Comparative Study Of Two-Particle Interaction In The Ground-State Of The Gradient Hamiltonian Model

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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) N X N 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. We have shown in this study, 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. This study reveals that when the Coulomb interaction is zero, that is, for free electron system, the variational parameters which describe the probability distribution of lattice electron system is the same.**

Keywords—Hubbard model, correlation time, ground state energy, interacting electrons, v ariational parameters and gradient Hamiltonian model.

I. 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 [2] 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 [3] various important quantities such as momentum distribution and correlation functions, which require an explicit form of the wave function, have not been properly explored [4].

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 [5].

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 [6].

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 [7].

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 [8].

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 [9].

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 [10].

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 [11].

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 wave function 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.

A. 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.

II. Mathematical Theory.

A The single-band Hubbard Hamiltonian (HM).

The single-band Hubbard Hamiltonian (HM) [2] 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.

B. The gradient Hamiltonian model (GHM).

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:

$$H = -t \sum_{\langle ij \rangle \sigma} \left(C_{i\sigma}^{+} C_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - t^{d} \sum_{|i-j|} \tan \beta_{l} \qquad (2.$$

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.

C. The correlated variational approach (CVA) or trial wave function.

The correlated variational approach established by [12] 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) N X N lattices can be found in [13] and [14]. However, because of the complexity of the lattice basis set we are only going to enumerate the relevant information that are suitable to our present study in the tables below.

D. Method of determining the lattice separations for various 2D N X N square lattices.

Let us consider the coordinates of a 2D N X N square lattice which is represented as (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 $\sqrt{(|x_1 - x_2|a)^2 + (|y_1 - y_2|a)^2}$, 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 lattice separation angle is given by $\tan\beta_l = \left(\frac{y_2 - y_1}{x_2 - x_1}\right)$.

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

Lattice separation length l and d_l			Total number of pair electronic states for different 2D N x N square lattices $\|x_1y_1\uparrow, x_2y_2\downarrow\rangle$				
l	$\|\Psi_l\rangle$	d_l	11 x 11	9 x 9	7 x 7	5 x 5	3 x 3
0	$\|\psi_0\rangle$	0	$\|11\uparrow, 11\downarrow\rangle$	$\|11\uparrow, 11\downarrow\rangle$	$\|11\uparrow, 11\downarrow\rangle$	$\|11\uparrow, 11\downarrow\rangle$	$\|11\uparrow, 11\downarrow\rangle$
1	$\|\psi_1\rangle$	a	$\|11\uparrow, 12\downarrow\rangle$	$\|11\uparrow, 12\downarrow\rangle$	$\|11\uparrow, 12\downarrow\rangle$	$\|11\uparrow, 12\downarrow\rangle$	$\|11\uparrow, 12\downarrow\rangle$
2	$\|\psi_2\rangle$	$\sqrt{2}a$	$\|11\uparrow, 22\downarrow\rangle$	$\|11\uparrow, 22\downarrow\rangle$	$\|11\uparrow, 22\downarrow\rangle$	$\|11\uparrow, 22\downarrow\rangle$	$\|11\uparrow, 22\downarrow\rangle$
3	$\|\psi_3\rangle$	$2a$	$\|11\uparrow, 13\downarrow\rangle$	$\|11\uparrow, 13\downarrow\rangle$	$\|11\uparrow, 13\downarrow\rangle$	$\|11\uparrow, 13\downarrow\rangle$	--
4	$\|\psi_4\rangle$	$\sqrt{5}a$	$\|11\uparrow, 23\downarrow\rangle$	$\|11\uparrow, 23\downarrow\rangle$	$\|11\uparrow, 23\downarrow\rangle$	$\|11\uparrow, 23\downarrow\rangle$	--
			$\|11\uparrow, 32\downarrow\rangle$	$\|11\uparrow, 32\downarrow\rangle$	$\|11\uparrow, 32\downarrow\rangle$	$\|11\uparrow, 32\downarrow\rangle$	--
5	$\|\psi_5\rangle$	$\sqrt{8}a$	$\|11\uparrow, 33\downarrow\rangle$	$\|11\uparrow, 33\downarrow\rangle$	$\|11\uparrow, 33\downarrow\rangle$	$\|11\uparrow, 33\downarrow\rangle$	--
6	$\|\psi_6\rangle$	$3a$	$\|11\uparrow, 14\downarrow\rangle$	$\|11\uparrow, 14\downarrow\rangle$	$\|11\uparrow, 14\downarrow\rangle$	--	--
7	$\|\psi_7\rangle$	$\sqrt{10}a$	$\|11\uparrow, 24\downarrow\rangle$	$\|11\uparrow, 24\downarrow\rangle$	$\|11\uparrow, 24\downarrow\rangle$	--	--
8	$\|\psi_8\rangle$	$\sqrt{13}a$	$\|11\uparrow, 34\downarrow\rangle$	$\|11\uparrow, 34\downarrow\rangle$	$\|11\uparrow, 34\downarrow\rangle$	--	--
9	$\|\psi_9\rangle$	$\sqrt{18}a$	$\|11\uparrow, 44\downarrow\rangle$	$\|11\uparrow, 44\downarrow\rangle$	$\|11\uparrow, 44\downarrow\rangle$	--	--
10	$\|\psi_{10}\rangle$	$4a$	$\|11\uparrow, 15\downarrow\rangle$	$\|11\uparrow, 15\downarrow\rangle$	--	--	--
11	$\|\psi_{11}\rangle$	$\sqrt{17}a$	$\|11\uparrow, 25\downarrow\rangle$	$\|11\uparrow, 25\downarrow\rangle$	--	--	--
12	$\|\psi_{12}\rangle$	$\sqrt{20}a$	$\|11\uparrow, 35\downarrow\rangle$	$\|11\uparrow, 35\downarrow\rangle$	--	--	--
13	$\|\psi_{13}\rangle$	$\sqrt{25}a$	$\|11\uparrow, 45\downarrow\rangle$	$\|11\uparrow, 45\downarrow\rangle$	--	--	--
14	$\|\psi_{14}\rangle$	$\sqrt{32}a$	$\|11\uparrow, 55\downarrow\rangle$	$\|11\uparrow, 55\downarrow\rangle$	--	--	--
15	$\|\psi_{15}\rangle$	$5a$	$\|11\uparrow, 16\downarrow\rangle$	--	--	--	--
16	$\|\psi_{16}\rangle$	$\sqrt{26}a$	$\|11\uparrow, 26\downarrow\rangle$	--	--	--	--
17	$\|\psi_{17}\rangle$	$\sqrt{29}a$	$\|11\uparrow, 36\downarrow\rangle$	--	--	--	--
18	$\|\psi_{18}\rangle$	$\sqrt{34}a$	$\|11\uparrow, 46\downarrow\rangle$	--	--	--	--
19	$\|\psi_{19}\rangle$	$\sqrt{41}a$	$\|11\uparrow, 56\downarrow\rangle$	--	--	--	--
20	$\|\psi_{20}\rangle$	$\sqrt{50}a$	$\|11\uparrow, 66\downarrow\rangle$	--	--	--	--

Table 2.2: Relevant information derived from the basis set of the geometry of 2D N X N square lattice. The table gives the Lattice Separation l and actual lattice separation distance d_l .

