Original Research Article

ANALYSIS OF ELECTRON CORRELATION IN THE MODIFIED SINGLE-BAND HUBBARD MODEL

Abstract

The major characteristic of the single-band Hubbard model (HM) is to redistribute electrons at a uniform lattice separation distance within the molecular lattice. Hence, it is only linearly dependent on lattice separations distance. Thus the single-band Hubbard model does not consider the lattice gradient encountered by interacting electrons as they hop from one lattice point to another. The linear dependence of the single-band HM only on lattice separations would certainly not provide a thorough understanding of the interplay between interacting electrons. Consequently, we have in this study developed a gradient Hamiltonian model to solve the associated defects pose by the limitations of the single band Hubbard model. Thus, we utilized the single-band HM and the gradient Hamiltonian model to study the behaviour of two interacting electrons on a two dimensional (2D) 9X9 square lattice. It is revealed in this study that the results of the ground-state energies produced by the gradient Hamiltonian model are more favourable when compared to those of the single-band Hubbard model. We have also shown in this work, that the repulsive Coulomb interaction which in part leads to the strong electronic correlations, would indicate that the two electron system prefer not to condense into s-wave superconducting singlet state (s = 0), at high positive values of the interaction strength.

Keywords: gradient Hamiltonian model, correlation time, single-band Hubbard model, ground-state energy, interacting electrons and variational parameters.

1.0 Introduction.

The single band Hubbard model (HM) is the simplest Hamiltonian containing the essence of strong correlation. Notwithstanding its apparent simplicity, our understanding of the physics of the Hubbard model is still limited. In fact, although its thermodynamics was clarified by many authors (Takahashi, 1977) various important quantities such as momentum distribution and correlation functions, which require an explicit form of the wave function, have not been properly explored (Ogata and Shiba, 1992).

The single band Hubbard model (HM) is linearly dependent only on lattice separations. However, it does not consider the lattice gradient encountered by interacting electrons as they hop from one lattice site to another. The linear dependence of the Hubbard model only on the lattice separations would certainly not provide a true comprehensive quantum picture of the interplay between the two interacting electrons. It is clear that one of the major consequences of the HM is to redistribute the electrons along the lattice sites when agitated. However, we have in this study, extended the Hubbard model by including gradient parameters in order to solve the associated defects pose by the limitations of the single-band HM.

A particle like an electron, that has charge and spin always feels the presence of a similar particle nearby because of the Coulomb and spin interactions between them. So long as these interactions are taken into account in a realistic model, the motion of each electron is said to be correlated. The physical properties of several materials cannot be described in terms of any simple independent electron picture; rather the electrons behave cooperatively in a correlated manner (Stintzing and Zwerger, 1997). The interaction between these particles depends then in some way on their relative positions and velocities. We assume for the sake of simplicity that their interaction does not depend on their spins.

Electron correlation plays an important role in describing the electronic structure and properties of molecular systems. Dispersion forces are also due to electron correlation. The theoretical description of strongly interacting electrons poses a difficult problem. Exact solutions of specific models usually are impossible, except for certain one-dimensional models. Fortunately, such exact solutions are rarely required when comparing with experiment (Xi - Wen et al, 2013).

Most measurements, only probe correlations on energy scales small compared to the Fermi energy so that only the low – energy sector of a given model is of importance. Moreover, only at low energies can we hope to excite only a few degrees of freedom, for which a meaningful comparison to theoretical predictions can be attempted (Johannes, 2008).

One of the first steps in most theoretical approaches to the electronic structure of molecules is the use of mean – field models or orbital models. Typically, an orbital model such as Hartree – Fock self – consistent – field theory provides an excellent starting point which accounts for the bulk (≈ 99 %) of the total energy of the molecule (Hehre et al. 1986).

However, the component of the energy left out in such a model, which results from the neglect of instantaneous interactions (correlations) between electrons, is crucial for the description of chemical bond formation. The term "electron correlation energy'' is usually defined as the difference between the exact non-relativistic energy of the system and the Hartree – Fock (HF) energy. Electron correlation is critical for the accurate and quantitative evaluation of molecular energies (Knecht et. al., 2014).

Interacting electrons are key ingredients for understanding the properties of various classes of materials, ranging from the energetically most favourable shape of small molecules to the magnetic and superconductivity instabilities of lattice electron systems, such as high-T_c superconductors and heavy fermions compounds (van Bemmel et al. 1994).

In probability theory and statistics, correlation, also called correlation coefficient, indicates the strength and direction of a linear relationship between two random variables. In general statistical usage, correlation or co-relation refers to the departure of two variables from independence, although correlation does not imply causation (Fleig, 2012).

Electron correlation effects, as defined above, are clearly not directly observable. Correlation is not a perturbation that can be turned on or off to have any physical consequences. Rather, it is a measure of the errors that are inherent in HF theory or orbital models. This may lead to some ambiguities. While HF is well – defined and unique for closed – shell molecules, several versions of HF theory are used for open-shell molecules (Krishnan and James, 1996).

The organization of this paper is as follows. In section 2 we provide the method of this study by giving a brief description of the single - band Hubbard Hamiltonian and the gradient Hamiltonian model. We also present in this section an analytical solution for the two particles interaction in a 9 X 9 cluster of the square lattice. In section 3 we present results emanating from this study. The result emanating from this study is discussed in section 4. This paper is finally brought to an end with concluding remarks in section 5 and this is immediately followed by list of references.

1.1 Research Methodology

In this study, we applied the gradient Hamiltonian model on the correlated trial wave-function. The action of the gradient Hamiltonian model on the correlated trial wave-function is thus studied by means of variational technique.

2.0 Mathematical Theory

2.1 The single-band Hubbard Hamiltonian (HM).

The single-band Hubbard Hamiltonian (HM) (Hubbard. J, 1963) reads;

$$H = -t \sum_{\langle ij\rangle\sigma} \left(C^{+}_{i\sigma} C_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (2.1)$$

where $\langle i, j \rangle$ denotes nearest-neighbour (NN) sites, $C^{+}_{i\sigma}\left(C_{j\sigma}\right)$ is the creation (annihilation) operator with electron spin $\sigma = \uparrow$ or $\downarrow$ at site i, and $n_{i\sigma} = C^{+}_{i\sigma} C_{i\sigma}$ is usually known to be the occupation number operator, $h.c.\,(C^{+}_{j\sigma} C_{i\sigma})$ is the hermitian conjugate . The transfer integral t_{ij} is written as $t_{ij} = t$, which means that all hopping processes have the same probability. The parameter U is the on-site Coulomb interaction. It is worth mentioning that in principle, the parameter U is positive because it is a direct Coulomb integral.

