# The Ground- State Analytical Solution of Two-Interacting Electrons in a Two-Dimensional Square Lattice

Edison A. Enaibe[1*] Daniel A. Babaiwa[2] and Osafile Omosede[1]
1Department of Physics, Federal University of Petroleum Resources,P.M.B. 1221 Effurun, Nigeria.
2. Department of Science Laboratory Technology, Auchi Polytechnic, Auchi, Nigeria.
*E – mail: aroghene 70@yahoo.com

**Abstract**
In this work, we developed the unit step model as an approximate solution to the single-band Hubbard Hamiltonian to solve variationally strongly correlated interacting elections on a two-dimensional (2D) square lattice. We also showed primarily how to derive possible electronic states available for several 2D N x N square lattices, although, with special emphasis on a 2D 5 x 5 square lattice. The results emerging from our present study was compared with the results of Gutzwiller variational approach (GVA) and correlated variational approach (CVA), at the large limit of the Coulomb interaction strength (U/4t).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. 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 (non-interacting), the variational parameters which describe the probability distribution of lattice electron system is the same. The spectra intensity increases with increase in the interaction strength and it decreases to zero when the interaction strength is made negatively large.

**Keywords**: unit step Hamiltonian, Hubbard Hamiltonian, 3D cubic lattice, interaction strength, total energy, lattice separation.

## 1.0 Introduction

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 (Domaski *et al.* 1996). In spite of the enormous successes of the approach 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 (Rycerz & Spalek 2001).

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 (Stintzing & Zwerger 1997).

The Hubbard model was originally proposed as a simple model to describe the physics of metallic ferromagnetism. Apart from the fact that it exhibits anti-ferromagnetism, it also gives rise to ferromagnetism for large values of the on-site Coulomb repulsion within mean field theory as well as within other approximations (Jaklic & Prelovsek 1993). However, subsequent work has shown that an on-site Coulomb repulsion by itself will not give rise to metallic ferromagnetism except in special situations, such as a single hole in a half-filled band or special lattice geometries (Guerrero *et al.* 1998, Samuel *et al.* 2005).

It appears in general, that electrons of anti-parallel spin can more easily avoid paying the price of on-site Coulomb repulsion by developing spatial correlations rather than by spin polarization, contrary to the predictions of mean field theory (Wang 1996). 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 (Balatsky 1990).

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. However, even when the Hubbard model is conceptually simple, this model is very difficult to solve in general, with few tractable limits (Elric *et al.* 1993, Vallejo *et al.* 2003).

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 2D N x N lattices of the Hubbard model. Although, we demonstrated the effectiveness of the unit step model to a 5 x 5 square lattice.

The passage from an exact approach to a variational approach becomes necessary because of the large uncontrollable matrix size which results from the dimensional increase in the lattice size. Any variational approach is an approximation to an exact treatment. In view of the fact that the many-body problem in condensed matter physics is quite complicated it is not unusual in the study of highly correlated electron systems to encounter approximation methods.

The Hubbard model has the following features: (i) the model exhibits non-fermi liquid (FL) (quantum liquid in which the spin fluctuation is unmodified by interaction) behaviour as long as U > 0 for a finite particle density, (ii) there is no correspondence between the states of free and interacting particles even at nearly zero density, (iii) it allows double occupancy at a given site, (iv) consequent upon (iii) the size of the Hilbert space for a given cluster is much larger than for the *t* - *J* model, (v) the model exhibits anti-ferromagnetism rather than ferromagnetism, (vi) the Hubbard Hamiltonian becomes very cumbersome to handle when the size of the Hilbert space of a given dimensional lattice increases (Marsiglo 1997).

The results emerging from our present study was compared with the results of Gutzwiller variational approach (1963) and correlated variational approach 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 wave function to be utilized. We also present in this section an analytical solution for the two particles interaction on a 2D 5 x 5 square lattice using the unit step model. 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 an appendix and lists of references.

### 2.1 Mathematical Theory

The single-band Hubbard Hamiltonian (Marsiglo 1997, Weng *et al.* 1997) reads;

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

where $\langle i, j \rangle$ denotes nearest-neighbour (NN) sites, $C^{+}_{i\sigma}\left(C_{j\sigma}\right)$ is the creation (annihilation) operator with spin $\sigma = \uparrow or \downarrow$ at site $i$, and $n_{i\sigma} = C^{+}_{i\sigma} C_{i\sigma}$ is the occupation number operator, and of course $h.c. \, (C^{+}_{j\sigma} C_{i\sigma})$ 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.

### 2.2 The correlated variational approach (CVA)

The trial wave function for the correlated variational approach which was adopted by Chen and Mei (1989) is of the form

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

Where, $X_i$ $\left( i = 0, 1, 2,...,\right)$ are variational parameters and $\left| i\sigma, j\sigma \right\rangle$ 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 on finite-size lattice provided the two basic conditions stated below are duly followed.

