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A VARIATIONAL THEORY OF QUASI-PARTICLES IN A 3D N x N x N CUBIC LATTICE

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Abstract

The single-band Hubbard Hamiltonian study faces a serious limitation and difficulty as we move away from finite - size lattices to larger N - dimensional lattices. Thus there is the needto develop the means of overcoming the finite - size lattice defects as we pass on to a higher dimension.In this work, a quantitative approximation to the one-band Hubbard model is presented using a variational analytic approach. The goal of this work, therefore, is to explore quantitatively the lowest ground-state energy and the pairing correlations in 3D N x N x N lattices of the Hubbard model. We developed the unit step model as an approximate solution to the single-band Hubbard Hamiltonian to solve variationallythe correlation of two interacting elections on a three-dimensional cubic lattice. We also showed primarily how to derive possible electronic states available for several even and odd3D lattices, although, this work places more emphasis on a 3D 5 x 5 x 5 lattice. The results emerging from our present study compared favourablywith the results of Gutzwillervariational approach (GVA) and correlated variational approach (CVA), at thelarge limit of the Coulomb interaction strength (U/4t). It is revealed 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.

Keywords:

Unit Step Hamiltonian; Hubbard Hamiltonian; 3D cubic lattice; interaction strength; totalenergy; lattice separation.

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1.0. Introduction.

The most important problem associated with the applicability of the models of highly correlated electron systems is the nature of the ground-state of the correlated systems, what types of particles are condensed and what the structure of the excitations of this ground-state are, and the exact nature of the interaction between particles which can be studied using pair correlation functions [1].

The suggestion that the Hubbard Hamiltonian plays the key role to understanding the high temperature superconductors has stimulated interest in the physics of strongly correlated electron systems and many methods have been used to study the Hubbard model and approximations to it [2]. However, even when the Hubbard model is conceptually simple, this model is very difficult to solve in general, with few tractable limits [3].

In recent years, the Hubbard model has received increasing attention for its relevance for high-T_c superconductivity, antiferromagnetism, and ferromagnetism, thus playing a central role in the theoretical investigation of strongly correlated systems [4].In spite of the enormous successes of the approach [5] based on the effective single particle wave equation for many 3-dimensional metals and semiconductors, the understanding of the so-called correlated fermionic systems is still lacking.

This is because in their description of the electronic states the role of the long-range Coulomb interaction is crucial, as the charge screening becomes less effective. An electron located at a given lattice site would always feel the presence of another electron which is located at a different lattice site. This interaction is due to the presence of spin and charge between them. So long as this relationship exists the electrons are said to be correlated.

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.

Interacting electrons [6] 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 fermion compounds.

We also showed primarily how to derive possible electronic states available for several 3D N x N x N cubic lattices, although, this work place special interest and emphasis on a 3D 5 x 5 x 5 cubic lattice. The results emerging from our present study was compared with the results of Gutzwillervariational approach (GVA) [7] and correlated variational approach (CVA) [8]at large limit of the Coulomb interaction strength ($U/4t \approx 50$).The approximation to the Hubbard Hamiltonian study is actually necessary because of the strong limitation and difficulty pose by the Hubbard Hamiltonian as we move away from finite - size lattices to larger N - dimensional lattices. Thus this work has provided a means of overcoming the finite - size lattice defects as we pass on to a higher and larger dimension.

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 trail wavefunction to be utilized. We also present in this section an analytical solution for the two particles interaction in a 5x 5 x 5 cluster of the simple cubic 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.

2.0 Mathematical Theory.

The single-band Hubbard Hamiltonian [9] reads;

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

where $\langle i, j\rangle$ denotes nearest-neighbour (NN) sites, $C^{+}_{i\sigma}\left(C_{j\sigma}\right)$ is the creation (annihilation) operator with spin $\sigma = \uparrow or \downarrow$ at site i, and $n_{i\sigma} = C^{+}_{i\sigma} C_{i\sigma}$ is 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, this method is applicable only to smaller dimensional lattice system, since the dimension of the Hamiltonian matrix increases very rapidly with the number of sites and number of particles.

2.1 The correlated variational trial wave function (CVA)

The correlated variational trial wave function (CVA) given by Chen and Mei [8] is of the form

$$\left|\Psi\right\rangle = \sum_{i} X\left(i, i\right)\left\{ \left| i\uparrow, i\downarrow \right\rangle \right\} + \sum_{i \neq j} X_{|i-j|} \left\{ \left| i\uparrow, j\downarrow \right\rangle - \left| i\downarrow, j\uparrow \right\rangle \right\} \qquad (2.2)$$

where $X_i\ (i = 0, 1, 2, ...,)$ are variational parameters and $|\, i\sigma, j\sigma \rangle$ is the eigen state of a given electronic state, l is the lattice separation.

With a careful application of the two equations above we can conveniently solve for the wave function and hence the ground-state energy of the two interacting electrons provided the two important conditions stated below are duly followed.

(i) the field strength tensor

$$\langle i \,|\, j \rangle = \delta_{ij} \begin{cases} 1 & iff \quad i = j \\ 0 & iff \quad i \neq j \end{cases} \qquad (2.3)$$

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

$$|\, i \uparrow, j \downarrow \rangle = -|\, j \downarrow, i \uparrow \rangle \qquad (2.4)$$

However, to overcome the finite - size lattice defects,we developed the unit step model as an approximate solution to the Hubbard Hamiltonian in other to solveeffectively any higher and larger dimensional lattices.

Now let us consider for example two electrons interacting on a three-dimensional (3D) N x N x N lattice. If one electron is at site (x, y, z) and the second one is at site (x_1, y_1, z_1) ,then the state will be $|(xyz)\sigma, (x_1 y_1 z_1)\bar{\sigma}\rangle$ where the relative spins of the two electronsare $\sigma(\bar{\sigma}) = \uparrow (\downarrow)$ .The 3D 5 x 5 x 5 cubic lattice is similar to that of 3D 3 x 3 x 3 simple cubic lattice, except that instead of five planar lattices for 3D 3 x3 x 3, it is nine in the case of 3D 5 x 5 x 5 cubic lattice. However because of the limited space we cannot present the lattice geometry figuratively in this work. Consequently, we are only going to present some of the relevant information necessary for this study.We have generally summarized the details of the two electrons interaction on the 3D 5 x 5 x 5 cluster of the cubic lattice in table 2.1 below.