2.2 The gradient Hamiltonian model (GHM).

The single band Hubbard model (HM) has some limitations as it is only linearly dependent on lattice separations. It does not consider the lattice gradient encountered by interacting electrons as they hop from one lattice point to another within the cluster lattice. The linear dependence of the single-band HM only on lattice separations would certainly not provide a thorough understanding of the interplay between interacting electrons. Consequently, we have in this work, extended the single-band Hubbard model by introducing gradient displacement parameters. We hope that the inclusion of the gradient displacement parameters will help to resolve the associated defects pose by the limitations of the single-band HM on application to the determination of some quantum quantities. The gradient Hamiltonian model read as follows:

$$H = -t \sum_{\langle ij \rangle \sigma} \left(C_{i\sigma}^{+} C_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - t^{d} \sum_{|i-j|} \tan \beta_l \tag{2.2}$$

Now, $t_{ij}^{d} = t^{d}$ is the diagonal kinetic hopping term or transfer integral between two lattice sites, $\tan \beta_l$ is the angle between any diagonal lattice and l represent the diagonal lattice separations while the other symbols retain their usual meaning.

2.3 The correlated variational trial wave function (CVTWF)

The correlated trial wave function given by Chen and Mei (1989) is of the form

$$\left| \Psi \right\rangle = \sum_{i} X_i \left| \, i\uparrow, i\downarrow \right\rangle + \sum_{i \neq j} X_{\,|i-j|} \left\{ \left| \, i\uparrow, j\downarrow \right\rangle - \left| \, i\downarrow, j\uparrow \right\rangle \right\} \tag{2.3}$$

where $X_i \;\left(i = 0, 1, 2, \ldots, \right)$ are the variational parameters and $\left| \, i\sigma, j\sigma \right\rangle$ is the eigen state of a given electronic state, l is the lattice separation. The variational parameters indicate the probability of electrons being found or located at any of the lattice sites. However, because of the symmetry property of (2.3) we can recast it as follows.

$$\left| \Psi \right\rangle = \sum_{l} X_l \left| \, \Psi_l \right\rangle \tag{2.4}$$

In this current study the complete details of the basis set of the two dimensional (2D) N X N lattices can be found in (Akpojotor *et al*. 2002) and Enaibe (2003). However, because of the complexity of the lattice basis set we are only going to enumerate in the tables below the relevant information that are suitable to our study.

Let us consider the coordinates of a 2D N X N square lattice which is represented by (x_1, y_1) and (x_2, y_2). Suppose one electron is located at the first coordinate while the other electron is located at the second coordinate. Then we can write that the diagonal lattice separation is given by the expression $\sqrt{\left(|x_1 - x_2|a\right)^2 + \left(|y_1 - y_2|a\right)^2}$, also for linear lattice separation it is either $|x_1 - x_2| = 1a, 2a \ldots$ and $|y_1 - y_2| = 0$ or $|y_1 - y_2| = 1a, 2a, \ldots$ and $|x - x_1| = 0$), while for the on-site lattice separation we have that $|x_1 - x_2| = |y_1 - y_2| = 0$, then the corresponding diagonal lattice separation angle is given by $\tan \beta = (\Delta y / \Delta x)$.

The various values of $\tan \beta_l$ are enumerated in Table 2.2. The reader should note that there are two basic separations in lattice separation $l = 4$ or diagonal lattice separation distance $d = \sqrt{5}a$. There are also a total of 11 diagonal lattice separations while linear lattice separations are neglected in the second summation of (2.2).

Table 2.1: Relevant information derived from the basis set of the geometry of 2D 9 x 9 square lattice.

Lattice separation l and actual lattice separation distance d_l		Total number of nearest neighbour sites at a separation length l	Pair wave function $\|\Psi_l\rangle$	Total number of Pair electronic states	Number of different pair electronic states at lattice separation l	Representative 2 D Pair electronic states for each separation l $\|x_1 y_1 \uparrow, x_2 y_2 \downarrow\rangle$
l	Separation Distance d_l	σ_l	$\|\Psi_l\rangle$	$\langle\Psi_l\|\Psi_l\rangle$	$(\sigma_l \times N^2)$	
0	0	1	$\|\psi_0\rangle$	81	$1\times 81 = 81$	$\|11\uparrow, 11\downarrow\rangle$
1	a	4	$\|\psi_1\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 12\downarrow\rangle$
2	$\sqrt{2}a$	4	$\|\psi_2\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 22\downarrow\rangle$
3	$2a$	4	$\|\psi_3\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 13\downarrow\rangle$
*4	$\sqrt{5}a$	8	$\|\psi_4\rangle$	648	$4\times 81 = 324$	$\|11\uparrow, 23\downarrow\rangle$
					$4\times 81 = 324$	$\|11\uparrow, 32\downarrow\rangle$
5	$\sqrt{8}a$	4	$\|\psi_5\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 33\downarrow\rangle$
6	$3a$	4	$\|\psi_6\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 14\downarrow\rangle$
7	$\sqrt{10}a$	8	$\|\psi_7\rangle$	648	$8\times 81 = 648$	$\|11\uparrow, 24\downarrow\rangle$
8	$\sqrt{13}a$	8	$\|\psi_8\rangle$	648	$8\times 81 = 648$	$\|11\uparrow, 34\downarrow\rangle$
9	$\sqrt{18}a$	4	$\|\psi_9\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 44\downarrow\rangle$
10	$4a$	4	$\|\psi_{10}\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 15\downarrow\rangle$
11	$\sqrt{17}a$	8	$\|\psi_{11}\rangle$	648	$8\times 81 = 648$	$\|11\uparrow, 25\downarrow\rangle$
12	$\sqrt{20}a$	8	$\|\psi_{12}\rangle$	648	$8\times 81 = 648$	$\|11\uparrow, 35\downarrow\rangle$
13	$\sqrt{25}a$	8	$\|\psi_{13}\rangle$	648	$8\times 81 = 648$	$\|11\uparrow, 45\downarrow\rangle$
14	$\sqrt{32}a$	4	$\|\psi_{14}\rangle$	324	$4\times 81 = 324$	$\|11\uparrow, 55\downarrow\rangle$
Total number of electronic states $N = 9$; $(N\times N)^2$=6561				6561	6561	6561

*Note that there are two basic diagonal separations length in $l = 4$.

Table 2.2: Relevant information derived from the basis set of the geometry of 2D 9 x 9 square lattice.