(i) the field strength tensor

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

(ii) the Marshal rule for non-conservation of parity [14]

$$\left| i\uparrow, j\downarrow \right\rangle = -\left| j\downarrow, i\uparrow \right\rangle \tag{2.4}$$

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 solve effectively any higher and larger dimensional lattices.
Now let us consider for example two electrons interacting on a two dimensional (2D) N x N lattice. If one electron is at site $(x, y)$ and the second one is at site $(x_1, y_1)$, then the state will be $\left| xy\sigma, x_1y_1\bar{\sigma} \right\rangle$ where the relative spins of the two electrons are $\sigma(\bar{\sigma}) = \uparrow (\downarrow)$. In consideration of the lattice symmetry for the 2D 5 x 5 cluster as shown in the appendix, we have generally summarized the details of the two electrons interaction on the 2D 5 x 5 cluster of a square lattice in table 2.1 below.

**Table 2.1:** The summary of the relevant information derived from the analytical geometry of the 2D 5 x 5 cluster on a square lattice lattice.

| Lattice separation $l$ Between the two electrons and actual separation distance $d$ | | Pair wave function $\left\|\psi_l\right\rangle$ | Number of pair electronic states at lattice separation $l$ $\left\langle\psi_l\middle\|\psi_l\right\rangle$ | Pair electronic states $\left\|i\uparrow, j\downarrow\right\rangle$ |
|---|---|---|---|---|
| $l$ | $d$ | | | |
| 0 | 0 | $\left\|\psi_0\right\rangle$ | 25 | $\left\|11\uparrow,11\downarrow\right\rangle, \ldots, \left\|55\uparrow,55\downarrow\right\rangle$ |
| 1 | $a$ | $\left\|\psi_1\right\rangle$ | 100 | $\left\|11\uparrow,12\downarrow\right\rangle, \ldots, \left\|54\uparrow,55\downarrow\right\rangle$ |
| 2 | $\sqrt{2}a$ | $\left\|\psi_2\right\rangle$ | 100 | $\left\|11\uparrow,22\downarrow\right\rangle, \ldots, \left\|45\uparrow,51\downarrow\right\rangle$ |
| 3 | $2a$ | $\left\|\psi_3\right\rangle$ | 100 | $\left\|11\uparrow,13\downarrow\right\rangle, \ldots, \left\|53\uparrow,55\downarrow\right\rangle$ |
| 4 | $\sqrt{5}a$ | $\left\|\psi_4\right\rangle$ | 200 | $\left\|11\uparrow,23\downarrow\right\rangle, \ldots, \left\|43\uparrow,55\downarrow\right\rangle$<br>or<br>$\left\|11\uparrow,32\downarrow\right\rangle, \ldots, \left\|34\uparrow,55\downarrow\right\rangle$ |
| 5 | $\sqrt{8}a$ | $\left\|\psi_5\right\rangle$ | 100 | $\left\|11\uparrow,33\downarrow\right\rangle, \ldots, \left\|35\uparrow,53\downarrow\right\rangle$ |
| Total number of electronic states N = 5 ; ( $N^2$ x $N^2$ ) or $(N \text{ x } N)^2$ | | | 625 | 625 |

**Table 2.2:** Summary of how to generate the respective lattice separation length and distance that is available for the two interacting electrons in the 2D 5 x 5 square lattice

| Lattice separation $l$ Between the two electrons and actual separation distance $d$ | | Total number of sites at a separation length $l$ | Description of lattice separation $l$ | Method for determining the lattice separation length $l$ |
|---|---|---|---|---|
| $l$ | $d$ | | | |
| 0 | 0 | 1 | On-site with no separation | $\lvert x-x_1\rvert = 0$ or $\lvert y-y_1\rvert = 0$ |
| 1 | $a$ | 4 | Linear lattice length<br>$a$ | $\lvert x-x_1\rvert = 0$ or $\lvert y-y_1\rvert = 1$<br>$\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 0$ |
| 2 | $\sqrt{2}a$ | 4 | Diagonal with one nearest neighbour sites<br>$\sqrt{(\lvert x-x_1\rvert a)^2 + (\lvert y-y_1\rvert a)^2}$ | $\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 1$ |
| 3 | $2a$ | 4 | Linear lattice length<br>$(a+a)$ | $\lvert x-x_1\rvert = 0$ or $\lvert y-y_1\rvert = 2$<br>$\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 0$ |
| 4 | $\sqrt{5}a$ | 8 | Diagonal lattice length<br>$\sqrt{(\lvert x-x_1\rvert a)^2 + (\lvert y-y_1\rvert a)^2}$ | $\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 1$<br>$\lvert x-x_1\rvert = 1$ or $\lvert y-y_1\rvert = 2$ |
| 5 | $\sqrt{8}a$ | 4 | Diagonal lattice length<br>$\sqrt{(\lvert x-x_1\rvert a)^2 + (\lvert y-y_1\rvert a)^2}$ | $\lvert x-x_1\rvert = 2$ or $\lvert y-y_1\rvert = 2$ |

The above conditions stated in table 2.1, generally hold except for boundary sites, where coordinates of y remain invariant along x axis and coordinates of x are also invariant along y axis. In which case, when calculating the separation length, 5 is taken as 0, for off boundary sites along x and y axis.