Table 2.1: Relevant information derived from the geometry of the 3D 5 x 5 x 5 cluster on a cubic lattice.

Lattice Separation l and actual separation distance d		Total number of sites at a separation length l	Pair wave function $\|\Psi_l\rangle$	Number of different pair electronic states at lattice separation l $(\lambda_l \times N^3)$	Representative Pair electronic states $\|i\uparrow, j\downarrow\rangle$
l	Separation Distance d	λ_l			
0	0	1	$\|\Psi_0\rangle$	125	$\|111\uparrow, 111\downarrow\rangle$
1	a	6	$\|\Psi_1\rangle$	750	$\|111\uparrow, 211\downarrow\rangle$
2	$\sqrt{2}a$	12	$\|\Psi_2\rangle$	1500	$\|111\uparrow, 221\downarrow\rangle$
3	$\sqrt{3}a$	8	$\|\Psi_3\rangle$	1000	$\|111\uparrow, 222\downarrow\rangle$
4	$2a$	6	$\|\Psi_4\rangle$	750	$\|111\uparrow, 311\downarrow\rangle$
5	$\sqrt{5}a$	24	$\|\Psi_5\rangle$	3000	$\|111\uparrow, 321\downarrow\rangle$
6	$\sqrt{6}a$	24	$\|\Psi_6\rangle$	3000	$\|111\uparrow, 322\downarrow\rangle$
7	$\sqrt{8}a$	12	$\|\Psi_7\rangle$	1500	$\|111\uparrow, 331\downarrow\rangle$
8	$\sqrt{9}a$	24	$\|\Psi_8\rangle$	3000	$\|111\uparrow, 332\downarrow\rangle$
9	$\sqrt{12}a$	8	$\|\Psi_9\rangle$	1000	$\|111\uparrow, 333\downarrow\rangle$
Total number of electronic states $N = 5$; $(N \times N)^3$ or $(N \times N \times N)^2$				15625	15625

Table 2.2: The summary of the relevant information derived from the analytical geometry of the 3D 5 x 5x5 cluster on a cubic lattice.

Lattice separation l Between the two electrons and actual separation distance d		Number of different pair electronic states at lattice separation l $(\lambda_l \times N^3)$	Description of lattice separation l and actual separation distance d (comprises of both linear and diagonal lattice length)	Method for determining the lattice separation length l and actual separation distance d
l	d			
0	0	(1 x 125)	On-site with no separation	$\lvert x-x_1\rvert = 0$ or $\lvert y-y_1\rvert = 0$ $\lvert z-z_1\rvert = 0$
1	a	(6 x 125)	Linear lattice length a	$\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 0$ $\lvert z-z_1\rvert = 0$
2	$\sqrt{2}a$	(12 x 125)	Diagonal lattice length $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 1$ $\lvert z-z_1\rvert = 0$
3	$\sqrt{3}a$	(8 x 125)	Diagonal lattice length $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 1$ $\lvert z-z_1\rvert = 1$
4	$2a$	(6 x 125)	Linear latticelength $(a+a)$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 0$ $\lvert z-z_1\rvert = 0$
5	$\sqrt{5}a$	(24 x 125)	Diagonal latticelength $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 1$ $\lvert z-z_1\rvert = 0$
6	$\sqrt{6}a$	(24 x 125)	Diagonal latticelength $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 1$ $\lvert z-z_1\rvert = 1$
7	$\sqrt{8}a$	(12 x 125)	Diagonal latticelength $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 2$ $\lvert z-z_1\rvert = 0$
8	$\sqrt{9}a$	(24 x 125)	Diagonal latticelength $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 2$ $\lvert z-z_1\rvert = 1$
9	$\sqrt{12}a$	(8 x 125)	Diagonal latticelength $\sqrt{(\lvert x-x_1\rvert a)^2+(\lvert y-y_1\rvert a)^2+(\lvert z-z_1\rvert a)^2}$	$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 2$ $\lvert z-z_1\rvert = 2$

The above conditions stated in table 2.1, generally hold except for boundary sites, where coordinates of y and z remain invariant along x axis; and the coordinates of x and y are also invariant along z axis; and finally x and z remain invariant along y axis. In which case, when calculating the separation length, 6 is taken as 0, for off boundary sites along, x , y and z axis respectively.Thisrequirement is a consequence of theperiodic boundary conditions.

Example, $\left|111\uparrow,611\downarrow\right\rangle = \left|111\uparrow,011\downarrow\right\rangle$, then $\left|x-x_1\right|=1$ or $\left|y-y_1\right|=0$ and $\left|z-z_1\right|=0$, this is a state in separation $l=1$. Also when determining the lattice separation length withthe conditions stated in the last column of table 2.1, the order of the coordinate states of the separation difference does not matter. For instance, site co-ordinate($x\,y\,z$) $\Rightarrow$ (210) = (120) = (201) again ($x\,y\,z$) $\Rightarrow$ (221) = (122) = (212).Hence when calculating the separation length or distance co-ordinates; (x, y, z) , (y, x, z) and (z, y, x) are the same state since the model we have developed in this work does not recognize conservationof parity. This makes the operation with the new model we have adopted in this study very easy and straightforward.

Table 2.3: Electronic states available to the two interacting electrons in a 3D N x N x Neven cubic lattice

Lattice dimension Even	Central lattice site from the selected origin Even	Number of separation length l Even	Number of electronic state	Number of on-site electrons
3D $(N\times N\times N)$	$\left(\frac{N}{2},\frac{N}{2},\frac{N}{2}\right)$	$\left(\frac{(N+6)(N+4)(N+2)}{48}\right)$	$(N\times N)^3$	$(N\times N\times N)$ N^3
4 X 4 x 4	(2 , 2, 2)	10	4096	64
6 X 6 x 6	(3 , 3, 3)	20	46656	216
8 X 8 x 8	(4 , 4, 4)	35	262144	512
10 X 10 x 10	(5 , 5, 5)	56	1000000	1000
12 x 12 x 12	(6 , 6, 6)	84	2985984	1728

Table 2.4:Electronic states available to the two interacting electrons in a 3D N x N x N odd cubic lattice

Lattice dimension Odd	Central lattice site from the selected origin Odd	Number of separation length l Odd	Number of electronic state	Number of on-site electrons
3D $(N\times N\times N)$	$\left(\frac{N+1}{2},\frac{N+1}{2},\frac{N+1}{2}\right)$	$\left(\frac{(N+5)(N+3)\,(N+1)}{48}\right)$	$(N\times N)^3$	$(N\times N\times N)$ N^3
3 X 3 x 3	(2 , 2, 2)	4	729	27
5 X 5 x 5	(3 , 3, 3)	10	15625	125
7 X 7 x 7	(4 , 4, 4)	20	117649	343
9 X 9 x 9	(5 , 5, 5)	35	531441	729
11 x 11 x 11	(6 , 6, 6)	56	1771561	1331

Details of how to calculate the respective actual separation distance for various separation lengths between the two interacting electrons in a 3D N x N x Nsimple cubiclattice can be found in [10 ,11].

