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Many Electron Highly Simplified Correlated Variational Approach to Mott Insulator State at Half-filling

Godfrey E. Akpojotor

**Theoretical and Computational Condensed Matter Physics,
Physics Department, Delta State University, Abraka 330106, Nigeria**

Abstract

The field of correlated electrons represents the frontier of our understanding of the electronic properties of solids. Most often, the mathematical and computational tools to investigate strongly correlated systems are complex, thereby making it difficult to following the research in this field. It is therefore necessary to develop simplified mathematical tools to give useful insight into these strongly correlated systems. The purpose of this study is to extend our earlier formulation of a highly simplified correlated variational approach (HSCVA) for strongly correlated two electrons on two sites in all three dimensions to many electrons. The standard Hubbard model is studied to investigate the effect of on-site interaction strength, U/4t on the variational parameters at various electron densities. The usual Mott insulator state at half-filling is elegantly obtained. The possibility of enhancing and extending the many electron HSCVA to larger lattices and other models is then discussed.

1.0 Introduction

The few particle studies usually provide very useful insight into the study of strongly correlated systems as well as provide a quick means to test the results obtained from infinite particle interaction in complex system. However, there are still relatively poor mathematical tools to analytically investigate the low-density limits [1-3]. The reason is that as we increase the number of particles and probably the sizes of the systems as well as the dimension, the computation become too complex to handle. One example is the correlated variational approach (CVA) which has been very successful in its application to the two-electron Hubbard and extended Hubbard models in all three dimensions (D = 1, 2, 3) [4-7]. The beauty of the CVA is that it yields amenable matrix sizes even for large lattices and therefore have helped in overcoming the finite-size lattice effect in studying strongly correlated systems. Further, we have shown that in the highly simplified correlated variational approach (HSCVA) version [5,7], the creation and annihilation operators can be replaced by statistical operators which by merely adding and subtracting 1 or 2 provide the same itinerant behaviour for the kinetic part of the Hubbard model and Hubbard-like models. And as been pointed out in previous studies [7, 8], this formulation makes it possible to clearly observe the roles of the interaction matrix one decides to include in the kinetic part. However, like other few particles problem, the CVA hence the HSCVA version application to lattices beyond two electrons have been very challenging (see Ref.[1] for a number of studies for 4 electrons]. One major problem is how to avoid repetitive states when choosing the basis states as well as the product of the activated states [6]. A more critical study of the formation of the HSCVA however, indicates that the problem of repetitive basis states can be suppressed and therefore the approach can be extended to study systems with more than two electrons. This is the purpose of this current study which is to demonstrate the many electrons interaction within the HSCVA to study strongly correlated systems. Our focus here is to investigate if the ground state of the Hubbard model is a Mott insulator state as has been observed both theoretically [9,10] and experimentally [11, 12]. The Mott insulator state occurs when all the conduction elections are tied to the atomic sites. This means the charge degree of freedom will be localized at these atomic sites thereby leaving the spin and orbital degrees of freedom to combine to produce various ordering patterns. This is the basic property of the transition oxides and by extension the high temperature superconducting copper oxides [9, 13, 14]. It is this observation of the Mott insulating state in the Hubbard model that first engendered interest in using it to explore high temperature superconducting cuprates [15-17]. Therefore, investigating the Mott insulator state in

Corresponding author: E-mail: -, Tel.: +2348066602677

the many electron Hubbard interaction in the HSCVA is a necessary precursory step. The study is structured as follows. In the section II, a brief review of the HSCVA will be done for the two-electron interaction in the Hubbard model so as to determine the salient features of the formation that can be used to extend it to many electrons. The application of the many electron HSCVA will be done for four lattice sites at various electron density in Section III. Here the electron density n = N_p/N where N_p is the number of electrons and N is the number of lattice sites determines the electronic filling level (= N_p/N_e) where N_e = 2N is the maximum number of electrons that can occupy N. The results will be presented and discussed in Section IV and this will be followed by a conclusion.

