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# SPIN AND MAGNETIC CORRELATION IN THE ONE: DIMENSIONAL HUBBARD MODEL

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**ABSTRACT:** *The description of a solid at a microscopic level is complex, involving the interaction of a huge number of its constituents, such as ions or electrons. The Hubbard model used in this research describes interacting electrons in narrow energy bands, with application to problems as diverse as high – Tc superconductivity, band magnetism and the metal-insulator transition. This research seeks to solve one of the most challenging problems in Theoretical physics which is to describe electronic correlations. In this research the t – U Hubbard model is used to solve analytically and numerically using the exact diagonalization techniquesThis research work focused on the spin interaction and magnetic behavior of some systems and it is therefore an investigation into the various phenomena seen in the phase diagram of ferromagnetic systems. We studied the 2 electrons on 2 sites, 2 electrons on 3 sites and 2 electrons on 4 sites all in One-Dimension (1-D), where the onsite coulomb repulsion, U, and the hopping matrix element, t, were varies to determine their magnetic phase diagram.This results obtained shows that, as the values of the onsite coulomb repulsion, U, increases in all the lattice systems studied, the electronic correlation that favours ferromagnetism gets stronger, but there were no clear transition, and at some point the lattices loss its antiferromagnetic properties, hence the instability of ferromagnetism were established. It was also observed that as the hopping matrix element, t, increases the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties but beyond the transition point the lattice began to gain a much stronger antiferromagnetism, hence the ferromagnetism is unstable.*

**KEYWORDS:** Ferromagnetism, Antiferromagnetism, Singlet State, Triplet State, Hubbard Model

## INTRODUCTION

Magnetic phenomena have been known and exploited for many centuries. The earliest experiences with the magnetism involved Magnetite, the only material that occurs naturally in a magnetic state. The Hubbard Hamiltonian offers the simplest insight on how the interactions between electrons give rise to insulating, magnetic, and even novel superconducting effects in a solid. It was written down (Gutzwiller, 1963; Kanamori, 1963; Hubbard, 1963; Sherman 2020; Zhuo *et al* 2020) in the early 1960's and initially applied to the behavior of the transition – metal monoxides (FeO, NiO, CoO), compounds which are anti-ferromagnetic insulators, yet had been predicted to be metallic by methods which treat strong interactions less carefully.

Over the intervening years, it has been applied to many systems, from 'heavy fermions' and the Cerium volume collapse transition in the 1980's, to high temperature superconductors in the

1990's. Indeed, it is an amazing feature of the Hubbard Hamiltonian that, despite its simplicity, it exhibits behavior relevant to many of the most subtle and beautiful properties of solid state systems. We focus here for the most part on the Hubbard Hamiltonian with variants like that allows us to introduce other fundamental concepts in many – body physics, such as the competition between magnetic order and singlet formation. Randomness can be simply introduced into the Hubbard Hamiltonian, so it can be used as a starting point for investigations of the interplay of interactions and disorder in metal – insulator transitions and, recently, many-body localization.

It has been studied by the full range of analytic techniques developed by the condensed – matter community, from static mean – field approaches and the much richer dynamical mean – field theory, to diagrammatic approaches of various degrees of sophistication (the random phase approximation and parquet approach), as well as expansions in the degeneracy of the number of 'flavors' (spin, orbital angular momentum). It has also been extensively attacked with numerical methods like quantum Monte Carlo (QMC) but results on Exact Diagonalization (ED) (which we will outline here) are scarce. The aim of this research is to investigate the Hubbard Model and observe the effect of magnetic ground state properties. The objectives of this work are to: elucidate the nature of the ground state and the magnetic properties of the Hubbard Model; determine the effect of the Hamiltonian matrix parameters on electrons interacting in 1-D; demonstrate the role of onsite coulomb repulsion *U*, and the hopping matrix element *t* in the Hamiltonian matrix and to investigate the parameter range giving rise to the ferromagnetic phases.

