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QUANTITATIVE EVALUATION OF THE CORRELATION TIME AND VARIATIONAL GROUND-STATE ENERGY OF TWO INTERACTING ELECTRONS ON (2D) 5 X 5 SQUARE LATTICE

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ABSTRACT

In this work, we utilized two types of Hamiltonian model to study the behaviour of two interacting electrons on a two dimensional (2D) 5X5 square lattice. The Hamiltonian is the single band Hubbard model and the gradient Hamiltonian model. The single band Hubbard model is only linearly dependent on lattice separations. However, it does not consider the lattice gradient encountered by interacting electrons as they hop from one lattice point to another. 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. The results of the ground-state energies produced by the gradient Hamiltonian model are more favourable when compared to those of the Hubbard model. It is also established in this study that high negative interaction strength decreases the correlation time between the two electrons as they hop from one lattice position to another.

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

1.0 INTRODUCTION.

There has been dramatic progress in the development of electron correlation techniques for the accurate treatment of the structures and energies of molecules. 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 [1]. 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.

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 [2] various important quantities such as momentum distribution and correlation functions, which require an explicit form of the wave function, have not been properly explored [3].

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 point 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.

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 [4].

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 [5].

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 ($\approx 99\%$) of the total energy of the molecule [6].

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 [7].

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 [8].

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 [9].

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 [10].

It is clearly not possible to give a comprehensive account of all the different theories and applications within the space available. We have to give brief and somewhat qualitative descriptions of the different methods that have been developed to describe electron correlation effects. Some of the several methods of taking the electron correlation into account are: Couple cluster, Hartree – Fock and Many body perturbation theory or Moller – Plesset perturbation theory [11], [12].

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 trial wavefunction to be utilized. We also present in this section an analytical solution for the two particles interaction in a 5X5 cluster of the square lattice. In section 3 we present numerical results. 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 correlation time and ground-state energies of the two interacting electrons which is the result of 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) [9] 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, $C_{i\sigma}^{+}(C_{j\sigma})$ is the creation (annihilation) operator with 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. The exact diagonalization of (2.1) is the most desirable one. However, the method of exact diagonalization is applicable only to a small-finite dimensional

lattice system, since the dimension of the Hamiltonian matrix increases very rapidly with the number of sites and number of particles.

2.2 The gradient Hamiltonian model.

The single band Hubbard model (HM) has some limitations as it is linearly dependent only on lattice separations. It does not consider the lattice gradient encountered by interacting electrons as they hop from one lattice point to another. The linear dependence of the Hubbard model 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 HM when applied in the determination of some quantum quantities. The gradient Hamiltonian model read as follows:

$$H = -t \sum_{\langle ij \rangle \sigma} \left(C_{i\sigma}^{+} C_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - t^{v} \sum_{|i-j|} \sin\theta -$$

$$t^{h} \sum_{|i-j|} \cos\alpha - t^{d} \sum_{|i-j|} \left(\tan\lambda + \tan\beta + \tan\gamma + \ldots + \tan\eta \right) \qquad (2.2)$$

Now, t^{v}, t^{h} and t^{d} are the corresponding vertical, horizontal and diagonal kinetic hopping terms of the interacting electrons while the other symbols retain their usual meaning.

2.3 The correlated variational trial wave function.

The correlated variational trial wavefunction.given by [13] is of the form

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

Where X_i $(i = 0, 1, 2, \ldots,)$ are variational parameters and $|\, i\sigma, j\sigma\rangle$ is the eigen state of a given electronic state, l is the lattice separation. However, because of the symmetry property of (2.3) we can recast it as follows.

$$|\Psi\rangle = \sum_{l} X_{l} \,|\, \Psi_{l}\rangle \qquad (2.4)$$

In this current study the complete details of the basis set of the two dimensional (2D) 5X5 lattices can be found in [14]. 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 present study. Table 2.1 – 2.3 shows the linear dependence of the two hopping electrons in the vertical v, horizontal h and diagonal d on the lattice angles respectively. For instance, consider lattice separation $l = 1$ along the vertical plane, one electron is located at lattice site 1,1 $\Rightarrow$ (x, y) while the other one can hop from 1,1 to 1,2 (which is vertical) and from 1,1 to 2,1 (which is horizontal). Then

lattice separation $l = 2$, one electron is located at lattice site $(1,1) \Rightarrow (x, y)$ while the other electron can hop from $1,1$ to $2,2$ (which is diagonal). We have also that from the geometry of the 5X5 square lattice the gradient or the angles between the two interacting electrons are as follows: $\theta = 90^0$, $\alpha = 180^0$, $\lambda = 45^0$, $\beta = 63^0$ and $\gamma = 26.6^0$ this is given in the tables below.

Table 2.1: Relevant information derived from the basis set of the geometry of 2D 5 x 5 square lattice.

