has attracted a lot of scientific interest in this HF material and related compounds. Despite its long history, only recently a whole variety of new physical phases have been observed which was possible by the intriguing development of experimental techniques. By substituting *Si* by *Ge* in the parent compound $CeCu_2Si_2$, a continuous change from a HF superconducting phase to an antiferromagentic state was observed. An even more complex phase diagram has been found in pure $CeCu_2Si_2$ by applying high pressure. These two superconducting phases with different pairing mechanisms have been found besides an antiferromagnetic and a HF phase. Furthermore, a transition between intermediate and integral valence states has been observed (Hubsch and Becker, 2006).

However, a spectacular series of discoveries and developments in *f*-electron superconductors took place at the same time. While in the first twelve years following the discovery of HF superconductivity in $CeCu_2Si_2$ only five more HF superconductors could be identified, over twenty five additional systems have been found in the past fifteen years. By now over thirty systems are known, about half of which were discovered in the past seven years alone. This illustrates the speed of development the field of *f*-electron superconductivity has picked up despite its long tradition. As a result there is growing appreciation that superconducting phases of *f*-electron compounds frequently exist at the border of competing and coexisting forms of spin order. For the majority of systems, including the original HF superconductors, an interplay with antiferromagnetism (AFM) is observed. However,there are also several examples of superconductivity that coexists with ferromagnetism (FM). Further examples include superconductivity at the border of polar order and near electron localization transitions.

Finally, several HF superconductors have even been discovered with non-centrosymmetric crystal structures and coexistent antiferromagnetic order. The large variety of systems found so far establishes unconventional f – electron superconductivity as a rather general phenomenon. It also suggests the existence of further unimagined forms of superconductivity (Pleiderer, 2009).

The objective of this paper is to draw attention to another phenomenon in *Ce* compound ($CeCu_2Si_2$), namely magnetic instability also capable of generating superconductivity. In this case the pairing is mediated by electron-electron interaction, or localized f electron and conduction election interaction. It is the view of the authors that this scenario is of widespread importance and must be taken into account for a complete understanding of the behaviour of all *Ce* – based HF compounds. We emphasized the heavy fermion nature of these superconductors; those *Ce* compounds in which the f – electrons play little role in their superconductivity do not concern us for the purposes of this discussion.

The outline of this paper is as follows. In section 2 we formulate the problem by the introduction of the Hamiltonian model. The Exact Diagonalization (ED) calculation of seventy basis electronic states is presented in section 3. The numerical results are presented and discussed in section 4 and this is followed by summary and conclusion.

2. Model formulation

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 single site impurity Anderson model (SIAM) as indicated by Anderson (1961), Enaroseha *et al* (2011) and Streltsov *et al* (2011):

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

where $C^{+}_{i\sigma}(C_{i\sigma})$ create (annihilate) conduction electrons with spin σ (= ↑, ↓) at site i, and $f^{+}_{i\sigma}(f_{i\sigma})$ create (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 study 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 the Hamiltonian in Eq.(2.1), $n^{f}_{\uparrow} = f^{+}_{i\uparrow}f_{\uparrow}$, $n_{f\sigma} = f^{+}_{\sigma}f_{\sigma}$ and $n^{f}_{\downarrow} = f^{+}_{i\downarrow}f_{\downarrow}$. A significant feature of this model is the hybridization term V, which allows the f–electrons in HF systems to become mobile, despite the fact that they are separated by a great distance. Generalizing the SIAM to a lattice of localized orbital, f, we obtained the so-called Periodic Anderson Model (PAM). The Hamiltonian, H, of the PAM is given by

$$H = -t\Big(\sum_{\langle i,j\rangle,\sigma} C^{+}_{i\sigma}C_{i+1\sigma} + C^{+}_{i+1\sigma}C_{i\sigma}\Big) + E_f\sum_{i\sigma} n^{f}_{i\sigma} + Un^{f}_{i\uparrow}n^{f}_{i\downarrow} + V\sum_{i\sigma}(C^{+}_{i\sigma}f_{i\sigma} + f^{+}_{i\sigma}C_{i\sigma}) \tag{2.2}$$

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.

