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NUMERICAL METHODS FOR STRONGLY CORRELATED ELECTRONS IN ONE DIMENSIONAL FINITE SIX SITES SYSTEM.

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ABSTRACT

In recent years, the Hubbard model has been subjected to a renewed attention because of its relevance for High-$T_c$superconductivity, quantum antiferromagnetism, and ferromagnetism thus playing a central role in theoretical investigations of strongly correlated systems. In this paper, we present a numerical exact diagonalization NED of the Hubbard model and a theoretical exact simulation (TES)with the view to obtaining the groundstate-energy spectrum of two electron interaction on a finite six sites lattice system. The extended Hubbard model with nearest and next-nearest neighbour kinetic hopping terms was first applied on the eigenstates available to the two electrons six sites system. The application of the Hubbard model on the various electron eigenstates generated 36×36 *eigenvalue matrix which was solved by numerical exact diagonalization. The results of the ground-state energies from the numerical exact diagonalization were compared with the results obtained from the theoretical exact simulation. The comparison of both methods showed that there is a good correlation between the two results. It is established here that there is a strong correlation between the two electrons at very low negative values of the Coulomb interaction strength* $U/4t$*.Whereas high values of positive Coulomb interaction strength promotes high kinetic energy between two interacting electrons, since the electrons are now free to hop from one atomic site to another.*

1.0 Introduction

One of the outstanding problems in solid state physics is a detailed understanding of electron correlations and tt requires going beyond the independent electron approximation. Certainly, a considerable progress has been made in the past towards this goal [1]. However, only in exceptional cases can one claim to understand quantitatively correlation effects. There are many examples of physical phenomena that originate from the correlated motion of electrons. The simplest example is of Van der Waals forces between neutral atoms. When two atoms are brought close together, the electronic charge cloud of one atom interacts with the charge cloud of the other so that the electrons avoid each other [2,3].

Another outstanding example of correlation effect is the phenomenon of superconductivity where particularly long-range electron correlations lead to the Cooper-pair instability. The theory of superconductivity which is based on this pair correlation is able to make quantitative statements about a large number of measurable quantities in the superconducting state of the system without having to treat the remaining electron correlations [4,5].

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Despite remarkable efforts the understanding of the physics of correlated electron systems is still far from complete. Even in one spatial dimension where the Hubbard Hamiltonian provides the opportunity to study correlation effects in an integrable model [6,7], apparently simple quantities like the asymptotic of correlation functions have been calculated only in certain limits. A better description of the electronic properties of metals is given by the extended Hubbard model. Where the standard Hubbard model only takes nearest neighbour hopping t and local interaction U into account, the extended Hubbard model introduces the next-nearest neighbour hopping t' and nearest neighbour interactions V between electrons on two different sites [8,9].

These are the so called non-local interactions. The non-local interaction strength between site i and j is denoted by V_{ij}. These types of model were used to describe for example charge ordering, a special ordering of the electrons that arises from the interactions between lattice sites and that cannot be described by the usual single-band Hubbard model [10,11]. Plasmons are other phenomena that can only be described using non-local interactions.

With the inclusion of long-range (non-local) part of the potential V the off-site terms and additional kinetic hopping term t' to the single-band Hubbard model, we obtain the extended Hubbard model. To what extent the inclusion of the off-site terms relevant to the description and understanding of strongly correlated systems is still a matter of current debate in the literature, and the general issue is a difficult one [12].

The Hubbard model has been very successful in describing a variety of effects. One of these effects is the metal-insulator phase transition. For high positive ratio of Coulomb interaction to the nearest neighbour hopping integral U/t, some metal are insulators, whereas for very low negative U/t some of the metals can conduct electricity, the transition from one phase to the other occur at some critical ratio of $\frac{U}{t}$ [13].

We need numerical methods to address the following: to (i) validate predictions from a theory (ii) understand the physics when theory fails and to serve as a guide toward a new theory (iii) find new phases or study phases that are analytically intractable (iv) compare competing orders (v) make quantitative predictions for experiments.