Lattice Separation l and actual lattice separation distance d_l			Pair wave function $\left| \Psi_l \right\rangle$ $1A^0 = 10^{-10} m$	NN number of sites at a separation length l	Total number of Pair electronic states	Angle between two diagonal lattice separation and their ratio		Representative 2 D Pair electronic states for each separation l $\left| x_1 y_1 \uparrow, x_2 y_2 \downarrow \right\rangle$
l	Separation Distance d		Separation Distance (m)	σ_l	$\left\langle \Psi_l \middle| \Psi_l \right\rangle$	$\tan \beta_l$	D_l	
0	$\left| \psi_0 \right\rangle$	0	0	1	81	--	--	$\left| 11 \uparrow, 11 \downarrow \right\rangle$
1	$\left| \psi_1 \right\rangle$	a	1×10^{-10}	4	324	--	--	$\left| 11 \uparrow, 12 \downarrow \right\rangle$
2	$\left| \psi_2 \right\rangle$	$\sqrt{2}a$	$\sqrt{2} \times 10^{-10}$	4	324	1	0.0494	$\left| 11 \uparrow, 22 \downarrow \right\rangle$
3	$\left| \psi_3 \right\rangle$	$2a$	2×10^{-10}	4	324	--	--	$\left| 11 \uparrow, 13 \downarrow \right\rangle$
*4	$\left| \psi_4 \right\rangle$	$\sqrt{5}a$	$\sqrt{5} \times 10^{-10}$	8	324	2	0.0494	$\left| 11 \uparrow, 23 \downarrow \right\rangle$
					324	0.5	0.0494	$\left| 11 \uparrow, 32 \downarrow \right\rangle$
5	$\left| \psi_5 \right\rangle$	$\sqrt{8}a$	$\sqrt{8} \times 10^{-10}$	4	324	1	0.0494	$\left| 11 \uparrow, 33 \downarrow \right\rangle$
6	$\left| \psi_6 \right\rangle$	$3a$	3×10^{-10}	4	324	--	--	$\left| 11 \uparrow, 14 \downarrow \right\rangle$
7	$\left| \psi_7 \right\rangle$	$\sqrt{10}a$	$\sqrt{10} \times 10^{-10}$	8	648	3	0.0988	$\left| 11 \uparrow, 24 \downarrow \right\rangle$
8	$\left| \psi_8 \right\rangle$	$\sqrt{13}a$	$\sqrt{13} \times 10^{-10}$	8	648	1.5	0.0988	$\left| 11 \uparrow, 34 \downarrow \right\rangle$
9	$\left| \psi_9 \right\rangle$	$\sqrt{18}a$	$\sqrt{18} \times 10^{-10}$	4	324	1	0.0494	$\left| 11 \uparrow, 44 \downarrow \right\rangle$
10	$\left| \psi_{10} \right\rangle$	$4a$	4×10^{-10}	4	324	--	--	$\left| 11 \uparrow, 15 \downarrow \right\rangle$
11	$\left| \psi_{11} \right\rangle$	$\sqrt{17}a$	$\sqrt{17} \times 10^{-10}$	8	648	4	0.0988	$\left| 11 \uparrow, 25 \downarrow \right\rangle$
12	$\left| \psi_{12} \right\rangle$	$\sqrt{20}a$	$\sqrt{20} \times 10^{-10}$	8	648	2	0.0988	$\left| 11 \uparrow, 35 \downarrow \right\rangle$
13	$\left| \psi_{13} \right\rangle$	$\sqrt{25}a$	$\sqrt{25} \times 10^{-10}$	8	648	1.33	0.0988	$\left| 11 \uparrow, 45 \downarrow \right\rangle$
14	$\left| \psi_{14} \right\rangle$	$\sqrt{32}a$	$\sqrt{32} \times 10^{-10}$	4	324	1	0.0494	$\left| 11 \uparrow, 55 \downarrow \right\rangle$
Total number of electronic states $N = 9$; $(N \times N)^2 = 6561$					6561			

The ratio D_l is found from the division of the pair electronic states in each separation by the total number of electronic states.

Table 2.3: Relevant information derived from the diagonal basis set of the geometry of 2D 9 x 9 lattice.

Diagonal Lattice separation l	Diagonal lattice Pair wave function	Actual diagonal lattice separation distance d_l	Actual separation distance d_l x 10^{-10} (m)	Diagonal Lattice $y(\phi_l)$ (Degree)	Diagonal Lattice $y(\phi_l)$ (Radian)	Diagonal pair electronic states for each separation
2	$\lvert \psi_2 \rangle$	$\sqrt{2}a$	1.414	$\beta_2 (45^0)$	0.7855	$\lvert 11\uparrow, 22\downarrow \rangle$
*4	$\lvert \psi_4 \rangle$	$\sqrt{5}a$	2.236	$\beta_4^1 (63.43^0)$	1.1072	$\lvert 11\uparrow, 23\downarrow \rangle$
				$\beta_4^2 (26.56^0)$	0.4636	$\lvert 11\uparrow, 32\downarrow \rangle$
5	$\lvert \psi_5 \rangle$	$\sqrt{8}a$	2.828	$\beta_5 (45^0)$	0.7855	$\lvert 11\uparrow, 33\downarrow \rangle$
7	$\lvert \psi_7 \rangle$	$\sqrt{10}a$	3.162	$\beta_7 (71.56^0)$	1.2492	$\lvert 11\uparrow, 24\downarrow \rangle$
8	$\lvert \psi_8 \rangle$	$\sqrt{13}a$	3.605	$\beta_8 (56.31^0)$	0.9829	$\lvert 11\uparrow, 34\downarrow \rangle$
9	$\lvert \psi_9 \rangle$	$\sqrt{18}a$	4.242	$\beta_9 (45^0)$	0.7855	$\lvert 11\uparrow, 44\downarrow \rangle$
11	$\lvert \psi_{11} \rangle$	$\sqrt{17}a$	4.123	$\beta_{11} (75.96^0)$	1.3259	$\lvert 11\uparrow, 25\downarrow \rangle$
12	$\lvert \psi_{12} \rangle$	$\sqrt{20}a$	4.472	$\beta_{12} (63.43^0)$	1.1072	$\lvert 11\uparrow, 35\downarrow \rangle$
13	$\lvert \psi_{13} \rangle$	$\sqrt{25}a$	5-000	$\beta_{13} (53.12^0)$	0.9272	$\lvert 11\uparrow, 45\downarrow \rangle$
14	$\lvert \psi_{14} \rangle$	$\sqrt{32}a$	5.656	$\beta_{14} (45^0)$	0.7855	$\lvert 11\uparrow, 55\downarrow \rangle$

Now when the correlated variational trial wave-function given by (2.4) is written out in full on account of the information enumerated in Tables 2.1 and 2.2 we get

$$\lvert \Psi \rangle = X_0 \lvert \psi_0 \rangle + X_1 \lvert \psi_1 \rangle + X_2 \lvert \psi_2 \rangle + X_3 \lvert \psi_3 \rangle + X_4 \lvert \psi_4 \rangle + X_5 \lvert \psi_5 \rangle + X_6 \lvert \psi_6 \rangle + X_7 \lvert \psi_7 \rangle + X_8 \lvert \psi_8 \rangle + X_9 \lvert \psi_9 \rangle + X_{10} \lvert \psi_{10} \rangle + X_{11} \lvert \psi_{11} \rangle + X_{12} \lvert \psi_{12} \rangle + X_{13} \lvert \psi_{13} \rangle + X_{14} \lvert \psi_{14} \rangle \tag{2.5}$$