3. Exact Calculation of the Anderson Model on Four Site System

Considering a system of four interacting electrons and keeping seventy basis electronic states with thirty-six states with net zero (the antiferromagnetic states), thirty-two states with net spin ±1 and two states with net spin ±2 (the ferromagnetic states). Expanding the SIAM Hamiltonian in Eq. (2.1) completely we have

$$\begin{aligned} H_{SIAM} = t\Big(&C^{+}_{1\uparrow}C_{2\uparrow} + C^{+}_{2\uparrow}C_{2\uparrow} + C^{+}_{1\downarrow}C_{2\downarrow} + C^{+}_{2\downarrow}C_{\downarrow} + C^{+}_{2\uparrow}C_{3\uparrow} + C^{+}_{3\uparrow}C_{2\uparrow} + C^{+}_{2\downarrow}C_{3\downarrow} + C^{+}_{3\downarrow}C_{2\downarrow} + C^{+}_{3\uparrow}C_{4\uparrow} + C^{+}_{4\uparrow}C_{3\uparrow} + \\ &C^{+}_{3\downarrow}C_{4\downarrow} + C^{+}_{4\downarrow}C_{3\downarrow} + C^{+}_{1\uparrow}C_{4\uparrow} + C^{+}_{4\uparrow}C_{1\uparrow} + C^{+}_{\downarrow}C_{4\downarrow} + C^{+}_{4\downarrow}C_{1\downarrow}\Big) + E_f\Big(f^{+}_{1\uparrow}f_{1\uparrow} + f^{+}_{1\downarrow}C_{1\downarrow}\Big) + U\ f^{+}_{1\uparrow}f_{1\uparrow}f^{+}_{1\downarrow}f_{1\downarrow} + \\ &V\Big(C^{+}_{1\uparrow}f_{1\uparrow} + f^{+}_{1\uparrow}C_{1\uparrow} + C^{+}_{1\downarrow}f_{1\downarrow} + f^{+}_{1\downarrow}C_{1\downarrow}\Big) \end{aligned} \tag{3.1}$$

Using the same formalism in obtaining expanded Hamiltonian in Eq. (3.1), we can also obtain the expanded Hamiltonians for sites 2, 3 and 4 of the SIAM. Generalizing the SIAM, it follows that for the PAM, we have the Hamiltonian in Eq.(3.2) by expanding the Hamiltonian in Eq. (2.2) completely:

$$H_{PAM}=t\left(C_{1\uparrow}^{+}C_{2\uparrow}+C_{2\uparrow}^{+}C_{2\uparrow}+C_{1\downarrow}^{+}C_{2\downarrow}+C_{2\downarrow}^{+}C_{\downarrow}+C_{2\uparrow}^{+}C_{3\uparrow}+C_{3\uparrow}^{+}C_{2\uparrow}+C_{2\downarrow}^{+}C_{3\downarrow}+C_{3\downarrow}^{+}C_{2\downarrow}+C_{3\uparrow}^{+}C_{4\uparrow}+C_{4\uparrow}^{+}C_{3\uparrow}+C_{3\downarrow}^{+}C_{4\downarrow}+C_{4\downarrow}^{+}C_{3\downarrow}+C_{1\uparrow}^{+}C_{4\uparrow}+C_{4\uparrow}^{+}C_{1\uparrow}+C_{\downarrow}^{+}C_{4\downarrow}+C_{4\downarrow}^{+}C_{1\downarrow}\right)+E_f\left(f_{1\uparrow}^{+}f_{1\uparrow}+f_{1\downarrow}^{+}C_{1\downarrow}+f_{2\uparrow}^{+}f_{2\uparrow}+f_{2\downarrow}^{+}C_{2\downarrow}+f_{3\uparrow}^{+}f_{3\uparrow}+f_{3\downarrow}^{+}C_{3\downarrow}+f_{4\uparrow}^{+}f_{4\uparrow}+f_{4\downarrow}^{+}C_{4\downarrow}\right)+U\left(f_{1\uparrow}^{+}f_{1\uparrow}f_{1\downarrow}^{+}f_{1\downarrow}+f_{2\uparrow}^{+}f_{2\uparrow}f_{2\downarrow}^{+}f_{2\downarrow}+f_{3\uparrow}^{+}f_{3\uparrow}f_{3\downarrow}^{+}f_{3\downarrow}+f_{4\uparrow}^{+}f_{4\uparrow}f_{4\downarrow}^{+}f_{4\downarrow}\right)+V\left(C_{1\uparrow}^{+}f_{1\uparrow}+f_{1\uparrow}^{+}C_{1\uparrow}+C_{1\downarrow}^{+}f_{1\downarrow}+f_{1\downarrow}^{+}C_{1\downarrow}+C_{2\uparrow}^{+}f_{2\uparrow}+f_{2\uparrow}^{+}C_{2\uparrow}+C_{2\downarrow}^{+}f_{2\downarrow}+f_{2\downarrow}^{+}C_{1\downarrow}C_{3\uparrow}^{+}f_{3\uparrow}+f_{3\uparrow}^{+}C_{3\uparrow}+C_{3\downarrow}^{+}f_{3\downarrow}+f_{3\downarrow}^{+}C_{3\downarrow}+C_{4\uparrow}^{+}f_{4\uparrow}+f_{4\uparrow}^{+}C_{4\uparrow}+C_{4\downarrow}^{+}f_{4\downarrow}+f_{4\downarrow}^{+}C_{4\downarrow}\right). \quad (3.2)$$