## 2.0 MODEL AND METHODOLOGY

The single – band Hubbard model (Hubbard, 1963) was originally introduced as a model for ferromagnetism of itinerant electrons. The model is given by

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \text{H. C.}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (2.1)$$

where $\hat{c}_{i\sigma}^{\dagger}$ $(c_{i\sigma})$ creates (annihilates) an electron with spin $\sigma = \uparrow, \downarrow$, $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger} \hat{c}_{i\sigma}$ is the number operator, and $\langle ij \rangle$ denotes nearest neighbors. This is the simplest possible correlation model for electrons on a lattice. However, rigorous evidence for itinerant ferromagnetism in this model is very limited. One of the most important results is Nagaoka's theorem, (Nagaoka, 1966) which states that if the Hubbard repulsion *U*, is infinite, the ground state has maximum total spin on certain lattices in the case of precisely one hole. The physical mechanism behind Nagaoka's theorem is the following. If $U = \infty$ the ground state of (2.1) is macroscopically degenerate. This degeneracy is lifted by the motion of the hole since it is energetically favorable for it to move in a background of fully aligned spins (provided the lattice allows for motion of the hole around loops). A simpler proof of Nagaoka's theorem was later given by Tasaki (1989) who also showed that additional density-dependent interactions do not alter this result.

Several other mechanisms leading to ferromagnetism in the Hubbard model have been discussed since then. Lieb (1989) proved that the ground state is ferromagnetic for bipartite lattices with different numbers of sites in each sublattice. Mielke (1991) and Tasaki (1992) proved the stability of ferromagnetism for special lattices with flat bands.

Recently, Muller – Hartmann (1995) studied ferromagnetism at low particle density in dimension d=1. He included next-nearest- neighbor hopping in such a way that the band has two minima. At low density, the on-site repulsion $U$ generates a ferromagnetic exchange coupling between particles in these two pockets. Clearly, it is still a long way to a true understanding of itinerant ferromagnetism in solids. It is quite obvious that the single-band Hubbard model is not a *generic* model for ferromagnetism. So far, either the assumption of a special kind of hopping or of $U = \infty$ or both, was necessary to prove the stability of ferromagnetism.

The method of solution used in this work is the Exact Diagonalization (ED) technique. 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 particles states, and all the eigenvalues and eigenvectors found (Carter, 2004). From these the interacting wave-function can be constructed using the eigenvector corresponding to the singlet and triplet states energies by means of Lehmann representation (Mahan, 2000). To obtain the eigenvalue and eigenvector of the lattice system, the matrix elements were evaluated with the help of an analytical diagonalization routine provided by Wolfram Mathematica 12.0 software. Having obtained the results of the eigensystems, the lowest of the eigenvalues provides the ground state energy of the system. To obtain the wave-function, the corresponding eigenvector to the eigen value is used.

## 3.0 RESULTS

### 3.1 CALCULATIONS FOR 2 ELECTRONS ON A 2 SITE LATTICE SYSTEM (1-D)

Considering a system of two interacting electrons on two sites.

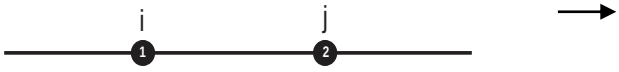


Fig 1.1a: Two electrons on two sites i and j

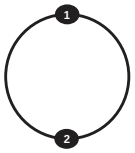


Fig 1.1b: Cyclic lattice, to avoid edge effect

Periodic boundary condition is imposed to avoid edge effect, giving rise to a cyclic lattice.
The possible electronic states of 2 electrons on 2 sites are 6.
*Generating the states we have:*

$$|1\rangle = |1\uparrow 1\downarrow\rangle,\ |2\rangle = |2\uparrow 2\downarrow\rangle,\ |3\rangle = |1\uparrow 2\downarrow\rangle,\ |4\rangle = |1\downarrow 2\uparrow\rangle,\ |5\rangle = |1\uparrow 2\uparrow\rangle,\ |6\rangle = |1\downarrow 2\downarrow\rangle.$$

*From the (2.1), the expanded Hamiltonian is given by:*

$$H = -t\left(C^{+}_{i\uparrow}C_{i+1\uparrow} + C^{+}_{i+1\uparrow}C_{i\uparrow} + C^{+}_{i\downarrow}C_{i+1\downarrow} + C^{+}_{i+1\downarrow}C_{i\downarrow}\right) + U\left(C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{i\downarrow}C_{i\downarrow} + C^{+}_{i+1\uparrow}C_{i+1\uparrow}C^{+}_{i+1\downarrow}C_{i+1\downarrow}\right) \quad (3.1)$$

*Using the basis electronic states to act on the Hamiltonian, the summary of the interaction is given by:*

$$H|1\rangle = t|4\rangle - t|3\rangle + U|1\rangle,\ H|2\rangle = -t|3\rangle + t|4\rangle + U|2\rangle,\ H|3\rangle = -t|2\rangle - t|1\rangle,$$
$$H|4\rangle = t|1\rangle + t|2\rangle,\quad H|5\rangle = 0,\ H|6\rangle = 0 \qquad (3.2)$$