Lattice separation length l and d_l			11 x 11 $\langle\psi_l\|\psi_l\rangle$	9 x 9 $\langle\psi_l\|\psi_l\rangle$	7 x 7 $\langle\psi_l\|\psi_l\rangle$	5 x 5 $\langle\psi_l\|\psi_l\rangle$	3 x 3 $\langle\psi_l\|\psi_l\rangle$
l	$\|\Psi_l\rangle$	d_l	$(\sigma_l \times N^2)$	$(\sigma_l \times N^2)$	$(\sigma_l \times N^2)$	$(\sigma_l \times N^2)$	$(\sigma_l \times N^2)$
0	$\|\psi_0\rangle$	0	$1\times121=121$	$1\times81=81$	$1\times49=49$	$1\times25=25$	$1\times9=9$
1	$\|\psi_1\rangle$	a	$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	$4\times9=36$
2	$\|\psi_2\rangle$	$\sqrt{2}a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	$4\times9=36$
3	$\|\psi_3\rangle$	$2a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	--
4	$\|\psi_4\rangle$	$\sqrt{5}a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	--
			$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	--
5	$\|\psi_5\rangle$	$\sqrt{8}a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	$4\times25=100$	--
6	$\|\psi_6\rangle$	$3a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	--	--
7	$\|\psi_7\rangle$	$\sqrt{10}a$	$8\times121=968$	$8\times81=648$	$8\times49=392$	--	--
8	$\|\psi_8\rangle$	$\sqrt{13}a$	$8\times121=968$	$8\times81=648$	$8\times49=392$	--	--
9	$\|\psi_9\rangle$	$\sqrt{18}a$	$4\times121=484$	$4\times81=324$	$4\times49=196$	--	--
10	$\|\psi_{10}\rangle$	$4a$	$4\times121=484$	$4\times81=324$	--	--	--
11	$\|\psi_{11}\rangle$	$\sqrt{17}a$	$8\times121=968$	$8\times81=648$	--	--	--
12	$\|\psi_{12}\rangle$	$\sqrt{20}a$	$8\times121=968$	$8\times81=648$	--	--	--
13	$\|\psi_{13}\rangle$	$\sqrt{25}a$	$8\times121=968$	$8\times81=648$	--	--	--
14	$\|\psi_{14}\rangle$	$\sqrt{32}a$	$4\times121=484$	$4\times81=324$	--	--	--
15	$\|\psi_{15}\rangle$	$5a$	$4\times121=484$	--	--	--	--
16	$\|\psi_{16}\rangle$	$\sqrt{26}a$	$8\times121=968$	--	--	--	--
17	$\|\psi_{17}\rangle$	$\sqrt{29}a$	$8\times121=968$	--	--	--	--
18	$\|\psi_{18}\rangle$	$\sqrt{34}a$	$8\times121=968$	--	--	--	--
19	$\|\psi_{19}\rangle$	$\sqrt{41}a$	$8\times121=968$	--	--	--	--
20	$\|\psi_{20}\rangle$	$\sqrt{50}a$	$4\times121=484$	--	--	--	--
$(N\ X\ N)^2$			14641	6561	2401	625	81

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

Lattice separation length l and d_l			Total number of pair electronic states for different 2D N x N square lattices $\langle\psi_l\|\psi_l\rangle$						
l	$\|\Psi_l\rangle$	d_l	$\|x_1y_1\uparrow, x_2y_2\downarrow\rangle$	Number of NN σ_l	11 X 11	9 X 9	7 X 7	5 X 5	3 X 3
0	$\|\psi_0\rangle$	0	$\|11\uparrow, 11\downarrow\rangle$	1 (on-site)	121	81	49	25	9
1	$\|\psi_1\rangle$	a	$\|11\uparrow, 12\downarrow\rangle$	4 (linear)	484	324	196	100	36
2	$\|\psi_2\rangle$	$\sqrt{2}a$	$\|11\uparrow, 22\downarrow\rangle$	4(diagonal)	484	324	196	100	36
3	$\|\psi_3\rangle$	$2a$	$\|11\uparrow, 13\downarrow\rangle$	4 (linear)	484	324	196	100	--
4	$\|\psi_4\rangle$	$\sqrt{5}a$	$\|11\uparrow, 23\downarrow\rangle$	4(diagonal)	484	324	196	100	--
			$\|11\uparrow, 32\downarrow\rangle$	4(diagonal)	484	324	196	100	--
5	$\|\psi_5\rangle$	$\sqrt{8}a$	$\|11\uparrow, 33\downarrow\rangle$	4(diagonal)	484	484 324	196	100	--
6	$\|\psi_6\rangle$	$3a$	$\|11\uparrow, 14\downarrow\rangle$	4 (linear)	484	324	196	--	--
7	$\|\psi_7\rangle$	$\sqrt{10}a$	$\|11\uparrow, 24\downarrow\rangle$	8 (diagonal)	968	648	392	--	--
8	$\|\psi_8\rangle$	$\sqrt{13}a$	$\|11\uparrow, 34\downarrow\rangle$	8 (diagonal)	968	648	392	--	--
9	$\|\psi_9\rangle$	$\sqrt{18}a$	$\|11\uparrow, 44\downarrow\rangle$	4(diagonal)	484	324	196	--	--
10	$\|\psi_{10}\rangle$	$4a$	$\|11\uparrow, 15\downarrow\rangle$	4 (linear)	484	324	--	--	--
11	$\|\psi_{11}\rangle$	$\sqrt{17}a$	$\|11\uparrow, 25\downarrow\rangle$	8 (diagonal)	968	648	--	--	--
12	$\|\psi_{12}\rangle$	$\sqrt{20}a$	$\|11\uparrow, 35\downarrow\rangle$	8 (diagonal)	968	648	--	--	--
13	$\|\psi_{13}\rangle$	$\sqrt{25}a$	$\|11\uparrow, 45\downarrow\rangle$	8 (diagonal)	968	648	--	--	--
14	$\|\psi_{14}\rangle$	$\sqrt{32}a$	$\|11\uparrow, 55\downarrow\rangle$	4(diagonal)	484	324	--	--	--
15	$\|\psi_{15}\rangle$	$5a$	$\|11\uparrow, 16\downarrow\rangle$	4 (linear)	484	--	--	--	--
16	$\|\psi_{16}\rangle$	$\sqrt{26}a$	$\|11\uparrow, 26\downarrow\rangle$	8 (diagonal)	968	--	--	--	--
17	$\|\psi_{17}\rangle$	$\sqrt{29}a$	$\|11\uparrow, 36\downarrow\rangle$	8 (diagonal)	968	--	--	--	--
18	$\|\psi_{18}\rangle$	$\sqrt{34}a$	$\|11\uparrow, 46\downarrow\rangle$	8 (diagonal)	968	--	--	--	--
19	$\|\psi_{19}\rangle$	$\sqrt{41}a$	$\|11\uparrow, 56\downarrow\rangle$	8 (diagonal)	968	--	--	--	--
20	$\|\psi_{20}\rangle$	$\sqrt{50}a$	$\|11\uparrow, 66\downarrow\rangle$	4(diagonal)	484	--	--	--	--
$(N\ X\ N)^2$					14641	6561	2401	625	81