Example, $|11\uparrow,51\downarrow\rangle = |11\uparrow,01\downarrow\rangle$, then $|x-x_1| = 1$ or $|y-y_1| = 0 \Rightarrow (1,0) \Rightarrow (0,1)$, and this is a state in $l = 1$. Hence when calculating the separation length or distance co-ordinates; $(x,y)$ and $(y,x)$ are the same state since the model we have developed in this work does not recognize parity conservation.

**Table 2.3:** Electronic states available to the two interacting electrons in a 2D N x N even square lattice

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

**Table 2.4:** Electronic states available to the two interacting electrons in a 2D N x N odd square lattice

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

Details of how to calculate the respective actual separation distance for various separation lengths between the two interacting electrons in a 2D N x N square lattice can be found in (Akpojotor *et al*. 2002).

## 2.3 The Unit Step Hamiltonian in 2D N x N square 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 or -1. The U part can only act on the on-site electrons (double occupancy) while it is zero otherwise. Also from the geometry of the 2D 5 x 5 square lattice (see appendix) we can recast (2.2) as

$$\left|\Psi\right\rangle = \sum_{l=0}^{l} X_l \left|\Psi_l\right\rangle \tag{2.5}$$

where $\left|\Psi_l\right\rangle$ are the eigen states for a given separation, $l$ 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 $\left|(i\,j)\uparrow,(k\,l)\downarrow\right\rangle$. Then the operation of the Unit step Hamiltonian in 2D (even or odd) square lattice is define as

$$\begin{aligned} H\left|(i\,j)\uparrow,\ (k\,l)\downarrow\right\rangle = -t\Big\{ & \left|(i\pm1)\,j\uparrow,(k\,l)\downarrow\right\rangle + \left|i\,(j\pm1)\uparrow,(k\,l)\downarrow\right\rangle + \\ & \left|(i\,j)\uparrow,(k\pm1)\,l\downarrow\right\rangle + \left|(i\,j)\uparrow,k\,(l\pm1)\downarrow\right\rangle\Big\} \\ & +U.1.\left|(i\,i)\uparrow,(i\,i)\downarrow\right\rangle \end{aligned} \tag{2.6}$$

$$\begin{aligned} H\left|(i\,j)\uparrow,\ (k\,l)\downarrow\right\rangle = -t\Big\{ & \left|(i+1)\,j\uparrow,(k\,l)\downarrow\right\rangle + \left|(i-1)\,j\uparrow,(k\,l)\downarrow\right\rangle + \\ & \left|i\,(j+1)\uparrow,(k\,l)\downarrow\right\rangle + \left|i\,(j-1)\uparrow,(k\,l)\downarrow\right\rangle + \\ & \left|(i\,j)\uparrow,(k+1)\,l\downarrow\right\rangle + \left|(i\,j)\uparrow,(k-1)\,l\downarrow\right\rangle + \\ & \left|(i\,j)\uparrow,k\,(l+1)\downarrow\right\rangle + \left|(i\,j)\uparrow,k\,(l-1)\downarrow\right\rangle\Big\} \\ & +U\left|(i\,i)\uparrow,(i\,i)\downarrow\right\rangle \end{aligned} \tag{2.7}$$

## 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 2D 10 x 10 square lattice where there are a total of 10000 pair electronic states; $H\left|\Psi_l\right\rangle :\ l = 0,1,2,3,\ldots,10000$. While for 2D 9 x 9 square lattice where there are a total of 6561 pair electronic states; then $H\left|\Psi_l\right\rangle :\ l = 0,1,2,3,\ldots,6561$. 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 Hamiltonian 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 the pair electronic states one after the other as the case demands, we rather use (2.6) to act on only one single electronic in each separation and sum the result. We know that $\langle\Psi|H|\Psi\rangle$ 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 $|\Psi_l\rangle$ 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.

$$H|\Psi\rangle = H\sum_{l} X_l|\Psi_l\rangle = -t\sum_{(jl)}\left\{\frac{n\,X_l\,\langle\Psi_l|\Psi_l\rangle|\Psi_j\rangle}{\langle\Psi_j|\Psi_j\rangle}\right\} + U\sum_{l} X_l|\Psi_l\rangle \tag{2.8}$$

where $n$ is the total number of states generated within a given lattice separation, $\langle\Psi_l|\Psi_l\rangle$ is the inner product of the state acted on by the unit step Hamiltonian, $\langle\Psi_j|\Psi_j\rangle$ 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, $|\Psi_j\rangle$ 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