2.0 Brief Review of the HSCVA for the two-electron Hubbard Interaction

The formulation of the correlated variational approach for the two-electron ground state problem on an arbitrary large torus was initiated for one dimension (1D) and two dimension (2D) in Ref [4]. It was then extended to three dimension (3D) by Enaibe and Idiodi [18]. In the CVA, the variational ground state energy has to be minimized with respect to the variational parameters to obtain several algebraic equations which can then be expressed as the matrix representation of the two-electron Hubbard interaction in the lattice system being studied. To avoid this minimization process which become more tedious with increase in the lattice sites as well as dimension, the HSCVA was formulated by developing a general expression for the direct matrix representation of the two-electron Hubbard interaction in ID, 2D, and 3D lattices and it is given by [5, 7],

$$H_{L_{CX}L_X}[X_{L_{CX}}]=\left[E_{\delta L_{CX}L_X}-4\left(\frac{U}{4t}\right)_{\delta_{0L_{CX}}\delta_{0L_X}}+T_{L_{CX}L_X}\right][X_{L_{CX}}]=[0] \qquad (1)$$

where H is the Hubbard model, $X_{L_{CX}}$ are the variational parameters which are functions of the various separation, L_{CX} of the basis states, E is the energy spectrum and U/4t is the ratio of the Coulomb potential, U to the hopping term, t. Obviously the salient features required to apply the HSCVA are (1) identify the possible separations, L_{CX} for the lattice system under study (2) select the first basis state ($\frac{N}{2}\uparrow, \frac{N}{2}\downarrow$) hence the electronic configuration of all the basis states (3) activate the basis states for the various separation using the kinetic part of the Hubbard Hamiltonian and (4) identify the new states from the activation of the basis states using the Kinetic part of the Hubbard Hamiltonian, their various separations L_x and the number of such new states T_{L_X}

The standard Hubbard model also known as the t-U Hamiltonian is given by

$$H = H_t + H_U \qquad (2a)$$

with H_t being the kinetic part:

$$H_t = -t\left\{\sum_{\langle i,j\rangle,\sigma} c^{+}_{i\sigma}c_{\ j\bar{\sigma}} + H.C\right\} \qquad (2b)$$

and H_U being the Coulombic interaction part which is the origin of electron correlation:

$$H_U = U\sum_i \eta_{i\uparrow}\eta_{i\downarrow} \ . \qquad (2c)$$

It is important to point out that Eq.(2b) is obtained from the overlap of two atomic Wannier orbitals $\varphi_{i\sigma}(r)$ on site i and $\varphi_{j\sigma}(r)$ on site j [9]:

$$t = \int dr\varphi^{*}_{i\sigma}(r)\frac{1}{2m}\nabla^2\varphi_{j\sigma}(r)$$

where m is the electron mass and Planck constant ħ is set to unity. Thus in Eqs. (2b), the $c^{+}_{i\sigma}, c_{i\bar{\sigma}}$ are the creation and annihilation operators respectively, for an election of spin $\sigma(\bar{\sigma})$ in the Wannier state on the i*th*(j*th)* lattice site(s). The notation $\langle i, j\rangle$ means nearest neighbours, while t is the electronic hopping parameter between nearest neighbour sites *i* and j. H. C. denotes Hermitian conjugation and its inclusion in the Hamiltonian guarantees that the expectation values of the dynamical quantities will be real.

Similarly, Eq.(2c) is obtained from a two electron Coulombic intrasite interaction:

$$U = \int dr\ dr'\varphi^{*}_{i\sigma}(r)\varphi_{i\sigma}(r)\frac{e^2}{|r-r'|}\varphi^{*}_{i-\sigma}(r')\varphi_{i-\sigma}(r').$$

Thus in Eq. (2c), the $\eta_{i\uparrow}\eta_{i\downarrow}$ is the number operators for two electrons. It follows then that the Hubbard model was developed effectively from two electrons on two sites with on-site Coulombic interaction.