2.3 The Unit Step Hamiltonian in 3D N x N x N cluster of the cubic lattice.

The approximation to the Hubbard Hamiltonian study is actually necessary because of the strong limitation and difficulty pose by the Hubbard Hamiltonian as we move away from finite - size lattices to larger N - dimensional lattices. Thus this work has provided a means of overcoming the finite - size lattice defects as we pass on to a higher dimension.

The unit step model takes advantage of the symmetry of the Hubbard model given by (2.1). The kinetic hopping term (t) can only distribute the electrons within only nearest-neighbour (NN) sites in a given lattice according to ±1. The U part can only act on the on-site electrons (double occupancy) while it is zero otherwise. Generally, from the geometry of the 1D, 2D and 3D lattices, we can recast the guessed trail wave functiongiven by (2.2) as

$$\left|\Psi\right\rangle = \sum_{l=0}^{l} X_l \; \left|\Psi_l\right\rangle \text{(2.5)}$$

$$\left\langle\Psi\middle|\Psi\right\rangle = \sum_{l=0}^{l} X_l^2 \; \left\langle\Psi_l\middle|\Psi_l\right\rangle \text{(2.6)}$$

where $\left|\Psi_l\right\rangle$ are the eigen states for a given separation, *N* is the total number of separations. Now suppose we let i, j, k, l, m and n represent the eigen state of a given lattice site such that for the 3D cluster on a simple cubic lattice it will be $\left|(ijk)\uparrow,(lmn)\downarrow\right\rangle$. Then

$$\begin{aligned}
H\left|(ijk)\uparrow,(lmn)\downarrow\right\rangle = -t\Big\{ & \left|(i\pm1)\; jk\uparrow,(lmn)\downarrow\right\rangle + \left|i\,(j\pm1)\,k\uparrow,\;(lmn)\downarrow\right\rangle + \\
& \left|ij\;(k\pm1)\uparrow,(\,lmn\,)\downarrow\right\rangle + \left|(ijk)\uparrow,(\,l\pm1\,)\,mn\downarrow\right\rangle + \\
& \left|(ijk)\uparrow,\;l(m\pm1)n\downarrow\right\rangle + \left|(ijk)\uparrow,\;lm\,(n\pm1\,)\downarrow\right\rangle\Big\} \\
& + U\left|(\,i\,i\,i\,)\uparrow,(\,i\,i\,i\,)\downarrow\right\rangle \text{(2.7)}
\end{aligned}$$

$$\begin{aligned}
H\left|(ijk)\uparrow,(lmn)\downarrow\right\rangle = -t\Big\{ & \left|(i+1)\,jk\uparrow,\;(lmn)\downarrow\right\rangle + \left|(i-1)\;j\,k\uparrow,(lmn)\downarrow\right\rangle + \\
& \left|i\,(j+1)\,k\uparrow,(lmn)\downarrow\right\rangle + \left|i\,(j-1)\,k\uparrow,(lmn)\downarrow\right\rangle + \\
& \left|ij\;(k+1)\uparrow,\;(lmn)\downarrow\right\rangle + \left|ij\;(k-1)\uparrow,\;(lmn)\downarrow\right\rangle + \\
& \left|(ijk)\uparrow,\;(l+1)\,mn\downarrow\right\rangle + \left|(ijk)\uparrow,\;(l-1)m\,n\downarrow\right\rangle + \\
& \left|(ijk)\uparrow,\;l\,(m+1)\,n\downarrow\right\rangle + \left|(ijk)\uparrow,\;l\,(m-1)\,n\downarrow\right\rangle + \\
& \left|(ijk)\uparrow,\;lm\,(n+1)\downarrow\right\rangle + \left|(ijk)\uparrow,\;lm\,(n-1)\downarrow\right\rangle\Big\} \\
& + U\left|(\,i\,i\,i\,)\uparrow,(\,i\,i\,i\,)\downarrow\right\rangle \text{(2.8)}
\end{aligned}$$

2.4 On the evaluation of the unit step Hamiltonian.

The N - dimensional unit step Hamiltonian contains the kinetic hopping term *t* and the on-site Coulomb repulsion term U. In practice the U term makes a contribution only when all lattice sites are equal (double occupancy). It is zero for inter-site lattice.The implementation of the Hubbard model on the trail wave function would demand using (2.1) to run through all pair electronic states one after the other. That is, for 3D 5 x 5 x 5 cubic lattice where there are a total of 15625 pair electronic states we shall be contending with ; $H\left|\Psi_l\right\rangle :\; l = 0,1,2,3,\ldots,15625$. While for 3D 6 x 6 x 6 simple cubic lattice where there are a total of 46656 pair electronic states; then $H\left|\Psi_l\right\rangle :\; l = 0,1,2,3,\ldots,46656$. This process as we all know is actually cumbersome and it will be very difficult to handle without error.

The advantage of the unit step model as an approximation to the single band Hubbard Hamiltonian, which we presented in this work is that instead of using (2.1) to run through all pair electronic states one after the other as the case demands, we rather use (2.7) to act on only one single electronic in each separation and sum the result. We know that $\left\langle\Psi\middle|H\middle|\Psi\right\rangle$ is always a commuting or Hermitian matrix. The eigen vectors of the Hermitian matrix are orthogonal and form a complete set, i.e., to say that any vector of this space is a linear combination of vectors of this set.