$$H|\Psi\rangle = HX_0|\Psi_0\rangle + HX_1|\Psi_1\rangle + HX_2|\Psi_2\rangle + HX_3|\Psi_3\rangle + HX_4|\Psi_4\rangle + HX_5|\Psi_5\rangle \tag{2.9}$$

$$\begin{aligned} H|\Psi_0\rangle = H|11\uparrow,11\downarrow\rangle = -tX_0\Big\{ & |21\uparrow,11\downarrow\rangle^1 + |51\uparrow,11\downarrow\rangle^1 + |12\uparrow,11\downarrow\rangle^1 + |15\uparrow,11\downarrow\rangle^1 + \\ & |11\uparrow,21\downarrow\rangle^1 + |11\uparrow,51\downarrow\rangle^1 + |11\uparrow,12\downarrow\rangle^1 + |11\uparrow,15\downarrow\rangle^1\Big\} + UX_0|\Psi_0\rangle \end{aligned} \tag{2.10}$$

Where for clarity of purpose the superscripts only indicate the respective separations generated. Also note that in the process of applying this technique, for instance, if ( $i$ + 1 ) = 6 or ( $i$ - 1 ) = 0, since there is no 6 or 0 in the information provided by the lattice geometry in table 2.1, then 6 ( = 1) and 0 ( = 5 ) because of the requirements of the repeated boundary conditions. It is obvious from the parentheses of (2.10) that all the 8 new eigen states generated are of the same separation $l = 1$ and therefore having eigen state $|\psi_1\rangle$. Hence

$$H|\Psi_0\rangle = -t\,\{8|\Psi_1\rangle\} + UX_0|\Psi_0\rangle \tag{2.11}$$

By comparing this result with the equation (2.8), then $n = 8$, $j = 1$ and $l = 0$ as a result

$$H|\Psi_0\rangle = -tX_0\left(\frac{8\times\langle\Psi_0|\Psi_0\rangle\times|\Psi_1\rangle}{\langle\Psi_1|\Psi_1\rangle}\right) + UX_0|\Psi_0\rangle \tag{2.12}$$

$$H|\Psi_0\rangle = -tX_0\left(\frac{8\times 25\times|\Psi_1\rangle}{100}\right) + UX_0|\Psi_0\rangle = -tX_0\,(2|\Psi_1\rangle) + UX_0|\Psi_0\rangle \tag{2.13}$$

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 little different from the first one. Thus, when the unit step Hamiltonian acts on the eigen state in separation $l = 1$ we get,

$$\begin{aligned} H|\Psi_1\rangle = H|11\uparrow,12\downarrow\rangle = -t\Big\{ & |21\uparrow,12\downarrow\rangle^2 + |51\uparrow,12\downarrow\rangle^2 + |12\uparrow,12\downarrow\rangle^0 + \\ & |15\uparrow,12\downarrow\rangle^3 + |11\uparrow,22\downarrow\rangle^2 + |11\uparrow,52\downarrow\rangle^2 + |11\uparrow,13\downarrow\rangle^3 + |11\uparrow,11\downarrow\rangle^0\Big\} \end{aligned} \tag{2.14}$$

$$H|\Psi_1\rangle = -t\,\{2|\Psi_0\rangle + 4|\Psi_2\rangle + 2|\Psi_3\rangle\} \tag{2.15}$$

We can now revert to (2.8) for the summation technique. Hence

$$H\left|\,\Psi_1\,\right\rangle = -t\,X_1\left(\frac{2\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\,\Psi_0\,\right\rangle}{\left\langle\Psi_0\middle|\Psi_0\right\rangle}+\frac{4\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\,\Psi_2\,\right\rangle}{\left\langle\Psi_2\middle|\Psi_2\right\rangle}+\frac{2\times\left\langle\Psi_1\middle|\Psi_1\right\rangle\times\left|\,\Psi_3\,\right\rangle}{\left\langle\Psi_3\middle|\Psi_3\right\rangle}\right) \tag{2.16}$$

$$H\left|\,\Psi_1\,\right\rangle = -t\,X_1\left(\frac{2\times 100\times\left|\,\Psi_0\,\right\rangle}{25}+\frac{4\times 100\times\left|\,\Psi_2\,\right\rangle}{100}+\frac{2\times 100\times\left|\,\Psi_3\,\right\rangle}{100}\right) \tag{2.17}$$

$$H\left|\,\Psi_1\,\right\rangle = -t\,X_1\left\{8\left|\Psi_0\right\rangle+4\left|\Psi_2\right\rangle+2\left|\Psi_3\right\rangle\right\} \tag{2.18}$$

Also by a similar algebraic subroutine, when the unit step Hamiltonian acts on the eigen state in separation $l = 2, 3, 4$ and $5$, we get respectively after a careful simplification the below equations.