Lattice Separation l and Pair wave function $\lvert \Psi_l \rangle$		Representative Pair electronic states $\lvert i\uparrow, j\downarrow \rangle$	Method of determining the projection between any two separations	Calculation of the angle between any two separations	Calculation of the lattice separation length l $\lvert xy\uparrow, x_1y_1\downarrow \rangle$
l	$\lvert \Psi_l \rangle$	$\lvert xy\uparrow, x_1y_1\downarrow \rangle$			
0	$\lvert \Psi_0 \rangle$ (0)	$\lvert 11\uparrow, 11\downarrow \rangle$	Zero projection	On-site with no separation	$\lvert x - x_1 \rvert = 0$ $\lvert y - y_1 \rvert = 0$
1	$\lvert \Psi_1 \rangle$ (a)	$\lvert 11\uparrow, 12\downarrow \rangle$	Vertical Linear lattice length a	$\sin\theta\,(\theta = 90^0)$	$\lvert x - x_1 \rvert = 1a$ $\lvert y - y_1 \rvert = 0$
		$\lvert 11\uparrow, 21\downarrow \rangle$	Horizontal Linear lattice length a	$\cos\alpha\,(\alpha = 180^0)$	
2	$\lvert \Psi_2 \rangle$ $(\sqrt{2}a)$	$\lvert 11\uparrow, 22\downarrow \rangle$	Diagonal $\sqrt{(\lvert x - x_1 \rvert a)^2 + (\lvert y - y_1 \rvert a)^2}$	$\tan\lambda\,(\lambda = 45^0)$ $\frac{opp}{adj} = \frac{2a}{2a} = 1$	$\lvert x - x_1 \rvert = 1a$ $\lvert y - y_1 \rvert = 1a$
3	$\lvert \Psi_3 \rangle$ $(2a)$	$\lvert 11\uparrow, 13\downarrow \rangle$	Vertical Linear lattice length $(a + a)$	$\sin\theta\,(\theta = 90^0)$	$\lvert x - x_1 \rvert = 2a$ $\lvert y - y_1 \rvert = 0$
		$\lvert 11\uparrow, 31\downarrow \rangle$	Horizontal Linear lattice length $(a + a)$	$\cos\alpha\,(\alpha = 180^0)$	
4	$\lvert \Psi_4 \rangle$ $(\sqrt{5}a)$	$\lvert 11\uparrow, 23\downarrow \rangle$	Diagonal $\sqrt{(\lvert x - x_1 \rvert a)^2 + (\lvert y - y_1 \rvert a)^2}$	$\tan\beta\,(\beta = 63^0)$ $\frac{opp}{adj} = \frac{2a}{a} = 2$	$\lvert x - x_1 \rvert = 1a$ $\lvert y - y_1 \rvert = 2a$
		$\lvert 11\uparrow, 32\downarrow \rangle$	Diagonal $\sqrt{(\lvert x - x_1 \rvert a)^2 + (\lvert y - y_1 \rvert a)^2}$	$\tan\gamma\,(\gamma = 26.6^0)$ $\frac{opp}{adj} = \frac{1a}{2a} = 0.5$	$\lvert x - x_1 \rvert = 2a$ $\lvert y - y_1 \rvert = 1a$
5	$\lvert \Psi_5 \rangle$ $(\sqrt{8}a)$	$\lvert 11\uparrow, 33\downarrow \rangle$	Diagonal $\sqrt{(\lvert x - x_1 \rvert a)^2 + (\lvert y - y_1 \rvert a)^2}$	$\tan\lambda\,(\lambda = 45^0)$ $\frac{opp}{adj} = \frac{2a}{2a} = 1$	$\lvert x - x_1 \rvert = 2a$ $\lvert y - y_1 \rvert = 2a$

Table 2.2: Relevant information derived from the basis set of the geometry of 2D 5 x 5 square lattice.

Lattice Separation l and actual lattice separation distance d		Total number of nearest neighbour sites at a separation length l	Pair wave function $\lvert \Psi_l \rangle$	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 $\lvert xy\uparrow, x_1y_1\downarrow\rangle$
l	Separation Distance d	σ_l	$\lvert \Psi_l \rangle$	$\langle \Psi_l \lvert \Psi_l \rangle$	$(\sigma_l \times N^2)$	
0	0	1	$\lvert \Psi_0 \rangle$	25	$1\times 25 = 25$	$\lvert 11\uparrow, 11\downarrow\rangle$
1	a	4	$\lvert \Psi_1 \rangle$	100	$4\times 25 = 100$	$\lvert 11\uparrow, 12\downarrow\rangle$
2	$\sqrt{2}a$	4	$\lvert \Psi_2 \rangle$	100	$4\times 25 = 100$	$\lvert 11\uparrow, 22\downarrow\rangle$
3	$2a$	4	$\lvert \Psi_3 \rangle$	100	$4\times 25 = 100$	$\lvert 11\uparrow, 13\downarrow\rangle$
4	$\sqrt{5}a$	8	$\lvert \Psi_4 \rangle$	200	$8\times 25 = 200$	$\lvert 11\uparrow, 23\downarrow\rangle$ $\lvert 11\uparrow, 32\downarrow\rangle$
5	$\sqrt{8}a$	4	$\lvert \Psi_5 \rangle$	100	$4\times 25 = 100$	$\lvert 11\uparrow, 33\downarrow\rangle$
Total number of electronic states $N = 5;\ (N\times N)^2$					625	625

Table 2.3: Relevant information derived from the basis set of the geometry of 2D 5 x 5 square lattice.