Note that NN is the nearest neighbour.

Table 2.4: Relevant information on the angular displacement derived from the basis set of the geometry of 2D N x N square lattice for only diagonal lattice sites.

Lattice separation length l		11 x 11 $\langle\psi_l\|\psi_l\rangle$		9 x 9 $\langle\psi_l\|\psi_l\rangle$		7 x 7 $\langle\psi_l\|\psi_l\rangle$		5 x 5 $\langle\psi_l\|\psi_l\rangle$		3 x 3 $\langle\psi_l\|\psi_l\rangle$	
l	$\|\Psi_l\rangle$	D_l	$\tan\beta_l$	D_l	$\tan\beta_l$	D_l	$\tan\beta_l$	D_l	$\tan\beta_l$	D_l	$\tan\beta_l$
2	$\sqrt{2}a$	0.0331	1.00	0.0494	1.0	0.0816	1.00	0.1600	1.00	0.0124	1.00
4	$\sqrt{5}a$	0.0331	2.00	0.0494	2.0	0.0816	2.00	0.1600	2.00	--	--
		0.0331	0.50	0.0494	0.5	0.0816	0.50	0.1600	0.50	--	--
5	$\sqrt{8}a$	0.0331	1.00	0.0494	1.0	0.0816	1.00	0.1600	1.00	--	--
7	$\sqrt{10}a$	0.0661	3.00	0.0988	3.0	0.1633	3.00	--	--	--	--
8	$\sqrt{13}a$	0.0661	1.50	0.0988	1.5	0.1633	1.50	--	--	--	--
9	$\sqrt{18}a$	0.0331	1.00	0.0494	1.0	0.0816	1.00	--	--	--	--
11	$\sqrt{17}a$	0.0661	4.00	0.0988	4.00	--	--	--	--	--	--
12	$\sqrt{20}a$	0.0661	2.00	0.0988	2.00	--	--	--	--	--	--
13	$\sqrt{25}a$	0.0661	1.33	0.0988	1.33	--	--	--	--	--	--
14	$\sqrt{32}a$	0.0331	1.00	0.0494	1.00	--	--	--	--	--	--
16	$\sqrt{26}a$	0.0661	5.00	--	--	--	--	--	--	--	--
17	$\sqrt{29}a$	0.0661	2.50	--	--	--	--	--	--	--	--
18	$\sqrt{34}a$	0.0661	1.66	--	--	--	--	--	--	--	--
19	$\sqrt{41}a$	0.0661	1.25	--	--	--	--	--	--	--	--
20	$\sqrt{50}a$	0.0331	1.00	--	--	--	--	--	--	--	--

The ratio D_l is found from the division of the pair electronic states in each separation by the total number of electronic states. For example, $D_2 = 324/6561 = 0.0494$.

Table 2.5: Electronic states available to the two interacting electrons in a 2D N X N even square lattice

Lattice Dimension	Dimension of matrix	Central lattice site Even	Number of separation length l Even	Number of electronic state	Number of on-site electrons
2D $(N \times N)$	N x N	$\left(\frac{N}{2}, \frac{N}{2}\right)$	$\left(\frac{(N+4)(N+2)}{8}\right)$	$(N \times N)^2$	$(N \times N)$
4 X 4	6 x 6	(2 , 2)	6	256	16
6 X 6	10 x 10	(3 , 3)	10	1296	36
8 X 8	15 x 15	(4 , 4)	15	4096	64
10 X 10	21 x 21	(5 , 5)	21	10000	100
12 X 12	28 x 28	(6 , 6)	28	20736	144

Table 2.6: Electronic states available to the two interacting electrons in a 2D N X N odd square lattice.

Lattice Dimension	Dimension of matrix	Central lattice site Odd	Number of separation length l Odd	Number of electronic state	Number of on-site electrons
2D $(N \times N)$	N x N	$\left(\frac{N+1}{2}, \frac{N+1}{2}\right)$	$\left(\frac{(N+3)(N+1)}{8}\right)$	$(N \times N)^2$	$(N \times N)$
3 X 3	3 x 3	(2 , 2)	3	81	9
5 X 5	6 x 6	(3 , 3)	6	625	25
7 X 7	10 x 10	(4 , 4)	10	2407	49
9 X 9	15 x 15	(5 , 5)	15	6561	81
11 X 11	21 x 21	(6 , 6)	21	14641	121

E. Evaluation of the quantum state functions $\langle \Psi | \Psi \rangle$ and $\langle \Psi | H | \Psi \rangle$ of the two interacting electrons.