$$H\left|\,\Psi_2\,\right\rangle = -t\,X_2\left\{4\left|\Psi_1\right\rangle+2\left|\Psi_4\right\rangle\right\} \tag{2.19}$$

$$H\left|\,\Psi_3\,\right\rangle = -t\,X_3\left\{2\left|\Psi_1\right\rangle+2\left|\Psi_4\right\rangle\right\} \tag{2.20}$$

$$H\left|\,\Psi_4\,\right\rangle = -t\,X_4\left\{4\left|\Psi_2\right\rangle+4\left|\Psi_3\right\rangle+4\left|\Psi_5\right\rangle\right\} \tag{2.21}$$

$$H\left|\,\Psi_5\,\right\rangle = -t\,X_5\left\{2\left|\Psi_4\right\rangle\right\} \tag{2.22}$$

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 one after the other. Hence in accordance with (2.8) and (2.9) we get

$$\left|\,\Psi\,\right\rangle = X_0\left|\,\Psi_0\,\right\rangle+X_1\left|\,\Psi_1\,\right\rangle+X_2\left|\,\Psi_2\,\right\rangle+X_3\left|\,\Psi_3\,\right\rangle+X_4\left|\,\Psi_4\,\right\rangle+X_5\left|\,\Psi_5\,\right\rangle \tag{2.23}$$

$$\begin{aligned}H\left|\,\Psi\,\right\rangle = -t\{&2X_0\left|\,\Psi_1\,\right\rangle+8X_1\left|\,\Psi_0\,\right\rangle+4X_1\left|\,\Psi_2\,\right\rangle+2X_1\left|\,\Psi_3\,\right\rangle+4X_2\left|\,\Psi_1\,\right\rangle+2X_2\left|\,\Psi_4\,\right\rangle+2X_3\left|\,\Psi_1\,\right\rangle+\\&2X_3\left|\,\Psi_4\,\right\rangle+4X_4\left|\,\Psi_2\,\right\rangle+4X_4\left|\,\Psi_3\,\right\rangle+4X_4\left|\,\Psi_5\,\right\rangle+2X_5\left|\,\Psi_4\,\right\rangle\}\;+\;UX_0\left|\,\Psi_0\,\right\rangle\end{aligned} \tag{2.24}$$

With the use of (2.3) and the information provided in table 3.1, we can eventually establish after multiplying through (2.21) and (2.22) by the complex conjugate of (2.5) that

$$\left\langle\Psi\middle|\Psi\right\rangle = X_0^2\left\langle\Psi_0\middle|\Psi_0\right\rangle+X_1^2\left\langle\Psi_1\middle|\Psi_1\right\rangle+X_2^2\left\langle\Psi_2\middle|\Psi_2\right\rangle+X_3^2\left\langle\Psi_3\middle|\Psi_3\right\rangle+X_4^2\left\langle\Psi_4\middle|\Psi_4\right\rangle+X_5^2\left\langle\Psi_5\middle|\Psi_5\right\rangle \tag{2.25}$$

$$\left\langle\Psi\middle|\Psi\right\rangle = 25\left(X_0^2+4X_1^2+4X_2^2+4X_3^2+8X_4^2+4X_5^2\right) \tag{2.26}$$

$$\begin{aligned}\left\langle\Psi\middle|H\middle|\Psi\right\rangle = -(25)(4t)\{&4X_0X_1+8X_1X_2+4X_1X_3+8X_2X_4+8X_3X_4+8X_4X_5+\\&2X_3^2+4X_4^2+4X_5^2-(U/4t)X_0^2\}\end{aligned} \tag{2.27}$$

### 2.5 The variational method

The variational method consists in evaluating the integral

$$E_g\left\langle\Psi\middle|\Psi\right\rangle = \left\langle\Psi\middle|H\middle|\Psi\right\rangle = \left\langle\Psi\middle|H_t+H_u\middle|\Psi\right\rangle \tag{2.28}$$

Where $E_g$ is the correlated ground state energy and $\Psi$ is the guessed trial wave function. We can now differentially minimize (2.26) after the substitution of (2.24) and (2.25) as follows.

$$\left\langle\Psi\middle|\Psi\right\rangle\frac{\partial E_g}{\partial X_i}+E_g\frac{\partial}{\partial X_i}\left\langle\Psi\middle|\Psi\right\rangle = \frac{\partial}{\partial X_i}\left\langle\Psi\middle|H\middle|\Psi\right\rangle \tag{2.29}$$

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

$$\frac{\partial E_g}{\partial X_i} = 0 \qquad ; \quad \forall\; i = 0, 1, 2, 3 \tag{2.30}$$

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

$$\left[A-\lambda_l\,I\right]\vec{X}_l = 0 \tag{2.31}$$

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

$$\begin{pmatrix} E-4u & 8 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 \\ 0 & 4 & E & 0 & 4 & 0 \\ 0 & 2 & 0 & E+2 & 4 & 0 \\ 0 & 0 & 2 & 2 & E+2 & 2 \\ 0 & 0 & 0 & 0 & 4 & E+4 \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.32}$$