Exact diagonalization is usually a very simple method for solving finite-size matrix, it does not necessarily require any computer. But what happens when we now increase the number of lattice sites? The problem becomes complicated as the dimension of the Hilbert space, and consequently the size of the matrix, increase with the number of sites$N$. In this case even for writing the matrix elements of a $N^2 \times N^2$ square matrix, the computational time and memory required is prohibitive [14]. Exact solutions are possible by direct diagonalization of the many-body problem on small systems, the so-called small cluster technique. This method suffers from uncontrolled finite-size effects and cannot be extrapolated to the thermodynamic limit in any obvious way [15,16].

The preliminary purpose of this study is to present a theoretical exact simulation of a two electrons six-site lattice system. This is a semi-quantitative method for solving electron correlation and the relationship with the groundstate energy as we move from finite-size lattice to a more complex higher lattice sites. This study will therefore provide a means of solving the groundstate energies with ease without first writing down the much complicated matrix.

1.1. Research Methodology. We first applied the extended Hubbard model to act on the various electron states available to the two electrons six sites lattice. The application of the Hubbard model on the eigenstates of the two interacting electrons generated a16×16 eigen value matrix which was solved by numerical exact diagonalization. After this we developed the theoretical exact simulation approach which was patterned after the result of two electrons two-site system.

This paper is outlined as follows. Section one gave a brief introduction of the work under study. The mathematical theory work is given in section two. The results emerging from this study is presented in section three. The outcome of the results is discussed in section four and the work is finally brought to an end by concluding remarks in section five and this is immediately followed by the list of references.

2.0 Mathematical Theory

The Hamiltonian corresponding to the extended Hubbard model is given by:

$$H = -t\sum_{\langle i\,j\rangle\sigma}\left(C_{i\sigma}^{+}C_{j\sigma}+h.c.\right) - t'\sum_{\langle\langle i\,j\rangle\rangle\sigma}\left(C_{i\sigma}^{+}C_{j\sigma}+h.c.\right) +$$

$$U\sum_{i} n_{i\uparrow}\,n_{i\downarrow} + V_{ij}\sum_{\sigma\sigma'}\sum_{\langle i\,j\rangle} n_{i}\,n_{j} \tag{2.1}$$

where t is the amplitude of a nearest- neighbour NN hopping energy term,t' is the amplitude of a next - nearest- neighbour (NNN) hopping energy term while U is the usual Hubbard on-site interaction. The $C_{i\sigma}^{+}$ or $C_{j\sigma}$ is the creation or annihilation operator of electron with spin σ and the summation $\langle i\,j\rangle$ runs over nearest-neighbour NN pairs and $\langle\langle i\,j\rangle\rangle$ runs over next-nearest-neighbour NNN pairs. The $h.c = C_{j\sigma}^{+}C_{i\sigma}$ is the hermitian conjugate and the inclusion makes the dynamical quantities real, the term U in the Hamiltonian accounts for the dominant part of the Coulomb repulsion, $n_{i\uparrow}\,n_{i\downarrow}$ is the on-site occupation number operator and $n_{i}\;n_{j}$ is the nearest neighbour occupation number operator, finally, V_{ij} is nearest neighbour (NN) density-density interaction.

$$V_{ij} = \begin{cases} V \;if\;\; i\;and\;\; j\;nearest\;neighbour \\ 0\;\; otherwise \end{cases} \tag{2.2}$$

Let us also define the amount of particles on site i as $n_{i} = n_{i\uparrow} + n_{i\downarrow}$ and $n_{j} = n_{j\uparrow} + n_{j\downarrow}$ so that we show the following:

$$n_{i}\,n_{j} = (n_{i\uparrow} + n_{i\downarrow})\;(n_{j\uparrow} + n_{j\downarrow}) = n_{i\uparrow}\,n_{j\uparrow} + n_{i\uparrow}\,n_{j\downarrow} + n_{i\downarrow}n_{j\uparrow} + n_{i\downarrow}\;n_{j\downarrow} \tag{2.3}$$

$$n_{i}\,n_{j} = \sum_{\sigma,\sigma'} n_{i\sigma}\,n_{j\sigma'} \tag{2.4}$$

We also know that $n_{i\uparrow}\,n_{i\uparrow} = n_{i\downarrow}n_{i\downarrow} = n_{j\uparrow}n_{j\uparrow} = n_{j\downarrow}n_{j\downarrow} = 0$ and since we cannot have two electrons with the same spin on one site, also the Hubbard model does not account for parallel spin of electrons.

