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GENERATION OF LOCALIZED MAGNETIC ORDER USING 4-ELECTRONS ON A 2X2 SQUARE LATTICE (2-D): APPLICATION OF THE PERIODIC ANDERSON MODEL

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ABSTRACT

The magnetic order on the formation of localized magnetic moment for the Anderson model using the exact diagonalization technique on a four interacting electronic system in two dimension (2-D) was studied in this research work.

The result obtained shows remarkable degree of agreement with experimental and other theoretical technique discussed in the literature.

Our result establish a spin singlet ground state and the first excited state was always a singlet for all the lattice system studied. While increasing the value of t favours Anti-ferromanetism (AFM) to Ferromagnetism (FM) magnetic order, increasing u shows magnetic instability with a coexistence of Anti-ferromagnetism (AFM) and Ferromagnetism(FM), while increasing the values of V, a constant hybridization or semiconducting gap (i.e. $\Delta \sim 0.21$) is obtained

KEYWORDS: Anderson model, transition, hybridization, Singlet state, triplet state

INTRODUCTION

One of the most important challenges in theoretical physics is to develop a quantitative understanding of the process by which electrons interacts with each other using the various electronic states to acts on a given Hamiltonian. When an electron interacts with each other, it is accelerated by the surface potential well in which it can gain up to a few electron-Volts of kinetic energy. However, to adsorb on a surface the atomic state of the interacting system, referred to as the adsorbate hereafter, must lose sufficient energy to prevent it from escaping from the surface potential well. This lost energy can be dissipated into various channels, for example lattice vibrations (phonons), chemiluminescence (photons), exo-electrons (electrons ejected from the surface) and electron – hole pairs (electronic excitations within the surface). Phenomena such as chemiluminescence and exo-electron excitation require substantial amounts of energy to be transferred to a single electron and are therefore generally only seen in extremely exothermic reactions such as the oxidation of alkali metal surfaces [1]. The lower energy dissipation channels of phonon and electron-hole pair excitation, however,

are expected to be ubiquitous.

The purpose of this research is to ascertain the level of electrons excitation in relation to generation of localized magnetic order. The Anderson model [2] plays an important role in this regard. Despite its simplicity and many years of study, the physics of the Anderson model remains unknown [3]; surprisingly simple facts, such as whether it hosts antiferromagnetic or ferromagnetic ground state, though resolved but are still under investigation in higher dimensions.. Recently, the limit of *infinite* dimensions has allowed considerable progress, and provided insight into its behaviour in lower dimensions. The focus here is the 2D system, and we aim to survey its phase diagram, concentrating on magnetism, as *we* varied the Hamiltonian's parameters..

A metal contains a sea of mutually-repelling electrons in close proximity to each other; strangely, their interactions are usually unimportant, and merely manifest themselves solely as a renormalization of the electron's mass. Effective electron masses vary from close to the vacuum value (in *f*-electron metals, such as Cerium), to being hundreds or thousands of times the bare mass in heavy-fermion materials such as $CeCu_2Si_2$, where there is a large effective electronic interaction in the tight f -electron orbitals. The ordinary behaviour of these electrons is described by the *Fermi liquid theory* of Landau[4]; non-interacting electrons fill up modes in momentum space, yielding a *Fermi surface* the locus of points in momentum-space that are filled last. At low temperature, the properties of the system depend only on small excitations around this surface. Here we discuss one of the more successful many-body theories: Fermi-liquid theory proposed by [4,5,6,7,8]. However, it is useful to begin by considering a model which is the simplest possible for a system of fermionic electrons, namely the free-electron model. We investigate some properties of this model and acknowledge its unexpected successes as an explanation of the metallic state before moving on to realise the explanation for this success, leading to Fermi-liquid theory itself.

The Notion of the Quasiparticle with respect to the success of the free-electron model can be explained via an argument based on the idea of adiabatic continuity [9]. Let us first start with the now familiar non-interacting electron gas in its ground state, constructed as explained above. We imagine we have a knob which we can use to tune the interactions between the electrons from off (which is obviously the point we begin at) to an interaction strength which represents the realistic situation for electrons. Let us start to adiabatically turn the interactions on and allow the system to slowly evolve. The ground state of an interacting electron gas may be constructed by the adiabatic 'turning-on' of interactions between the free electrons of the non-interacting system's ground state. Furthermore, any arbitrary excited state of the interacting system could be constructed by exciting a number of electrons of the non-interacting gas into a state above the Fermi surface, leaving an equal number of holes behind, and then allowing the system to evolve adiabatically by turning our knob to a directly corresponding excited state of the interacting system. The crux of all this is that the free electron model's success is explained by the fact that, although wavefunctions of the interacting system are markedly different from those of the free-electron system from which they are adiabatically derived, the wavefunctions' labels (that is, momentum and spin) remain robust during the adiabatic transition. The one-to-one correspondence of the non-interacting system's electron configuration (whether excited or not) to that of the interacting system provides the realistic theoretical predictions which previously were puzzling. The new interacting system is made up of fermionic particles (therefore there exists a Fermi surface) which we shall call quasiparticles. These particles are not exact eigenstates of the system; hence they have a finite lifetime. Where in the non-interacting case we talked of free electrons being labeled via their momenta $\boldsymbol{k}$ and spin σ , we now talk of fermionic quasiparticles which share these labels.