For the SIAM, site 1 and 4 provides the same result while sites 2 and 3 provide the same result. This is due to side effects as open boundary condition can only be consider in the SIAM. Because of the complex nature of the matrices, the eigenvalues, eigenvectors and the wavefunction for a particular case was considered; where E_f =1, U = 1, V = 2 and t =1. The matrices were solved using numerically. For the Sites 1 and 4, the ground state energy of the singlet states is given by E_s = -3.47636 while that of the triplet states is given by E_t = -2.17032. This is an AFM ordering (Akpojotor, 2013). For the Sites 2 and 3, the singlet states ground state energy is given by E_s = -3.55822. For the triplet states, the ground state energy is given by,E_t = -2.03618. This is also an AFM ordering.To avoid edge effect in the PAM, periodic boundary condition is imposed, giving rise to a cyclic lattice. The ground state energy of the singlet states is given by E_s = 8.01647 and ground state energy of the triplet states is given by E_t = 10.3869. This is also an AFM ordering

4. Presentation and discussion of results

A numerical analysis carried out to obtain the series coefficients for the ground state energies in order to determine the magnetic instability and transition from antiferromagnetism to superconductivity are given by Tables 1, 2 and 3 with the corresponding graphs given by Figs. 1, 2 and 3 respectively. The energy units of the results presented below are in electron – volts (eV)

From the computations, we observed from Table 1 and Fig. 1 that as the value of the on-site Coulomb repulsion, U is increased from -10, the lattice system which was originally AFM becomes unstable just immediately after the point U = 10.0, this magnetic instability of the system is in agreement with theoretical results obtained by Rice and Ueda (1986) and Gebhard (1991). Rice and Ueda (1986) applied the Gutzwiller approximation and derived a lower bound for the existence of AFM from the ratio of magnetic exchange energy and kondo energy and found that the AFM state becomes unstable against FM ordering as $U\rightarrow\infty$. Gebhard (1991) investigated the Gutzwiller – correlated wavefunction using Gutzwiller approximation and also obtained magnetic instability as $U\rightarrow\infty$. Hence it is compelling as indicated in this study that the results obtained here are in qualitative agreement with other theoretical techniques. The interplay between AFM and HF Superconductivity was experimentally observed by increasing the *Cu* content in agreement with the results obtained by Pfleiderer (2009) that used neutron scattering (NS) and High Hydrostatic Pressure (HHP) experiments to show that the excess *Cu* tends to favour superconductivity in $CeCu_2Si_2$. Further, Pfleiderer (2009) observed that the HF superconductivity at the boundary of AFM and FM may be obtained: for Cu deficient the AFM (Metal) state is stabilized and superconductivity destroyed, while the AFM is destabilized and the superconductivity stabilized for Cu excess. Increasing the Cu content in $CeCu_2Si_2$ in the NS and HHP experiments is like increasing the parameter values of U in the SIAM and PAM which destabilized magnetism as $U\rightarrow\infty$; hence superconductivity in $CeCu_2Si_2$ at the boundary of AFM and FM is somehow related to the magnetic properties or instability observed in $CeCu_2Si_2$ at the boundary of AFM and FM in this study.