Lattice Separation l and actual lattice separation distance d			Pair wave function $\lvert \Psi_l \rangle$ $1A^0 = 10^{-10}m$	Total number of sites at a separation length l	Total number of Pair electronic states	Possible number of lattice separation hopping terms	Representative 2 D Pair electronic states for each separation l $\lvert xy\uparrow, x_1y_1\downarrow\rangle$
l	Separation Distance d		Separation Distance (m)	σ_l	$\langle \Psi_l \lvert \Psi_l \rangle$		
0	$\lvert \Psi_0 \rangle$	0	0	1	25	0 (on-site)	$\lvert 11\uparrow, 11\downarrow\rangle$
1	$\lvert \Psi_1 \rangle$	a	1×10^{-10}	4	50	2 (vertical)	$\lvert 11\uparrow, 12\downarrow\rangle$
					50	2 (horizontal)	$\lvert 11\uparrow, 21\downarrow\rangle$
2	$\lvert \Psi_2 \rangle$	$\sqrt{2}a$	$\sqrt{2}\times 10^{-10}$	4	100	4 (diagonal)	$\lvert 11\uparrow, 22\downarrow\rangle$
3	$\lvert \Psi_3 \rangle$	$2a$	2×10^{-10}	4	50	2 (vertical)	$\lvert 11\uparrow, 13\downarrow\rangle$
					50	2 (horizontal)	$\lvert 11\uparrow, 31\downarrow\rangle$
4	$\lvert \Psi_4 \rangle$	$\sqrt{5}a$	$\sqrt{5}\times 10^{-10}$	8	100	4 (diagonal)	$\lvert 11\uparrow, 23\downarrow\rangle$
					100	4 (diagonal)	$\lvert 11\uparrow, 32\downarrow\rangle$
5	$\lvert \Psi_5 \rangle$	$\sqrt{8}a$	$\sqrt{8}\times 10^{-10}$	4	100	4 (diagonal)	$\lvert 11\uparrow, 33\downarrow\rangle$
Total number of electronic states $N = 5;\ (N\times N)^2 = 625$						25	625

When we carefully apply equations (2.2) and (2.3) and considering the information provided in Tables 2.1 – 2.3 above we can conveniently solve for the wave function and the total energy of the two interacting electrons. However, to get at these two quantum quantities the two important conditions stated below must be duly followed.

(i) the field strength tensor

$$\langle i \mid j \rangle = \delta_{ij} \begin{cases} 1 & iff \quad i = j \\ 0 & iff \quad i \neq j \end{cases} \tag{2.5}$$

(ii) the Marshal rule for non-conservation of parity [15]

$$\mid i\uparrow,\ j\downarrow\rangle = -\mid j\downarrow,\ i\uparrow\rangle \tag{2.6}$$

Hence the following two basic equations can be established, $\langle\Psi|\Psi\rangle$ and $\langle\Psi|H|\Psi\rangle$ which we are to be employed in the variational calculation.

$$|\Psi\rangle = X_0|\Psi_0\rangle + X_1|\Psi_1\rangle + X_2|\Psi_2\rangle + X_3|\Psi_3\rangle + X_4|\Psi_4\rangle + X_5|\Psi_5\rangle \tag{2.7}$$

$$\langle\Psi|\Psi\rangle = 25\left(X_0^2 + 4X_1^2 + 4X_2^2 + 4X_3^2 + 8X_4^2 + 4X_5^2\right) \tag{2.8}$$

$$\begin{aligned} H|\Psi\rangle = -t\Big\{&2X_0|\Psi_1\rangle + 12X_1|\Psi_0\rangle + 4X_1|\Psi_2\rangle + 2X_1|\Psi_4\rangle + 8X_2|\Psi_1\rangle + 6X_2|\Psi_3\rangle + 2X_2|\Psi_5\rangle + \\ &4X_3|\Psi_2\rangle + 2X_3|\Psi_6\rangle + 2X_4|\Psi_1\rangle + 2X_4|\Psi_4\rangle + 2X_4|\Psi_5\rangle + 8X_5|\Psi_4\rangle + 4X_5|\Psi_6\rangle + 4X_5|\Psi_7\rangle + \\ &4X_5|\Psi_2\rangle + 4X_6|\Psi_5\rangle + 2X_5|\Psi_5\rangle + 4X_6|\Psi_8\rangle + 2X_6|\Psi_6\rangle + 6X_6|\Psi_3\rangle + 2X_7|\Psi_5\rangle + 4X_7|\Psi_7\rangle + \\ &2X_7|\Psi_8\rangle + 4X_8|\Psi_7\rangle + 4X_8|\Psi_6\rangle + 4X_8|\Psi_8\rangle + 6X_8|\Psi_9\rangle + 2X_9|\Psi_8\rangle + 6X_9|\Psi_9\rangle\Big\} + UX_0|\Psi_0\rangle \\ &- t^v X_1|\Psi_1\rangle\sin\theta - t^v X_3|\Psi_3\rangle\sin\theta - t^h X_1|\Psi_1\rangle\cos\alpha - t^h X_3|\Psi_3\rangle\cos\alpha \\ &- t^d X_2|\Psi_2\rangle\tan\lambda - t^d X_5|\Psi_5\rangle\tan\lambda - t^d X_4|\Psi_4\rangle\tan\beta - t^d X_4|\Psi_4\rangle\tan\gamma \end{aligned} \tag{2.9}$$