The material of this paper is structured as follows: In the next section we briefly introduce the model Hamiltonian, and present our results in Section 3. Discussion, Concluding remark and comparison with experimental results and other theoretical techniques were offered in Section 4.

2.0 MODEL AND METHODOLOGY

Considering, materials where "quantum impurity ions" are put on a lattice. Generalizing the single channel impurity Anderson model (2.1) to a lattice of localized orbital, *f,* and one obtains the so-called periodic Anderson model (PAM). The PAM as proposed by [9,10] is given by

$$H=-t\sum_{\langle ij\rangle\sigma}(C^{+}_{i\sigma}C_{i+1\sigma}+C^{+}_{i+1\sigma}C_{i\sigma})+E_f\sum_{i\sigma}n^{f}_{i\sigma}+U\sum_{i}n^{f}_{i\uparrow}n^{f}_{i\downarrow}+V\sum_{i,\sigma}(C^{+}_{i\sigma}f_{i\sigma}+f^{+}_{i\sigma}C_{i\sigma}) \tag{2.1}$$

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. t represents hopping matrix element, $\langle ij\rangle$ denotes nearest neighbour interactions. E_f is the energy of the localized f orbital, while U and V stands for onsite coulomb repulsion and hybridization respectively.

3.0 RESULTS

CALCULATION FOR A SYSTEM OF 4-ELECTRONS ON A 2X2 SQUARE LATTICE (2-D) USING THE PERIODIC ANDERSON HAMILTONIAN.

Consider the periodic Anderson Hamiltonian (2.1), for a system of four interacting electrons on a 2x2 square lattice (2-D), leads to the extended Hamiltonian with seventy basis electronic states having 36 states with net spin 0, 32 states with net spin ±1, and 2 states with net spin ±2.

Numerical analyses carried out to obtain the series coefficients for the ground state energies in order to determine the magnetic phase transition and Hybridization gap are given in Fig. 4.1, 4.2 and 4.3 respectively.

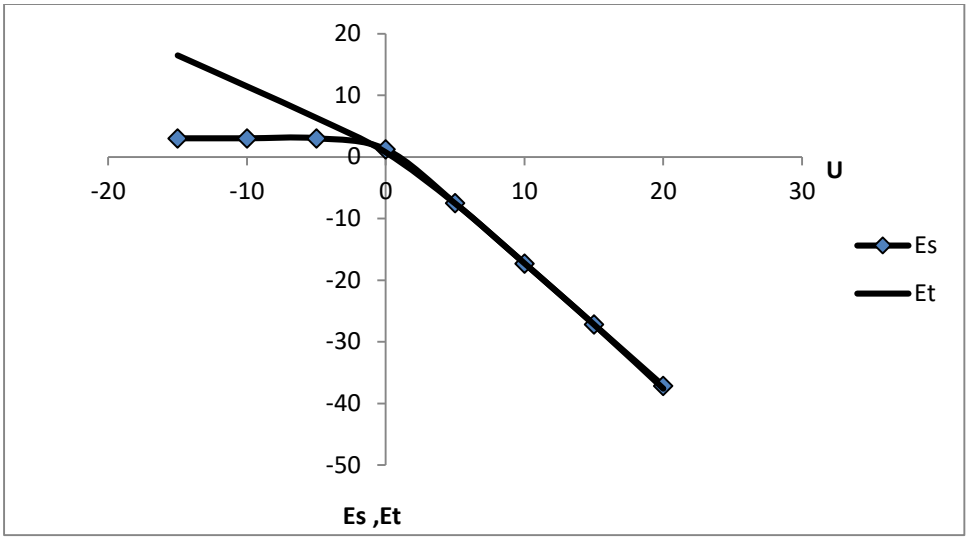

Fig. 4.1: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against U; showing the transition between E_s and E_t for a system of 4 electrons on 2 x 2 square lattice sites using the PAM (2-D).