$$H = -t\sum_{\langle i\,j\rangle\sigma}\left(C_{i\sigma}^{+}C_{j\sigma}+C_{j\sigma}^{+}C_{i\sigma}\right) - t'\sum_{\langle\langle i\,j\rangle\rangle\sigma}\left(C_{i\sigma}^{+}C_{j\sigma}+C_{j\sigma}^{+}C_{i\sigma}\right) +$$

$$U\sum_{i} n_{i\uparrow}\,n_{i\downarrow} + V_{ij}\sum_{\langle i\,j\rangle} n_{i\sigma}\,n_{j\sigma'} \tag{2.5}$$

2.1. The Groundstate Energies of the two interacting Electrons by Numerical exact Diagonalization. Numerical exact diagonalization (NED) which yields exact solutions is the most powerful technique, since no approximations are made, but they rarely occur in thermodynamic limits. The most common problems that are exactly solvable are the finite-size one-dimensional or quasi-one-dimensional system

Table 2.0.The Hilbert space derived from the geometry of the two electrons six sites system.

Lattice separation l between the two electrons		Pair wave function	Number of different electronic states at lattice separation l	Representative pair electronic states
i	Actual separation distance	$\lvert\Psi_{i}\rangle$	$\langle\Psi_{i}\rvert\Psi_{i}\rangle$	$\lvert i\uparrow, i\downarrow\rangle$ and $\lvert i\uparrow, j\downarrow\rangle$
1	0	$\lvert\Psi_{0}\rangle$	6	$\lvert 1\uparrow, 1\downarrow\rangle\cdots\lvert 6\uparrow, 6\downarrow\rangle$

2	a	$\lvert\Psi_1\rangle$	12	$\lvert 1\uparrow,2\downarrow\rangle\cdots\lvert 6\downarrow,1\uparrow\rangle$
3	$2a$	$\lvert\Psi_2\rangle$	12	$\lvert 1\uparrow,3\downarrow\rangle\cdots\lvert 6\downarrow,2\uparrow\rangle$
4	$3a$	$\lvert\Psi_3\rangle$	6	$\lvert 1\uparrow,4\downarrow\rangle\cdots\lvert 3\downarrow,6\uparrow\rangle$
			There are a total of 36 electron eigenstates	

where $\lvert i\uparrow,i\downarrow\rangle$ represents the eigenstates of the two electrons on the same site, while $\lvert i\uparrow, j\downarrow\rangle$ and $\lvert i\downarrow, j\uparrow\rangle$ are the eigenstates of the two electrons when they are on different lattice sites. When the Hubbard model given by (2.1) is used to act on the various electron states provided in Table 2.0, i.e., $H\lvert\Psi_\lambda\rangle\ \lambda = 1,2,3,\ \cdots,36$ we shall get an eigen value problem of the form: $\lvert Q-\lambda I\rvert\vec{X}=0$, where Q is a 36×36 matrix, the eigenvalue or the energy is represented by λ, the I is the identity matrix which must be of the same size as Q and $\vec{X}$ is the corresponding eigenvectors. For a non-trivial solution we know that $\lvert A-\lambda I\rvert = 0$ since $\vec{X}\neq 0$. Thus we get

$$Q = 36\times 36 = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = 0 \tag{2.6}$$

The above equation holds provided: $\langle i\rvert j\rangle = \delta_{ij}\begin{cases} 1 \ if \ \ i = j \\ 0 \ if \ \ i \neq j \end{cases}$. (2.7)

Because of limited space we separated the 36×36 matrix into four parts A, B, C and D. Each of the part matrix has the same dimension 18×18. The respective dimensional matrix is displayed below.