$$\begin{aligned} \langle\Psi|H|\Psi\rangle = &-(25)(4t)\Big\{4X_0X_1 + 8X_1X_2 + 4X_1X_3 + 8X_2X_4 + 8X_3X_4 + 8X_4X_5 + 2X_3^2 + 4X_4^2 + \\ &4X_5^2 - (U/4t)X_0^2\Big\} - t^v X_1|\Psi_1\rangle\sin\theta - t^v X_3|\Psi_3\rangle\sin\theta - t^h\Big\{X_1^2\langle\Psi_1|\Psi_1\rangle + X_3^2\langle\Psi_3|\Psi_3\rangle\Big\}\cos\alpha - \\ &t^d\Big\{X_2^2\langle\Psi_2|\Psi_2\rangle\tan\lambda + X_5^2\langle\Psi_5|\Psi_5\rangle\tan\lambda + X_4^2\langle\Psi_4|\Psi_4\rangle\tan\beta + X_4^2\langle\Psi_4|\Psi_4\rangle\tan\gamma\Big\} \end{aligned} \tag{2.10}$$

$$\begin{aligned} \langle\Psi|H|\Psi\rangle = &-(25)(4t)\Big\{4X_0X_1 + 8X_1X_2 + 4X_1X_3 + 8X_2X_4 + 8X_3X_4 + 8X_4X_5 + \\ &2X_3^2 + 4X_4^2 + 4X_5^2 - (U/4t)X_0^2\Big\} - t^v\Big\{50X_1^2 + 50X_3^2\Big\}\sin\theta - t^h\Big\{50X_1^2 + 50X_3^2\Big\}\cos\alpha \\ &- t^d\Big\{100X_2^2\tan\lambda + 100X_5^2\tan\lambda + 100X_4^2\tan\beta + 100X_4^2\tan\gamma\Big\} \end{aligned} \tag{2.11}$$

Again we should know that the values of $\langle\Psi_i|\Psi_i\rangle$ are stated in Tables 2.2 - 2.3.

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

$$E_g \langle \Psi | \Psi \rangle = \langle \Psi | H | \Psi \rangle = \left\langle \Psi \middle| H_t + H_u + H_{t^v} + H_{t^h} + H_{t^d} \middle| \Psi \right\rangle \tag{2.12}$$

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.

$$\langle \Psi | \Psi \rangle \frac{\partial E_g}{\partial X_i} + E_g \frac{\partial}{\partial X_i} \langle \Psi | \Psi \rangle = \frac{\partial}{\partial X_i} \langle \Psi | H | \Psi \rangle \tag{2.13}$$

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

$$\frac{\partial E_g}{\partial X_i} = 0 \qquad ; \quad \forall\, i = 0, 1, 2, 3 \tag{2.14}$$

By substituting (2.8) and (2.11) into (2.12) and also dividing top and bottom by $25t$ we get

$$E\left(X_0^2 + 4X_1^2 + 4X_2^2 + 4X_3^2 + 8X_4^2 + 4X_5^2\right) = -\{16X_0X_1 + 32X_1X_2 + 16X_1X_3 + 32X_2X_4 + 32X_3X_4 + 32X_4X_5 + 8X_3^2 + 16X_4^2 + 16X_5^2 - 4(U/4t)X_0^2\} - V\left(2X_1^2 \sin\theta\right) - H\left(2X_1^2\right)\cos\alpha - D\left(4X_2^2 \tan\lambda\right) - V\left(2X_3^2 \sin\theta\right) - H\left(2X_3^2 \cos\alpha\right) - D\left(4X_4^2 \tan\beta\right) - D\left(4X_4^2 \tan\gamma\right) - D\left(4X_5^2 \tan\lambda\right) \tag{2.15}$$