When we carefully use equations (2.2) to act on equation (2.3) and with proper information provided in Tables 2.1 and 2.3 above we can conveniently solve for the wave function and the total energy possess by the two interacting electrons. However, to get at these two significant quantum quantities there are two important conditions which must be duly followed. The conditions are as follows:

(i) the field strength tensor

$$\langle i \mid j \rangle = \delta_{i\,j} \begin{cases} 1 & iff \quad i = j \\ 0 & iff \quad i \neq j \end{cases} \tag{2.6}$$

(ii) the Marshal rule for non-conservation of parity (Weng et al., 1997)

$$\lvert\, i\uparrow,\ j\downarrow \rangle = -\lvert\, j\downarrow, i\uparrow \rangle \tag{2.7}$$

Hence we can establish that the inner product $\langle \Psi | \Psi \rangle$ of the variational guess trial wave function is given by

$$\langle \Psi | \Psi \rangle = X_0^2 \langle \psi_0 | \psi_0 \rangle + X_1^2 \langle \psi_1 | \psi_1 \rangle + X_2^2 \langle \psi_2 | \psi_2 \rangle + X_3^2 \langle \psi_3 | \psi_3 \rangle + X_4^2 \langle \psi_4 | \psi_4 \rangle + X_5^2 \langle \psi_5 | \psi_5 \rangle + X_6^2 \langle \psi_6 | \psi_6 \rangle + X_7^2 \langle \psi_7 | \psi_7 \rangle + X_8^2 \langle \psi_8 | \psi_8 \rangle + X_9^2 \langle \psi_9 | \psi_9 \rangle + X_{10}^2 \langle \psi_{10} | \psi_{10} \rangle + X_{11}^2 \langle \psi_{11} | \psi_{11} \rangle + X_{12}^2 \langle \psi_{12} | \psi_{12} \rangle + X_{13}^2 \langle \psi_{13} | \psi_{13} \rangle + X_{14}^2 \langle \psi_{14} | \psi_{14} \rangle \tag{2.8}$$

$$\langle \Psi | \Psi \rangle = 81 \left\{ X_0^2 + 4X_1^2 + 4X_2^2 + 4X_3^2 + 4X_4^2 + 4X_5^2 + 4X_6^2 + 8X_7^2 + 8X_8^2 + 4X_9^2 + 4X_{10}^2 + 8X_{11}^2 + 8X_{12}^2 + 8X_{13}^2 + 4X_{14}^2 \right\} \tag{2.9}$$

$$\begin{aligned}
H\left|\Psi\right\rangle = -t\{&2X_0\left|\psi_1\right\rangle+8X_1\left|\psi_0\right\rangle+4X_1\left|\psi_2\right\rangle+2X_1\left|\psi_3\right\rangle+2X_2\left|\psi_4\right\rangle+4X_2\left|\psi_1\right\rangle+2X_3\left|\psi_1\right\rangle+\\
&2X_3\left|\psi_4\right\rangle+2X_3\left|\psi_6\right\rangle+4X_4\left|\psi_2\right\rangle+4X_4\left|\psi_3\right\rangle+4X_4\left|\psi_5\right\rangle+2X_4\left|\psi_7\right\rangle+2X_5\left|\psi_4\right\rangle+2X_5\left|\psi_8\right\rangle+2X_6\left|\psi_3\right\rangle+\\
&2X_6\left|\psi_7\right\rangle+2X_6\left|\psi_{10}\right\rangle+2X_7\left|\psi_4\right\rangle+4X_7\left|\psi_6\right\rangle+2X_7\left|\psi_8\right\rangle+2X_7\left|\psi_{11}\right\rangle+4X_8\left|\psi_5\right\rangle+2X_8\left|\psi_7\right\rangle+4X_8\left|\psi_9\right\rangle+\\
&2X_8\left|\psi_{12}\right\rangle+2X_9\left|\psi_8\right\rangle+2X_9\left|\psi_{13}\right\rangle+2X_{10}\left|\psi_6\right\rangle+2X_{10}\left|\psi_{10}\right\rangle+2X_{10}\left|\psi_{11}\right\rangle+2X_{11}\left|\psi_7\right\rangle+4X_{11}\left|\psi_{10}\right\rangle+\\
&2X_{11}\left|\psi_{11}\right\rangle+2X_{11}\left|\psi_{12}\right\rangle+2X_{12}\left|\psi_8\right\rangle+2X_{12}\left|\psi_{11}\right\rangle+2X_{12}\left|\psi_{12}\right\rangle+2X_{12}\left|\psi_{13}\right\rangle+4X_{13}\left|\psi_9\right\rangle+2X_{13}\left|\psi_{12}\right\rangle+\\
&2X_{13}\left|\psi_{13}\right\rangle+4X_{13}\left|\psi_{14}\right\rangle+2X_{14}\left|\psi_{13}\right\rangle+4X_{14}\left|\psi_{14}\right\rangle-U\,X_0\left|\psi_0\right\rangle\}\\
\\
-t^d\{&X_2\tan^2\beta_2\left|\psi_2\right\rangle+X_4(\tan^2\beta_4^1\left|\psi_4\right\rangle+\tan^2\beta_4^2\left|\psi_4\right\rangle)+X_5\tan^2\beta_5\left|\psi_5\right\rangle+X_7\tan^2\beta_7\left|\psi_7\right\rangle+\\
&X_8\tan^2\beta_8\left|\psi_8\right\rangle+X_9\tan^2\beta_9\left|\psi_9\right\rangle+X_{11}\tan^2\beta_{11}\left|\psi_{11}\right\rangle+X_{12}\tan^2\beta_{12}\left|\psi_{12}\right\rangle+X_{13}\tan^2\beta_{13}\left|\psi_{13}\right\rangle+\\
&X_{14}\tan^2\beta_{14}\left|\psi_{14}\right\rangle\}
\end{aligned}\tag{2.10}$$