Consequent upon this, we use (2.6) to evaluate only a given eigen state from each of the given set $\left| \Psi_l \right\rangle$ and generalize the result since the vectors are commuting. Thus generally, when the unit step model acts on (2.5) we can sum the result as follows.

$$H \left| \Psi \right\rangle = H \sum_l X_l \left| \Psi_l \right\rangle = -t \sum_{(jl)} \left\{ \frac{n X_l \left\langle \Psi_l \middle| \Psi_l \right\rangle \left| \Psi_j \right\rangle}{\left\langle \Psi_j \middle| \Psi_j \right\rangle} \right\} + U \sum_l X_l \left| \Psi_l \right\rangle \quad (2.9)$$

where n is the total number of states generated within a given lattice separation, $\left\langle \Psi_l \middle| \Psi_l \right\rangle$ is the inner product of the state acted on by the unit step Hamiltonian, $\left\langle \Psi_j \middle| \Psi_j \right\rangle$ is the total number or the inner product of the new state generated after operating on the eigen state, l is the particular lattice separation, $\left| \Psi_j \right\rangle$ is the new state generated.

To understand completely how the unit step Hamiltonian works, we shall demonstrate it elementarily for only two cases and assume the same routine for the rest separations. Now

$$H \left| \Psi \right\rangle = H \sum X_l \left| \Psi_l \right\rangle \quad (2.10)$$

$$\begin{aligned} H \left| \Psi_0 \right\rangle = H \left| 111\uparrow,111\downarrow \right\rangle = -t \Big\{ & \left| 011\uparrow,111\downarrow \right\rangle^1 + \left| 211\uparrow,111\downarrow \right\rangle^1 + \left| 101\uparrow,111\downarrow \right\rangle^1 + \\ & \left| 121\uparrow,111\downarrow \right\rangle^1 + \left| 110\uparrow,111\downarrow \right\rangle^1 + \left| 112\uparrow,111\downarrow \right\rangle^1 + \left| 111\uparrow,011\downarrow \right\rangle^1 + \left| 111\uparrow,211\downarrow \right\rangle^1 + \\ & \left| 111\uparrow,101\downarrow \right\rangle^1 + \left| 111\uparrow,121\downarrow \right\rangle^1 + \left| 111\uparrow,110\downarrow \right\rangle^1 + \left| 111\uparrow,112\downarrow \right\rangle^1 \Big\} + U X_0 \left| \Psi_0 \right\rangle \quad (2.11) \end{aligned}$$

Where for clarity of purpose the superscripts only indicate the respective separations generated after activating the states with the unit step model. It is obvious from the parentheses of (2.11) that all the 12 new eigen states generated are of the same separation $l = 1$ and therefore having eigen state $\left| \Psi_1 \right\rangle$. The reader can confirm this by considering the last column of table 2.2. Thus

$$H \left| \Psi_0 \right\rangle = -t \left\{ 12 \left| \Psi_1 \right\rangle \right\} + U X_0 \left| \Psi_0 \right\rangle \quad (2.12)$$

Upon comparing this result with the equation (2.8), then $n = 12$, $j = 1$ and $l = 0$. Hence

$$H \left| \Psi_0 \right\rangle = -t X_0 \left(\frac{12 \times \left\langle \Psi_0 \middle| \Psi_0 \right\rangle \times \left| \Psi_1 \right\rangle}{\left\langle \Psi_1 \middle| \Psi_1 \right\rangle} \right) + U X_0 \left| \Psi_0 \right\rangle \quad (2.13)$$

$$H \left| \Psi_0 \right\rangle = -t X_0 \left(\frac{12 \times 125 \times \left| \Psi_1 \right\rangle}{750} \right) + U X_0 \left| \Psi_0 \right\rangle = -t X_0 \left(2 \left| \Psi_1 \right\rangle \right) + U X_0 \left| \Psi_0 \right\rangle \quad (2.14)$$

Now there is also the need for us to use the unit step Hamiltonian to act on the state in separation $l = 1$ instead of just generalising the effectiveness and accuracy of the unit step Hamiltonian with the result of only separation $l = 0$. The events of separation $l = 1$ would be a bit different.

$$\begin{aligned} H \left| \Psi_1 \right\rangle = H \left| 111\uparrow,211\downarrow \right\rangle = -t \Big\{ & \left| 011\uparrow,211\downarrow \right\rangle^4 + \left| 211\uparrow,211\downarrow \right\rangle^0 + \left| 101\uparrow,211\downarrow \right\rangle^2 + \\ & \left| 121\uparrow,211\downarrow \right\rangle^2 + \left| 110\uparrow,211\downarrow \right\rangle^2 + \left| 112\uparrow,211\downarrow \right\rangle^2 + \left| 111\uparrow,111\downarrow \right\rangle^0 + \left| 111\uparrow,311\downarrow \right\rangle^4 + \\ & \left| 111\uparrow,201\downarrow \right\rangle^2 + \left| 111\uparrow,221\downarrow \right\rangle^2 + \left| 111\uparrow,210\downarrow \right\rangle^2 + \left| 111\uparrow,212\downarrow \right\rangle^2 \Big\} \quad (2.15) \end{aligned}$$

We can now revert to (2.9) for the summation technique.

$$H\left|\ \Psi_1\ \right\rangle = -t\left\{2\left|\Psi_0\right\rangle + 8\left|\Psi_2\right\rangle + 2\left|\Psi_4\right\rangle\right\} \quad (2.16)$$

$$H\left|\ \Psi_1\ \right\rangle = -t\,X_1\left(\frac{2\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\ \Psi_0\ \right\rangle}{\left\langle\Psi_0\middle|\Psi_0\right\rangle} + \frac{8\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\ \Psi_2\ \right\rangle}{\left\langle\Psi_2\middle|\Psi_2\right\rangle} + \frac{2\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\ \Psi_4\ \right\rangle}{\left\langle\Psi_4\middle|\Psi_4\right\rangle}\right) \quad (2.17)$$

$$H\left|\ \Psi_1\ \right\rangle = -t\,X_1\left(\frac{2\times 750\times\left|\ \Psi_0\ \right\rangle}{125} + \frac{8\times 750\times\left|\ \Psi_2\ \right\rangle}{1500} + \frac{2\times 750\times\left|\ \Psi_4\ \right\rangle}{750}\right) \quad (2.18)$$

$$H\left|\ \Psi_1\ \right\rangle = -t\,X_1\left\{12\left|\Psi_0\right\rangle + 4\left|\Psi_2\right\rangle + 2\left|\Psi_4\right\rangle\right\} (2.19)$$

