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THEORETICAL EXACT CALCULATION OF THE GROUNDSTATE ENERGIES OF TWO ELECTRON INTERACTION IN 1D FOUR SITES SYSTEM

[1]Akpata Erhieyovwe and [2]Enaibe A. Edison

[1]Department of Physics, Delta State University, Abraka.
[2]Department of Physics, Federal University of Petroleum Resources, Effurun.

Abstract

There has been dramatic progress in the development of electron correlation techniques for the accurate treatment of atomic structures and energies of molecules. In this study, we consider a theoretical exact method for obtaining the ground-state energies of two interacting electrons on a one-dimensional four sites lattice system. We first applied the extended Hubbard model with nearest and next-nearest neighbour to act on the various electron sites available to the two electrons four sites lattice. The application of the Hubbard model on the electron states produced an 16×16 ***eigen value matrix which was solved by analytical exact diagonalization. The results of the ground-state energies from the theoretical exact method are compared with the ones obtained from the analytical exact diagonalization. The results compared favourably with one another. It is established here that there is a strong correlation between the two electrons at high negative values of the Coulomb interaction strength*** $U/4t$***. It is also shown in this study that the*** $-t+U+V$ ***extended Hubbard model is a better model to study correlation process and the ground-state energies it produced is minimum compared to the other forms of the Hubbard model.***

***Keywords*:** Electron correlation, Hubbard model, Coulomb interaction strength, density-density interaction, ground-state energies and total energies.

1.0 Introduction

In recent years, the Hubbard model has been subject 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 its simplest form the Hubbard model consists of a single-band tight-binding Hamiltonian, t, plus a periodic, on-site interaction term, U, which accounts for the dominant part of the Coulomb repulsion experienced by the electrons [1].

With the inclusion of long-range (non-local) part of the potential V the off-site terms and additional kinetic hopping term t', we obtain an 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 [2].

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 exponentially with the number of sites N. In this case even for writing the matrix elements of a $2^N \times 2^N$ square matrix, the computational time and memory required is prohibitive [3].

At present, there is no method that allows the general solution of a generic many-body Hamiltonian with a computational efforts scaling polynomial with the system size N. The complexity of the many-body problem is exponential, and this is the main reason why strong correlation is a difficult task.

The purpose of this preliminary paper is to present a theoretical exact diagonalization of a two electrons four-site lattice system. This is a semi-quantitative method for solving electron correlation and its bearing on the ground state energy as we move from finite-size lattice to a more complex higher lattice sites. This preliminary report will therefore provide a means of solving the ground state energies with ease without writing down the much complicated matrix.

Corresponding Author**:** Akpata E., Email: akpataleg@hotmal.com, Tel: +2348024515959

The many-body problem constitutes the quantum mechanical of a system with a large number of mutually interacting particles. The essence of the many-body problem involving the correlated motions of particle, that is, the response of the other particles in the system to the motion of a given particle. [4]. 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 [5]. 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.

The correlated motion of the electrons produces fluctuating dipole moments on each atom that attract each other with a potential that depends on the distance between them. Another example is an exciton in a semiconductor [6]. An exciton is formed by the correlated motion of an electron in the conduction band and a hole in the valence band that allow the particles to bind together into a complex.

The study of strongly correlated systems is becoming a subject of increasing interest due to the realistic possibility that in many physical materials, such as High-T_c superconductors, strong correlations between electrons may lead to an unexpected physical behaviour, that cannot be explained within the conventional schemes, such as, for instance, mean-field or Fermi liquid theory [7].

Since electrons are negatively charged particles there is a repulsive Coulomb interaction between them. The strength of these interactions between two electrons on one site is denoted by the local interaction strength. The study on the Hubbard model has been one of the most attractive fields in solid-state physics and the effect of electron correlations in the model has been investigated by using various methods [8] and [9].

Since electrons are fermions we cannot have more than one electron per site, which means the term only gives a contribution if there are two electrons on one site. This is exactly what we would expect for the interaction. Electrons in the Hubbard model can hop from their original site to another site. This event is called hopping and causes the electrons to be more delocalised over the lattice [10].

The various terms in the Hubbard Hamiltonian influence the localisation of the electrons differently. In order to see what the effects of the different terms are, it is insightful to consider a system with only four lattice sites. For simplicity we will ignore the correlations caused by the fermionic properties of the electrons (the exchange hole interactions) [11].