$$\begin{aligned}
\left\langle\Psi\right|H\left|\Psi\right\rangle = -t\{&2X_0\left\langle\psi_1|\psi_1\right\rangle+8X_1\left\langle\psi_0|\psi_0\right\rangle+4X_1\left\langle\psi_2|\psi_2\right\rangle+2X_1\left\langle\psi_3|\psi_3\right\rangle+2X_2\left\langle\psi_4|\psi_4\right\rangle+\\
&4X_2\left\langle\psi_1|\psi_1\right\rangle+2X_3\left\langle\psi_1|\psi_1\right\rangle+2X_3\left\langle\psi_4|\psi_4\right\rangle+2X_3\left\langle\psi_6|\psi_6\right\rangle+4X_4\left\langle\psi_2|\psi_2\right\rangle+4X_4\left\langle\psi_3|\psi_3\right\rangle+\\
&4X_4\left\langle\psi_5|\psi_5\right\rangle+2X_4\left\langle\psi_7|\psi_7\right\rangle+2X_5\left\langle\psi_4|\psi_4\right\rangle+2X_5\left\langle\psi_8|\psi_8\right\rangle+2X_6\left\langle\psi_3|\psi_3\right\rangle+2X_6\left\langle\psi_7|\psi_7\right\rangle+\\
&2X_6\left\langle\psi_{10}|\psi_{10}\right\rangle+2X_7\left\langle\psi_4|\psi_4\right\rangle+4X_7\left\langle\psi_6|\psi_6\right\rangle+2X_7\left\langle\psi_8|\psi_8\right\rangle+2X_7\left\langle\psi_{11}|\psi_{11}\right\rangle+4X_8\left\langle\psi_5|\psi_5\right\rangle+\\
&2X_8\left\langle\psi_7|\psi_7\right\rangle+4X_8\left\langle\psi_9|\psi_9\right\rangle+2X_8\left\langle\psi_{12}|\psi_{12}\right\rangle+2X_9\left\langle\psi_8|\psi_8\right\rangle+2X_9\left\langle\psi_{13}|\psi_{13}\right\rangle+2X_{10}\left\langle\psi_6|\psi_6\right\rangle+\\
&2X_{10}\left\langle\psi_{10}|\psi_{10}\right\rangle+2X_{10}\left\langle\psi_{11}|\psi_{11}\right\rangle+2X_{11}\left\langle\psi_7|\psi_7\right\rangle+4X_{11}\left\langle\psi_{10}|\psi_{10}\right\rangle+2X_{11}\left\langle\psi_{11}|\psi_{11}\right\rangle+2X_{11}\left\langle\psi_{12}|\psi_{12}\right\rangle+\\
&2X_{12}\left\langle\psi_8|\psi_8\right\rangle+2X_{12}\left\langle\psi_{11}|\psi_{11}\right\rangle+2X_{12}\left\langle\psi_{12}|\psi_{12}\right\rangle+2X_{12}\left\langle\psi_{13}|\psi_{13}\right\rangle+4X_{13}\left\langle\psi_9|\psi_9\right\rangle+2X_{13}\left\langle\psi_{12}|\psi_{12}\right\rangle+\\
&2X_{13}\left\langle\psi_{13}|\psi_{13}\right\rangle+4X_{13}\left\langle\psi_{14}|\psi_{14}\right\rangle+2X_{14}\left\langle\psi_{13}|\psi_{13}\right\rangle+4X_{14}\left\langle\psi_{14}|\psi_{14}\right\rangle-U\,X_0\left\langle\psi_0|\psi_0\right\rangle\}\\
\\
-t^d\{&X_2\tan^2\beta_2\left\langle\psi_2|\psi_2\right\rangle+X_4(\tan^2\beta_4^1\left\langle\psi_4|\psi_4\right\rangle+\tan^2\beta_4^2\left\langle\psi_4|\psi_4\right\rangle)+X_5\tan^2\beta_5\left\langle\psi_5|\psi_5\right\rangle+\\
&X_7\tan^2\beta_7\left\langle\psi_7|\psi_7\right\rangle+X_8\tan^2\beta_8\left\langle\psi_8|\psi_8\right\rangle+X_9\tan^2\beta_9\left\langle\psi_9|\psi_9\right\rangle+X_{11}\tan^2\beta_{11}\left\langle\psi_{11}|\psi_{11}\right\rangle+\\
&X_{12}\tan^2\beta_{12}\left\langle\psi_{12}|\psi_{12}\right\rangle+X_{13}\tan^2\beta_{13}\left\langle\psi_{13}|\psi_{13}\right\rangle+X_{14}\tan^2\beta_{14}\left\langle\psi_{14}|\psi_{14}\right\rangle\}
\end{aligned}\tag{2.11}$$

$$\begin{aligned}
\left\langle\Psi\right|H\left|\Psi\right\rangle = -(81)(t)\{&16X_0X_1+32X_1X_2+16X_1X_3+32X_2X_4+32X_3X_4+16X_3X_6+32X_4X_5+\\
&32X_4X_7+32X_5X_8+32X_6X_7+16X_6X_{10}+32X_7X_8+32X_7X_{11}+32X_8X_9+32X_8X_{12}+32X_9X_{13}+\\
&32X_{10}X_{11}+32X_{11}X_{12}+32X_{12}X_{13}+32X_{13}X_{14}+8X_{10}^2+16X_{11}^2+16X_{12}^2+16X_{13}^2+16X_{14}^2-4(U/4t)X_0^2\}\\
-(81)(t^d)\{&4X_2^2\tan\beta_2+4X_4^2(\tan\beta_4^1+\tan\beta_4^2)+4X_5^2\tan\beta_5+8X_7^2\tan\beta_7+8X_8^2\tan\beta_8+4X_9^2\tan\beta_9+8\\
&X_{11}^2\tan\beta_{11}+8X_{12}^2\tan\beta_{12}+8X_{13}^2\tan\beta_{13}+4X_{14}^2\tan\beta_{14}\}
\end{aligned}\tag{2.12}$$

Again we should understand that the values of $\left\langle\Psi_l\middle|\Psi_l\right\rangle$ is stated in Tables 2.1 - 2.2.

2.4 The variational theory

Configuration interaction is based on the variational principle in which the trial wave-function being expressed as a linear combination of Slater determinants. The expansion coefficients are determined by imposing that the energy should be a minimum. The variational method consists in evaluating the integral

$$E_g\left\langle\Psi|\Psi\right\rangle = \left\langle\Psi\right|H\left|\Psi\right\rangle = \left\langle\Psi\middle|H_t + H_u + H_{t^d}\middle|\Psi\right\rangle \tag{2.13}$$

Where E_g is the correlated ground-state energy while Ψ is the guessed trial wave function. We can now differentially minimize (2.14) using the below equations.

$$\langle \Psi | \Psi \rangle \frac{\partial E_g}{\partial X_i} + E_g \frac{\partial}{\partial X_i} \langle \Psi | \Psi \rangle = \frac{\partial}{\partial X_i} \langle \Psi | H | \Psi \rangle \tag{2.14}$$

Subject to the condition that the correlated ground state energy of the two interacting electrons is a constant of the motion, that is

$$\frac{\partial E_g}{\partial X_i} = 0 \qquad ; \quad \forall \; i = 0, 1, 2, 3 \tag{2.15}$$