$$A=\begin{pmatrix}
4u & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\
0 & 4u & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 4u & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 4u & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 4u & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 4u & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 \\
-1 & -1 & 0 & 0 & 0 & 0 & 4v & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 4v & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 \\
0 & -1 & -1 & 0 & 0 & 0 & 0 & 4s & 4v & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 1 & 0 & 0 & 0 & 4s & 0 & 0 & 4v & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 4s & 4v & 0 & 0 & 4s & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 4v & 4s & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 4v & 0 & 0 & 4s & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 4v & 4s & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 4v & 0 & 0 & 4s \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 4v & 4s & 0 \\
-1 & 0 & 0 & 0 & 0 & -1 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 4v & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 4v
\end{pmatrix}. \tag{2.8}$$

$$B=\begin{pmatrix}
-4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 \\
-4s & 4s & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -4s & 4s & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -4s & 4s & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -4s & 4s & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -4s & 0 & 0 & 4s & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -4s & 4s & 0 & 0 & 0 \\
-1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 0 & 0 & 4s \\
0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 4s & 0 \\
0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 0 & 0 & 0 & -4s & 0 \\
0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 0 & 0 & 0 & -4s \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & -4s & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & -4s & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & -4s & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & -4s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 4s & 0 & 0 & 0 & 4s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4s & 0 & 0 & 0 & 4s & 0
\end{pmatrix}. \quad (2.9)$$

$$C=\begin{pmatrix}
-4s & 0 & -4s & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4s & 0 & 4s & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -4s & 0 & -4s & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 4s & 0 & 4s & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -4s & 0 & -4s & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 4s & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -4s & 0 & -4s & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 4s & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\
-4s & 0 & 0 & 0 & -4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\
4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\
0 & -4s & 0 & 0 & 0 & -4s & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 4s & 0 & 0 & 0 & 4s & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & -4s & 0 & 0 & 0 & -4s & 0 & 0 & 4s & 0 & 0 & 0 & 4s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -4s & 0 & 0 & 0 & -4s & 4s & 0 & 0 & 0 & 4s & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & -4s & 0 & 0 & 0 & -4s & 0 & 0 & 4s & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & -4s & 0 & 0 & 0 & -4s & 4s & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & -4s & 0 & 0 & 0 & -4s & 0 & 0 & 4s \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & -4s & 0 & 0 & 0 & -4s & 4s & 0
\end{pmatrix}. \quad (2.10)$$

$$D=\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 4s & -1 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\
0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\
4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\
0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 1 & 0 & 0 & -1 & 0 \\
0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4s & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\
0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
0 & 0 & 4s & 0 & 0 & 0 & 4s & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
-1 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}. \quad (2.11)$$

where $u=U/4t$, $v=V/4t$ and $s=t'/4t$. For the purpose of clarity we need to define the terms: $u=U/4t$ (Coulomb interaction strength), $v=V/4t$ (NN density- density interaction strength) and $s=t'/4t$ (NNN hopping interaction strength). In this study, we used several arbitrary values of u to determine the total energy of the two interacting electrons with fixed attractive values of $v=-0.1$ and $s=-0.01$.Although, the choice of these values is not unique but depends on the individual researcher. The numerical exact diagonalization of the above 36×36 matrix given by (2.6) will give the total energies and the corresponding eigenvectors for each arbitrary$u$.

2.2. The groundstate energies of the two interacting electrons by theoretical exact simulation. (TES)

In this section, theoretically we shall derive analytic equations that would give the total energy of two interacting electrons in one dimensional four-site system without using or passing through the lengthy numerical approach as seen in the previous section. This theoretical simulation is based on the choice of arbitrary values that we subscribed for the relevant variables in this study.

The theoretical exact simulation we have done in this study is actually derived from the known exact calculation of two electrons interaction on one dimensional two sites lattice system. We used α to denote the complementary value of the total energies for some interval δ of positive values of u, while for the negative values of u, depending on the given intervalδ we used β to complement the equation that would yield the total energies.

The positive values of the Coulomb interaction strength $U/4t$ ranges from: 0, 5, 10, 15, …, 45, 50, that is, the interval is 5. However, the negative values of the Coulomb interaction strength $U/4t$ is made up of twoparts of interval. The first part ranges from: -0.05, -0.5, -0.15, …, -0.7, that is, the interval is -0.05. While the second part ranges from: -1, -1.5, -2, … , -4, that means, it has an interval of -0.5. Thus there are specific values thatα and β will take in each of these intervals.

This iteration was done for several types of the extended Hubbard model: (i) $-t-t'+U$ (where $V=0$), (ii) $-t+U$ (where $t'=V=0$), (iii) $-t-t'+U+V$ and (iv) $-t+U+V$ (where $t'=0$). We should note that the values of α and β will also depend on the respective arbitrary values of the on-site Coulomb

interaction strength $U/4t$, hext-nearest neighbour interaction strength $t'/4t$ and the off-site nearest neighbour density-density interaction strength $V/4t$.