This paper is outlined as follows. In section one, we gave a brief introduction of the work under study. The mathematical formulation of the theoretical work is given in section two. The results emerging from this study is shown in section three. We discussed the outcome of the results in section four and the work was brought to an end by concluding remark in section five and this is immediately followed by the lists of references.

2.0. Presentation of Results.

Table 2.0: Results of analytical exact diagonalization of matrix (4.6) using arbitrary values of the Coulomb interaction strength $U/4t$ between the two-interacting electrons four sites system.

Variation in the interaction strength			Total Energy E Analytical exact diagonalization values AEDV			
$U/4t$	$V/4t$	$t'/4t$	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	-2.7666	-2.8482	-2.9694	-3.0566
45.00	-0.1	-0.01	-2.7685	-2.8504	-2.9714	-3.0590
40.00	-0.1	-0.01	-2.7708	-2.8531	-2.9740	-3.0619
35.00	-0.1	-0.01	-2.7738	-2.8566	-2.9772	-3.0656
30.00	-0.1	-0.01	-2.7778	-2.8612	-2.9815	-3.0705
25.00	-0.1	-0.01	-2.7834	-2.8676	-2.9875	-3.0773
20.00	-0.1	-0.01	-2.7916	-2.8771	-2.9963	-3.0874
15.00	-0.1	-0.01	-2.8052	-2.8927	-3.0109	-3.1041
10.00	-0.1	-0.01	-2.8316	-2.9232	-3.0392	-3.1363
5.00	-0.1	-0.01	-2.9054	-3.0076	-3.1176	-3.2250
0.00	-0.1	-0.01	-3.8400	-4.0000	-4.0450	-4.2050
-0.01	-0.1	-0.01	-3.8501	-4.0101	-4.0546	-4.2146
-0.05	-0.1	-0.01	-3.8917	-4.0516	-4.0941	-4.2540
-0.10	-0.1	-0.01	-3.9470	-4.1065	-4.1464	-4.3060
-0.15	-0.1	-0.01	-4.0060	-4.1649	-4.2022	-4.3613
-0.20	-0.1	-0.01	-4.0690	-4.2270	-4.2617	-4.4200
-0.25	-0.1	-0.01	-4.1362	-4.2930	-4.3250	-4.4822
-0.30	-0.1	-0.01	-4.2077	-4.3629	-4.3923	-4.5482
-0.35	-0.1	-0.01	-4.2837	-4.4371	-4.4639	-4.6182

-0.40	-0.1	-0.01	-4.3644	-4.5156	-4.5398	-4.6922
-0.45	-0.1	-0.01	-4.4498	-4.5984	-4.6203	-4.7703
-0.50	-0.1	-0.01	-4.5401	-4.6858	-4.7053	-4.8528
-0.55	-0.1	-0.01	-4.6352	-4.7778	-4.7950	-4.9396
-0.60	-0.1	-0.01	-4.7352	-4.8744	-4.8893	-5.0309
-0.65	-0.1	-0.01	-4.8400	-4.9755	-4.9885	-5.1267
-0.70	-0.1	-0.01	-4.9496	-5.0813	-5.0923	-5.2269
-1.00	-0.1	-0.01	-5.7002	-5.8064	-5.8091	-5.9194
-1.50	-0.1	-0.01	-7.2226	-7.2915	-7.2893	-7.3617
-2.00	-0.1	-0.01	-8.9429	-8.9879	-8.9854	-9.0327
-2.50	-0.1	-0.01	-10.7649	-10.7957	-10.7937	-10.8259
-3.00	-0.1	-0.01	-12.6428	-12.6648	-12.6634	-12.6864
-3.50	-0.1	-0.01	-14.5542	-14.5706	-14.5696	-14.5866
-4.00	-0.1	-0.01	-16.4870	-16.4995	-16.4989	-16.5119

Table 2.1: Comparison of the calculated analytical exact diagonalization values (AEDV) and the theoretical exact values (TEV) of the total energies E for the various extended Hubbard models.