Where $E = E_g / t$ (is the total energy of the two interacting electrons), while $V = t^v / t$, $H = t^h / t$ and $D = t^d / t$ are the ratios of the vertical, horizontal and diagonal kinetic hopping to the total number of lattice separations or total kinetic hopping sites respectively. In this work, we take the values of $V = t^v / t = 100/625 = 0.16$, $H = t^h / t = 100/625 = 0.16$ and $D = t^d / t = 400/625 = 0.64$. This is just the number of states contain within each of the separation (vertical. Horizontal and diagonal) divided by the total pair electronic states in the lattice. When (2.13) is successively applied to (2.15) we get the following corresponding equations.

$$2E\,X_0 = -16X_1 + 8(U/4t)\,X_0 \tag{2.16}$$

$$8E\,X_1 = -16X_0 - 32X_2 - 16X_3 - V(4X_1 \sin\theta) - H(4X_1 \cos\alpha) \tag{2.17}$$

$$8E\,X_2 = -32X_1 - 32X_4 - D(8X_2 \tan\lambda) \tag{2.18}$$

$$8E\,X_3 = -16X_1 - 32X_4 - 16X_3 - V(4X_3 \sin\theta) - H(4X_3 \cos\alpha) \tag{2.19}$$

$$16E\,X_4 = -32X_2 - 32X_3 - 32X_4 - 32X_5 - D(8X_4 \tan\beta) - D(8X_4 \tan\gamma) \tag{2.20}$$

$$8E\,X_5 = -32X_4 - 32X_5 - D(8X_5 \tan\lambda) \tag{2.21}$$

We can carefully transform the resulting (2.16) – (2.21) into a homogeneous eigen value problem of the form

$$\left[A - \lambda_l I\right]\vec{X}_l = 0 \tag{2.22}$$

Where A is an NXN matrix which takes the dimension of the number of separations, λ_l is the eigen value (total energy E) to be determined, I is the identity matrix which is also of the same order as A, $\vec{X}_i$ are the various eigen vectors or simply the variational parameters corresponding to each eigen value. After some algebraic subroutine we get the matrix.

$$\begin{pmatrix} E-4u & 8 & 0 & 0 & 0 & 0 \\ 2 & E+M & 4 & 2 & 0 & 0 \\ 0 & 4 & E+N & 0 & 4 & 0 \\ 0 & 2 & 0 & E+2+P & 4 & 0 \\ 0 & 0 & 2 & 2 & E+2+K & 2 \\ 0 & 0 & 0 & 0 & 4 & E+4+L \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.23}$$

That is, for the sake of clarity we have introduced the symbols: $M = 0.5V\sin\theta + 0.5H\cos\alpha$, $N = D\tan\lambda$, $P = 0.5V\sin\theta + 0.5H\cos\alpha$, $K = 0.5D\tan\beta + 0.5D\tan\gamma$ and $L = D\tan\lambda$. Suppose we put $M = N = P = K = L = 0$, then we realize the results of the single band Hubbard model. Consequently, after careful substitution of the actual values of M, N P K and L, we get after substitution matrix below.

$$\begin{pmatrix} E-4u & 8 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 \\ 0 & 4 & E+0.64 & 0 & 4 & 0 \\ 0 & 2 & 0 & E+2 & 4 & 0 \\ 0 & 0 & 2 & 2 & E+2.8 & 2 \\ 0 & 0 & 0 & 0 & 4 & E+4.64 \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.24}$$

Where $u = U/4t$ 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. From the matrix given by (2.26) we can now determine the total energy 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 which can be internal $F(t)$ or external $\zeta(t)$, agitating the motion of the electrons can be characterized by some correlation time τ which measures roughly the mean time between two successive maxima (or minima) of the fluctuating function $F(t)$ or $\zeta(t)$. 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 t over all systems of the lattice may be written as

$$y\ (x,\phi;t) = \frac{1}{N}\sum_{l=1}^{N-1}\sum_{l=1}^{N-1}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle \qquad (2.25)$$

Where $x_l\,(l=1,2,\ldots,5)$ and $\phi_l\,(l=1,2,\ldots,5)$ which may correspond to vertical v, horizontal h or diagonal d. 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

$$\bar{v} = \frac{d}{dt}\langle y\ (x,\phi;t)\rangle = \frac{d}{dt}\left(\frac{1}{N}\sum_{l=1}^{N-1}\sum_{l=1}^{N-1}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle\right) \qquad (2.26)$$

$$\bar{v} = \frac{d}{dt}\langle y\ (x,\phi;t)\rangle = \frac{1}{N}\sum_{l=1}^{N-1}\sum_{l=1}^{N-1}\left(\frac{d}{dt}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle\right) \qquad (2.27)$$

$$\bar{v} = \frac{d}{dt}\langle y\ (x,\phi;t)\rangle = \left\langle\frac{d}{dt}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle\right\rangle \qquad (2.28)$$

$$\bar{v} = \frac{d}{dt}\langle y\ (x,\phi;t)\rangle = \langle y(\phi_l,t)\rangle\frac{d}{dt}\langle y(x_l,t)\rangle + \langle y(x_l,t)\rangle\frac{d}{dt}\langle y(\phi_l,t)\rangle \qquad (2.29)$$