Also by a similar algebraic subroutine, when the unit step Hamiltonian acts on the eigen state in separation $l = 2$, $3, \dots, 9$, after a careful simplification with the use of (2.9) we finally get

$$H\left|\Psi\right\rangle = -t\left\{2X_0\left|\Psi_1\right\rangle + 12X_1\left|\Psi_0\right\rangle + 4X_1\left|\Psi_2\right\rangle + 2X_1\left|\Psi_4\right\rangle + 8X_2\left|\Psi_1\right\rangle + 6X_2\left|\Psi_3\right\rangle + 2X_2\left|\Psi_5\right\rangle\right.$$
$$4X_3\left|\Psi_2\right\rangle + 2X_3\left|\Psi_6\right\rangle + 2X_4\left|\Psi_1\right\rangle + 2X_4\left|\Psi_4\right\rangle + 2X_4\left|\Psi_5\right\rangle + 8X_5\left|\Psi_4\right\rangle + 4X_5\left|\Psi_6\right\rangle + 4X_5\left|\Psi_7\right\rangle + 4X_5\left|\Psi_2\right\rangle +$$
$$4X_6\left|\Psi_5\right\rangle + 2X_5\left|\Psi_5\right\rangle + 4X_6\left|\Psi_8\right\rangle + 2X_6\left|\Psi_6\right\rangle + 6X_6\left|\Psi_3\right\rangle + 2X_7\left|\Psi_5\right\rangle + 4X_7\left|\Psi_7\right\rangle + 2X_7\left|\Psi_8\right\rangle +$$
$$\left.4X_8\left|\Psi_7\right\rangle + 4X_8\left|\Psi_6\right\rangle + 4X_8\left|\Psi_8\right\rangle + 6X_8\left|\Psi_9\right\rangle + 2X_9\left|\Psi_8\right\rangle + 6X_9\left|\Psi_9\right\rangle\right\} + UX_0\left|\Psi_0\right\rangle \quad (2.20)$$

When we multiplying from the left of (2.20) with the result of the summation of (2.5) and using the field constraint (2.3) we get

$$\left\langle\Psi\middle|H\middle|\Psi\right\rangle = -t\{12X_0X_1\left\langle\Psi_0\middle|\Psi_0\right\rangle + 2X_0X_1\left\langle\Psi_1\middle|\Psi_1\right\rangle + 8X_1X_2\left\langle\Psi_1\middle|\Psi_1\right\rangle + 2X_1X_4\left\langle\Psi_1\middle|\Psi_1\right\rangle +$$
$$4X_1X_2\left\langle\Psi_2\middle|\Psi_2\right\rangle + 4X_2X_3\left\langle\Psi_2\middle|\Psi_2\right\rangle + 4X_2X_5\left\langle\Psi_2\middle|\Psi_2\right\rangle + 6X_2X_3\left\langle\Psi_3\middle|\Psi_3\right\rangle + 6X_3X_6\left\langle\Psi_3\middle|\Psi_3\right\rangle +$$
$$2X_1X_4\left\langle\Psi_4\middle|\Psi_4\right\rangle + 2X_4^2\left\langle\Psi_4\middle|\Psi_4\right\rangle + 8X_4X_5\left\langle\Psi_4\middle|\Psi_4\right\rangle + 2X_2X_5\left\langle\Psi_5\middle|\Psi_5\right\rangle + 2X_4X_5\left\langle\Psi_5\middle|\Psi_5\right\rangle +$$
$$2X_5^2\left\langle\Psi_5\middle|\Psi_5\right\rangle + 4X_5X_6\left\langle\Psi_5\middle|\Psi_5\right\rangle + 2X_5X_7\left\langle\Psi_5\middle|\Psi_5\right\rangle + 2X_3X_6\left\langle\Psi_6\middle|\Psi_6\right\rangle + 4X_5X_6\left\langle\Psi_6\middle|\Psi_6\right\rangle +$$
$$2X_6^2\left\langle\Psi_6\middle|\Psi_6\right\rangle + 4X_6X_8\left\langle\Psi_6\middle|\Psi_6\right\rangle + 4X_5X_7\left\langle\Psi_7\middle|\Psi_7\right\rangle + 4X_7^2\left\langle\Psi_2\middle|\Psi_2\right\rangle + 4X_7X_8\left\langle\Psi_7\middle|\Psi_7\right\rangle +$$
$$4X_6X_8\left\langle\Psi_8\middle|\Psi_8\right\rangle + 2X_7X_8\left\langle\Psi_8\middle|\Psi_8\right\rangle + 4X_8^2\left\langle\Psi_8\middle|\Psi_8\right\rangle + 2X_8X_9\left\langle\Psi_8\middle|\Psi_8\right\rangle + 6X_8X_9\left\langle\Psi_9\middle|\Psi_9\right\rangle +$$
$$6X_9^2\left\langle\Psi_9\middle|\Psi_9\right\rangle\} + U\,X_0^2\left\langle\Psi_0\middle|\Psi_0\right\rangle \quad (2.21)$$

Also we can establish from (2.6) that

$$\left\langle\Psi\middle|\Psi\right\rangle = X_0^2\left\langle\Psi_0\middle|\Psi_0\right\rangle + X_1^2\left\langle\Psi_1\middle|\Psi_1\right\rangle + X_2^2\left\langle\Psi_2\middle|\Psi_2\right\rangle + X_3^2\left\langle\Psi_3\middle|\Psi_3\right\rangle + X_4^2\left\langle\Psi_4\middle|\Psi_4\right\rangle + X_5^2\left\langle\Psi_5\middle|\Psi_5\right\rangle +$$
$$X_6^2\left\langle\Psi_6\middle|\Psi_6\right\rangle + X_7^2\left\langle\Psi_7\middle|\Psi_7\right\rangle + X_8^2\left\langle\Psi_8\middle|\Psi_8\right\rangle + X_9^2\left\langle\Psi_9\middle|\Psi_9\right\rangle \quad (2.22)$$

We can now substitute the values provided in table 2.1 into (2.21) and 2.22) and get after some direct simplification that

$$\left\langle\Psi\middle|H\middle|\Psi\right\rangle = -\ (125)\ (4t)\ \{6X_0X_1 + 24\,X_1X_2 + 6\,X_1X_4 + 24\,X_2X_3 + 24\,X_2X_5 +$$
$$24\,X_3X_6 + 24\,X_4X_5 + 28\,X_5X_6 + 24\,X_5X_7 + 28\,X_6X_8 + 24\,X_7X_8 + 24\,X_8X_9 + 3X +$$
$$12X_5^2 + 12X_6^2 + 12X_7^2 + 24X_8^2 + 12X_9^2 - \left(U/4t\right)X_0^2\} \quad (2.23)$$

$$\left\langle \Psi \middle| \Psi \right\rangle = 125\ (X_0^2 + 6X_1^2 + 12X_2^2 + 8X_3^2 + 6X_4^2 + 24X_5^2 + 24X_6^2 + 12X_7^2 + 24X_8^2 + 8X_9^2) \quad (2.24)$$

We can see that this technique is very straightforward as it limits the operation to only one eigen state in a given lattice separation instead of using the Hubbard Hamiltonian to operate on all the states consecutively.