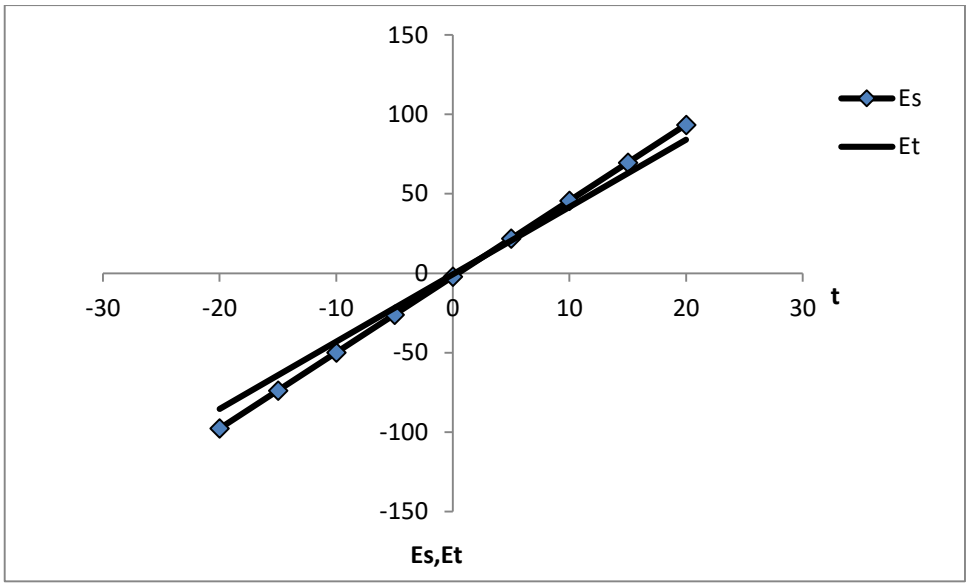

Fig. 4.2: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against t, showing the ferromagnetic alignment between E_s and E_t for a system of 4 electrons on 2 x 2 square lattice sites using PAM (2-D).

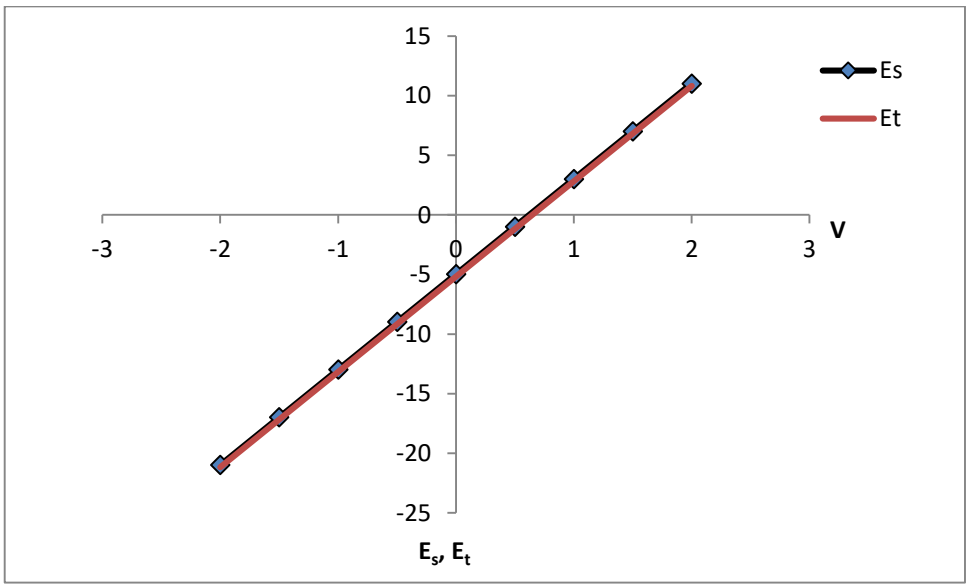

Fig. 4.3: Graph of Singlet (E_s) and Triplet (E_t) state energies plotted against V; showing a hybridization gap between E_s and E_t for a system of 4 electrons on 2 x 2 square lattice sites using PAM (2-D).

4.0 DISCUSSION OF RESULTS.

From the computations of Fig 4.1 shows that as U is increased, there is a magnetic instability in the system. This results obtained here are in agreement with some theoretical [11,12] and experimental results [13]. Horiuchi *et al* [11] applied a Variational Cluster Approach (VCA) based on the self-energy functional theory to Anderson model at quarter filling (2-D) and obtained magnetic instability of the AFM ordered state, and as $U\rightarrow\infty$, the gaps between E_s and E_t tends smoothly and merge, indicating the system tends to the non interacting band insulator or magnetic instability.