Taking into account the condition that only nearest neighbour is allowed, Eq. (2b) can be expanded for a four sites problem (i, j, k, l = 1, 2, 3, 4) as follows:

$$\begin{aligned} H_t = -t[&c_{1\uparrow}^{+}c_{2\uparrow} + c_{2\uparrow}^{+}c_{1\uparrow} + c_{1\downarrow}^{+}c_{2\downarrow} + c_{2\downarrow}^{+}c_{1\downarrow} + c_{1\uparrow}^{+}c_{4\uparrow} + c_{4\uparrow}^{+}c_{1\uparrow} + c_{1\downarrow}^{+}c_{4\downarrow} + c_{4\downarrow}^{+}c_{1\downarrow} + \\ &c_{2\uparrow}^{+}c_{3\uparrow} + c_{3\uparrow}^{+}c_{2\uparrow} + c_{2\downarrow}^{+}c_{3\downarrow} + c_{3\downarrow}^{+}c_{2\downarrow} + c_{3\uparrow}^{+}c_{4\uparrow} + c_{4\uparrow}^{+}c_{3\uparrow} + c_{3\downarrow}^{+}c_{4\downarrow} + c_{4\downarrow}^{+}c_{3\downarrow}] \end{aligned} \tag{3}$$

It is easy to see that irrespective of the number of electrons, the annihilation will be for one electron on one site of the basis state and the creation of one electron will be for the appropriate NN site on the condition that (1) if this NN site is vacant, then the electron can be created in it irrespective of its quantum characteristics and (2) if there is an electron already occupying this NN site, then the Pauli Exclusion principle requires that the electron to be created must not possess the same quantum characteristics as the first one. This is also expected for the Hermitian conjugate part. Thus the annihilation and creation operators and their Hermitian conjugates effectively deals with two electrons on two sites at any given instance until the operation of the full kinetic Hamiltonian is completed. Now each of these instances is similar to the observed scenario for the independent case of $N_p = 2$ on N = 2. Therefore the generalized equation developed for the $N_p = 2$ on N = 2 can be adopted by summing up all the possible instances for any numbers of electrons and sites in all three dimensions. All that is needful is to obtain the aforementioned salient features of the HSCVA.

Following the above line of observation, the wavefunction constructed for the $N_p = 2$ on N = 2 can also be extended for the many electron Hubbard interactions on lattices in all three dimensions. In previous work [5, 7], the wavefunction obtained for the $N_p = 2$ on N = 2 is

$$/\psi> = \sum_{i=1}^{N} X_{|i-i|}\,/i\uparrow, i\downarrow> + \sum_{<i,j>}^{N} X_{|i-j|}[/i\uparrow, j\downarrow> - /i\downarrow, j\uparrow>] \tag{4}$$

with i = j for on-site states (double occupancy) and i ≠ j for inter-site states. Therefore the lattice separation is given by $L = |i-i|$ for on-site states and $L = |i-j|$ for inter-site states where $L = L_{CX}$ for that of the basis states and $L = L_X$ for that of the new states. For the four site problem ((i, j, k, l), Eq. (4) can be extended to become

$$\begin{aligned} /\psi> &= \sum_{i=1}^{N} X_{|i-i|}\,/i\uparrow, i\downarrow> + \sum_{j=1}^{N} X_{|j-j|}\,/j\uparrow, j\downarrow> + \sum_{k=1}^{N} X_{|k-k|}\,/k\uparrow, k\downarrow> + \sum_{l=1}^{N} X_{|l-l|}\,/l\uparrow, l\downarrow> \\ &= \sum_{<i,j>}^{N} X_{|i-j|}[/i\uparrow, j\downarrow> - /i\downarrow, j\uparrow>] + \sum_{<i,l>}^{N} X_{|i-k|}[/i\uparrow, k\downarrow> - /i\downarrow, k\uparrow>] \\ &= + \sum_{<i,l>}^{N} X_{|i-l|}[/i\uparrow, l\downarrow> - /i\downarrow, l\uparrow>] \quad + \sum_{<j,k>}^{N} X_{|j-k|}[/j\uparrow, k\downarrow> - /j\downarrow, k\uparrow>] \\ &\quad + \sum_{<j,l>}^{N} X_{|j-l|}[/j\uparrow, l\downarrow> - /j\downarrow, l\uparrow>] + \sum_{<k,l>}^{N} X_{|k-l|}[/k\uparrow, l\downarrow> - /k\downarrow, l\uparrow>] \end{aligned} \tag{5}$$