Hence upon the substitution of (2.9) and (2.12) into (2.14) and also dividing all through the resulting equation by $81t$ we get

$$\begin{aligned} &E \left\{ X_0^2 + 4X_1^2 + 4X_2^2 + 4X_3^2 + 4X_4^2 + 4X_5^2 + 4X_6^2 + 8X_7^2 + 8X_8^2 + 4X_9^2 + 4X_{10}^2 + 8X_{11}^2 + 8X_{12}^2 + 8X_{13}^2 + 4X_{14}^2 \right\} = \\ &-\{ 16X_0X_1 + 32X_1X_2 + 16X_1X_3 + 32X_2X_4 + 32X_3X_4 + 16X_3X_6 + 32X_4X_5 + 32X_4X_7 + 32X_5X_8 + \\ &32X_6X_7 + 16X_6X_{10} + 32X_7X_8 + 32X_7X_{11} + 32X_8X_9 + 32X_8X_{12} + 32X_9X_{13} + 32X_{10}X_{11} + 32X_{11}X_{12} + \\ &32X_{12}X_{13} + 32X_{13}X_{14} + 8X_{10}^2 + 16X_{11}^2 + 16X_{12}^2 + 16X_{13}^2 + 16X_{14}^2 - 4(U/4t)X_0^2 \} - \{ 4X_2^2 D_2 \tan\beta_2 + 4X_4^2 \\ &(D_4^1 \tan\beta_4^1 + D_4^2 \tan\beta_4^2) + 4X_5^2 D_5 \tan\beta_5 + 8X_7^2 D_7 \tan\beta_7 + 8X_8^2 D_8 \tan\beta_8 + 4X_9^2 D_9 \tan\beta_9 + 8X_{11}^2 D_{11} \tan\beta_{11} \\ &+ 8X_{12}^2 D_{12} \tan\beta_{12} + 8X_{13}^2 D_{13} \tan\beta_{13} + 4X_{14}^2 D_{14} \tan\beta_{14} \} \end{aligned} \tag{2.16}$$

Where $U/4t$ is the interaction strength between the two interacting electrons and $E = E_g/t$ is the total energy possess by the two interacting electrons as they hop from one lattice site to another. Also $D_l = t^d/t$ (l =2, 4, 5, 7, 8, 9, 11, 12, 13, 14) are the ratios of the individual diagonal kinetic hopping to the total number of lattice separations or total kinetic hopping sites respectively. For example, $D_2 = 324/6561$ (0.0494). Now with the use of (2.14) we can carefully transform the equation given by (2.16) into a homogeneous eigen value problem of the form

$$[A - \lambda_l I] X_l = 0 \tag{2.17}$$

Where A is an N X N matrix which takes the dimension of the number of separations, λ_l is the eigen value or the total energy E_l to be determined, I is the identity matrix which is also of the same order as A, X_i are the various eigen vectors or simply the variational parameters corresponding to each eigen value.

After careful simplifications we shall realize a 15 x 15 matrix from (2.17) and from the resulting matrix we can now determine the total energies and the corresponding variational parameters for various arbitrary values of the interaction strength.

2.5 CALCULATION OF THE CORRELATION TIME

The rate at which the force $F(t)$ agitating the motion of the electrons is can be characterized by some correlation time τ which measures roughly the mean time between two successive maxima (or minima) of the fluctuating function $F(t)$. Correlation time is quite small on a macroscopic scale. The ordinary statistical average of a function of position x_l and angular displacement ϕ_l at a given time over all systems of the lattice may be written as

$$y\,(x, \phi; t) = \frac{1}{N} \sum \sum \langle y(x_l, t) \rangle \langle y(\phi_l, t) \rangle \tag{2.18}$$

Where N is the total number of sites (l for only the diagonal separation length). The operations of taking a time derivative and taking an ensemble average commute since one can interchange the order of differentiation and summation. The Mean velocity of the interacting electrons

$$\bar{v} = \frac{d}{dt}\left\langle y\;(x,\phi\,;t)\right\rangle = \frac{d}{dt}\left(\frac{1}{N}\sum\sum\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle\right) \tag{2.19}$$

$$\bar{v} = \frac{d}{dt}\left\langle y\;(x,\phi\,;t)\right\rangle = \frac{1}{N}\sum\sum\left(\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle\right) \tag{2.20}$$

$$\bar{v} = \frac{d}{dt}\left\langle y\;(x,\phi\,;t)\right\rangle = \left\langle\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle\right\rangle \tag{2.21}$$

$$\bar{v} = \frac{d}{dt}\left\langle y\;(x,\phi\,;t)\right\rangle = \left\langle y\,(\phi_l\,,t)\right\rangle\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle + \left\langle y\,(x_l\,,t)\right\rangle\frac{d}{dt}\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.22}$$

The mean acceleration a of the interacting electrons becomes

$$a = \frac{d\bar{v}}{dt} = \frac{d^2}{dt^2}\left\langle y\;(x,\phi\,;t)\right\rangle = \frac{d}{dt}\left\langle y\,(\phi_l\,,t)\right\rangle\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle + \left\langle y\,(\phi_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle +$$

$$\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle\frac{d}{dt}\left\langle y\,(\phi_l\,,t)\right\rangle + \left\langle y\,(x_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.23}$$

$$a = \frac{d\bar{v}}{dt} = 2\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle + \left\langle y\,(\phi_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle + \left\langle y\,(x_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.24}$$

We can now multiply through (2.24) by μ (the reduced mass of the two interacting electrons). The multiplication will simply translate the acceleration of the two interacting electrons into force. It should also be made known that the force responsible for the acceleration of the electrons can be described as a sum of both the internal $F(t)$ and external $\zeta(t)$ forces. That is

$$\mu\left(2\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle + \left\langle y\,(\phi_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle + \left\langle y\,(x_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(\phi_l\,,t)\right\rangle\right) = \zeta(t) + F(t) \tag{2.25}$$

$$\mu\left(2\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle + \left\langle y\,(\phi_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle + \left\langle y\,(x_l\,,t)\right\rangle\frac{d^2}{dt^2}\left\langle y\,(\phi_l\,,t)\right\rangle\right) = \zeta(t) + F(t) \tag{2.26}$$

$$\mu\left(2\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle + \frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle\right) = \zeta(t) + F(t) \tag{2.27}$$