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 (2.30) 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 (2.5) in terms of only nearest neighbours site to a given separation length. Accordingly, $\langle \Psi_l | \Psi_l \rangle = 1, 4, 4, 4, 8$ and 4; $l = 0, 1, 2, 3, 4$ and 5, respectively, then we get

$$|\Psi\rangle = a_0|\Psi_0\rangle + a_1|\Psi_1\rangle + a_2|\Psi_2\rangle + a_3|\Psi_3\rangle + a_4|\Psi_4\rangle + a_5|\Psi_5\rangle \tag{2.33}$$

$$\langle\Psi|\Psi\rangle = a_0^2 + 4a_1^2 + 4a_2^2 + 4a_3^2 + 8a_4^2 + 4a_5^2 \tag{2.34}$$

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

Then this will make us redefine (2.26) as

$$\langle\Psi|\Psi\rangle = \sum_{l=0}^{5} \lambda_l\, a_l^2 \tag{2.35}$$

where $\lambda_l$ $(l = 0, 2, \dots, 5)$ 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

$$\widehat{f}(\omega) = \frac{\lambda_l\, a_l^2}{\sqrt{2\pi}} \int_0^\infty f(x)\, e^{-i\omega x}\, dx \tag{2.36}$$

However, the kernel $f(x)$ in the integrand is simply $x^2$, because the basis is a square of the lattice separation parameter, $\omega$ is the angular vibration of the two electrons. As a result, (2.36) becomes

$$\widehat{f}(\omega) = \frac{\lambda_l\, a_l^2}{\sqrt{2\pi}} \int_0^l x^2\, e^{-i\omega x}\, dx \tag{2.37}$$

$$\widehat{f}(\omega) = \frac{2\lambda_l\, a_l^2}{\omega^2\sqrt{2\pi}}\left(1 + l\, e^{-i\omega l} - e^{-i\omega l}\right) + i\frac{\lambda_l\, a_l^2}{\omega\sqrt{2\pi}}\left(l^2\, e^{-i\omega l}\right) \tag{2.38}$$

It is sometimes convenient to express the spectral intensity in terms of polar coordinate, so that $\widehat{f}(\omega) = \left(\frac{\lambda_l\, a_l^2}{\sqrt{2\pi}}\right)\left\{\frac{2}{\omega^2} + \frac{2l}{\omega^2}(\cos\omega l - i\sin\omega l) - \frac{2}{\omega^2}(\cos\omega l - i\sin\omega l) + i\frac{l^2}{\omega}(\cos\omega l - i\sin\omega l)\right\}$

(2.39)

$$\left|\widehat{f}(\omega)\right|^2 = \left(\frac{\lambda_l\, a_l^2}{\sqrt{2\pi}}\right)^2 \left\{\left(\frac{2}{\omega^2} + \frac{2l}{\omega^2}\cos\omega l - \frac{2}{\omega^2}\cos\omega l + \frac{l^2}{\omega}\sin\omega l\right)^2 + \left(\frac{2}{\omega^2}\sin\omega l + \frac{l^2}{\omega}\cos\omega l - \frac{2l}{\omega^2}\sin\omega l\right)^2\right\} \tag{2.40}$$

$$\left|\widehat{f}(\omega)\right|^2 = \left(\frac{\lambda_l a_l^2}{\sqrt{2\pi}}\right)^2 \left\{\frac{8}{\omega^4} + \frac{l^4}{\omega^2} - \frac{8l}{\omega^4} + \frac{4l^2}{\omega^4} + \frac{8l}{\omega^4}\cos\omega l + \frac{4l^2}{\omega^3}\sin\omega l - \frac{8}{\omega^4}\cos\omega l\right\} \tag{2.41}$$

Suppose we decide to vary (2.41) logarithmically, then after some arithmetic jamboree the resulting equation simplifies to

$$\ln\left|\hat{f}(\omega)\right|^2 = \ln\left(\frac{\lambda_l\, a_l^2}{\sqrt{2\pi}}\right)^2 + 8\ln l - 2\ln 4 - 5\ln\omega + \ln\sin\omega l \tag{2.42}$$

$$\ln\left|\hat{f}(\omega)\right|^2 = \ln\left\{\left(\frac{\lambda_l\, a_l^2}{\sqrt{2\pi}}\right)^2\left(\frac{l^8\sin\omega l}{\omega^5}\right)\right\} - 2.77 \tag{2.43}$$

$$\left|\hat{f}(\omega)\right|^2 = 0.06\left(\frac{\lambda_l\, a_l^2}{\sqrt{2\pi}}\right)^2\left(\frac{l^8}{\omega^5}\right)\sin\omega l \tag{2.44}$$