The mean acceleration a of the two interacting electrons becomes

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

$$\frac{d}{dt}\langle y(x_l,t)\rangle\frac{d}{dt}\langle y(\phi_l,t)\rangle + \langle y(x_l,t)\rangle\frac{d^2}{dt^2}\langle y(\phi_l,t)\rangle \qquad (2.30)$$

$$a = \frac{d\bar{v}}{dt} = 2\frac{d^2}{dt^2}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle + \langle y(\phi_l,t)\rangle\frac{d^2}{dt^2}\langle y(x_l,t)\rangle + \langle y(x_l,t)\rangle\frac{d^2}{dt^2}\langle y(\phi_l,t)\rangle \qquad (2.31)$$

We can now multiply through (2.31) by μ (the reduced mass of the two interacting electrons). The multiplication will simply translate the mean acceleration of the two interacting electrons into force. It should also be made

known that the force responsible for the mean acceleration of the two electrons can be described as a sum of both the internal $F(t)$ and external $\zeta(t)$ forces. That is

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

(2.32)

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

(2.33)

$$\mu\left(2\frac{d^2}{dt^2}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle+\frac{d^2}{dt^2}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle\right)=\zeta(t)+F(t) \qquad (2.34)$$

By integrating all through the equation given by (2.34) twice and with little simplification we get

$$\mu\left(2\frac{d}{dt}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle+\frac{d}{dt}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle\right)=\zeta\tau+\int F(t)dt \qquad (2.35)$$

$$3\mu\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle=\zeta\tau^2+\iint F(t)dt\,dt' \qquad (2.36)$$

$$3\mu\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle=\zeta\tau.\tau+\mu\iint\frac{d^2}{dt^2}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle dt\,dt' \qquad (2.37)$$

$$3\mu\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle=\zeta\tau.\tau+\mu\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle \qquad (2.38)$$

$$\zeta\tau.\tau=2\mu\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle \qquad (2.39)$$

$$\zeta\tau\,\bar{v}.\tau=2\mu\bar{v}\langle y(x_l,t)\rangle\langle y(\phi_l,t)\rangle \qquad (2.40)$$

$$E_l\,\tau_l=2\mu\,\bar{v}\,\langle y(x_l)\rangle\langle y(\phi_l)\rangle \qquad (2.41)$$

$$\tau_l=\frac{2\mu\,\bar{v}\,\langle y(x_l)\rangle\langle y(\phi_l)\rangle}{E_l} \qquad (2.42)$$

Where we have introduced the same constraint for both E_l and τ_l ($l=1,2,\ldots,5$) and also suppressed t in (2.42) for clarity of purpose. Thus $E_l=\zeta\,\tau\,\bar{v}$ is the correlated ground-state energy which we have assume as the same as the total energy of the two interacting electrons and it has a unit of kgm^2/s^2 or simply Joules J. Note that on the right hand side of (2.42), x_l has the dimension of length m in the atomic scale. That is one atomic spacing a is equal to 1 Amstrong A^0 ($1A^0=10^{-10}m$).

The Amstrong is the quantum mechanical analogue of length as 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 m/s which is equal to

-0.00028 m/s and finally the angular displacement ϕ_l is in radian. Hence the unit of the correlation time τ_l is seconds s.

To obtain the value for $y(x_l)$, the calculation is simply done as follows: $y(x_l) = X_l \times 10^{-10} \times d_l$ (meters), that is l =1, 2,…, 5 is the lattice separation constant) and d_l is the actual lattice distance ($1, \sqrt{2}, \ldots, \sqrt{8}$), also X_l are the variational parameters.

3.0 PRESENTATION OF RESULTS.

The results of the total energies emerging from the matrix given by (2.24) are shown in Table 3.1 while results of the correlation time τ which is given by equation (2.42) are enumerated in Tables 3.2 below. We should also note that the result of the single band HM with respect to the interaction strength corresponds to $V = H = D = 0$ while that of the gradient Hamiltonian model as a function of the interaction strength (present work) corresponds to $V = H = 0.16, D = 0.64$.