We shall in this work show clearly the operation of the gradient Hamiltonian given by (2.2) on (2.4) only for the case of 2D 7 X 7 square lattice and assume the same procedure for the other 2D N X N square lattices.

There are two basic quantum constraints or gauge which must be duly followed in this aspect of the work. The constraints are that:

(i) the field strength tensor

$$\langle i \mid j \rangle = \delta_{i\,j} \begin{cases} 1 & iff \quad i = j \\ 0 & iff \quad i \neq j \end{cases} \qquad (2.5)$$

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

$$\mid i\uparrow,\, j\downarrow \rangle = -\mid j\downarrow,\, i\uparrow \rangle \qquad (2.6)$$

Hence with these two basic constraints we can solve for the inner product $\langle \Psi | \Psi \rangle$ of the variational trial wave function and the activation of the Gradient Hamiltonian model on the trial wave function $\langle \Psi | H | \Psi \rangle$.

F. Determination of $\langle \Psi | \Psi \rangle$ and $\langle \Psi | H | \Psi \rangle$ for 2D 7 X 7 square lattices.

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 - 2.2 we get

$$\mid \Psi \rangle = X_0 \mid \psi_0 \rangle + X_1 \mid \psi_1 \rangle + X_2 \mid \psi_2 \rangle + X_3 \mid \psi_3 \rangle + X_4 \mid \psi_4 \rangle + X_5 \mid \psi_5 \rangle + X_6 \mid \psi_6 \rangle + X_7 \mid \psi_7 \rangle + X_8 \mid \psi_8 \rangle + X_9 \mid \psi_9 \rangle \qquad (2.7)$$

$$\langle \Psi | \Psi \rangle = X_0^2 \langle \psi_0 | \psi_0 \rangle + X_1^2 \langle \psi_1 | \psi_1 \rangle + X_2^2 \langle \psi_2 | \psi_2 \rangle + X_3^2 \langle \psi_3 | \psi_3 \rangle + X_4^2 \langle \psi_4 | \psi_4 \rangle + X_5^2 \langle \psi_5 | \psi_5 \rangle + X_7^2 \langle \psi_7 | \psi_7 \rangle + X_8^2 \langle \psi_8 | \psi_8 \rangle + X_9^2 \langle \psi_9 | \psi_9 \rangle \qquad (2.8)$$

$$\langle \Psi | \Psi \rangle = 49 \Big\{ X_0^2 + 4X_1^2 + 4X_2^2 + 4X_3^2 + 8X_4^2 + 4X_5^2 + 4X_6^2 + 8X_7^2 + 8X_8^2 + 4X_9^2 \Big\} \qquad (2.9)$$

When we carefully use equation (2.2) to act on equation (2.7), with the proper application of the information provided in Tables 2.1 and 2.3 we get as follows.

$$H|\Psi\rangle = -t\Big\{2X_0|\psi_1\rangle + 8X_1|\psi_0\rangle + 4X_1|\psi_2\rangle + 2X_1|\psi_3\rangle + 2X_2|\psi_4\rangle + 4X_2|\psi_1\rangle + 2X_3|\psi_1\rangle + 2X_3|\psi_4\rangle + 2X_3|\psi_6\rangle + 4X_4|\psi_2\rangle + 4X_4|\psi_3\rangle + 4X_4|\psi_5\rangle + 2X_4|\psi_7\rangle + 2X_5|\psi_4\rangle + 2X_5|\psi_8\rangle + 2X_6|\psi_3\rangle + 2X_6|\psi_6\rangle + 2X_6|\psi_7\rangle + 2X_7|\psi_4\rangle + 4X_7|\psi_6\rangle + 2X_7|\psi_7\rangle + 2X_7|\psi_8\rangle + 4X_8|\psi_5\rangle + 2X_8|\psi_7\rangle + 2X_8|\psi_8\rangle + 4X_8|\psi_9\rangle + 2X_9|\psi_8\rangle + 4X_9|\psi_9\rangle - U X_0|\psi_0\rangle\Big\}$$
$$-t^d \Big\{X_2 \tan\beta_2 \mid \psi_2\rangle + X_4 (\tan\beta_4^1 \mid \psi_4\rangle + \tan\beta_4^2 \mid \psi_4\rangle) + X_5 \tan\beta_5 \mid \psi_5\rangle + X_7 \tan\beta_7 \mid \psi_7\rangle + X_8 \tan\beta_8 \mid \psi_8\rangle + X_9 \tan\beta_9 \mid \psi_9\rangle\Big\} \qquad (2.10)$$

$$\langle\Psi|H|\Psi\rangle = -t\Big\{2X_0X_1\langle\psi_1|\psi_1\rangle + 8X_1X_0\langle\psi_0|\psi_0\rangle + 4X_1X_2\langle\psi_2|\psi_2\rangle + 2X_1X_3\langle\psi_3|\psi_3\rangle + 2X_2X_4\langle\psi_4|\psi_4\rangle + 4X_2X_1\langle\psi_1|\psi_1\rangle + 2X_3X_1\langle\psi_1|\psi_1\rangle + 2X_3X_4\langle\psi_4|\psi_4\rangle + 2X_3X_6\langle\psi_6|\psi_6\rangle + 4X_4X_2\langle\psi_2|\psi_2\rangle + 4X_4X_3\langle\psi_3|\psi_3\rangle + 4X_4X_5\langle\psi_5|\psi_5\rangle + 2X_4X_7\langle\psi_7|\psi_7\rangle + 2X_5X_4\langle\psi_4|\psi_4\rangle + 2X_5X_8\langle\psi_8|\psi_8\rangle + 2X_6X_3\langle\psi_3|\psi_3\rangle + 2X_6X_7\langle\psi_7|\psi_7\rangle +$$

$$+2X_7X_4\langle\psi_4|\psi_4\rangle+ 4X_7X_6\langle\psi_6|\psi_6\rangle+2X_7X_8\langle\psi_8|\psi_8\rangle+ 4X_8X_5\langle\psi_5|\psi_5\rangle+ 2X_8X_7\langle\psi_7|\psi_7\rangle+4X_8X_9\langle\psi_9|\psi_9\rangle+$$

$$2X_9X_8\langle\psi_8|\psi_8\rangle + 2X_{10}X_6\langle\psi_6|\psi_6\rangle+ 2X_{11}X_7\langle\psi_7|\psi_7\rangle+ 2X_{12}X_8\langle\psi_8|\psi_8\rangle+ 4X_{13}X_9\langle\psi_9|\psi_9\rangle -U\,X_0X_0\langle\psi_0|\psi_0\rangle\}$$