Thus (2.44) 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 angular vibration $\omega$ 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 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, 5) | | | | | |
|---|---|---|---|---|---|---|---|
| | | $X_0$ | $X_1$ | $X_2$ | $X_3$ | $X_4$ | $X_5$ |
| 50.00 | -7.7585 | 0.0131 | 0.3390 | 0.4242 | 0.4538 | 0.4837 | 0.5148 |
| 40.00 | -7.7602 | 0.0162 | 0.3399 | 0.4244 | 0.4537 | 0.4835 | 0.5143 |
| 30.00 | -7.7630 | 0.0214 | 0.3412 | 0.4247 | 0.4537 | 0.4830 | 0.5134 |
| 20.00 | -7.7684 | 0.0313 | 0.3438 | 0.4253 | 0.4535 | 0.4821 | 0.5117 |
| 10.00 | -7.7834 | 0.0587 | 0.3506 | 0.4266 | 0.4528 | 0.4794 | 0.5068 |
| 5.00 | -7.8084 | 0.1039 | 0.3613 | 0.4279 | 0.4508 | 0.4739 | 0.4978 |
| 1.00 | -7.9013 | 0.2631 | 0.3914 | 0.4240 | 0.4351 | 0.4462 | 0.4575 |
| 0.00 | -8.0000 | 0.4082 | 0.4082 | 0.4082 | 0.4082 | 0.4082 | 0.4082 |
| -1.00 | -8.3668 | 0.7235 | 0.3945 | 0.3176 | 0.2934 | 0.2695 | 0.2468 |
| -5.00 | -20.8086 | 0.9947 | 0.1005 | 0.0200 | 0.0114 | 0.0034 | 0.0008 |
| -10.00 | -40.4010 | 0.9987 | 0.0501 | 0.0050 | 0.0026 | 0.0004 | 0.0000 |
| -20.00 | -80.2001 | 0.9997 | 0.0250 | 0.0012 | 0.0006 | 0.0000 | 0.0000 |

**Table 3.2:** Shows the calculated values of the Spectra intensity for arbitrary value of $\omega$ For 2D 5 x 5 square lattice

| Interaction strength $U/4t$ | Spectra intensity $\left|\hat{f}(\omega)\right|^2$ ( $\omega$ =0.5) | | | | | |
|---|---|---|---|---|---|---|
| | $l=0$ | $l=1$ | $l=2$ | $l=3$ | $l=4$ | $l=5$ |
| 50.00 | 0.0000 | 0.0309 | 34.0995 | 1356.815 | 63786.98 | 80267.54 |
| 40.00 | 0.0000 | 0.0313 | 34.1635 | 1355.619 | 63681.55 | 79956.16 |
| 30.00 | 0.0000 | 0.0318 | 34.2602 | 1355.619 | 63418.54 | 79397.95 |
| 20.00 | 0.0000 | 0.0327 | 34.4542 | 1353.23 | 62947.18 | 78351.53 |
| 10.00 | 0.0000 | 0.0354 | 34.8774 | 1344.895 | 61548.84 | 75393.21 |
| 5.00 | 0.0000 | 0.0399 | 35.3045 | 1321.29 | 58772.55 | 70178.71 |
| 1.00 | 0.0000 | 0.0550 | 34.0348 | 1146.618 | 46189.79 | 50066.84 |
| 0.00 | 0.0000 | 0.0651 | 29.2383 | 888.2896 | 32353.38 | 31730.57 |
| -1.00 | 0.0000 | 0.0568 | 10.7147 | 237.0844 | 6146.994 | 4240.01 |
| -5.00 | 0.0000 | 0.0002 | 0.0002 | 0.00054 | 0.000156 | 4.68E-07 |
| -10.00 | 0.0000 | 1.4E-05 | 6.58E-07 | 1.46E-06 | 2.98E-08 | 0.0000 |
| -20.00 | 0.0000 | 9.16E-07 | 2.18E-09 | 4.15E-09 | 0.0000 | 0.0000 |

**Table 3.3:** 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 the 2D N x N square lattice

| 2D N x N Square Lattice | GVA<br>$E_N = -8(1-1/N^2)$ | CVA<br>$E_N = -8(1-\alpha/N^2)$<br>$\alpha = 0.6250$ | Present study<br>$E_N = -8(1-\alpha/N^2)$<br>$\alpha = 0.7546$ |
|---|---|---|---|
| 3 x 3 | -7.1111 | -7.4444 | -7.3292 |
| 5 x 5 | -7.6800 | -7.8000 | -7.7585 |
| 7 x 7 | -7.8367 | -7.8980 | -7.8768 |
| 9 x 9 | -7.9012 | -7.9382 | -7.9255 |
| 11 x 11 | -7.9339 | -7.9587 | -7.9501 |

## 4.0 Discussion of Results

The total energies and the variational parameters for the 2D 5 x 5 square lattice obtained from the matrix (2.32) of section 2 is shown in table 3.1. The table 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, (iii) $X_1$ increases until the interaction strength $U/4t = 0$ and then it starts to decrease as $U/4t$ is decreased, (iv) $X_2$ increases until the interaction strength $U/4t = 5$ and then it starts to decrease as $U/4t$ is decreased, (v) $X_3$, $X_4$ and $X_5$ 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 is zero, we observe a free electron system, 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, $X_0 \prec X_1 \prec X_2 \prec X_3 \prec X_4 \prec X_5$. Also for negative interaction strength we observe that $X_0 \succ X_1 \succ X_2 \succ X_3 \succ X_4 \succ X_5$.