Clearly, the possible separations for the basis states for N = 4 will be $L_{CX} = 0, 1, 2$.

Finally, one can easily see that using Eq.(3) to operate on a basis state of four electrons on four sites will yield the same new states as using our statistical hopperer, H_p [7], that is, for the state /1↑, 2↓, 3↑, 4↓> say,

$$\begin{aligned} H_t\,/1,\uparrow, 2\downarrow, 3\uparrow, 4\downarrow> = H_p\,/1,\uparrow, 2\downarrow, 3\uparrow, 4\downarrow> = /4\uparrow, 2\downarrow, 3\uparrow, 4\downarrow> + /2\uparrow, 2\downarrow, 3\uparrow, 4\downarrow> \\ + /1,\uparrow, 1\downarrow, 3\uparrow, 4\downarrow> + /1,\uparrow, 3\downarrow, 3\uparrow, 4\downarrow> + /1,\uparrow, 2\downarrow, 2\uparrow, 4\downarrow> + /1,\uparrow, 2\downarrow, 4\uparrow, 4\downarrow> \\ + /1,\uparrow, 2\downarrow, 3\uparrow, 3\downarrow> + /1,\uparrow, 2\downarrow, 3\uparrow, 1\downarrow> \end{aligned} \tag{6}$$

where the H_p is given for 1D in general as

$$\begin{aligned} H_P\,/i\uparrow, j\downarrow, /k\uparrow, l\downarrow, > = /(i\pm 1)\uparrow, j\downarrow, /k\uparrow, l\downarrow, > + /i\uparrow, (j\pm 1)\downarrow, /k\uparrow, l\downarrow, >, \\ + /i\uparrow, j\downarrow, (k\pm 1)\uparrow, l\downarrow, > + /i\uparrow, j\downarrow /k\uparrow, (l\pm 1)\downarrow> \end{aligned} \tag{7}$$

3.0 Application of the many electron HSCVA

The four atomic sites lattice can be filled with a maximum of eight electrons. This means one can have quarter filling (N_p = 2 on N = 4), half filling (N_p = 4 on N = 4), three quarter filling (N_p = 6 on N = 4) and 7/8 filling (N_p = 7 on N = 8).

(i) Quarter-filling: 2-electron interaction on 4 atomic sites (8 electronic sites)

The selected basis state for N = 4 is $\frac{N}{2}\uparrow, \frac{N}{2}\downarrow$ = /2↑, 2↓>. Therefore the basis states configuration and their separations will be /2↑, 2↓> with L_{CX} = 0, /2↑,3↓> with L_{CX} = 1 and /2↑,4↓> with L_{CX} = 2 as shown in Fig. 1.

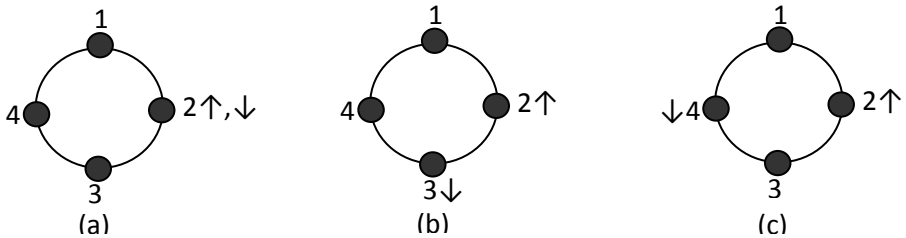

Fig. 1 The electronic configuration of the basis states for the various separation for N_p = 4 on N = 4.