Where $\zeta(t)$ is the external force. By integrating all through the equation given by (2.27) we get

$$\mu\left(2\frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle + \frac{d}{dt}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle\right) = \zeta\,\tau + \int F(t)\,dt \tag{2.28}$$

$$3\mu\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle = \zeta\,\tau^2 + \iint F(t)\,dt\,dt' \tag{2.29}$$

$$3\mu\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle = \zeta\,\tau.\tau + \mu\iint\frac{d^2}{dt^2}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle dt\,dt' \tag{2.30}$$

$$3\,\mu\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle = \zeta\,\tau.\tau + \mu\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.31}$$

$$\zeta\,\tau.\tau = 2\mu\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.32}$$

$$\zeta\,\tau\,\bar{v}.\tau = 2\mu\,\bar{v}\left\langle y\,(x_l\,,t)\right\rangle\left\langle y\,(\phi_l\,,t)\right\rangle \tag{2.33}$$

$$E_l\;\tau_l = 2\mu\,\bar{v}\left\langle y\,(x_l)\right\rangle\left\langle y\,(\phi_l)\right\rangle \tag{2.34}$$

$$\tau_l = \frac{2\mu\,\bar{v}\left\langle y\,(x_l)\right\rangle\left\langle y\,(\phi_l)\right\rangle}{E_l} \tag{2.35}$$

Where we have introduced the same constraint for both E_l and τ_l (l = 2, 4, 5, 7, 8, 9, 11, 12, 13, 14) and also suppressed t in (2.35) for clarity of purpose. Thus $E_l = \zeta\,\tau\,\bar{v}$ is the correlated ground-state energy which is the same as the total energy of the interacting electrons and it has a unit of kgm^2/s^2 or simply Joules J. The Amstrong is the quantum analogue of length in classical mechanics. The reduced mass μ has the usual unit of kg with a value of 9.1×10^{-31} kg, the unit of the mean velocity of electron $\bar{v}$ is -0.00028 m/s and finally the gradient parameter ϕ_l is in radian. Hence the unit of the correlation time τ_l is seconds S.

To obtain the value of $y(x_l)$ the calculation is simply done as follows: $y(x_l) = X_l \times d_l \times 10^{-10}$ (meters). This calculation would certainly convert the ordinary values of the variational parameters to the dimension of length meters.

3.0 Presentation of Results.

The results emerging from the matrix given by (2.17) are shown in Table 3.1 while results of the correlation time τ_l which is given by equation (2.35) are enumerated in Tables 3.2. We should also note that the result of the single-band HM with respect to the interaction strength is denoted as previous study while that of the gradient Hamiltonian model is denoted as present study.

Table3.1. shows the calculated values of the variational parameters X_l and the total energies E_l possess by the interacting electrons as a function of some arbitrary values of the interaction strength $u/4t$.

$u/4t$	Present and *Previous study	Total Energy E_l	Variational Parameters X_l (l = 0, 1, 2, 3, 4, 5, 6)						
			X_0	X_1	X_2	X_3	X_4	X_5	X_6
50	Present	-9.1542	0.0090	0.2353	0.3576	0.3530	0.5786	0.3365	0.2234
	Previous	-9.0412	0.0093	0.2426	0.3640	0.3596	0.5802	0.3374	0.2226
40	Present	-9.1551	0.0112	0.2359	0.3577	0.3531	0.5785	0.3364	0.2233
	Previous	-9.0422	0.0115	0.2432	0.3642	0.3596	0.5801	0.3373	0.2225
30	Present	-9.1565	0.0147	0.2367	0.3580	0.3531	0.5784	0.3362	0.2232
	Previous	-9.0437	0.0151	0.2441	0.3645	0.3597	0.5799	0.3371	0.2224
20	Present	-9.1592	0.0214	0.2384	0.3585	0.3532	0.5782	0.3358	0.2229
	Previous	-9.0466	0.0221	0.2458	0.3650	0.3597	0.5797	0.3367	0.2221
10	Present	-9.1666	0.0395	0.2427	0.3598	0.3534	0.5774	0.3347	0.2221
	Previous	-9.0546	0.0408	0.2503	0.3663	0.3598	0.5788	0.3355	0.2212
5	Present	-9.1784	0.0684	0.2495	0.3616	0.3534	0.5758	0.3328	0.2206
	Previous	-9.0673	0.0708	0.2573	0.3680	0.3597	0.5769	0.3334	0.2197
0	Present	-9.2549	0.2469	0.2857	0.3646	0.3457	0.5534	0.3140	0.2072
	Previous	-9.1511	0.2576	0.2946	0.3700	0.3505	0.5519	0.3127	0.2052
-1	Present	-9.3727	0.4704	0.3159	0.3471	0.3160	0.4931	0.2723	0.1786
	Previous	-9.2824	0.4909	0.3241	0.3486	0.3160	0.4848	0.2668	0.1741
-1.5	Present	-9.5956	0.7151	0.3214	0.2897	0.2476	0.3699	0.1949	0.1268
	Previous	-9.5312	0.7353	0.3245	0.2848	0.2419	0.3540	0.1853	0.1200
-2.0	Present	-10.3333	0.9172	0.2675	0.1693	0.1264	0.1677	0.0778	0.0501
	Previous	-10.3135	0.9215	0.2665	0.1651	0.1225	0.1591	0.0731	0.0471
-2.5	Present	-11.7220	0.9680	0.2084	0.0954	0.0625	0.0700	0.0271	0.0178
	Previous	-10.3135	0.9215	0.2665	0.1651	0.1225	0.1591	0.0731	0.0471
-5	Present	-20.8093	0.9946	0.1006	0.0206	0.0110	0.0065	0.0013	0.0012
	Previous	-20.8092	0.9946	0.1006	0.0206	0.0110	0.0065	0.0013	0.0012
-10	Present	-40.4010	0.9987	0.0501	0.0050	0.0026	0.0008	0.0001	0.0001
	Previous	-40.4010	0.9987	0.0501	0.0050	0.0026	0.0008	0.0001	0.0001
-15	Present	-60.2670	0.9994	0.0334	0.0022	0.0011	0.0002	0.0000	0.0000
	Previous	-60.2670	0.9994	0.0334	0.0022	0.0011	0.0002	0.0000	0.0000