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

$u/4t$	V	H	D	Total Energy $E_l = Eg/t$	Variational Parameters X_l ($l = 0, 1, 2, 3, 4, 5$)					
					X_0	X_1	X_2	X_3	X_4	X_5
50	0.16	0.16	0.64	-8.3103	0.0118	0.3062	0.4223	0.4162	0.5035	0.5487
	0	0	0	-7.7585	0.0131	0.3390	0.4242	0.4538	0.4837	0.5148
40	0.16	0.16	0.64	-8.3117	0.0146	0.3070	0.4225	0.4162	0.5033	0.5483
	0	0	0	-7.7602	0.0162	0.3399	0.4244	0.4537	0.4835	0.5143
30	0.16	0.16	0.64	-8.3139	0.0192	0.3081	0.4228	0.4162	0.5029	0.5475
	0	0	0	-7.7630	0.0214	0.3412	0.4247	0.4537	0.4830	0.5134
20	0.16	0.16	0.64	-8.3183	0.0281	0.3104	0.4233	0.4162	0.5022	0.5461
	0	0	0	-7.7684	0.0313	0.3438	0.4253	0.4535	0.4821	0.5117
10	0.16	0.16	0.64	-8.3300	0.0524	0.3163	0.4246	0.4159	0.5000	0.5420
	0	0	0	-7.7834	0.0587	0.3506	0.4266	0.4528	0.4794	0.5068
5.0	0.16	0.16	0.64	-8.3494	0.0919	0.3256	0.4262	0.4149	0.4958	0.5347
	0	0	0	-7.8084	0.1039	0.3613	0.4279	0.4508	0.4739	0.4978
0.0	0.16	0.16	0.64	-8.4877	0.3491	0.3704	0.4166	0.3897	0.4469	0.4646
	0	0	0	-8.0000	0.4082	0.4082	0.4082	0.4082	0.4082	0.4082
-1.0	0.16	0.16	0.64	-8.7328	0.6435	0.3807	0.3535	0.3118	0.3345	0.3269
	0	0	0	-8.3668	0.7235	0.3949	0.3176	0.2934	0.2695	0.2468
-1.5	0.16	0.16	0.64	-9.1847	0.8461	0.3368	0.2491	0.2025	0.1953	0.1719
	0	0	0	-8.9871	0.8838	0.3300	0.2110	0.1770	0.1442	0.1156
-2.0	0.16	0.16	0.64	-10.2160	0.9433	0.2613	0.1437	0.1039	0.0828	0.0594
	0	0	0	-10.1506	0.9508	0.2556	0.1261	0.0943	0.0643	0.0418
-5.0	0.16	0.16	0.64	-20.8097	0.9946	0.1007	0.0207	0.0115	0.0037	0.0009
	0	0	0	-20.8086	0.9947	0.1005	0.0200	0.0114	0.0034	0.0008
-10	0.16	0.16	0.64	-40.4011	0.9987	0.0501	0.0051	0.0027	0.0004	0.0000
	0	0	0	-40.4010	0.9987	0.0501	0.0050	0.0026	0.0004	0.0000
-15	0.16	0.16	0.64	-60.2670	0.9994	0.0334	0.0022	0.0012	0.0001	0.0000
	0	0	0	-60.2670	0.9994	0.0334	0.0022	0.0012	0.0001	0.0000

Table3.2. Shows the calculated values of the Correlation times τ fo r each separation as a function of the interaction strength $u/4t$. Correlation times τ for arbitrary interaction strength $u/4t = 50, 40$ and 30.

$u/4t$	Total Energy $E_l = Eg/t$	Angular description of lattice separation ϕ_l or ϕ_{vhd}	$y(\phi_l)$ (radian)	Collision Time for each separation (seconds s) $\tau_l (l = 1,2,3,4,5)$; $\tau_0 = 0$				
				τ_1 $\times 10^{-45}$	τ_2 $\times 10^{-45}$	τ_3 $\times 10^{-45}$	τ_4 $\times 10^{-45}$	τ_5 $\times 10^{-45}$
50	-8.3103	$v_1(\theta = 90^0)$	1.5710	2.9498	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	5.8996	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8767	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	8..0190	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	16.0380	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.2303	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.2054	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.4755
40	-8.3117	$v_1(\theta = 90^0)$	1.5710	2.9570	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	5.9140	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8776	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	8.0176	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	16.0354	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.2263	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.2036	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.4688
30	-8.3139	$v_1(\theta = 90^0)$	1.5710	2.9668	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	5.9337	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8789	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	8.0156	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	16.0310	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.2187	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.2003	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.4560

Table 3.3. c.t.d. Collision times τ for arbitrary interaction strength $u/4t = 20, 10$ and 5.

$u/4t$	Total Energy $E_l = Eg/t$	Angular description of lattice separation ϕ_l or ϕ_{vhd}	$y(\phi_l)$ (radian)	Collision Time for each separation (seconds s) $\tau_l (l = 1,2,3,4,5)$; $\tau_0 = 0$				
				τ_1 $\times 10^{-45}$	τ_2 $\times 10^{-45}$	τ_3 $\times 10^{-45}$	τ_4 $\times 10^{-45}$	τ_5 $\times 10^{-45}$
20	-8.3183	$v_1(\theta = 90^0)$	1.5710	2.9874	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	5.9748	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8808	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	8.0114	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	16.0226	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.2048	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.1942	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.4328
10	-8.3300	$v_1(\theta = 90^0)$	1.5710	3.0399	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	6.0798	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8856	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	7.9942	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	15.9886	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.1632	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.1757	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.3666
5.0	-8.3494	$v_1(\theta = 90^0)$	1.5710	3.1220	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	6.2440	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.8900	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	7.9564	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	15.9130	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	7.0866	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	3.1417	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	7.2507

Table 3.4. c. t. d. Collision times τ for arbitrary interaction strength, $u/4t = 0.0$, -1.0 and -1.5.