Exact diagonalization is usually a very simple method for solving finite-size matrix and the process yields the energy and the eigenvectors. The method of exact diagonalization does not necessarily require much of computational time and intensive memory for the exact solutions. However, what happens to the computational process when we now increase the number of lattice sites? The problem becomes complicated and prohibitive as the dimension of the Hilbert space describing the size of the matrix, increase with the number of sites$N$. Exact solutions are possible by direct diagonalization of the many-body problem on small finite-size systems. This method suffers from uncontrolled finite-size effects.

Therefore the purpose of this study is to present a theoretical exact simulation of a two electrons interaction in 1D six sites lattice system. This is a semi-quantitative method for solving electron correlation and the relationship with the groundstate energy as we move from finite-size lattice to a more complex higher lattice sites. This study will therefore provide a means of solving the groundstate energies of finite-size dimensional lattice with ease without writing down the much complicated matrix. However, in this study because of space we could not display the eigenvectors corresponding to the calculated eigen values.

We need numerical methods to address the following: to (i) validate predictions from a theory (ii) to understand the physics when theory fails and to serve as a guide toward a new theory (iii) find new phases or study phases that are analytically intractableThe table below shows the theoretical exact simulation of two electrons on one dimensional 1D six sites system.

Table 2.1: Theoretical exact simulation of the total energy $E$for two electrons on a six sites system. (model I: $-t - t' + U$).

Number of lattice site	Interval $\delta = U_1 - U_2$	Positive values of the Coulomb interaction strength $U/4t$ The extended Hubbard model: $-t - t' + U$
$6-$sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{t'}{4t} + \alpha\right\}$ $\alpha = 1.6616$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$ $E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{t'}{4t} + \beta\right\}$ $\beta = 0.9058$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta = 0.5653$ for interval of -0.5 ranging from [-1, -4]

Table 2.2: Theoretical exact simulation of the total energy E for two electrons on a six sites system. (model II: $-t+U$).

Number of lattice site	Interval $\delta = U_1 - U_2$	Positive values of the Coulomb interaction strength $U/4t$ The Hubbard model: $-t+U$
6 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t} + \alpha\right\}$ $\alpha = 1.7252$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$
		$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t} + \beta\right\}$ $\beta = 0.9494$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta = 0.4565$ for interval of -0.5 ranging from [-1, -4]

Table 2.3: Theoretical exact simulation of the total energy E for two electrons on a six sites system. (model III: $-t-t'+U+V$).

Number of lattice site	Interval $\delta = U_1 - U_2$	Positive values of the Coulomb interaction strength $U/4t$ The extended Hubbard model: $-t-t'+U+V$
6 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{V}{4t} - \frac{t'}{4t} + \alpha\right\}$ $\alpha = 1.5962$ for interval of 5 ranging from [5, 50]
	[0, -0.70]	Negative values of the Coulomb interaction strength $U/4t$

	$\delta = -0.05$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2}-\frac{U}{4t}-\frac{V}{4t}-\frac{t'}{4t}+\beta\right\}$ $\beta = 0.8761$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta = 0.4000$ for interval of -0.5 ranging from [-1, -4]

Table 2.4: Theoretical exact simulation of the total energy E for two electrons on a six sites system. (model IV:$-t + U + V$).

Number of lattice site	Interval $\delta = U_1 - U_2$	Positive values of the Coulomb interaction strength $U/4t$ The extended Hubbard model: $-t + U + V$
6 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2}-\frac{U}{4t}-\frac{V}{4t}+\alpha\right\}$ $\alpha = 1.662$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$
		$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2}-\frac{U}{4t}-\frac{V}{4t}+\beta\right\}$ $\beta = 0.9651$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta = 0.4759$ for interval of -0.5 ranging from [-1, -4]

3.0 Presentation of results.

Table 3.0. Summary of the results of the total energies E as a function of $U/4t$. The numerical exact diagonalization (NED) of two electrons six sites system of the matrix given by (2.6) for the various models applied in this study.