$$-t^d\ \{X_2^2\tan\beta_2\langle\ \psi_2|\ \psi_2\rangle+X_4^2(\tan\beta_4^1\langle\ \psi_4|\ \psi_4\rangle+\tan\beta_4^2\langle\ \psi_4|\ \psi_4\rangle)+$$

$$X_5^2\tan\beta_5\langle\psi_5|\psi_5\rangle+X_7^2\tan\beta_7\langle\psi_7|\psi_7\rangle+X_8^8\tan\beta_8\langle\psi_8|\psi_8\rangle+X_9^2\tan\beta_9\langle\psi_9|\psi_9\rangle\ \} \qquad (2.11)$$

$$\langle\Psi|H|\Psi\rangle=-49(t)\{16X_0X_1+32X_1X_2+16X_1X_3+32X_2X_4+32X_3X_4+16X_3X_6+32X_4X_5+$$

$$32X_4X_7+32X_5X_8+32X_6X_7+32X_7X_8+32X_8X_9+8X_6^2+16X_7^2+16X_8^2+16X_9^2-4(U/4t)X_0^2\}$$

$$8X_{10}^2+16X_{11}^2+16X_{12}^2+16X_{13}^2+16X_{14}^2-4(U/4t)X_0^2\}-49(t^d)\{4X_2^2\tan\beta_2+4X_4^2(\tan\beta_4^1+\tan\beta_4^2)+$$

$$4X_5^2\tan\beta_5+8X_7^2\tan\beta_7+8X_8^2\tan\beta_8+4X_9^2\tan\beta_9\ \} \qquad (2.12)$$

Again we should understand that the values of $\langle\Psi_l|\Psi_l\rangle$ is clearly stated in Tables 2.2 - 2.3.

G. Results of the $\langle\Psi|\Psi\rangle$ and $\langle\Psi|H|\Psi\rangle$ for the other 2D N X N square lattices.

We can now tactically follow the same procedure that led to the realization of equations (2.9) and (2.12) for the rest of the 2D N X N square lattices whose results are also clearly stated below.

(i) 2D 3 X 3 square lattice.

$$\langle\Psi|\Psi\rangle=9(X_0^2+4X_1^2+4X_2^2) \qquad (2.13)$$

$$\langle\Psi|H|\Psi\rangle=-9\{16X_0X_1+32X_1X_2+8X_1^2+16X_2^2-4(U/4t)X_0^2\}-9t^d(4X_2^2\tan\beta_2) \qquad (2.14)$$

(ii) 2D 5 X 5 square lattice.

$$\langle\Psi|\Psi\rangle=25(X_0^2+4X_1^2+4X_2^2+4X_3^2+8X_4^2+4X_5^2) \qquad (2.15)$$

$$\langle\Psi|H|\Psi\rangle=-(25)(4t)\{4X_0X_1+8X_1X_2+4X_1X_3+8X_2X_4+8X_3X_4+8X_4X_5+$$

$$2X_3^2+4X_4^2+4X_5^2-$$

$$(U/4t)X_0^2\}-$$

$$t^d\{X_2^2\langle\psi_2|\psi_2\rangle\tan\beta_2+X_4^2\langle\psi_4|\psi_4\rangle\tan\beta_4^1+X_4^2\langle\psi_4|\psi_4\rangle\tan\beta_4^2+X_5^2\langle\psi_5|\psi_5\rangle\tan\beta_5\} \qquad (2.16)$$

$$\langle\Psi|H|\Psi\rangle=-25(t)\ \{16X_0X_1+32X_1X_2+16X_1X_3+32X_2X_4+32X_3X_4+32X_4X_5+8X_3^2+16X_4^2+$$

$$16X_5^2-4(U/4t)X_0^2\}-25(t^d)\{4X_2^2\tan\beta_2+4X_4^2(\tan\beta_4^1+\tan\beta_4^2)+4X_5^2\tan\beta_5\ \} \qquad (2.17)$$

(iii) 2D 9 X 9 square lattice.

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

$$4X_{14}^2\} \qquad (2.18)$$

$$\langle\Psi|H|\Psi\rangle=-(81)(t)\{16X_0X_1+32X_1X_2+16X_1X_3+32X_2X_4+32X_3X_4+16X_3X_6+32X_4X_5+32X_4X_7+$$

$$32X_5X_8+32X_6X_7+16X_6X_{10}+32X_7X_8+32X_7X_{11}+32X_8X_9+32X_8X_{12}+32X_9X_{13}+32X_{10}X_{11}+32X_{11}X_{12}+$$

$$32X_{12}X_{13}+32X_{13}X_{14}+8X_{10}^2+16X_{11}^2+16X_{12}^2+16X_{13}^2+16X_{14}^2-4(U/4t)X_0^2\}-(81)(t^d)\{4X_2^2\tan\beta_2+4X_4^2(\tan\beta_4^1+$$

$$\tan\beta_4^2)+4X_5^2\tan\beta_5+8X_7^2\tan\beta_7+8X_8^2\tan\beta_8+4X_9^2\tan\beta_9+8X_{11}^2\tan\beta_{11}+8X_{12}^2\tan\beta_{12}+8X_{13}^2\tan\beta_{13}+4X_{14}^2$$

$$\tan\beta_{14}\} \qquad (2.19)$$

(iv) 2D 11 X 11 square lattice.