The numerical results in Table 2 and its corresponding graph in Fig. 2 for SIAM show that as the values of the on–site Coulomb repulsion of the f-electrons, U increases, the lattice is still AFM. For example, at U = -5.00, the system become unstable as AFM and FM tends to form magnetic glue. The results obtain in this study is in agreement with the theoretical results obtained by Tahvildar-Zadeh *et al.* (2008) and the experimental results obtained by Holmes *et al* (2007). In their study, Tahvildar-Zadeh*et al* (2008) applied a Quantum Monte Carlo (QMC) simulation and found that superconducting transition is indicated when the largest eigenvalue of the pairing matrix exceed one or unity. However, in the four electrons on four lattice sites of SIAM (1-D), the largest positive eigenvalue does not approach unity for any value of U studied. Instead, for relatively large value of U, a different type of magnetic instability was found: at a very large U, Tahvildar-Zadeh *et al* (2008) found generally that all eigenvalues are either small in magnitude or large and negative. As U is lowered, the positive eigenvalues grow slowly; however the most negative eigenvalues diverges at a U value upon lowering U further, the dominant eigenvalue (that with the largest absolute value) switches sign and become large (>>1) and positive, indicating a pairing instability of the system. The corresponding eigenvector yields information about

the superconducting order parameter. The dominant eigenvector of the pairing matrix has both negative and positive parts. Such an order parameter is compelling as it relates naturally to the complex phase diagram of the superconducting HF materials, in which the competition and sometimes the coexistence of AFM and superconductivity is observed. However, it is clear that the results obtained in this work correspond to the actual order parameter of the QMC simulation. The instability ceases for $E_s > E_t$ leading to a phase diagram which suggests re-entrance into the normal state (E_s and E_t distinctly separated) in the protracted screening regime. The shape of the lower phase boundary of the transition back to the normal metal is consistent with the decreasing U. This indicates that the system either loss the mechanism driving superconductivity or the system can gain more free energy by forming a Fermi liquid or magnetic glue (E_s and E_t merging together). It is compelling to relate the magnetic instability obtained in this study to superconductivity as the normal states relate to E_s and E_t distinctly separated, and E_s and E_t merging to form magnetic instability at the region where superconductivity is found.

Holmes *et al* (2007) investigated superconductivity in $CeCu_2Si_2$ using high pressure experiment and found that for decreasing pressure and Cu proportion, the superconductivity was weakened, and for large enough pressure and Cu proportion, the superconducting region could be split into two domes, near the AFM and FM region respectively. Hence, this region is related to the magnetic instability region obtain in this study. From Table 3 and Fig. 3, we observed 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.

Transition from AFM to HF Superconductivity was experimentally observed by Stockert *et al* (2011) that used inelastic neutron scattering experiment. Stockert *et al* (2011) adjusted a spectrometer in an experiment and measure inelastic neutron scattering in a compound of Cerium, Copper and Silicon ($CeCu_2Si_2$). This experiment reveals the magnetic fluctuations of the compound. According to the experiment, the superconductivity in $CeCu_2Si_2$ is caused by the magnetic interactions and shows how to change the electronic state of the material: a small deficiency in Cu causes the material to become AFM; with a tiny excess, it becomes a superconductor. The 4f-electrons of cerium atom in $CeCu_2Si_2$ are involved in both the superconductivity and magnetism. In the magnetic version of the material spins of the 4f- electrons, which turn them into bar magnets, give rise to the AFM order of the material: this can be imagined in a simple picture where the tiny magnets, lie next to each other with alternating north and south poles. In the superconducting version of $CeCu_2Si_2$, 4f-electrons flow into the reservoir from which Cooper pairs form electron pairs whose quantum properties make them visible to the crystal lattice and which can therefore move through it unhindered. Simultaneously, the AFM order disappears and the individual magnetic moment of the 4f-electrons are no longer visible to the outside. In this respect, $CeCu_2Si_2$ basically behaves as a conventional superconductor. The magnetic instability obtained in this work is somehow related to the superconductivity, as $CeCu_2Si_2$ transit from AFM on decreasing U is related (in this study) to copper deficient and increasing U that produces magnetic instability is related to superconductivity on copper tiny excess in the $CeCu_2Si_2$. This shows that excess Cu tends to favour superconductivity.