Variation in the interaction strength			Total Energy E Numerical Exact Diagonalization(NED)			
$U/4t$	$V/4t$	$t'/4t$	Model I $-t-t'+U$	Model II $-t+U$	Model III $-t-t'+U+V$	Model IV $-t+U+V$
50.00	-0.1	-0.01	-3.3637	-3.4707	-3.4329	-3.5448
45.00	-0.1	-0.01	-3.3643	-3.4714	-3.4336	-3.5457
40.00	-0.1	-0.01	-3.3650	-3.4723	-3.4345	-3.5468
35.00	-0.1	-0.01	-3.3659	-3.4735	-3.4356	-3.5482
30.00	-0.1	-0.01	-3.3672	-3.4751	-3.4371	-3.5500
25.00	-0.1	-0.01	-3.3689	-3.4772	-3.4393	-3.5526
20.00	-0.1	-0.01	-3.3715	-3.4804	-3.4424	-3.5564
15.00	-0.1	-0.01	-3.3757	-3.4857	-3.4476	-3.5627
10.00	-0.1	-0.01	-3.3841	-3.4960	-3.4578	-3.5750
5.00	-0.1	-0.01	-3.4078	-3.5252	-3.4867	-3.6096
0.00	-0.1	-0.01	-3.8400	-4.0000	-3.9823	-4.1416
-0.01	-0.1	-0.01	-3.8467	-4.0067	-3.9894	-4.1487
-0.05	-0.1	-0.01	-3.8752	-4.0350	-4.0195	-4.1782
-0.10	-0.1	-0.01	-3.9144	-4.0736	-4.0605	-4.2182
-0.15	-0.1	-0.01	-3.9580	-4.1162	-4.1057	-4.2619
-0.20	-0.1	-0.01	-4.0066	-4.1632	-4.1555	-4.3097
-0.25	-0.1	-0.01	-4.0606	-4.2149	-4.2101	-4.3619
-0.30	-0.1	-0.01	-4.1203	-4.2718	-4.2700	-4.4189
-0.35	-0.1	-0.01	-4.1862	-4.3341	-4.3354	-4.4808
-0.40	-0.1	-0.01	-4.2585	-4.4022	-4.4066	-4.5480
-0.45	-0.1	-0.01	-4.3375	-4.4764	-4.4837	-4.6206

-0.50	-0.1	-0.01	-4.4232	-4.5568	-4.5669	-4.6990
-0.55	-0.1	-0.01	-4.5156	-4.6435	-4.6563	-4.7831
-0.60	-0.1	-0.01	-4.6146	-4.7365	-4.7516	-4.8729
-0.65	-0.1	-0.01	-4.7200	-4.8357	-4.8530	-4.9686
-0.70	-0.1	-0.01	-4.8315	-4.9409	-4.9600	-5.0699
-1.00	-0.1	-0.01	-5.6091	-5.6845	-5.7087	-5.7864
-1.50	-0.1	-0.01	-7.1776	-7.2187	-7.2397	-7.2829
-2.00	-0.1	-0.01	-8.9219	-8.9467	-8.9623	-8.9883
-2.50	-0.1	-0.01	-10.7550	-10.7713	-10.7828	-10.7998
-3.00	-0.1	-0.01	-12.6381	-12.6495	-12.6582	-12.6701
-3.50	-0.1	-0.01	-14.5520	-14.5604	-14.5672	-14.5759
-4.00	-0.1	-0.01	-16.4861	-16.4925	-16.4980	-16.5046

Table 3.1: Comparison of the results of the total energies Eobtained from numerical exact diagonalization (NED) and theoretical exact simulation (TES) for the various models.