2.5 The variationaltheory.

The variational method consists in evaluating the integral

$$E_g \left\langle \Psi \middle| \Psi \right\rangle = \left\langle \Psi \middle| H \middle| \Psi \right\rangle = \left\langle \Psi \middle| H_t + H_u \middle| \Psi \right\rangle \quad (2.25)$$

Where E_g is the correlated ground state energy and Ψ is the guessed trial wave function. We can now differentially minimize (2.25) after the substitution of (2.23) and (2.24) as follows.

$$\left\langle \Psi \middle| \Psi \right\rangle \frac{\partial E_g}{\partial X_i} + E_g \frac{\partial}{\partial X_i} \left\langle \Psi \middle| \Psi \right\rangle = \frac{\partial}{\partial X_i} \left\langle \Psi \middle| H \middle| \Psi \right\rangle \quad (2.26)$$

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

$$\frac{\partial E_g}{\partial X_i} = 0 \qquad ; \quad \forall\ i = 0, 1, 2, 3 \quad (2.27)$$

we can transform the resulting equation into a homogeneous eigen value problem of the form

$$\left[A - \delta_l\, I \right] \vec{X}_l = 0 \quad (2.28)$$

Where A is an NXN matrix which takes the dimension of the number of separations, δ_l is the eigen value (total energy E) to be determined, I is the identity matrix which is also of the same order as the matrix A , $\vec{X}_i$ are the various eigen vectors or simply the variational parameters corresponding to each eigen value. Hence after a careful simplification we finallyestablish the below matrix.

$$\begin{pmatrix} E-4u & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & E & 8 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & E & 4 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 6 & E & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & E+2 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 2 & E+2 & 4 & 2 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 4 & E+2 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & E+4 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 2 & E+4 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & E+6 \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ X_9 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (2.29)$$

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. From the matrix given by (2.29) we can now determine the total energy and the corresponding variational parameters for various arbitrary values of the interaction strength.

2.6 Evaluation of the spectral intensity.

Suppose we write (2.6) in terms of only nearest neighbours site to a given separation length. Accordingly, $\left\langle \Psi_l \middle| \Psi_l \right\rangle = \lambda_i$ = 1, 6, 12, 8, 6, 24, 24, 12, 24 and 8 for $l =$ 0, 1, 2,…, 9 respectively, then

$$\left| \Psi \right\rangle = a_0 \left| \Psi_0 \right\rangle + a_1 \left| \Psi_1 \right\rangle + a_2 \left| \Psi_2 \right\rangle + a_3 \left| \Psi_3 \right\rangle + a_4 \left| \Psi_4 \right\rangle + a_5 \left| \Psi_5 \right\rangle \quad (2.30)$$

$$\left\langle \Psi \middle| \Psi \right\rangle = a_0^2 + 6a_1^2 + 12a_2^2 + 8a_3^2 + 6a_4^2 + 24a_5^2 + 24a_6^2 + 12a_7^2 + 24a_8^2 + 8a_9^2 \quad (2.31)$$

Where $a_l^2\ (l = 0, 1, \dots, 5)$ still represent the variational parameters.

Then this will make us redefine (2.6) as

$$\left\langle \Psi \middle| \Psi \right\rangle = \sum_{l=0}^{5} \lambda_l \, a_l^2 \qquad (2.32)$$

where $\lambda_l \ (l = 0, 2, \ldots, 5)$ are the respective weights or coefficients of the various basis of the lattice separation parameters a_l^2 .The spectral density $\widehat{f}\,(\omega)$ defines the distribution of the probability of values of the momentum possess by the two electrons to the total energy. That is

$$\widehat{f}\,(\omega) = \frac{\lambda_l \, a_l^2}{\sqrt{2\pi}} \int_0^{\infty} f(x)\, e^{-i\omega x}\, dx \qquad (2.33)$$

However, the kernel $f(x)$ in the integrand is simply x^2 , because the basis is a square of the lattice separation parameter, ω is the spatial vibration of the two electrons. As a result, (2.33) becomes

$$\widehat{f}\,(\omega) = \frac{\lambda_l \, a_l^2}{\sqrt{2\pi}} \int_0^{l} x^2 \, e^{-i\omega x}\, dx \qquad (2.34)$$

$$\widehat{f}\,(\omega) = \frac{2\lambda_l \, a_l^2}{\omega^2 \sqrt{2\pi}} \left(1 + l\, e^{-i\omega l} - e^{-i\omega l}\right) + i\,\frac{\lambda_l \, a_l^2}{\omega\sqrt{2\pi}} \left(l^2 \, e^{-i\omega l}\right) \quad (2.35)$$

It is sometimes convenient to express the spectral intensity in terms of polar coordinate, so that

$$\widehat{f}\,(\omega) = \left(\frac{\lambda_l \, a_l^2}{\sqrt{2\pi}}\right) \left\{ \frac{2}{\omega^2} + \frac{2l}{\omega^2}(\cos\omega l - i \sin\omega l) - \frac{2}{\omega^2}(\cos\omega l - i\sin\omega l) + i\,\frac{l^2}{\omega}(\cos\omega l - i\sin\omega l) \right\}$$