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.

As indicated in table 3.2, the spectra intensity for on-site electrons is zero for all values of the interaction strength. The table exhibits clearly that the variational parameter $X_1$ increases until $U/4t = 0$ and thereafter it starts to decrease while $X_2$ increases until when $U/4t = 10$ before it starts to decrease. The parameters $X_3$, $X_4$ and $X_5$ decreases consistently to zero as the interaction strength is decreased. This implies 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 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 that $\alpha$ varies with N, the number of lattice sites. For large N, $\alpha$ approaches the value of 0.7546 in this present study, while $\alpha$ is 0.6350 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 those of GVA and CVA.

## 5.0 Conclusion

The result of this work 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 and hence the highest potential. The model in this regime best describes ferromagnetism. Also 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. Generally, it is this coming together or correlation of electrons that is responsible for the many physical properties of materials in condensed matter physics, e.g. superconductivity, magnetism, super fluidity. 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*.

## Appendix

### TWO – DIMENSIONAL (2D) 5 X 5 SQUARE LATTICE :

### VARIATIONAL APPROACH

From the geometry of the 2D 5 X 5 square lattice as shown in fig. A1 we can therefore summarize the details of the two electrons interaction in table 2.1

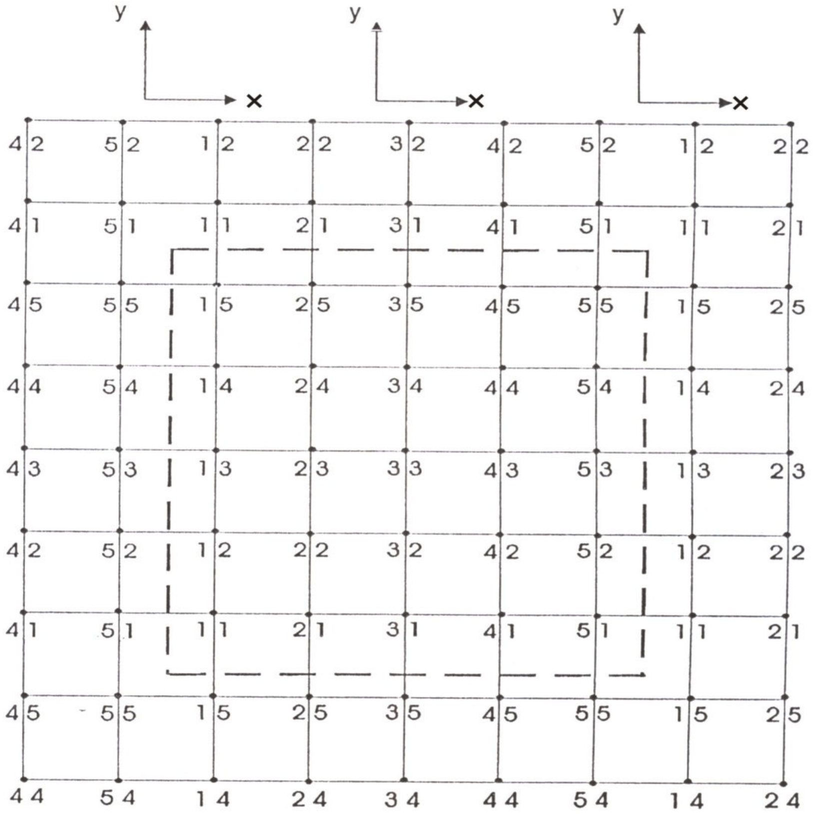

**FIG. A1 2D 5 X 5 square lattice with periodic boundary conditions. The inner dashed lines map out the actual lattice size of our study. The numbers represent co-ordinates of lattice sites.**

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Biography of the first Author: Edison A. Enaibe.

I was born on 26th April, 1970, in Benin City but my home town is Oginibo a town in Ughelli South Local Government Area of Delta State, Nigeria. I obtained all my University degrees from the Department of Physics, University of Benin, Benin – City, Edo State, Nigeria. The order of the degrees is as follows:

B.Sc. (Hons) Applied Physics, 1992/1993 academic session.
M.Sc. Theoretical Physics, 1997/1998 academic session.
Ph.D. Theoretical Physics (Condensed Matter Physics) , 2003/2004 academic session.

I am also a member of the following reputable Associations:

(i) Member of the National Association of Mathematical Physics (MNAMP) in 1995.
(ii) Member of the Nigerian Institute of Physics (MNIP) in 2001.
(iii) Member of the International AIDS Society in 2013.
(iv) Member of the International Organization of Scientific research (MIOSR) in 2013.

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