Coulomb interaction strength $U/4t$	Total Energy E Two electrons interaction on a one dimensional four sites lattice system							
	Model I $-t-t'+U$		Model II $-t+U$		Model III $-t-t'+U+V$		Model IV $-t+U+V$	
	AEDV	**TEV**	**AEDV**	**TEV**	**AEDV**	**TEV**	**AEDV**	**TEV**
50.00	-2.7666	-2.7598	-2.8482	-2.8482	-2.9694	-2.9692	-3.0566	-3.0514
45.00	-2.7685	-2.7620	-2.8504	-2.8504	-2.9714	-2.9714	-3.0590	-3.0536
40.00	-2.7708	-2.7648	-2.8531	-2.8532	-2.9740	-2.9742	-3.0619	-3.0564
35.00	-2.7738	-2.7683	-2.8566	-2.8567	-2.9772	-2.9778	-3.0656	-3.0600
30.00	-2.7778	-2.7731	-2.8612	-2.8615	-2.9815	-2.9826	-3.0705	-3.0648
25.00	-2.7834	-2.7797	-2.8676	-2.8681	-2.9875	-2.9893	-3.0773	-3.0715
20.00	-2.7916	-2.7897	-2.8771	-2.8781	-2.9963	-2.9994	-3.0874	-3.0816
15.00	-2.8052	-2.8064	-2.8927	-2.8947	-3.0109	-3.0162	-3.1041	-3.0984
10.00	-2.8316	-2.8395	-2.9232	-2.9279	-3.0392	-3.0497	-3.1363	-3.1319
5.00	-2.9054	-2.9378	-3.0076	-3.0262	-3.1176	-3.1490	-3.2250	-3.2312
0.00	-3.8400	-3.8391	-4.0000	-4.0000	-4.0450	-4.0444	-4.2050	-4.2041
-0.05	-3.8917	-3.9416	-4.0516	-4.1025	-4.0941	-4.1469	-4.2540	-4.3066
-0.10	-3.9470	-4.0490	-4.1065	-4.2099	-4.1464	-4.2544	-4.3060	-4.4141
-0.15	-4.0060	-4.1614	-4.1649	-4.3223	-4.2022	-4.3667	-4.3613	-4.5264
-0.20	-4.0690	-4.2787	-4.2270	-4.4396	-4.2617	-4.4838	-4.4200	-4.6435
-0.25	-4.1362	-4.4006	-4.2930	-4.5615	-4.3250	-4.6057	-4.4822	-4.7654
-0.30	-4.2077	-4.5271	-4.3629	-4.6880	-4.3923	-4.7321	-4.5482	-4.8918
-0.35	-4.2837	-4.6580	-4.4371	-4.8189	-4.4639	-4.8628	-4.6182	-5.0225
-0.40	-4.3644	-4.7931	-4.5156	-4.9540	-4.5398	-4.9978	-4.6922	-5.1575
-0.45	-4.4498	-4.9322	-4.5984	-5.0931	-4.6203	-5.1367	-4.7703	-5.2964
-0.50	-4.5401	-5.0751	-4.6858	-5.2360	-4.7053	-5.2794	-4.8528	-5.4391
-0.55	-4.6352	-5.2216	-4.7778	-5.3825	-4.7950	-5.4257	-4.9396	-5.5854
-0.60	-4.7352	-5.3714	-4.8744	-5.5323	-4.8893	-5.5754	-5.0309	-5.7351
-0.65	-4.8400	-5.5244	-4.9755	-5.6853	-4.9885	-5.7282	-5.1267	-5.8879
-0.70	-4.9496	-5.6803	-5.0813	-5.8413	-5.0923	-5.8839	-5.2269	-6.0436
-1.00	-5.7002	-5.7001	-5.8064	-5.8570	-5.8091	-5.8867	-5.9194	-6.0456
-1.50	-7.2226	-7.47721	-7.2915	-7.6341	-7.2893	-7.6623	-7.3617	-7.8212
-2.00	-8.9429	-9.3437	-8.9879	-9.5007	-8.9854	-9.5278	-9.0327	-9.6868
-2.50	-10.7649	-11.2568	-10.7957	-11.4138	-10.7937	-11.4401	-10.8259	-11.5991
-3.00	-12.6428	-13.1962	-12.6648	-13.3532	-12.6634	-13.3789	-12.6864	-13.5379
-3.50	-14.5542	-15.1517	-14.5706	-15.3087	-14.5696	-15.3341	-14.5866	-15.4931
-4.00	-16.4870	-17.1178	-16.4995	-17.2748	-16.4989	-17.2999	-16.5119	-17.4588

3.0 Discussion of Results

From table 2.0 the behaviour of the hopping kinetic energy is very easy to explain. As $U/4t$ increases positively, more hopping occurs, so the expectation value $(C^{+}_{i\sigma}C_{j\sigma})$ for kinetic hopping terms increases. When $U/4t$ itself decreases negatively then the hopping kinetic energy terms decrease, and this increases the tendency of the two electrons to come together or to be restricted to one site. The amount of doubly occupied sites increases for higher negative $/4t$. This means that the potential energy also increases.