(2.36)

$$\left|\widehat{f}\,(\omega)\right|^2 = \left(\frac{\lambda_l \, a_l^2}{\sqrt{2\pi}}\right)^2 \left\{ \left(\frac{2}{\omega^2} + \frac{2l}{\omega^2}\cos\omega l - \frac{2}{\omega^2}\cos\omega l + \frac{l^2}{\omega}\sin\omega l \right)^2 + \right.$$

$$\left. \left(\frac{2}{\omega^2}\sin\omega l + \frac{l^2}{\omega}\cos\omega l - \frac{2l}{\omega^2}\sin\omega l \right)^2 \right\} \qquad (2.37)$$

$$\left|\widehat{f}\,(\omega)\right|^2 = \left(\frac{\lambda_l a_l^2}{\sqrt{2\pi}}\right)^2 \left\{ \frac{8}{\omega^4} + \frac{l^4}{\omega^2} - \frac{8l}{\omega^4} + \frac{4l^2}{\omega^4} + \frac{8l}{\omega^4}\cos\omega l + \frac{4l^2}{\omega^3}\sin\omega l - \frac{8}{\omega^4}\cos\omega l \right\} \qquad (2.38)$$

Suppose we decide to vary (2.38) logarithmically, then after some arithmetic jamboree the resulting equation simplifies to

$$\ln\left|\,\widehat{f}(\omega)\right|^2 = \ln\left(\frac{\lambda_l \, a_l^2}{\sqrt{2\pi}}\right)^2 + 8\ln l - 2\ln 4 - 5\ln\omega + \ln\sin\omega l \quad (2.39)$$

$$\ln\left|\widehat{f}(\omega)\right|^2 = \ln\left\{ \left(\frac{\lambda_l \, a_l^2}{\sqrt{2\pi}}\right)^2 \left(\frac{l^8 \sin\omega l}{\omega^5}\right) \right\} - 2.77 \qquad (2.40)$$

$$\left|\widehat{f}(\omega)\right|^2 = 0.06 \left(\frac{\lambda_l \, a_l^2}{\sqrt{2\pi}}\right)^2 \left(\frac{l^8}{\omega^5}\right) \sin\omega l \qquad (2.41)$$

Thus (2.41) gives the spectral intensity of the two interacting electrons. The spectral intensity is made up of constant amplitude and an oscillating phase. The intensity is determined by the fifth power of the spatial angular vibration ω of the two interacting electrons.

3.0 Presentation of Results.

Table 3.1: Shows the calculated values of the total energy and the variational parameters for 3D 5 x 5 x 5 cubic lattice for various arbitrary values of the interaction strength.

Interaction strength $U/4t$	Total energy $E = E_g/t$	Variational parameters (X_l) (l = 0, 1, 2, 3, 4)				
		X_0	X_1	X_2	X_3	X_4
50.00	-11.9274	0.0153	0.2694	0.3159	0.3330	0.3278
30.00	-11.9295	0.0349	0.2712	0.3163	0.3328	0.3279
20.00	-11.9320	0.0357	0.2734	0.3169	0.3329	0.3281
10.00	-11.9385	0.0644	0.2789	0.3181	0.3325	0.3282
1.00	-11.9774	0.2296	0.3057	0.3195	0.3246	0.3231
0.25	-11.9928	0.2893	0.3132	0.3176	0.3191	0.3187
0.00	-12.0000	0.3162	0.3162	0.3162	0.3162	0.3162
-1.00	-12.0545	0.4901	0.3290	0.3000	0.2895	0.2927
-1.50	-12.1240	0.6433	0.3283	0.2722	0.2521	0.2582
-2.00	-12.3133	0.8340	0.2998	0.2068	0.1744	0.1843
-10.00	-40.6047	0.9994	0.0356	0.0036	0.0005	0.0019
-20.00	-80.3006	0.9998	0.0177	0.0009	0.0001	0.0005

Table 3.1c.t.d: Shows the calculated values of the total energy and the variational parameters for3D 5 x 5 x 5 cubic lattice for various arbitrary values of the interaction strength.

Interaction strength $U/4t$	Total energy $E = E_g/t$	Variational parameters (X_l) (l = 5, 6, 7, 8, 9)				
		X_5	X_6	X_7	X_8	X_9
50.00	-11.9274	0.3395	0.3460	0.3493	0.3528	0.3572
30.00	-11.9295	0.3392	0.3455	0.3487	0.3521	0.3563
20.00	-11.9320	0.3390	0.3451	0.3482	0.3514	0.3555
10.00	-11.9385	0.3380	0.3435	0.3463	0.3492	0.3528
1.00	-11.9774	0.3265	0.3280	0.3294	0.3304	0.3316
0.25	-11.9928	0.3197	0.3203	0.3206	0.3210	0.3213
0.00	-12.0000	0.3162	0.3162	0.3162	0.3162	0.3162
-1.00	-12.0545	0.2856	0.2817	0.2797	0.2777	0.2752
-1.50	-12.1240	0.2335	0.2372	0.2335	0.2297	0.2250
-2.00	-12.3133	0.1454	0.1510	0.1454	0.1395	0.1326
-10.00	-40.6047	0.0003	0.0001	0.0000	0.0000	0.0000
-20.00	-80.3006	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3.2: Shows the calculated values of the spectra intensity for arbitrary value of ω

For 3D 5 x 5 x 5 cubic lattice.

Interaction strength $U/4t$	Spectra intensity $\left|\hat{f}(\omega)\right|^2$ (ω=10)				
	$l=0$	$l=1$	$l=2$	$l=3$	$l=4$
50.00	0.0000	3.56E-07	0.000421	0.008649	0.0473
30.00	0.0000	3.61E-07	0.000422	0.008639	0.0473
20.00	0.0000	3.66E-07	0.000424	0.008644	0.0474
10.00	0.0000	3.81E-07	0.000427	0.008624	0.0474
1.00	0.0000	4.58E-07	0.000431	0.008219	0.0460
0.25	0.0000	4.81E-07	0.000425	0.007942	0.0447
0.00	0.0000	4.90E-07	0.000422	0.007799	0.0440
-1.00	0.0000	5.3E-07	0.00038	0.006537	0.0377
-1.50	0.0000	5.29E-07	0.000313	0.004957	0.0293
-2.00	0.0000	4.41E-07	0.00018	0.002372	0.0149
-10.00	0.0000	6.22E-09	5.47E-08	1.95E-08	1.59E-06
-20.00	0.0000	1.53E-09	3.42E-09	7.8E-10	1.10E-07

Table 3.2c.t.d: Shows the calculated values of the spectra intensity for arbitrary value of ω