$$\langle\Psi|\Psi\rangle=121\{X_0^2+4X_1^2+4X_2^2+4X_3^2+4X_4^2+4X_5^2+4X_6^2+8X_7^2+8X_8^2+4X_9^2+4X_{10}^2+8X_{11}^2+8X_{12}^2+8X_{13}^2+$$

$$4X_{14}^2 4X_{15}^2+8X_{16}^2+8X_{17}^2+8X_{18}^2+8X_{19}^2+4X_{20}^2 \Big\} \qquad (2.20)$$

$$\langle\Psi|H|\Psi\rangle = -121\,t\,\{16X_0X_1+32X_1X_2+16X_1X_3+32X_2X_4+32X_3X_4+16X_3X_6+32X_4X_5+32X_4X_7+$$

$$32X_5X_8+32X_6X_7+16X_6X_{10}+32X_7X_8+32X_7X_{11}+32X_8X_9+32X_8X_{12}+32X_9X_{13}+32X_{10}X_{11}+$$

$$16X_{10}X_{15}+32X_{11}X_{12}+32X_{11}X_{16}+32X_{12}X_{13}+32X_{12}X_{17}+32X_{13}X_{14}+32X_{13}X_{18}+32X_{14}X_{19}+32X_{15}X_{16}+$$

$$32X_{16}X_{17}+32X_{17}X_{18}+32X_{18}X_{19}+32X_{19}X_{20}+8X_{15}^2+16X_{16}^2+16X_{17}^2+16X_{18}^2+16X_{19}^2+16X_{20}^2-4\left(\frac{U}{4t}\right)X_0^2\Big\}$$

$$-(81)(t^d)\Big\{4X_2^2\tan\beta_2+4X_4^2(\tan\beta_4^1+\tan\beta_4^2)+4X_5^2\tan\beta_5+8X_7^2\tan\beta_7+8X_8^2\tan\beta_8+4X_9^2\tan\beta_9+8X_{11}^2\tan\beta_{11}+8$$

$$X_{12}^2\tan\beta_{12}+8X_{13}^2\tan\beta_{13}+4X_{14}^2\tan\beta_{14}+8X_{16}^2\tan\beta_{16}+$$

$$8X_{17}^2\tan\beta_{17}+8X_{18}^2\tan\beta_{18}+8X_{19}^2\tan\beta_{19}+4X_{20}^2\tan\beta_{20}\Big\} \qquad (2.21)$$

H. The variational theory of the two interacting electrons.

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

$$E_g\langle\Psi|\Psi\rangle=\langle\Psi|H|\Psi\rangle=\langle\Psi|H_t+H_u+H_{td}|\Psi\rangle \quad (2.22)$$

Where E_g is the correlated ground-state energy while Ψ is the guessed trial wave function. We can now differentially minimize (2.9) and (2.12) using the below equations.

$$\langle\Psi|\Psi\rangle\frac{\partial E_g}{\partial X_i}+E_g\frac{\partial}{\partial X_i}\langle\Psi|\Psi\rangle=\frac{\partial}{\partial X_i}\langle\Psi|H|\Psi\rangle \quad (2.23)$$

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

$$\frac{\partial E_g}{\partial X_i}=0 \quad ; \quad \forall\, i=0,1,2,3 \qquad (2.24)$$

Now in this work we are only going to evaluate that of 2D 7 X 7 lattices and assume the same procedure for the rest ones. Hence upon the substitution of (2.9) and (2.12) into (2.23) and also dividing all through the resulting equation by $81t$ we get the following equation.

$$E\ \Big\{X_0^2+4X_1^2+4X_2^2+4X_3^2+8X_4^2+4X_5^2+4X_6^2+8X_7^2+8X_8^2+4X_9^2\Big\}=-\{16X_0X_1+32X_1X_2+16X_1X_3+$$

$$32X_2X_4+32X_3X_4+16X_3X_6+32X_4X_5+32X_4X_7+32X_5X_8+32X_6X_7+32X_7X_8+32X_8X_9+8X_6^2+$$

$$16X_7^2+16X_8^2+16X_9^2-4(U/4t)X_0^2\Big\}-\Big\{4X_2^2D_2\tan\beta_2+4X_4^2(D_4^1\tan\beta_4^1+D_4^2\tan\beta_4^2)+4X_5^2D_5\tan\beta_5+$$

$$8X_7^2D_7\tan\beta_7+8X_8^2D_8\tan\beta_8+4X_9^2D_9\tan\beta_9\Big\} \qquad (2.25)$$

Where $U/4t=u$ 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) are the ratios of the individual diagonal kinetic hopping to the total number of lattice separations or total kinetic hopping sites respectively as stated in Table 2.4.

$$2EX_0=-16X_1+8(U/4t)X_0 \qquad (2.26)$$

$$8EX_1=-16X_0-32X_2-16X_3 \qquad (2.27)$$

$$8EX_2=-32X_1-32X_4-8D_2X_2\tan\beta_2 \qquad (2.28)$$

$$8EX_3=-16X_1-32X_4-16X_6 \qquad (2.29)$$

$$16EX_4=-32X_2-32X_3-32X_5-32X_7-8X_4(D_4^1\tan\beta_4^1+D_4^2\tan\beta_4^2)$$

(2.30)

$$8EX_5=-32X_4-32X_8-8D_5X_5\tan\beta_5 \quad (2.31)$$

$$8EX_6=-16X_3-32X_7-16X_6 \qquad (2.32)$$

$$16EX_7=-32X_4-32X_6-32X_8-32X_7-16D_7X_7\tan\beta_7$$

(2.33)

$$16EX_8=-32X_5-32X_7-32X_8-32X_9-16D_8X_8\tan\beta_8$$

(2.34)

$$8EX_9=-32X_8-32X_9-8D_9X_9\tan\beta_9 \quad (2.35)$$

However, we can carefully transform the equations given by (2.26) – (2.35) into a homogeneous eigen value problem of the form

$$[A-\lambda_l\,I]X_l=0 \qquad (2.36)$$

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. The values of D_l and $\tan\beta_l$ are clearly indicated in Table 2.4.

After careful simplifications we get a 10 x 10 matrix from (2.36) which is shown in equation (2.37) below. From the resulting matrix we can now determine the total energies or the ground-state energies, and the corresponding variational parameters for various arbitrary values of the interaction strength u .

$$\begin{pmatrix} E-4u & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & E+0.0816 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & E & 4 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 2 & E+0.102 & 2 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & E+0.0816 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & E+2 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 2 & E+2.4899 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & E+2.2449 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & E+4.0816 \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad (2.37)$$

We used Matlab 7.5 version in the computation of the total energies and variational parameters corresponding to various arbitrary values of the interaction strength u . The result emerging from this is shown in the next session.

III. Presentation of Results.

The results emerging from the matrix given by (2.37) are shown in Tables 3.1 and 3.2. The result of the single-band HM with respect to the interaction strength by [12] is denoted as previous study, while that of our study emerging from the application of the gradient Hamiltonian model is denoted as the present study. In this section we also compared our work with the ones emerging from the exact calculation using Guzwiller variational approach (GVA) [16] and the correlated variational approach (CVA) [12]. We also simulate the possible equation for exact calculation and also compared the result with our present study.