Adopting Eq.(7) to activate the basis states, we obtain

H_P /2↑,2↓>= /1↑,2↓>, /3↑,2↓>, /2↑,1↓>, /2↑,3↓>

H_P /2↑, 3↓>= /1↑,3↓>, /3↑,3↓>, /2↑,2↓>, /2↑,4↓>

H_P /2↑, 4↓>= /1↑, 4↓>+/3↑, 4↓>, /2↑, 3↓>, /2↑, 1↓>

Thus a table showing L_{CX}, L_X and $T_{L_{CX}L_X}$ can now be prepared as shown in Table 1. Taking into account these values in Eq.(1), the matrix representation of the Hubbard interaction for N_p = 2 on N = 4 will be

$$\begin{bmatrix} E-4(U/4t) & 4 & 0 \\ 2 & 0 & 2 \\ 0 & 4 & 0 \end{bmatrix}\begin{bmatrix} X_0 \\ X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (8)$$

Eq. (8) is solved numerically to obtain the ground state energy and the variational parameters as the on-site interaction strength, U/4t is increased from 0 to 20. The results are presented in Table 2 while a graph of the effect of increasing the U/4t from 0 to 20 on the variational parameters is shown in Fig. 6.

Table 1. A table showing the separation of the basis states, L_{CX}, separation of the new states from activation of the basis states, L_X and the number of new states with separation, $T_{L_{CX}L_X}$.

Separation of the basis states L_{CX}	Separation of the new states from activation of the basis states L_X	Number of new states new states with separation L_X $T_{L_{CX}L_X}$
0	1	4
1	0 2	2 2
2	1	4

(ii) Half-filling: 4-electron interaction on 4 atomic sites (8 electronic sites)

The four electron N_p = 4 on four sites N = 4 is half filling. The selected basis state for N = 4 is /2↑, 2↓>. Therefore the basis state configuration and their separations will be /2↑, 2↓> with L_{CX} = 0, /2↑,3↓> with L_{CX} = 1 and /2↑,4↓> with L_{CX} = 2. For configuration of the two remaining electrons, there are two possible types of the electronic configurations of the basis states as follows:

a. Starting with the basis state /2↑, 2↓, 1↑,3↓> as shown in as shown Fig 2.

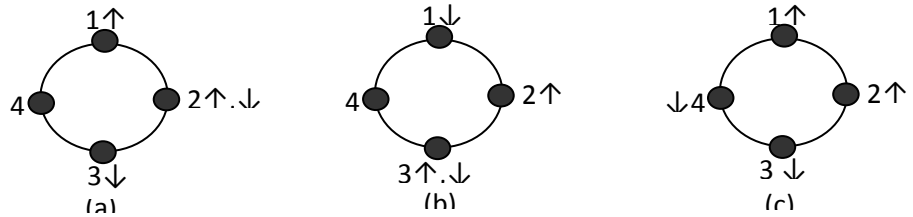

Fig. (2) The electronic configuration of the basis states for the various separation for $N_p = 4$ on N = 4 starting with the state /2↑,2↓,1↑,3↓>.

Observe that the spins of the last two sites in the case of the separation $L_c = 1$ have to be interchange in line with the Pauli Exclusion Principle. Because the emphasis of the HSCVA is on the separation, this interchange will not affect the outcome of the configuration since the number of electrons with spin-up and spin-down remain equal, that is: H_P /2↑, 3↓, 1↓, 3↑> = H_P / 2↓, 3↑, 1↑, 3↓>.