*Therefore the matrix representation of the entire Hamiltonian in this basis becomes:*

$$H = \begin{Bmatrix} U & 0 & -t & t & 0 & 0 \\ 0 & U & -t & t & 0 & 0 \\ -t & -t & 0 & 0 & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{Bmatrix} \qquad (3.3)$$

*For the singlet state we hav*

$$H = \begin{Bmatrix} U & 0 & -t & t \\ 0 & U & -t & t \\ -t & -t & 0 & 0 \\ t & t & 0 & 0 \end{Bmatrix} \qquad (3.4)$$

To obtain the eigenvector corresponding the minimum energy, we solve for $\vec{X}$ in the equation

$$(H_{ij} - \lambda I)\vec{X} = 0 \qquad (3.5)$$

*Where $\lambda = E_g$ = Minimum energy or ground state energy, I = Identity Matrix and $H_{ij}$ = Hamiltonian Matrix*

Hence (3.4) becomes

$$\begin{Bmatrix} U-\lambda & 0 & -t & t \\ 0 & U-\lambda & -t & t \\ -t & -t & 0-\lambda & 0 \\ t & t & 0 & 0-\lambda \end{Bmatrix} \begin{Bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \qquad (3.6)$$

$$H_{ij} - \lambda I \quad \begin{Bmatrix} U-\lambda & 0 & -t & t \\ 0 & U-\lambda & -t & t \\ -t & -t & 0-\lambda & 0 \\ t & t & 0 & 0-\lambda \end{Bmatrix} \qquad (3.7)$$

*The Eigenvalues are*

{18.4659, 15.0000, -3.46586, 0} (3.8)

*The ground state energy is;*

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$E_s = -3.46586$ (3.9)

*The corresponding ground state amplitudes for the singlet states are*

$|\varphi\rangle_s$ = {-0.433232|1 ↑ 1 ↓⟩ -0.433232|2 ↑ 2 ↓⟩ -1.00000|1 ↑ 2 ↓⟩ +1.00000|1 ↓ 1 ↑⟩ (3.10)

*For the triplet state we have:*

$$H = \begin{Bmatrix} 0 & 0 \\ 0 & 0 \end{Bmatrix} \quad (3.11)$$

*The g*round state energy is;

$E_t = 0$ (3.11)

## 3.2 CACULATION FOR 2 ELECTRONS ON 3 SITES LATTICE SYSTEM (1-D)

The number of possible electronic states for 2 electrons on 3 sites lattice is 15, and, the results of the interaction on using the 15 basis electronic states to act on the Hamiltonian are summarized in (3.15)

$$H = \begin{Bmatrix} U & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & U & 0 & -t & t & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & U & 0 & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 \\ -t & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -t & -t & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t & t & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 \end{Bmatrix} \quad (3.12)$$

*For the singlet state we have:*

$$H = \begin{Bmatrix} U & 0 & 0 & -t & t & 0 & 0 & 0 & 0 \\ 0 & U & 0 & -t & t & 0 & 0 & -t & t \\ 0 & 0 & U & 0 & 0 & 0 & 0 & -t & t \\ -t & -t & 0 & 0 & 0 & -t & 0 & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 & -t & 0 & 0 \\ 0 & 0 & 0 & -t & 0 & 0 & 0 & -t & 0 \\ 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & -t \\ 0 & -t & -t & 0 & 0 & -t & 0 & 0 & 0 \\ 0 & t & t & 0 & 0 & 0 & -t & 0 & 0 \end{Bmatrix} \quad (3.13)$$

*The Eigenvalues are*

$$\{5.85169, -5.47651, 3.08945, -2.82843, 2.82843, -2.58945, 0.5, 0.124817, -7.96826 \times 10^{-17}\} \quad (3.14)$$

*The ground state energy for the singlet state is*

$$E_s = -5.47651 \quad (3.15)$$

*The corresponding ground state amplitudes are*

$$|\varphi\rangle_s = \{-0.240343|1\uparrow 1\downarrow\rangle -0.480687|2\uparrow 2\downarrow\rangle -0.240343|3\uparrow 3\downarrow\rangle -0.359104|1\uparrow 2\downarrow\rangle$$
$$0.359104|1\downarrow 2\uparrow\rangle -0.262287|1\uparrow 3\downarrow\rangle 0.262287|1\downarrow 3\uparrow\rangle -0.359104|2\uparrow 3\downarrow\rangle$$

$$+0.359104|2\downarrow 3\uparrow\rangle \quad (3.16)$$

*For the triplet state we have:*

$$m = \begin{Bmatrix} 0 & 0 & -t & 0 & 0 & 0 \\ 0 & 0 & 0 & -t & 0 & 0 \\ -t & 0 & 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 & 0 & -t \\ 0 & 0 & -t & 0 & 0 & 0 \\ 0 & 0 & 0 & -t & 0 & 0 \end{Bmatrix} \quad (3.17)$$