Table3.1. shows the calculated values of the total energies E_l and the variational parameters X_l as a function of some arbitrary values of the interaction strength $u/4t$ for X_l ($l = 0, 1, 2, 3, 4$)

Interaction strength $u/4t$	Present and *Previous study	Total Energy E_l	Variational Parameters (2D 7 X 7 square lattice) X_l ($l = 0, 1, 2, 3, 4$)				
			X_0	X_1	X_2	X_3	X_4
50.00	Present	-8.0758	0.0080	0.2091	0.2682	0.3000	0.3269
	Previous	-7.8929	0.0086	0.2245	0.2820	0.3135	0.3319
40.00	Present	-8.0763	0.0100	0.2098	0.2686	0.3002	0.3269
	Previous	-7.8936	0.0107	0.2253	0.2823	0.3137	0.3319
30.00	Present	-8.0773	0.0132	0.2109	0.2691	0.3004	0.3270
	Previous	-7.8947	0.0142	0.2265	0.2829	0.3139	0.3319
20.00	Present	-8.0791	0.0193	0.2130	0.2701	0.3008	0.3271
	Previous	-7.8968	0.0208	0.2288	0.2841	0.3144	0.3320
10.00	Present	-8.0841	0.0364	0.2187	0.2729	0.3020	0.3273
	Previous	-7.9028	0.0393	0.2351	0.2871	0.3156	0.3321
5.00	Present	-8.0926	0.0650	0.2282	0.2773	0.3036	0.3273
	Previous	-7.9129	0.0704	0.2456	0.2920	0.3173	0.3320
0.00	Present	-8.1635	0.2868	0.2926	0.3012	0.3054	0.3158
	Previous	-8.0000	0.3162	0.3162	0.3162	0.3162	0.3162
-1.00	Present	-8.3544	0.6537	0.3558	0.2888	0.2550	0.2414
	Previous	-8.2439	0.6971	0.3698	0.2890	0.2491	0.2259
-1.50	Present	-8.9001	0.8888	0.3222	0.1995	0.1461	0.1175
	Previous	-8.8660	0.8973	0.3214	0.1938	0.1400	0.1082
-2.00	Present	-10.1060	0.9548	0.2514	0.1200	0.0754	0.0493
	Previous	-10.0987	0.9557	0.2507	0.1180	0.0742	0.0473
-2.50	Present	-11.6571	0.9747	0.2019	0.0783	0.0454	0.0248
	Previous	-11.6547	0.9749	0.2016	0.0775	0.0451	0.0242
-5.00	Present	-20.8078	0.9942	0.1004	0.0200	0.0104	0.0030
	Previous	-20.8077	0.9947	0.1004	0.0199	0.0103	0.0030
-10.00	Present	-40.4010	0.9987	0.0501	0.0050	0.0025	0.0004
	Previous	-40.4010	0.9987	0.0501	0.0050	0.0025	0.0004
-15.00	Present	-60.2670	0.9994	0.0334	0.0022	0.0011	0.0001
	Previous	-60.2670	0.9994	0.0334	0.0022	0.0011	0.0001

Table 3.2. Shows the calculated values of the total energies E_l and the variational parameters X_l as a function of some arbitrary values of the interaction strength $u/4t$ for X_l ($l = 5, 6, 7, 8, 9$)

Interaction strength $u/4t$	Present and *Previous study	Total Energy E_l	Variational Parameters (2D 7 X 7 square lattice) X_l ($l = 5, 6, 7, 8, 9$)				
			X_5	X_6	X_7	X_8	X_9
50.00	Present	-8.0758	0.3557	0.3485	0.3793	0.3841	0.3848
	Previous	-7.8929	0.3568	0.3490	0.3574	0.3722	0.3824
40.00	Present	-8.0763	0.3556	0.3484	0.3792	0.3839	0.3844
	Previous	-7.8936	0.3567	0.3489	0.3572	0.3719	0.3821
30.00	Present	-8.0773	0.3554	0.3483	0.3790	0.3835	0.3839
	Previous	-7.8947	0.3564	0.3488	0.3570	0.3715	0.3816
20.00	Present	-8.0791	0.3551	0.3481	0.3786	0.3828	0.3830
	Previous	-7.8968	0.3560	0.3485	0.3565	0.3707	0.3805
10.00	Present	-8.0841	0.3539	0.3473	0.3773	0.3808	0.3805
	Previous	-7.9028	0.3546	0.3476	0.3551	0.3684	0.3776
5.00	Present	-8.0926	0.3517	0.3458	0.3749	0.3771	0.3761
	Previous	-7.9129	0.3519	0.3457	0.3524	0.3641	0.3722
0.00	Present	-8.1635	0.3230	0.3221	0.3436	0.3368	0.3300
	Previous	-8.0000	0.3162	0.3162	0.3162	0.3162	0.3162
-1.00	Present	-8.3544	0.2200	0.2266	0.2324	0.2136	0.1999
	Previous	-8.2439	0.1971	0.2053	0.1959	0.1803	0.1699
-1.50	Present	-8.9001	0.0845	0.0928	0.0871	0.0687	0.0570
	Previous	-8.8660	0.0740	0.0827	0.0719	0.0559	0.0459
-2.00	Present	-10.1060	0.0259	0.0310	0.0252	0.0156	0.0104
	Previous	-10.0987	0.0241	0.0293	0.0223	0.0137	0.0090
-2.50	Present	-11.6571	0.0102	0.0133	0.0093	0.0047	0.0035
	Previous	-11.6547	0.0098	0.0129	0.0086	0.0043	0.0022
-5.00	Present	-20.8078	0.0006	0.0012	0.0005	0.0001	0.0000
	Previous	-20.8077	0.0006	0.0012	0.0005	0.0001	0.0000
-10.00	Present	-40.4010	0.0000	0.0001	0.0000	0.0000	0.0000
	Previous	-40.4010	0.0000	0.0001	0.0000	0.0000	0.0000
-15.00	Present	-60.2670	0.0000	0.0000	0.0000	0.0000	0.0000
	Previous	-60.2670	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3.3: Results of the ground-state energy obtained in present study compared with previous study.