Table 3.1. Extention. For $l = 1 - 14$

$u/4t$	Total Energy E_l	Variational Parameters X_l (l = 7, 8, 9, 10, 11, 12, 13, 14)							
		X_7	X_8	X_9	X_{10}	X_{11}	X_{12}	X_{13}	X_{14}
50	-9.1542	0.2592	0.1873	0.1222	0.1511	0.1585	0.1255	0.0908	0.0712
	-9.0412	0.2503	0.1823	0.1192	0.1463	0.1462	0.1181	0.0870	0.0690
40	-9.1551	0.2590	0.1872	0.1221	0.1510	0.1584	0.1254	0.0907	0.0711
	-9.0422	0.2502	0.1824	0.1191	0.1462	0.1461	0.1180	0.0869	0.0690
30	-9.1565	0.2589	0.1870	0.1219	0.1508	0.1582	0.1252	0.0906	0.0709
	-9.0437	0.2500	0.1822	0.1190	0.1460	0.1459	0.1178	0.0868	0.0688
20	-9.1592	0.2585	0.1866	0.1216	0.1505	0.1578	0.1249	0.0902	0.0706
	-9.0466	0.2496	0.1818	0.1186	0.1456	0.1455	0.1174	0.0864	0.0685
10	-9.1666	0.2575	0.1856	0.1206	0.1495	0.1568	0.1239	0.0894	0.0699
	-9.0546	0.2485	0.1807	0.1176	0.1446	0.1445	0.1165	0.0856	0.0677
5	-9.1784	0.2556	0.1838	0.1191	0.1478	0.1550	0.1223	0.0880	0.0686
	-9.0673	0.2466	0.1788	0.1160	0.1430	0.1427	0.1148	0.0841	0.0664
0	-9.2549	0.2391	0.1692	0.1073	0.1349	0.1411	0.1100	0.0778	0.0598
	-9.1511	0.2294	0.1635	0.1037	0.1296	0.1290	0.1024	0.0736	0.0572
-1	-9.3727	0.2048	0.1416	0.0871	0.1115	0.1162	0.0890	0.0614	0.0461
	-9.2824	0.1934	0.1344	0.0823	0.1051	0.1042	0.0811	0.0567	0.0429
-1.5	-9.5956	0.1437	0.0954	0.0555	0.0734	0.0759	0.0564	0.0372	0.0268
	-9.5312	0.1316	0.0875	0.0505	0.0668	0.0658	0.0494	0.0328	0.0238
-2.0	-10.3333	0.0546	0.0323	0.0162	0.0234	0.0237	0.0161	0.0093	0.0059
	-10.3135	0.0496	0.0293	0.0145	0.0211	0.0204	0.0139	0.0081	0.0051
-2.5	-11.7220	0.0180	0.0090	0.0037	0.0061	0.0059	0.0035	0.0017	0.0009
	-10.3135	0.0496	0.0293	0.0145	0.0211	0.0204	0.0139	0.0081	0.0051
-5	-20.8093	0.0008	0.0002	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
	-20.8092	0.0008	0.0002	0.0000	0.0002	0.0001	0.0000	0.0000	0.0000
-10	-40.4010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	-40.4010	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-15	-60.2670	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	-60.2670	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

*The previous study was carried out by Chen and Mei (1989).

Table 3.2. Shows the calculated values of the Correlation time τ_l for only the diagonal separations as a function of the interaction strength $u/4t = U$ for different values of the corresponding total energy E_l .

Diagonal lattice separation l	Diagonal lattice separation $y(\phi_l)$ (degree)	Correlation time τ_l for only the diagonal separations in (seconds) as a function of the total energy E_l and for some selected U .						
		U	50	20	5	-1	-2	-2.5
		E_l	-9.1542	-9.1592	-9.1784	-9.3727	-10.3333	-11.7220
		τ_l	$\times10^{-45}$	$\times10^{-45}$	$\times10^{-45}$	$\times10^{-45}$	$\times10^{-45}$	$\times10^{-45}$
2	$\beta_2\,(45^0)$	τ_2	1.106	1.108	1.115	1.048	0.513	0.230
*4	$\beta_4^1\,(63.43^0)$	τ_4^1	3.987	3.981	3.957	3.319	1.133	0.377
	$\beta_4^2\,(26.56^0)$	τ_4^2	2.064	2.062	2.058	2.015	1.828	1.612
5	$\beta_5\,(45^0)$	τ_5	2.081	2.075	2.052	1.644	0.472	0.131
7	$\beta_7\,(71.56^0)$	τ_7	2.849	2.841	2.803	2.199	0.588	0.154
8	$\beta_8\,(56.31^0)$	τ_8	1.847	1.839	1.808	1.364	0.312	0.069
9	$\beta_9\,(45^0)$	τ_9	1.133	1.127	1.101	0.788	0.147	0.026
11	$\beta_{11}\,(75.96^0)$	τ_{11}	2.411	2.399	2.352	1.726	0.353	0.070
12	$\beta_{12}\,(63.43^0)$	τ_{12}	1.729	1.720	1.681	1.198	0.217	0.037
13	$\beta_{13}\,(53.12^0)$	τ_{13}	1.171	1.163	1.132	0.773	0.117	0.017
14	$\beta_{14}\,(45^0)$	τ_{14}	0.881	0.873	0.846	0.557	0.072	0.009

4.0 Discussion of Results

It is shown in Table 3.1 that as the interaction strength between the two electrons is decreased the total energies possess by the electrons also decrease and this is consistent with the two models we have employed in this study. However, our present model yielded lower results of the total energies which are quite preferable since the electrons would prefer to settle down in the region of minimum potential. The negative values of the total energies show that the interaction between the two electrons is attractive and not repulsive.

The table also revealed that for higher positive interaction strength the variational parameters for larger separations are greater than those of the lower ones. This is as a result of the fact that electrons prefer to stay far apart as possible so that the chance of finding them close to one another is reduced at high positive values of the interaction strength.

Also from the table we found that for lower negative interaction strength the variational parameters for larger separations are smaller than those of the lower ones. Thus when the interaction strength is increased more negatively the two electrons now prefer to stay very close to one another instead of remaining far apart from one another. Hence the chance of finding the electrons close to one another is increased at high negative values of the interaction strength.

It is clear from the table that the results of the total energies for both models converge to the same value in the large negative interaction strength. The variational parameters also vanish or go to zero at a high negative value of the interaction strength and this is around $u/4t \leq -5$.

It is shown in Tables 3.2 that in the positive region of the interaction strength $u/4t$, the correlation time τ_2 initially increases in value as the interaction strength is decreased before it starts to decrease consistently with respect to negative increase in the interaction strength, this is around the value of $u/4t \leq -1$.

Finally, the correlation times for the other diagonal lattice separations (τ_4, τ_5, τ_5 … τ_{14}) consistently decreases for regimes of both positive and negative interaction strength. However, the values of the correlation times in the negative regime are much lower than those in the positive regime. Thus high negative interaction strength decreases the correlation time between electrons as they hop from one lattice site to another.

5.0 Conclusion

In this work, we utilized two types of Hamiltonian model to study the behaviour of two interacting electrons on a two dimensional (2D) 9 X 9 square lattice. The Hamiltonian is the single-band Hubbard model and the gradient Hamiltonian model. Obviously, the total energies of the two interacting electrons produced by the gradient Hamiltonian model are consistently lower than those of the original single-band Hubbard model. Thus the inclusion of the gradient parameters into the single band HM yielded better results of the ground-state energies. Hence the lower ground-state energy results produced by our new model are quite compactable with quantum requirements. Generally, it is established in this work that electron correlation is highly favoured within the limits of high negative interaction strength.

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