*The Eigenvalues are:*

$$\{-2.82843, -2.82843, 2.82843, -2.82843, 0, 0.\} \quad (3.18)$$

*The ground state energy for the triplet state is:*

$$E_t = -2.82843 \quad (3.19)$$

*The corresponding ground state amplitudes are*

$$|\varphi\rangle_t = \{1.00000|1\downarrow 2\downarrow\rangle +1.41421|1\downarrow 3\downarrow\rangle +1.00000|2\downarrow 3\downarrow\rangle\} \quad (3.20)$$

## CACULATION FOR 2 ELECTRONS ON 4 SITES LATTICE SYSTEM (1-D)

The number of possible electronic states for 2 electrons on 3 sites lattice is 28 and results of the interaction on using the 15 basis electronic states (3) to act on the Hamiltonian matrix

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$$H = \begin{Bmatrix}
U & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & U & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & U & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & t & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & U & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-t & -t & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
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0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -t & 0 & 0
\end{Bmatrix} \tag{3.21}$$

*The Eigenvalues are:*

$$\{3.40077, -3.09956, 2.45426, -2.23607, 2.23607, -2.05347, 1.42794, 1.18687,$$

$$-1.10683, 1.00000, \quad -0.999999, -0.80919, 0.5, 0.099211,$$

$$-2.33279 \times 10^{-16}, 7.26911 \times 10^{-18}\} \tag{3.22}$$

*The ground state energy is:*

$E_s$ = *-3.09956* (3.23)

*The corresponding ground state amplitudes are*

$|\varphi\rangle_s$ = {-0.124514|1 ↑ 1 ↓⟩ -0.328902|2 ↑ 2 ↓⟩ -0.328902|3 ↑ 3 ↓⟩

-0.124514|4 ↑ 4 ↓⟩ -0.224098|1 ↑ 2 ↓⟩ +0.224098|1 ↓ 2 ↑⟩

-0.241189|1 ↑ 3 ↓⟩ +0.241189|1 ↓ 3 ↑⟩ -0.155628|1 ↑ 4 ↓⟩

+0.155628|1 ↓ 4 ↑⟩ -0.367853|2 ↑ 3 ↓⟩ +0.367853|2 ↓ 3 ↑⟩

-0.241189|2 ↑ 4 ↓⟩ +0.241189|2 ↓ 4 ↑⟩ -0.224098 +0.224098|3 ↓ 4 ↑⟩} (3.24)

*For the triplet state we have:*

*The Eigenvalues are:*

{ -2.23607, -2.23607, 2.23607, 2.23607,-1,-1,1,1,0,0,0,0} (3.25)

*The ground state energy is:*

$E_t$ = -2.23607 (3.26)

*The corresponding ground state amplitudes are*

$|\varphi\rangle_t$ = {1.00000|1 ↓ 2 ↓⟩ +2.23607|1 ↓ 3 ↓⟩ +2.00000|1 ↓ 4 ↓⟩

+2.00000|2 ↓ 3 ↓⟩ +2.23607|2 ↓ 4 ↓⟩ +1.00000|3 ↓ 4 ↓⟩ (3.27)

**PRESENTATION AND 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. It is important to note that the 1-D results of the Hubbard model are available but the present calculation is the first where the Exact-Diagonalization (ED) technique had been applied with graphical representation using Mathematica 12.0 software to solve the Hamiltonian matrix.

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 ferromagnetism phase is that the lowest energy of the triplet state, $E_t$ must be smaller than that of the singlet state, $E_s$ i.e. $E_t < E_s$ (Amadon and Hirsch, 1996). If the singlet state provide 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 state provide the ground state energy.

The value at which $E_t = E_s$ give rise to a transition from antiferromagnetic phase to a magnetic phase or vice-versa. The point is called the transition point, $T_p$. However the magnetic phase transition from antiferromagnetism to ferromagnetism is expected to occur when $E_t \sim E_s$ (Moller and Wolfle, 1993). The electronic spin configuration of the antiferromagnetism and ferromagnetism has direct comparison with the experimental Metallic and Insulating phase, where

a phase transition occurs from antiferromagnetism to ferromagnetism theoretically is equivalent to metal to insulation transition (MIT) or Mott transition.