In general, the activation of these basis states will yield

H_P /2↑,2↓,1↑,3↓>= /3↑,2↓,1↑,3↓> , /2↑,1↓,1↑,3↓>, /2↑, 2↓,/4↑,3↓>, /2↑,2↓ /1↑,4↓>

H_P /2↑, 3↓,1↓,3↑> = /1↑, 3↓, 1↓,3↑>, /2↑,2↓,1↓,3↑>, /2↑, 4↓,1↓,3↑>, /2↑, 3↓,2↓,3↑>
/2↑, 3↓,4↓,3↑>, /2↑, 3↓,1↓,4↑>

H_P /2↑, 4↓, 1↑,3↓>= /3↑, 4↓,1↑,3↓>, /2↑, 1↓,1↑,3↓>, /2↑, 4↓, 4↑,3↓>, /2↑, 4↓, 1↑,2↓>

The L_{CX}, L_X and $T_{L_{CX}L_X}$ are obtained and then taking into account Eq.(1), the matrix representation of the Hubbard interaction for $N_p = 4$ on N = 4 starting with the basis state /2↑, 2↓, 1↑,3↓> will be

$$\begin{bmatrix} E+3-4(U/4t) & 6 & 3 \\ 3 & 6 & 3 \\ 4 & 6 & 2 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (9)$$

Eq. (9) is solved numerically and the results depicted graphically showing the effect of increasing the U/4t from 0 to 20 on the variational parameters for Np = 4 on N = 4 starting with the basis state /2↑, 2↓, 1↑,3↓> as shown in Fig. 7.

b. Starting with basis state /2↑,2↓,1↑,4↓> as shown in Fig.3. It is pertinent to quickly point out that the third type of configuration with basis state /2↑,2↓,3↑,4↓> will yield the same results as that with the basis state /2↑,2↓,1↑,4↓> and therefore will not be demonstrated separately.

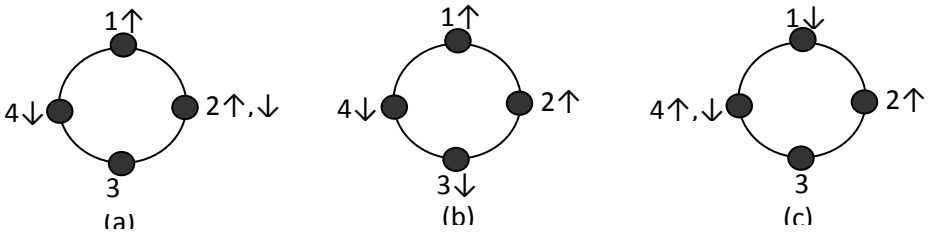

Fig. 3 The electronic configuration of the basis states for the various separation for $N_p = 4$ on N = 4 starting the with state /2↑,2↓,1↑,4↓> .

Again observe that the spins of the last two sites in the case of the separation $L_c = 2$ have to be interchanged in line with the Pauli Exclusion Principle. Because the emphasis of the HSCVA is on the separation, this interchange will not affect the outcome of the configuration since the number of electrons with spin-up and spin-down remain equal.

The activation of these basis states will yield

H_P /2↑, 2↓,1↑,4↓>= /3↑,2↓,1↑,4↓>, /2↑,1↓,1↑,4↓>, /2↑,3↓,1↑,4↓>, /2↑,2↓,4↑,4↓>, /2↑,2↓,1↑,1↓>, /2↑,2↓,1↑,3↓>

H_P /2↑,3↓,1↑,4↓> = /3↑,3↓,1↑,4↓>, /2↑,2↓,1↑,4↓>, /2↑,3↓,4↑,4↓>, /2↑,3↓,1↑,1↓>

H_P /2↑, 4↓, 1↓, 4↑>= /1↑, 4↓, 1↓, 4↑>, /3↑, 4↓, 1↓, 4↑>, /2↑, 3↓, 1↓, 4↑>, /2↑, 4↓, 2↓, 4↑>, /2↑, 4↓, 1↓, 1↑>, /2↑, 4↓, 1↓, 3↑>