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 positive higher U/4t electrons can have enough kinetic energy to doubly occupy a site. The $-t+U+V$ has the least non degenerate energy values while the $-t-t'+U$ model has the highest non degenerate energy values. Thus it may be decided that the $-t+U+V$ model is a better model to discuss the mechanics of electron correlations, since it produced the minimum energy and hence the minimum potential energy.

Table 2.1 provides the comparison of the values obtained from the analytical exact diagonalization and the theoretical exact calculations. The results compared favourably with one another particularly in the positive regime of the Coulomb interaction strength $U/4t$. The trend of non-degeneracy in the total energies, the consistent negative increase in the total energies of the two interacting electrons as $U/4t$ is decreased, is the same for the various models we applied in this study.

4.0 Research Methodology

We first applied the extended Hubbard model to act on the various electron states available to the two electrons four sites lattice. The application of the Hubbard model generated a 16×16 eigenvalue matrix which was solved by analytical exact diagonalization. Thereafter we formulated the theoretical exact approach which was patterned after the result of two electrons two-site system.

4.1 Mathematical Theory

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

$$H=-t\sum_{\langle i\,j\rangle\sigma}\left(C^{+}_{i\sigma}C_{j\sigma}+h.c.\right)-t'\sum_{\langle\langle i\,j\rangle\rangle\sigma}\left(C^{+}_{i\sigma}C_{j\sigma}+h.c.\right)+ U\sum_{i}n_{i\uparrow}n_{i\downarrow}+V_{ij}\sum_{\langle i\,j\rangle}n_i\,n_j \tag{4.1}$$

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.

$$V_{ij}=\begin{cases} V\ if\ \ i\ and\ \ j\ are nearest\ neighbours \\ 0\ \ otherwise \end{cases} \tag{4.2}$$

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:

$$n_i\,n_j=(n_{i\uparrow}+n_{i\downarrow})\ (n_{j\uparrow}+n_{j\downarrow})=n_{i\uparrow}\,n_{j\uparrow}+n_{i\uparrow}\,n_{j\downarrow}+n_{i\downarrow}n_{j\uparrow}+n_{i\downarrow}\,n_{j\downarrow} \tag{4.3}$$

$$n_i\,n_j=\sum_{\sigma,\sigma'}n_{i\sigma}\,n_{j\sigma'} \tag{4.4}$$

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. The Hamiltonian effectively annihilates an electron on its original site and creates an electron on another site. The amount of energy gained by this delocalisation of the electrons is given by the hopping amplitude t.

4.2. The Ground State Energies of the Two Interacting Electrons by Analytical Exact Diagonalization.

From the geometry of the two electrons four sites system we can write the summary of the Hilbert space available to the two-electron eigenstates, and this information is provided in the table below.

Table 4.0: Information derived from the geometry of the two electrons four sites lattice sites.

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	$\lvert\Psi_0\rangle$	4	$\lvert 1\uparrow, 1\downarrow\rangle, \lvert 2\uparrow, 2\downarrow\rangle$ $\lvert 3\uparrow, 3\downarrow\rangle, \lvert 4\uparrow, 4\downarrow\rangle$
2	a	$\lvert\Psi_1\rangle$	8	$\lvert 1\uparrow,2\downarrow\rangle, \lvert 1\downarrow,2\uparrow\rangle$ $\lvert 2\uparrow,3\downarrow\rangle, \lvert 2\downarrow,3\uparrow\rangle$ $\lvert 3\uparrow,4\downarrow\rangle, \lvert 3\downarrow,4\uparrow\rangle$ $\lvert 4\uparrow,1\downarrow\rangle, \lvert 4\downarrow,1\uparrow\rangle$
3	$2a$	$\lvert\Psi_2\rangle$	4	$\lvert 1\uparrow,3\downarrow\rangle, \lvert 1\downarrow,3\uparrow\rangle$ $\lvert 2\uparrow,4\downarrow\rangle, \lvert 2\downarrow,4\uparrow\rangle$
			There are a total of 16 electron eigen states	