For 3D 5 x 5 x 5 cubic lattice

Interaction strength $U/4t$	Spectra intensity $\left|\hat{f}(\omega)\right|^2$ (ω = 10)				
	$l=5$	$l=6$	$l=7$	$l=8$	$l=9$
50.00	0.4264	2.2124	9.8245	74.9198	59.0826
30.00	0.4256	2.2060	9.7908	74.6228	58.7852
20.00	0.4251	2.2009	9.7627	74.3264	58.5215
10.00	0.4226	2.1805	9.6565	73.3986	57.6360
1.00	0.3943	1.9882	8.7370	65.7082	50.9173
0.25	0.3781	1.8959	8.2764	62.0225	47.8033
0.00	0.3699	1.8477	8.0508	60.1815	46.2978
-1.00	0.3017	1.4665	6.2994	46.4185	35.0698
-1.50	0.2017	1.0398	4.3902	31.7586	23.4423
-2.00	0.0782	0.4213	1.70233	11.7135	8.1418
-10.00	3.33E-07	1.8481E-07	0	0	0
-20.00	0	0	0	0	0

Table 3.3: Comparison of the large limit of the interaction strength ($U/4t = 50$) of the ground state energy obtained in this study with GVA and CVA for even 3D N x N x N simple cubic lattice

3D $N \times N \times N$ Even	GVA $E_N = -12(1 - 1/N^3)$	CVA $E_N = -12(1 - \alpha/N^3)$ $\alpha = 0.4165$	Presentstudy $E_N = -12(1 - \alpha/N^3)$ $\alpha = 0.3872$
4x4x4	-11.8125	-11.9219	-11.9274
6x6x6	-11.9444	-11.9769	-11.9785
8 x 8 x 8	-11.9765	-11.9902	-11.9909
10 x 10 x 10	-11.9880	-11.9950	-11.9953
12 x 12 x12	-11.9930	-11.9971	-11.9973

Table 3.4: Comparison of the large limit of the interaction strength ($U/4t = 50$) of the ground state energy obtained in this Present study with GVA and CVA for odd 3D N x N x Ncubic lattice

3D N x N x N Simple cubic Lattice Odd	GVA $E_N = -12(1 - 1/N^3)$	CVA $E_N = -12(1 - \alpha/N^3)$ $\alpha = 0.4167$	Present study $E_N = -12(1 - \alpha/N^3)$ $\alpha = 0.7563$
3 x 3 x3	-11.5556	-11.8148	-11.6639
5 x 5 x 5	-11.9040	-11.9599	-11.9274
7 x 7 x 7	-11.9650	-11.9854	-11.9735
9 x 9 x 9	-11.9835	-11.9931	-11.9875
11 x 11 x 11	-11.9909	-11.9962	-11.9932

4.0 Discussion of Results.

The total energies and the variational parameters obtained for the 3D 5 x 5 x 5simple cubic lattice is shown in table 3.1. The table shows that (i) the total energy possess by the two electrons is non-degenerate and it generally decreases as the interaction strength is decreased, (ii) X_0 increases as the interaction strength is decreased, (iii) X_1 increases until the interaction strength $U/4t$ = -1 and then it starts to decrease as $U/4t$ is decreased,(iv) X_2 increases until the interaction strength $U/4t$ =0.25 and then it starts to decrease as $U/4t$ is decreased, (v) X_3decreases consistently when $U/4t$ =10(vi)X_4 decreases consistently when $U/4t$ =1,(vii) X_5, X_6,X_7 X_8 and X_9 decreases consistently as $U/4t$ is decreased.

The table exhibits clearly that the variational parameters for any given system are of equal weights when $U/4t$ = 0. This implies that the probability of double occupancy is the same as single occupancy. When the interaction strength iszero, we observe a free electron systems, the two electrons are not under the influence of any given potential they are free to hop to any preferable lattice site. It is clear from the table that for positive interaction strength, $X_0 \prec X_1 \prec X_2 \prec X_3 \prec X_4 \prec X_5 \prec X_6 \prec X_7 \prec X_8 \prec X_9$. Also for negative interaction strength we observe that $X_0 \succ X_1 \succ X_2 \succ X_3 \succ X_4 \succ X_5 \succ X_6 \succ X_7 \succ X_8 \succ X_9$.

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.

Table 3.2 shows the absolute values of the spectra intensity which is computed in the radian mode.There is correspondence in the interpretation of the results of the spectra intensity and those of the variational parameters. Although, the relevance of the resultsare determine by the value of the spatial frequency. For on-site electrons the spectra intensity is zero for all values of the interaction strength. The spectra intensity for the various separation lengths goes to zero when the interaction strength is made negatively large. With the exception of separation length l_9, the spectra intensity for a particular value of interaction strength increases according to $l_0 \prec l_1 \prec l_2 \prec l_3 \prec l_4 \prec l_5 \prec l_6 \prec l_7 \prec l_8$.

The decrease in the value of the spectra intensity at lattice separation l_9, means that the farther the electrons are apart the less the affinity they have for each other.The result in the table shows that high values of positive interaction strength increase the momentum of the two electrons. While high negative interaction strength decreases the momentum of the two interacting electrons.

As shown in table 3.1, the difference in values of the total energies as the interaction strength is made positively large is very small, as a result we assume $U/4t$ = 50 to be large enough to typify the large limit of the interaction strength. It is evident from table 3.3 and 3.4 that α varies with N, the number of lattice sites. In the work of Chen and Mei, for large N, α approaches the value of 0.4165 for even 3D lattice while in our work α is 0.3872. Also for odd 3D lattice α approaches the value of 0.4167 in the work of Chen and Mei, while in this study α is 0.7563. Generally,the result of the ground state energies for various 3D N x N x N simple cubic lattice obtained in this present study agreessuitably enough with those of GVA and CVA.

5.0 Conclusion

This work has provided a means of overcoming the finite - size lattice defects as we pass on to a higher dimension. The result of thepresent study demonstrates that positive on-site interaction strength ($U/4t$), makes the two interacting electrons to stay away from each other as far apart as possible in order to gain the lowest energy. The model in this regime best describes ferromagnetism. For sufficiently large and negative on-site interaction strength ($U/4t$) the electrons prefer to stay close together in order to gain the lowest energy and hence the minimum potential. The model in this regime favours Cooper pairing. We have investigated 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 *U/4t*.We have also in this study extended the work of Chen and Mei which was limited to one-and two-dimensional (ID and 2D) lattice to three-dimensional (3D) lattice.

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