5. Summary and Conclusion

For the lattice systems studied in this paper, the ground state energy is always a spin singlet and the first excited state is always a singlet for both the SIAM and PAM. The results obtained here show a magnetic instability which is the bedrock of Superconductivity as $U \rightarrow \infty$ for the SIAM and PAM as indicated by results obtained by various workers (Stockert *et al.,* 2011, Holmes *et al.,* 2011, Rice and Ueda, 1986). This simply means that U suppresses all ferromagnetic tendencies and enhances magnetic instability (superconductivity). Thus the U behave here as Cu. It is pertinent to emphasize that in this study, systems with holes and important modification of the on-site Coulomb repulsion energy were not considered, which hopefully will become possible in the near future.

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References

Akpojotor, G.E. (2008) Possible propagation of the Zhang-Rice singlet as a probable Cooper channel in the CuO2 planes, Physics Letters A 372, 6992 - 6995.

Akpojotor G. E. (2011) 100 years of superconductivity: the past, the present and the future quest for a generalized theory, J. of NAMP 19, 623 – 630.

Akpojotor G. E. (2012) Ultracold atoms in superlattices as quantum simulators for a spin ordering model and phenomena, Adv. in Phys. Theories and Applications 6, 15-23.

Akpojotor G. E. (2013) Superexchange Driven Singlet-Triplet Transition in Quantum Dots Array Embedded in Kagome Lattice System. Adv. in Phys. Theories and Applications 17, 69-77.

Anderson P.W. (1961) Localized Magnetic States in a Metal. Phys. Rev.124 : 41- 53.

Bardeen J., Cooper L. N. and Schrieffer J. R. (1957).Theory of Superconductivity, .Phys. Rev. 108, 1175 – 1205.

Demler E., Hanke W. and Zhang S. C. (2004). SO(5) Theory of Antiferromagnetism and Superconductivity. arXiv:cond-mat/0405038v1.

Enaroseha O. O. E, Iyorzor B. E., and Idiodi J. O. A. (2011). Mott Transition of Cerium Compound $CeCu_2Si_2$ in the Anderson Model. J. NAMP. 19, 565–570.

Gebhard F. (1991) Equivalennce of Variational and Slave Boson Mean Field Treatments of the Periodic Anderson Model. Phys. Rev. B 44, 992 – 1003.

Hirsch, J.E. (2009). BCS theory of superconductivity: it is time to question its validity, Phys. Scr. 80: 0357021 (11pp).

Holmes A. T., Jaccard D., and Miyake K. (2007) Valence Instability and Superconductivity in Heavy Fermion System.J. Phys. Soc. Jpn76, 051002 – 051012.

Hubsch A. and Becker K. W. (2006) Valence Transition in the Periodic Anderson Model. Eur. Phy. J. B 53, 345 – 353.

Nascimbene, S., Chen, Y.-A., Atala, M., Aidelsburger, M, Trotzky, S., Paredes, B. and Bloch, I. (2012) Experimental realization of plaquette resonating valence bond states with ultracold atoms in optical superlattices, arXiv:1202.6361.

Pfleiderer Christian (2009) Superconducting phase of f electron compounds. Rev. Mod. Phy.81, 1551 – 1726.

Rice T. M. and Ueda K. (1986). Gutzwiller Method for Heavy-Electrons. Phys. Rev. B 34, 6420 – 6427.

Schmalian J. (2011) In Bardeen Cooper and Schrieffer: 50 YEARS (edited by L. N. Cooper and D. Feldman) World Scientific Publishing Co Pte Ltd, Singapore.