The discussion of results are organized as follows: in section 4.2, the system of 2 electrons on 2-sites were discussed; section 4.3 discussed the system of 2 electrons on 3-sites; while section 4.4 discussed the system of 2 electrons on 4-sites.

## RESULTS FOR THE SYSTEM OF 2 ELECTRONS ON 2-SITES

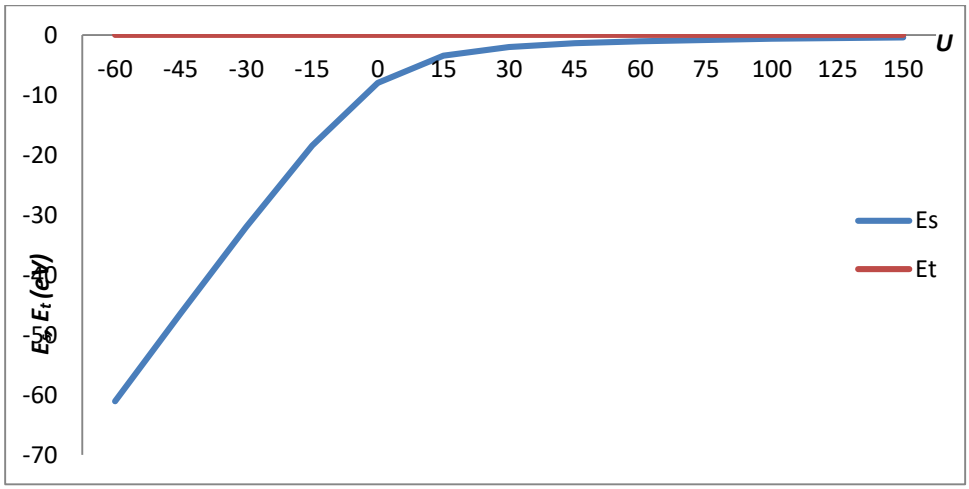


**Fig 4.1a:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *U* for system of 2 electrons on 2 sites.

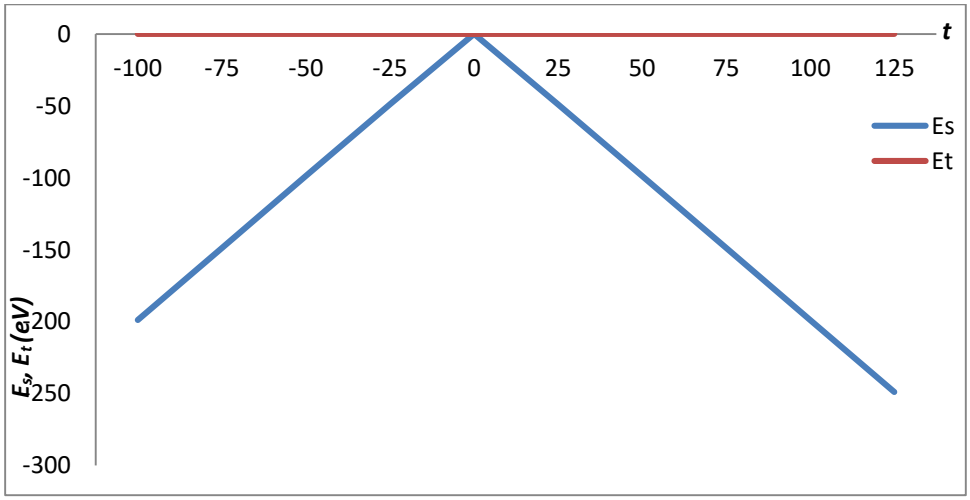


**Fig 4.1b:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *t* for system of 2 electrons on 2 sites.

**Discussion of the Results of 2 Electrons on 2 Site System**

From computations, we observed, from figure 4.1a that as the values of the on-site interactions strength, *U*, increased from -60, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 150, which is the transition point $T_p$ ($E_t$=$E_s$). And beyond this point there was no clear transition, hence the ferromagnetism is unstable. This is not in agreement with the Nagaoka's theorem.

Also it was observed from figure 4.1b that as the value of the hoping term, *t* increased from -100, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 0 which is the transition point $T_p$ ($E_t$=$E_s$). Beyond this point the lattice began to gain a much stronger antiferromagnetism, hence the ferromagnetism is unstable.