When the Hubbard model given by (4.1) is used to act on the various electron states provided in Table 2.0, i.e., $H\lvert\Psi_\lambda\rangle$ $\lambda = 1, 2, 3, \cdots, 16$ we shall get an eigen value problem of the form: $\lvert A-\lambda I\rvert\vec{X}=0$. But for a non-trivial solution $\lvert A-\lambda I\rvert=0$ provided $\vec{X}\neq 0$. Hence we get the following matrix.

$$A=\begin{pmatrix}
U & 0 & 0 & 0 & -t & t & 0 & 0 & 0 & 0 & -t & t & -2t' & 2t' & 0 & 0\\
0 & U & 0 & 0 & -t & t & -t & t & 0 & 0 & 0 & 0 & 0 & 0 & -2t' & 2t\\
0 & 0 & U & 0 & 0 & 0 & -t & t & -t & t & 0 & 0 & -2t' & 2t' & 0 & 0\\
0 & 0 & 0 & U & 0 & 0 & 0 & 0 & -t & t & -t & t & 0 & 0 & -2t' & 2t'\\
-t & -t & 0 & 0 & V & 0 & 0 & 2t' & 0 & 0 & 0 & 2t' & -t & 0 & 0 & t\\
t & t & 0 & 0 & 0 & V & 2t' & 0 & 0 & 0 & 2t' & 0 & 0 & -t & t & 0\\
0 & -t & -t & 0 & 0 & 2t' & V & 0 & 0 & 2t' & 0 & 0 & -t & 0 & -t & 0\\
0 & t & t & 0 & 2t' & 0 & 0 & V & 2t' & 0 & 0 & 0 & 0 & -t & 0 & -t\\
0 & 0 & -t & -t & 0 & 0 & 0 & 2t' & V & 0 & 0 & 2t' & 0 & t & -t & 0\\
0 & 0 & t & t & 0 & 0 & 2t' & 0 & 0 & V & 2t' & 0 & t & 0 & 0 & -t\\
-t & 0 & 0 & -t & 0 & 2t' & 0 & 0 & 0 & 8s & V & 0 & 0 & t & 0 & t\\
t & 0 & 0 & t & 2t' & 0 & 0 & 0 & 2t' & 0 & 0 & V & t & 0 & t & 0\\
-2t' & 0 & -2t' & 0 & -t & 0 & -t & 0 & 0 & t & 0 & t & 0 & 0 & 0 & 0\\
2t' & 0 & 2t' & 0 & 0 & -t & 0 & -t & t & 0 & t & 0 & 0 & 0 & 0 & 0\\
0 & -2t' & 0 & -2t' & 0 & t & -t & 0 & -t & 0 & 0 & t & 0 & 0 & 0 & 0\\
0 & 2t' & 0 & 2t' & t & 0 & 0 & -t & 0 & -t & t & 0 & 0 & 0 & 0 & 0
\end{pmatrix}\begin{pmatrix}X_1\\X_2\\X_3\\X_4\\X_5\\X_6\\X_7\\X_8\\X_9\\X_{10}\\X_{11}\\X_{12}\\X_{13}\\X_{14}\\X_{15}\\X_{16}\end{pmatrix}=\begin{pmatrix}0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\end{pmatrix} \quad (4.5)$$

Also the constraint $\langle i\rvert j\rangle=\delta_{ij}$ must be duly followed. The above generic eigenvalue matrix can be simplified by dividing through it by t and with further algebraic rearrangement for the purpose of simplicity we realize:

$$\begin{pmatrix} 4u & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 1 & -8s & 8s & 0 & 0 \\ 0 & 4u & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -8s & 8s \\ 0 & 0 & 4u & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & -8s & 8s & 0 & 0 \\ 0 & 0 & 0 & 4u & 0 & 0 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & -8s & 8s \\ -1 & -1 & 0 & 0 & 4v & 0 & 0 & 8s & 0 & 0 & 0 & 8s & -1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & 4v & 8s & 0 & 0 & 0 & 8s & 0 & 0 & -1 & 1 & 0 \\ 0 & -1 & -1 & 0 & 0 & 8s & 4v & 0 & 0 & 8s & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 & 8s & 0 & 0 & 4v & 8s & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & -1 & -1 & 0 & 0 & 0 & 8s & 4v & 0 & 0 & 8s & 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 8s & 0 & 0 & 4v & 8s & 0 & 1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 & 0 & 8s & 0 & 0 & 0 & 8s & 4v & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 8s & 0 & 0 & 0 & 8s & 0 & 0 & 4v & 1 & 0 & 1 & 0 \\ -8s & 0 & -8s & 0 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 8s & 0 & 8s & 0 & 0 & -1 & 0 & -1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -8s & 0 & -8s & 0 & 1 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 8s & 0 & 8s & 1 & 0 & 0 & -1 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (4.6)$$