Stockert O., J. Arndt, E. Faulhaber, C. Geibel, H. S. Teevan, S. Kirchner, M. Loewenhaupt, K. Schmalzl, W. Schmidt, Q. Si, and F. Steglich (2011). Magnetically Driven Superconductivity in $CeCu_2Si_2$.Nature Physics7, 119 – 124.

Streltsov S. V., Shorikov A. O., and Anisimov V. I. (2011). Applicability of Anderson and Hubbard Model for Ce Metal and Cerium Heavy Fermion Compound. arXiv 1009.3382 v1

Tahvildah-Zadeh A. N., Hettler M. H., and Jarrell M. (2008).Superconducting Instability in the Periodic Anderson Model.Submitted to Phys. Rev. Lett.Retrieved from http//www.arXiv:cond-mat/9804162v1.

Table 1: Singlet (E_s) and Triplet (E_t) state energies as U varies and other parameters remaining constant, Using the SIAM at sites 1 and 4.

t (Hopping matrix element of the conduction electron)	**V** (On-site hybridization element between *f* orbital and *C* band)	**E_f** (Energy of the localized *f* orbital)	**U** (On-site Coulomb repulsion of the *f* electrons)	**E_s** (Singlet state energies)	**E_t** (Triplet state energies)
0.50	0.375	5.00	-10.00	-1.52	-0.83
0.50	0.375	2.50	-5.00	-1.60	-0.92
0.50	0.375	0.00	0.00	-1.94	-1.30
0.50	0.375	-2.50	5.00	-3.55	-3.29
0.50	0.375	-5.00	10.00	-5.86	-5.73
0.50	0.375	-7.50	15.00	-8.29	-8.21
0.50	0.375	-10.00	20.00	-10.76	-10.70
0.50	0.375	-12.50	25.00	-13.24	-13.19
0.50	0.375	-15.00	30.00	-15.73	-15.69
0.50	0.375	-17.50	35.00	-18.22	-18.18
0.50	0.375	-20.00	40.00	-20.71	-20.68

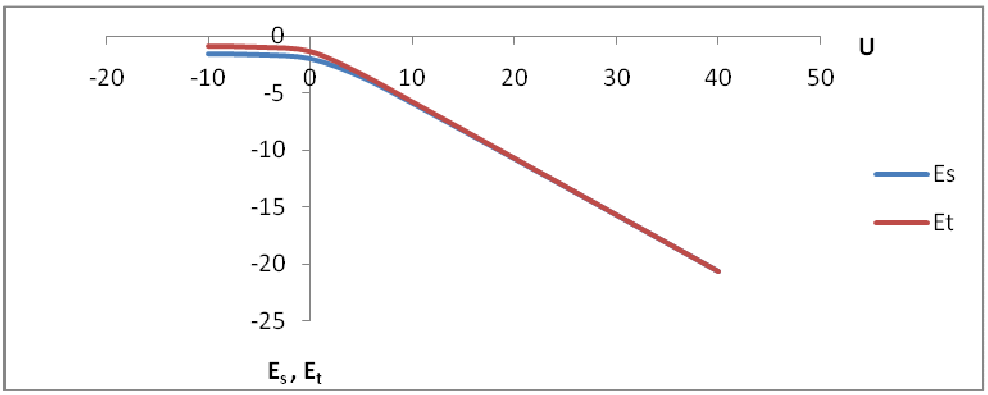

Fig. 1 (Colour online)**:** Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U for a system of 4 electrons on 4 lattice sites at sites 1 and 4 using the SIAM (1-D).