Coulomb strength	Total Energy E 2 – electrons on a 1D 6 – lattice system							
$U/4t$	Model I $-t-t'+U$		Model II $-t+U$		Model III $-t-t'+U+V$		Model IV $-t+U+V$	
	NED	**TES**	**NED**	**TES**	**NED**	**TES**	**NED**	**TES**
50.00	-3.3637	-3.3632	-3.4707	-3.4704	-3.4329	-3.4326	-3.5448	-3.5442
45.00	-3.3643	-3.3654	-3.4714	-3.4726	-3.4336	-3.4348	-3.5457	-3.5464
40.00	-3.3650	-3.3682	-3.4723	-3.4754	-3.4345	-3.4376	-3.5468	-3.5492
35.00	-3.3659	-3.3717	-3.4735	-3.4789	-3.4356	-3.4412	-3.5482	-3.5528
30.00	-3.3672	-3.3765	-3.4751	-3.4837	-3.4371	-3.4460	-3.5500	-3.5576
25.00	-3.3689	-3.3831	-3.4772	-3.4903	-3.4393	-3.4527	-3.5526	-3.5643
20.00	-3.3715	-3.3931	-3.4804	-3.5003	-3.4424	-3.4628	-3.5564	-3.5744
15.00	-3.3757	-3.4098	-3.4857	-3.5169	-3.4476	-3.4796	-3.5627	-3.5912
10.00	-3.3841	-3.4429	-3.4960	-3.5501	-3.4578	-3.5131	-3.5750	-3.6247
5.00	-3.4078	-3.5412	-3.5252	-3.6484	-3.4867	-3.6124	-3.6096	-3.7240

0.00	-3.8400	-3.8317	-4.0000	-3.8994	-3.9823	-3.9820	-4.1416	-4.1401
-0.05	-3.8752	-3.9342	-4.0350	-4.0019	-4.0195	-4.0845	-4.1782	-4.2426
-0.10	-3.9144	-4.0416	-4.0736	-4.1093	-4.0605	-4.1920	-4.2182	-4.3501
-0.15	-3.9580	-4.1540	-4.1162	-4.2217	-4.1057	-4.3043	-4.2619	-4.4624
-0.20	-4.0066	-4.2713	-4.1632	-4.3390	-4.1555	-4.4214	-4.3097	-4.5795
-0.25	-4.0606	-4.3932	-4.2149	-4.4609	-4.2101	-4.5433	-4.3619	-4.7014
-0.30	-4.1203	-4.5197	-4.2718	-4.5874	-4.2700	-4.6697	-4.4189	-4.8278
-0.35	-4.1862	-4.6506	-4.3341	-4.7183	-4.3354	-4.8004	-4.4808	-4.9585
-0.40	-4.2585	-4.7857	-4.4022	-4.8534	-4.4066	-4.9354	-4.5480	-5.0935
-0.45	-4.3375	-4.9248	-4.4764	-4.9925	-4.4837	-5.0743	-4.6206	-5.2324
-0.50	-4.4232	-5.0677	-4.5568	-5.1354	-4.5669	-5.2170	-4.6990	-5.3751
-0.55	-4.5156	-5.2142	-4.6435	-5.2819	-4.6563	-5.3633	-4.7831	-5.5214
-0.60	-4.6146	-5.3640	-4.7365	-5.4317	-4.7516	-5.5130	-4.8729	-5.6711
-0.65	-4.7200	-5.5170	-4.8357	-5.5847	-4.8530	-5.6658	-4.9686	-5.8239
-0.70	-4.8315	-5.6729	-4.9409	-5.7407	-4.9600	-5.8215	-5.0699	-5.9796
-1.00	-5.6091	-5.9791	-5.6845	-5.7414	-5.7087	-5.8555	-5.7864	-5.9872
-1.50	-7.1776	-7.7562	-7.2187	-7.5185	-7.2397	-7.6311	-7.2829	-7.7628
-2.00	-8.9219	-9.6227	-8.9467	-9.3851	-8.9623	-9.4966	-8.9883	-9.6284
-2.50	-10.7550	-11.535	-10.7713	-11.2982	-10.7828	-11.4089	-10.7998	-11.5407
-3.00	-12.6381	-13.475	-12.6495	-13.2376	-12.6582	-13.3477	-12.6701	-13.4795
-3.50	-14.5520	-15.430	-14.5604	-15.1931	-14.5672	-15.3029	-14.5759	-15.4347
-4.00	-16.4861	-17.3968	-16.4925	-17.1592	-16.4980	-17.2687	-16.5046	-17.4004