The results obtained in this research are in agreement with the results obtained by Koma and Tasaki (1992), in their work on the Hubbard model in One Dimension where the finite range hopping ($t \to \infty$) rules out long range spin-order or superconductivity at finite temperature ($t \to \infty$). This also confirmed that any lattice model with $U(1)$ symmetry in 1-D cannot have superconductivity or magnetic long range as $t \to \infty$.

However this result is not in agreement with the Nagaoka's theorem.

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## RESULTS FOR THE SYSTEM OF 2 ELECTRONS ON 3-SITES

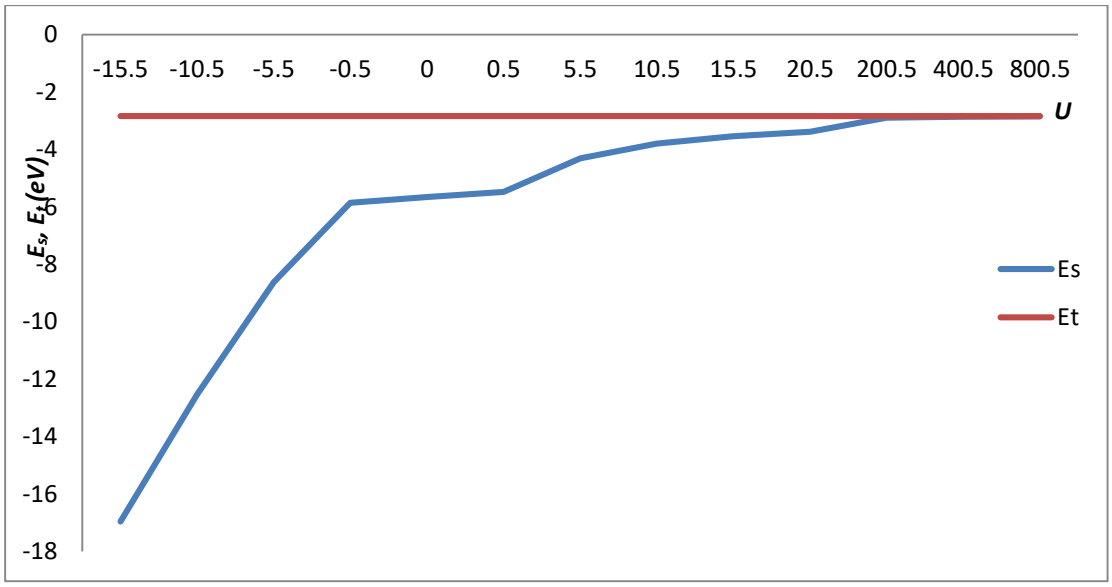


**Fig 4.2a:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *U* for system of 2 electrons on 3 sites.

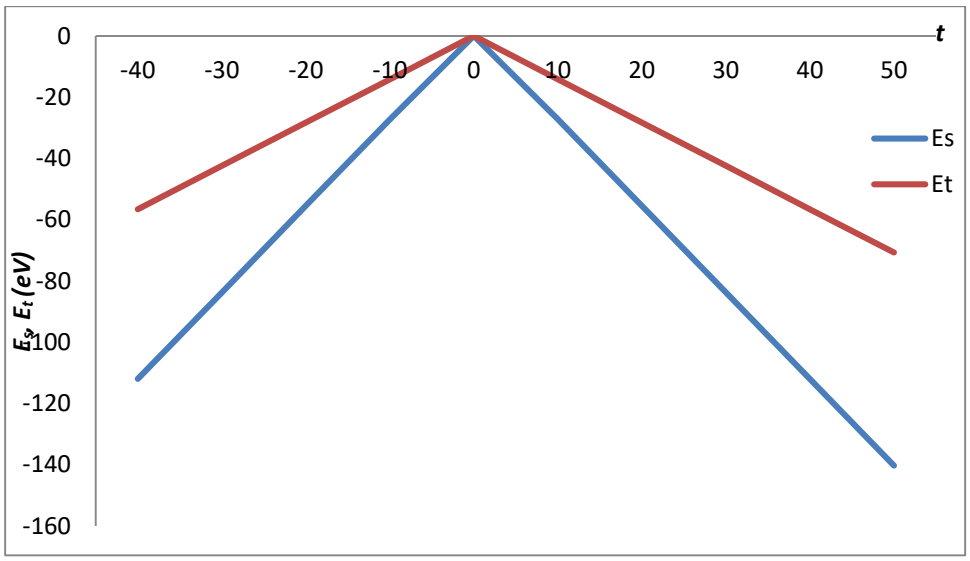


**Fig 4.2b:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *t* for system of 2 electrons on 3 sites.

**Discussion of the Results 2 Electrons on 3 Site System**

From computations, we observed, from figure 4.2a that as the values of the on-site coulomb repulsion interaction strength, *U*, increased from -15.5, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 800.50, which is the transition point $T_p$ ($E_s = E_t$), and beyond this point there was no clear transition, hence ferromagnetism is unstable.