Perez and Araujo [12] study the magnetic and superconducting instabilities with the infinite coulomb repulsion U in the random phase approximation (RPA), and found that AFM occur in a very small region as $U\rightarrow\infty$, as both AFM and superconductivity are controlled by the same interaction parameter U, which in turn, depends on hybridization only. This result is in qualitative agreement in this study as $U\rightarrow\infty$.

Using the muon-spin relaxation experiment (μSR) [13] found superconductivity at the boundary of AFM and FM in $CeCu_2Si_2$ at atmospheric pressure. The phase transition is studied in several samples of $CeCu_2Si_2$ with varying Cu stoichiometries, where Cu excess tends to favour superconductivity and with Cu deficiency favouring AFM. Thus in $CeCu_2Si$, there appear to be competition between magnetism and superconductivity as superconductivity is found between the boundary of AFM and FM which is related to magnetic instability in this study.

In Fig. 4.2 shows that, as the values of t increases, the system that was initially AFM losses its properties and becomes FM, showing a smooth phase transition in agreement with experimental results obtained by Muller *et al* [14].

Fig 4.3 shows that when the values of V increases, a constant hybridization or semiconducting gap (i.e. $\Delta \sim 0.21$) is obtained, this is in agreement with results obtained by Zhu and Zhu [15].

CONCLUSION

In this research, the Exact-Diagonalization technique has been employed to provide information on the behavior of four interacting electrons in 2-D lattices. The lattices considered in this thesis are small in size. It is not obvious that the results obtained for larger lattices in the literature are applicable here. the system studied is 4 electrons on a 2 X 2 square lattice for the PAM. Finite sized lattices with open boundary condition and periodic or cyclic boundary conditions were specifically considered, and the dynamics of the interacting electrons was described by the Hamiltonians used.

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.

REFERENCES

[1] Greber T. (1997).. "Charge-transfer induced particle emission in gas surface reactions."Surface Science Report., 28 pp 1 – 2

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

[3] Laughlin R. B. and D. Pines (2000). The Theory of Everything. Proc. National Academy of Science U.S.A. ***97***, 28 -31

[4] Pines D. and Nozieres P. (1989). *The Theory of Quantum Liquids.* Addison Wesley Advanced Books Classic, California, U. S. A.

[5] Rodrigo A. F, Costa N. C., Dos Dantos R, and Palva T(2022). The 2 – D Attractive Hubbard Model BCS – BEC Crossover. Sumitted to Phys. Rev. B. Retrived from ariv:2201.02156 on the 25th January 2022

[6] Baym G. and Pethick C. J. (1991). *Landau Fermi Liquid Theory: Concepts and Application.* John Wiley and Sons, U. S. A.

[7] Zheng R, He R. and Lu Z (2021). Order Parameter for the Multichannel Kondo Model at Quantum Criticality. Phys. Rev. B. 103, 045111 – 045116.

[8] Yang F (2022). Localization for Magnetic Quantum Walks. Sumitted to Phys. Rev. B. Retrived from ariv:2201.05779 on the 24th January 2022

[9] Anderson P.W. (1984). *Basic Notions of Condensed Matter Physics.* Addison Wesley, U. S. A.

[10]. Enaroseha O. E. Omamoke, Obed Oyibo, and N. Okpara. (2021). Analysis of Ground State Properties of Interacting Electrons in the Anderson Model. *The Journal of Applied Sciences Research,* 8(1), 15-27.

[11] Horiuchi S., Kudo S., Shirakawa T., and Ohta Y. (2008). Antiferromagnetism Vs Kondo Screening in the Two Orbital Periodic Anderson Model at Half-filling: Variational Cluster Approach. *Phys. Rev. B* ***78***: 155128 – 155133; Retrieved from http//www.arXiv:cond-mat/0808 – 0448.

[12] Perez N. M. R. and Araujo M. A. N. (2002). Magnetic and Superconducting Instability in the Periodic Anderson Model: RPA Study. *J. Phys. Condens. Matt.* ***14***, 5575 - 5583

[13] Heffner R. H. and Norman M. R. (1996). Heavy Fermion Superconductivity. *Comments on Cond. Matt. Phys.* ***17***, 361 – 406.

[14] Muller D. A., Shashkov D., Benedek R., Yang L. H., Silcox J., and Seidman D. (1998). Atomic Scale Observation of Metal Induced Gap States at {222} MgO/Cu Interface. *Phys. Rev. Lett.* ***80***, 4741 - 4743

[15] Zhu L. and Zhu J. (2011). Magnetic Field Induced Phase Transitions in the Two-Impurity Anderson Model. Submitted to *Phys. Rev. Lett.* Retrieved from http//www.arXiv 1011.6629 v1 [cond-mat.str-el].