Interaction strength $u/4t$	Present and *Previous study	Total Energy E_l 2D N X N Square lattices				
		3 X 3	5 X 5	7 X 7	9 X 9	11 X 11
50.00	Present	-7.2140	-8.3103	-8.0758	-8.0925	-8.0811
	Previous	-7.1525	-7.7585	-7.8929	-7.9411	-7.9633
40.00	Present	-7.2210	-8.3117	-8.0763	-8.0928	-8.0813
	Previous	-7.1596	-7.7602	-7.8936	-7.9414	-7.9635
30.00	Present	-7.2324	-8.3139	-8.0773	-8.0932	-8.0816
	Previous	-7.1712	-7.7630	-7.8947	-7.9420	-7.9638
20.00	Present	-7.2544	-8.3183	-8.0791	-8.0942	-8.0821
	Previous	-7.1936	-7.7684	-7.8968	-7.9431	-7.9644
10.00	Present	-7.3144	-8.3300	-8.0841	-8.0968	-8.0837
	Previous	-7.2546	-7.7834	-7.9028	-7.9461	-7.9662
5.00	Present	-7.4126	-8.3494	-8.0926	-8.1012	-8.0863
	Previous	-7.3546	-7.8084	-7.9129	-7.9513	-7.9693
0.00	Present	-8.0445	-8.4877	-8.1635	-8.1409	-8.1115
	Previous	-8.0000	-8.0000	-8.0000	-8.0000	-8.0000
-1.00	Present	-8.7740	-8.7328	-8.3544	-8.2829	-8.2297
	Previous	-8.7446	-8.3668	-8.2439	-8.1878	-8.1580
-1.50	Present	-9.5119	-9.1847	-8.9001	-8.8564	-8.8397
	Previous	-9.4931	-8.9871	-8.8660	-8.8348	-8.8268
-2.00	Present	-10.6040	-10.2160	-10.1060	-10.0974	-10.0949
	Previous	-10.5941	-10.1506	-10.0987	-10.0926	-10.0919
-2.50	Present	-12.0048	-11.7464	-11.6571	-11.6550	-11.6543
	Previous	-12.0000	-11.7218	-11.6547	-11.6533	-11.6532
-5.00	Present	-20.8919	-20.8097	-20.8078	-20.8078	-20.8077
	Previous	-20.8916	-20.8086	-20.8077	-20.8077	-20.8077
-10.00	Present	-40.4213	-40.4011	-40.4010	-40.4010	-40.4010
	Previous	-40.4213	-40.4010	-40.4010	-40.4010	-40.4010
-15.00	Present	-60.2759	-60.2670	-60.2670	-60.2670	-60.2670
	Previous	-60.2759	-60.2670	-60.2670	-60.2670	-60.2670

Table 3.4: comparison of the large limit of the interaction strength ($u = 50$) of the ground-state energy.

2D N X N Square Lattice	GVA $E_N = -8(1 - 1/N^2)$	CVA $E_N = -8(1 - \alpha/N^2)$ $\alpha = 0.6250$	Present study (Exact) $E_N = -8(1 - \alpha/N^2)$ $\alpha = 0.8843$	Present study Variational calculation
3 X 3	-7.1111	-7.4444	-7.2140	-7.2140
5 X 5	-7.6800	-7.8000	-7.7170	-8.3103
7 X 7	-7.8367	-7.8980	-7.8556	-8.0758
9 X 9	-7.9012	-7.9382	-7.9127	-8.0925
11 X 11	-7.9339	-7.9587	-7.9415	-8.0811

IV. Discussion of Results.

The total energies and the variational parameters for the 2D 7 X 7 square lattice obtained from the matrix (2.37) is shown in Tables 3.1 and 3.2. The tables shows that (i) the total energy possess by the two electrons is non-degenerate and it decreases as the interaction strength is decreased, (ii) X_0 increases as the interaction strength is decreased. The other variational parameters first increase before they start to decrease as the interaction strength is made more negatively large.

We infer from this result that when the interaction strength is made more negatively large, then the electrons now prefer to remain close together (Cooper pairing). This is represented by the greater value of X_0 (double occupancy). Generally, it is this coming together or correlation of electrons that is responsible for the many physical properties of condensed matter physics, e.g. superconductivity, magnetism, super fluidity. However, in the positive regime of the interaction strength, the two electrons prefer to stay far apart as possible and the event is synonymous with ferromagnetism.

One remarkable result of the CVA as shown in Table 3.1 is the values of the variational parameters obtained when the interaction strength between the two electrons is zero ($u = 0$). In this case, the variational parameters produced by the single-band HM have the same values. This implies that the probability of double occupancy is the same as single occupancy. When $u = 0$ we observe a free electron system (non-interacting); the two electrons are not under the influence of any given potential they are free to hop to any preferable lattice site.

However, the variational parameters produced by the gradient Hamiltonian model when $u = 0$ are not equal. The interpretation of this is that even in the absence of interaction strength or potential function $u = 0$ 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 can also be assumed that the linear dependence of the electrons on the uniform lattice separations and the gradient could be the reason for the unequal variational parameters.

The difference in values of the total energies for some 2D N X N square lattices is shown in Table 3.3. In a particular lattice dimension the values of the ground-state energies obtained in our present study consistently decreases negatively as the interaction strength is decreased. The values of the total energies are also smaller than those of the previous study carried out by Chen and Mei. In the regime when the interaction strength $u \leq -1.0$, the result of the total energies of the previous study consistently increases negatively in value as we move from a lower dimensional lattice to higher ones, and the result of our present study is also consistent with this trend.

The result of the total energies for some 2D N X N square lattices is shown in Table 3.4. It is clear from the table that as the interaction strength is made positively large the difference in values of the total energies is very small, as a result we assume that u = 50 is large enough to typify the large limit of the interaction strength. It is evident from the table that α varies with N, the number of lattice sites. For large N, α approaches the value of 0.8843 in this present study, while α is 0.6250 in the work of Chen and Mei. The result of the ground- state energies for various 2D N x N square lattices obtained in this present study agrees suitably enough with the results of GVA and CVA.

V. Conclusion.

In this work, we utilized two types of Hamiltonian model to study the behaviour of two interacting electrons on a two dimensional (2D) N X N square lattice. The Hamiltonian are the single-band HM and the gradient Hamiltonian model. 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 HM. Thus the inclusion of the gradient parameters in the single band-HM yielded better results of the ground-state energies. Hence the lower ground-state energy results of our new model are quite more compactable with quantum variational requirements; that the ground-state energy should be a minimum. 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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