The reader should note that for the purpose of clarity and convenience we have used $u = U/4t$ (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 analytical exact diagonalization of the above 16×16 matrix will produce the total energies and the corresponding eigenvectors for each arbitrary u. However, because of lack of space we are prohibited from presenting the eigenvectors in this paper.

4.3. Theoretical Exact Calculation of the Ground State Energies of the Two Interacting Electrons.

In this section, analytically we shall derive the equation that would give the total energy of two interacting electrons in one dimensional four-site system without using or passing through the lengthy analytical approach. This theoretical formulation is based on the choice of arbitrary values that we subscribed for the relevant variables in this study. The table below shows the theoretical exact calculation of two – electrons in one dimensional 1D lattice four – site.

The theoretical calculation 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 intervalδ of positive values of u, while for the negative values of u, depending on the given interval δ we used β to complement the equation to produce the total energies. 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 $t' = 0$).

Table 4.1: Theoretical Exact Calculation of the Total Energy E for 2 – Electrons on a 1D 4 – Lattice 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: $-t - t' + U$
4 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1 + \left(\frac{U}{4t}\right)^2 + \left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{t'}{4t} + \alpha\right\}$ $\alpha \approx 1.3599$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$
		$E = -2\left\{\sqrt{1 + \left(\frac{U}{4t}\right)^2 + \left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{t'}{4t} + \beta\right\}$ $\beta \approx 0.9095$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta \approx 0.4258$ for interval of -0.5 ranging from [-1, -4]

Table 4.2: **Theoretical Exact Calculation of the Total Energy E for 2 – Electrons on a 1D 4 – Lattice 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: $-t+U$
4 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t} + \alpha\right\}$ $\alpha \approx 1.4141$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$ $E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2} - \frac{U}{4t} + \beta\right\}$ $\beta \approx 1$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta \approx 0.5143$ for interval of -0.5 ranging from [-1, -4]

Table 4.3: Theoretical Exact Calculation of the Total Energy $E$for 2 – Electrons on a 1D 4 – Lattice 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: $-t-t'+U+V$
4 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{V}{4t} - \frac{t'}{4t} + \alpha\right\}$ $\alpha \approx 1.3645$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$ $E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2+\left(\frac{t'}{4t}\right)^2} - \frac{U}{4t} - \frac{V}{4t} - \frac{t'}{4t} + \beta\right\}$ $\beta \approx 0.9072$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta \approx 0.4156$ for interval of -0.5 ranging from [-1, -4]

Table 4.4: Theoretical Exact Calculation of the Total Energy E for 2 – Electrons on a 1D 4 – Lattice 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: $-t+U+V$
4 −sites	[5, 50] $\delta = 5$	$E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2} - \frac{U}{4t} - \frac{V}{4t} + \alpha\right\}$ $\alpha \approx 1.4156$ for interval of 5 ranging from [5, 50]
	[0, -0.70] $\delta = -0.05$	Negative values of the Coulomb interaction strength $U/4t$ $E = -2\left\{\sqrt{1+\left(\frac{U}{4t}\right)^2+\left(\frac{V}{4t}\right)^2} - \frac{U}{4t} - \frac{V}{4t} + \beta\right\}$ $\beta \approx 0.9971$ for interval of -0.05 ranging from [0, -0.70]
	[-1, -4] $\delta = -0.5$	$\beta \approx 0.5051$ for interval of -0.5 ranging from [-1, -4]

5.0 Conclusion

This is a preliminary report that provides a theoretical exact method of calculating the groundstate energies of two interacting electrons on a one dimensional four sites lattice 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 analytical computation and this approach will also eventually minimize computational errors. The first thing to notice is that all energies are negative and non-degenerate. This arises from the fact that the electron energy levels are defined relative to the Fermi energy.

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