Also it was observed from figure 4.2b that as the value of the hoping term, *t*, increased from -40, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 0 which is the transition point $T_p$ ($E_s = E_t$). Beyond this point the lattice began to gain a much stronger antiferromagnetism, hence ferromagnetism is unstable.

This result agreed with the results obtained by Hohenberg (1967), where he studied superconductivity / long range crystalline order were derived in one-dimension (1-D).

**RESULTS FOR THE SYSTEM OF 2 ELECTRONS ON 4-SITES**

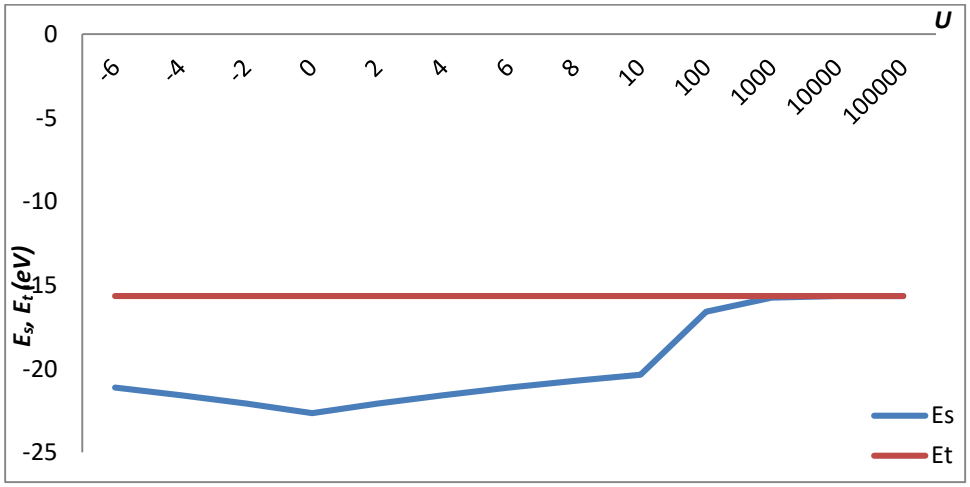


**Fig 4.4a:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *U* for system of 2 electrons on 4 sites.

*t*

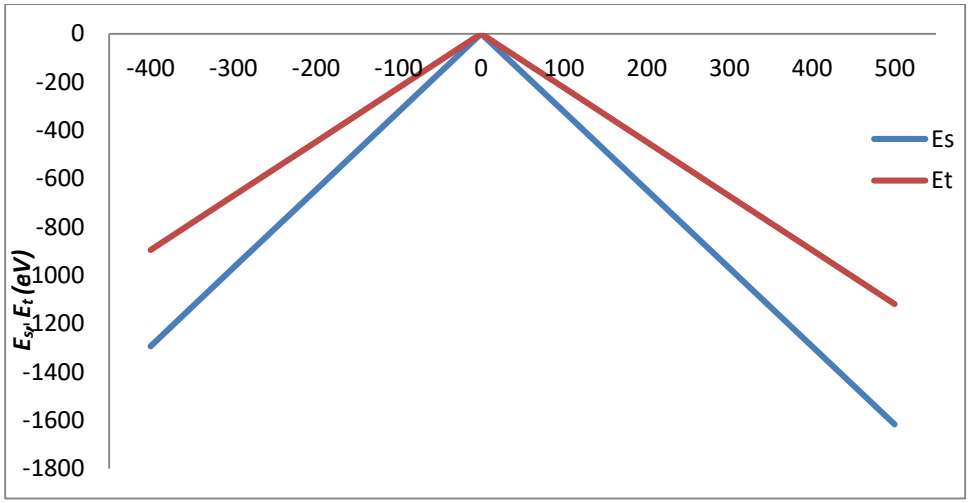


**Fig 4.3b:** Graph of Singlet ($E_s$) and Triplet ($E_t$) state energies against *t* for system of 2 electrons on 4 sites.

**Discussion of the Results 2 Electrons on 4 Site System**

The plot on figure 4.3a shows that as the value of the on-site coulomb repulsion interaction strength, *U,* increased from -6.0, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 100000, which is the transition point $T_p$ ($E_s$=$E_t$), and beyond this point there was no clear transition, hence the ferromagnetism is unstable.