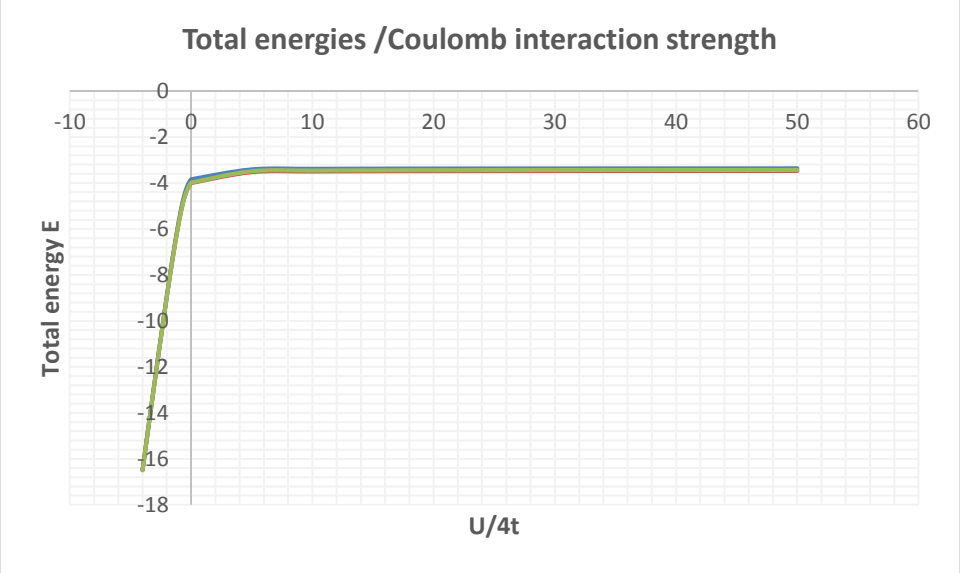

Figure 3.1: Shows the spectrum of the total energies$E$ as a function of the Coulomb interaction strength $U/4t$ for the four types of Hubbard model. This is just the graphical representation of the four model results shown in Table 3.0.

4.0 Discussion of Results

Table 3.0 shows energy expectation values as a function of $U/4t$. From the table it is observed that the ground state energies are negative and non-degenerate, this is because the electron energy levels were defined relative to the Fermi energy level. The negative groundstate energies mean attraction (correlation) between the two interacting electrons. We can see that as U/t increases, the potential energy decreases. For high positiveU/t it is unfavourable for the electrons to be together on one site, that means, as we increase $U/4t$positively the fraction of doubly occupied sites will decrease. In other words, the term $n_{i\uparrow}n_{i\downarrow}$ goes to zero as we positively increase $U/4t$ and this causes the potential energy to decrease.

It is also shown in the table that the total energies consistently decreases negatively as the Coulomb interaction strength $U/4t$is made to decrease and the values of the energies are non- degenerate. For high positive U/4t electrons can have enough hopping kinetic energy not to doubly occupy a site. While there is a tendency for on-site occupancy by the two electrons when the Coulomb interaction strength $U/4t$ is made negatively high, the $-t+U+V$ has the least values of non-degenerate energies while the $-t-t'+U$ model has the highest values of non-degenerate energies.

Table 3.1 provides the comparison of the results obtained from the numerical exact diagonalization and the theoretical exact simulation. The results compared favourably with one another particularly in the positive regime of the Coulomb interaction strength$U/4t$. The negative decrease in the total energies of the two interacting electrons as $U/4t$ is decreased is consistent with the various models we applied in this study.

Figure 3.1 shows energy expectation values as a function of $U/4t$. The graph shows a very good correlation between the four types of Hubbard model we applied in this study. The energy spectrum of these models is almost a continuous one. It is also observed in the graph that the groundstate energies have negative values and with steepest gradient in the region of high negative values of the on-site Coulomb interaction $U/4t$. The gradient goes to zero in the region of high positive values of the on-site Coulomb interaction $U/4t$.

5.0 Conclusion

This study provides a theoretical exact method for calculating the groundstate energies of two interacting electrons on a one dimensional six sites system. This method in theory and practice can be generally extended to solve the groundstate of two electrons interaction on $n-$dimensional lattice sites without

going through the rigours of numerical computations. This approach will also eventually minimize computational errors. It is revealed in this study that the groundstate energies generally have negative values and with steepest gradient in the region of high negative values of the on-site Coulomb interaction $U/4t$. The gradient goes to zero in the region of high positive values of the on-site Coulomb interaction $U/4t$. It is shown that not only are the energies negative but they are also non-degenerate. This arises from the fact that the electron energy levels are defined relative to the Fermi energy.

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