$u/4t$	Total Energy $E_l = Eg/t$	Angular description of lattice separation ϕ_l or ϕ_{vhd}	$y(\phi_l)$ (radian)	Collision Time for each separation (seconds s) $\tau_l\,(l = 1,2,3,4,5)$; $\tau_0 = 0$				
				τ_1 $\times 10^{-45}$	τ_2 $\times 10^{-45}$	τ_3 $\times 10^{-45}$	τ_4 $\times 10^{-45}$	τ_5 $\times 10^{-45}$
0.0	-8.4877	$v_1(\theta = 90^0)$	1.5710	3.4937	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	6.9874	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.7785	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	7.3516	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	14.7030	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	6.2836	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	2.7857	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	6.1974
-1.0	-8.7328	$v_1(\theta = 90^0)$	1.5710	3.4901	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	6.9802	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	2.2916	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	5.7168	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	11.4338	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	4.5712	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	1.8126	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	4.2381
-1.5	-9.1847	$v_1(\theta = 90^0)$	1.5710	2.9357	--	--	--	--
		$h_1(\alpha = 180^0)$	3.1420	5.8714	--	--	--	--
		$d_2(\lambda = 45^0)$	0.7855	--	1.5353	--	--	--
		$v_3(\theta = 90^0)$	1.5710	--	--	3.5302	--	--
		$h_3(\alpha = 180^0)$	3.1420	--	--	7.0604	--	--
		$d_4(\beta = 63^0)$	1.0473	--	--	--	2.5377	--
		$d_4(\gamma = 26.6^0)$	0.4643	--	--	--	1.1250	--
		$d_5(\lambda = 45^0)$	0.7855	--	--	--	--	2.1190

4.0 DISCUSSION OF RESULTS

Upon comparing the matrices given by (2.23) and (2.24) it is obvious that the vertical and the horizontal gradient which we have introduced in the single band HM do not really make any significant contribution to the kinetic hopping of the two interacting electrons. Hence they do not have any influence on the diagonal elements of the matrix. This is simply because $\cos 180^0$ (-1) and $\sin 90^0$(+1). It is therefore clear that only the diagonal gradient contained in the single band HM that makes absolute contribution to the interacting electrons. However, the introduction of the vertical and the horizontal parameter makes the gradient Hamiltonian model more general and well defined.

It is shown in Table 3.1 that as the interaction strength between the two electrons is decreased the total energy possess by the electrons also decrease and this is consistent with the two models we have employed in this study. However, our present model which is the gradient Hamiltonian model yielded lower results of the variational total energy which is quite preferable since the electrons would prefer to settle down in the region of minimum potential.

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 a result of the fact that the electrons prefer to stay far apart as possible so that the probability of finding them close to one another is reduced.

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 probability of finding the electrons close to one another is increased for high negative values of the interaction strength ($u/4t$).

One remarkable result produced by our work is the values of the variational parameters obtained when the interaction strength between the two electrons is zero ($u/4t = 0$). In this case, the variational parameters produced by the single band Hubbard model are the same, that is when $V = H = D = 0$. This is shown in Table 3.1. The interpretation of this is that in the absence of interaction strength the two electrons have equal probability of being found on any of the lattice separations.

However, the variational parameters produced by the gradient Hamiltonian model are not the same. The interpretation of this is that even in the absence of interaction strength or potential function $u/4t = 0$ there is still an existing residual potential field between the two interacting electrons hence the unequal probability of being found on any of the lattice separations.

It is clear from the table that the results for both models converge to the same value in the large negative U limit. Also the values of the total energies obtained corresponding to each of the interaction strength are negative and non degenerate. The negative values of the total energies show that the interaction between the two electrons is attractive and not repulsive.

It is clear from Tables 3.2, 3.3 and 3.4 that in the positive region of the interaction strength $u/4t$, the correlation time τ_1 increases in value as the interaction strength is decreased, while it decreases in value when the interaction strength is made more negative. This condition is consistent for both vertical and horizontal gradient hopping of the two electrons. Also, the correlation time τ_2 increases with respect to positive values of the interaction strength before it starts to decrease consistently around the value of $u/4t \leq 5$.

Finally the correlation times for τ_3, τ_4 and τ_5 consistently decreases for both regimes of positive and negative the interaction strength. However, the values of the correlation times in the negative regime are much lower than those in the positive regime. Thus generally, high negative interaction strength decreases the correlation time between electrons as they respond to the internal or external agitation forces.

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) 5X5 square lattice. The Hamiltonian are the single band Hubbard model in which case $t^v = t^h = t^d = 0$ and the gradient Hamiltonian model that is, with the inclusion of t^v, t^h and t^d. Obviously, the total energies of the two interacting electrons as a function of the interaction strength 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 high negative interaction strength decreases the correlation time between the interacting electrons. Also our study revealed that both the single band HM and the gradient Hamiltonian model converge to the same values of total energies and variational parameters in the large negative values of the interaction strength.

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