The plot on figure 4.3b also shows that as the value of the hoping term, *t,* increased from -400, the electronic correlation that favours ferromagnetism get stronger and the lattice begins to loss antiferromagnetic properties until point 0 which is the transition point $T_p$ ($E_s$=$E_t$). Beyond this point the lattice began to gain a much stronger antiferromagnetism, hence the ferromagnetism is unstable.

## SUMMARY, CONCLUSION AND RECOMMENDATION

### Summary

For all the lattice systems studied in this work, the ground state was always a spin singlet i.e, $E_s$ > $E_t$. Consequently, the singlet state provides the lowest energy in all the lattice systems studied, hence the result obtained in all the lattice systems studied favours zero spin polarization (antiferromagnetic). The results shows that increasing the values of *t* above the transition point

when other parameters remain constant always resulted in stronger antiferromagnetism; alo increasing the values *U* before the transition point when other parameters are constant favors ferromagnetism as the lattice begins to loss its antiferromagnetic properties.

## Conclusion

In this research work the Exact-Diagonalization technique has been employed to provide information on the behavior of two interacting electrons on two sites, two interacting electrons on three sites and two interacting electrons on four sites all in one-dimensional lattice system (1-D) The features of the Hubbard model as far as considered here are peculiar to the One-Dimensional model. Although the Hubbard model was proposed in the middle of the last century, and solved for the 1-D case back in 1968, it still offers numerous possibilities for active research work. It is hoped that this work will contribute to the spread of interest in this model and its applicability.

## Recommendation

We recommend that the One-Dimensional lattice systems with higher number of electrons and sites be employed to study the Hubbard model. In addition, lattice systems with holes should be investigated alongside with additional parameters e.g. the extended Hubbard model.

## REFERENCES

Amadon J.C. and Hirsch J.E. (1996): *Metallic ferromagnetism in the Single Band Model: Effect of Band filling and Coulumb Interactions*. Physical Review, B 54**:** 6364-6375

Carter E. C. (2004): *Anisotropic Phenomena in Strongly Correlated Electron System.* PhD thesis submitted to the School of Physics and Astronomy, University of Birmingham, U. K.

Gutzwiller, M.C. (1963): *Effect of Correlation on the Ferromagnetism of Transition Metals*, Physical Review Letter, 10(5): 159

Hohenberg, P.C. (1967): *Existence of Long-Range Order in One and Two Dimensions*, Physical Review 158(2): 383.

Hubbard, J. (1963): *Electron correlations in narrow energy bands,* Proceedings of the Royal Society A, 276(1365), 238-257

Kanamori, J. (1963): *Electron Correlation and Ferromagnetism of Transition Metals,* Progress of Theoretical Physics, 30(3): 275-289

Koma, T. and Tasaki, H. (1992): *Decay of superconducting and magnetic correlations in one and two-dimensional Hubbard models,* Physical Review Letters, 68(21): 3248-3251.

Lieb, E. H. (1989): *Two Theorems on the Hubbard Model.* Physical Review B. **62,** 1201-1204

Mahan G. D. (2000): *Many Particle Physics*. Third Edition, Kluwer Academic/Plenum, New York, U.S.A.

Mielke, A. (1991): *Ferromagnetic ground states for the Hubbard model on line graphs*, Journal of Physics A, 24(2): L73-L77.

Moller B. and Wolfle P. (1993): *Magnetic Order in the Periodic Anderson Model.* Physical Review, B 48: 10320-10326

Muller-Hartmann, E. (1995): *Ferromagnetism in Hubbard models: Low density route*, Journal of Low Temperature Physics, 99(3-4): 349–354.

Nagaoka, Y. (1966): *Ferromagnetism in a narrow, almost half-filled s band*, Physical Review, 147(1): 392-405

Sherman, A. (2020): *Spin and charge fluctuations in the two-band Hubbard model.* The European Physical Journal B 93, 168-172.

*http://doi.org/10.1140/epjb/e2020-10221-4*

Tasaki, H. (1989): *Extension of Nagaoka's theorem on the large U Hubbard Model,* Physical Review B, 40(13): 9192-9193

Zhuo Y., Feng Z., Yong-Xin Y., Wang C. and Ho K. (2020): *Ground state wave functions for single-band Hubbard models from the Gutzwiller conjugate gradient minimisation theory.* Molecular Physics, DOI: 10.1080/00268976.2020.1797917