Table 2: Singlet (E_s) and Triplet (E_t) state energies as U varies and other parameters remaining constant, Using the SIAM at sites 2 and 3.

t	**V**	**E_f**	**U**	**E_s**	**E_t**
0.50	0.375	5.00	-10.00	-1.49	-0.79
0.50	0.375	2.50	-5.00	-1.59	-0.86
0.50	0.375	0.00	0.00	-2.01	-1.23
0.50	0.375	-2.50	5.00	-3.55	-3.21
0.50	0.375	-5.00	10.00	-5.81	-5.66
0.50	0.375	-7.50	15.00	-8.23	-8.13
0.50	0.375	-10.00	20.00	-10.69	-10.62
0.50	0.375	-12.50	25.00	-13.17	-13.12
0.50	0.375	-15.00	30.00	-15.65	-15.61
0.50	0.375	-17.50	35.00	-18.14	-18.11
0.50	0.375	-20.00	40.00	-20.64	-20.61

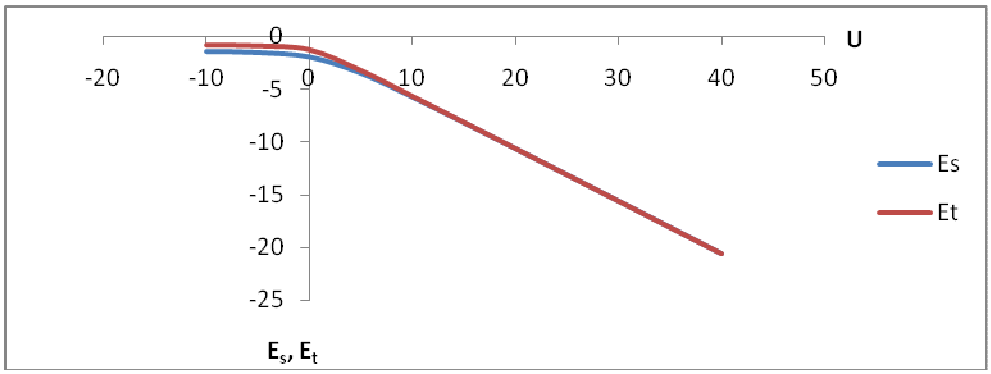

Fig. 2 (Colour online)**:** Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U for a system of 4 electrons on 4 lattice sites at sites 2 and 3 using the SIAM (1-D).

Table 3: Singlet (E_s) and Triplet (E_t) state energies as U 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	2.71	11.73
0.50	0.375	2.50	-5.00	2.44	6.76
0.50	0.375	0.00	0.00	0.54	1.97
0.50	0.375	-2.50	5.00	-7.51	-7.00
0.50	0.375	-5.00	10.00	-17.23	-17.00
0.50	0.375	-7.50	15.00	-27.17	-27.00
0.50	0.375	-10.00	20.00	-37.13	-37.00
0.50	0.375	-12.50	25.00	-47.10	-47.00
0.50	0.375	-15.00	30.00	-57.09	-57.00
0.50	0.375	-17.50	35.00	-67.07	-67.00
0.50	0.375	-20.00	40.00	-77.06	-77.00

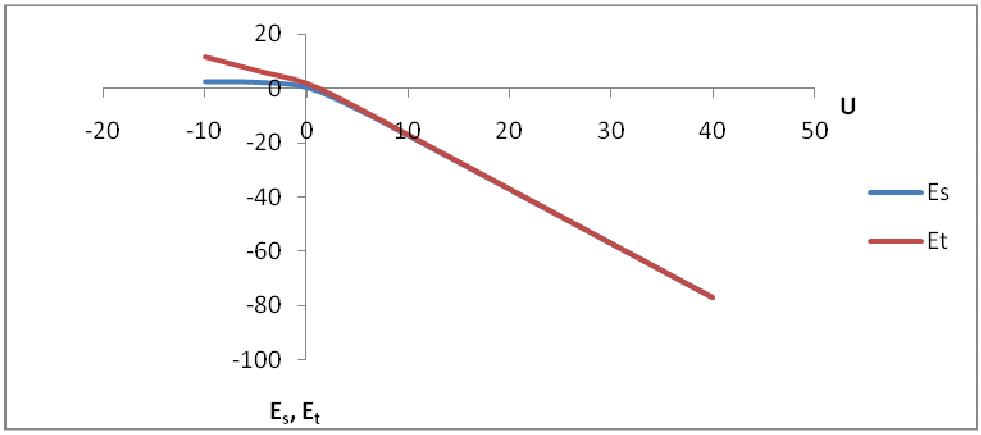

Fig. 3 (Colour online)**:** Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U for a system of 4 electrons on 4-sites using the PAM (1-D).