The L_{CX}, L_X and $T_{L_{CX}L_X}$ are obtained and then taking into account Eq.(1), the matrix representation of the Hubbard interaction for $N_p = 4$ on N = 4 starting with the basis state /2↑,2↓,1↑,4↓> will be

$$\begin{bmatrix} E+3-4(U/4t) & 6 & 3 \\ 4 & 6 & 2 \\ 3 & 6 & 3 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (10)$$

Eq. (10) is solved numerically and the results depicted graphically showing the effect of increasing the U/4t from 0 to 20 on the variational parameters for Np = 4 on N = 4 starting with the basis state /2↑, 2↓, 1↑, 4↓> as shown in Fig. 8

(iii) Three-quarter-filling: 6-electron interaction on 4 atomic sites (8 electronic sites)

The six electron $N_p = 6$ on four sites N = 4 is three quarter filling and there is only one type of the electronic configurations and that starting with the basis state /2↑, 2↓,1↑,1↓,3↑,4↓> as shown in Fig. 4.

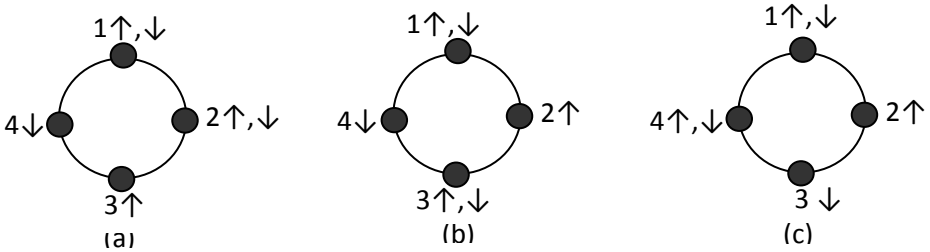

Fig. 4 The electronic configuration of the basis states for the various separation for $N_p = 6$ on N = 4.

Again observe that the spins of the last two sites in the case of the separation $L_c = 2$ have to be interchanged in line with the Pauli Exclusion Principle. Because the emphasis of the HSCVA is on the separation, this interchange will not affect the outcome of the configuration since the number of electrons with spin-up and spin-down remain equal.

The activation of these basis states will yield

H_P /2↑, 2↓,1↑,1↓,3↑,4↓> = /2↑, 3↓,1↑,1↓,3↑,4↓>, /2↑, 2↓,4↑,1↓,3↑,4↓> , /2↑, 2↓,1↑,1↓,4↑,4↓>, /2↑, 2↓,1↑,1↓,3↑,3↓>

H_P /2↑, 3↓,1↑,1↓,3↑,4↓>= /2↑,2↓,1↑,1↓,3↑,4↓>, /2↑,3↓,4↑,1↓,3↑,4↓>, /2↑,3↓,1↑,2↓,3↑,4↓>, /2↑,3↓,1↑,1↓,4↑,4↓>

H_P /2↑, 4↓, 1↑,1↓,3↓,4↑>= /3↑, 4↓, 1↑,1↓,3↓,4↑>, /2↑, 4↓, 1↑,2↓,3↓,4↑>, /2↑, 4↓, 1↑,1↓,2↓,4↑>, /2↑, 4↓, 1↑,1↓,3↓,3↑>

The L_{CX}, L_X and $T_{L_{CX}L_X}$ are obtained and then taking into account Eq.(1), the matrix representation of the Hubbard interaction for $N_p = 6$ on N = 4 will be

$$\begin{bmatrix} E+4-4(U/4t) & 8 & 4 \\ 4 & 8 & 3 \\ 4 & 7 & 4 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (11)$$

Eq. (11) is solved numerically and the results depicted graphically showing the effect of increasing the U/4t from 0 to 20 on the variational parameters for Np = 6 on N = 4 as shown in Fig. 9.

iv. 7/8-filling: 6-electron interaction on 4 atomic sites (8 electronic sites) - One Electron Removal Approach

The seven electron $N_p = 7$ on four sites N = 4 is 7/8 filling and it is also known as the first electron removal (FER) approach in theoretical and experimental studies of the high T_C superconducting cuprates [19, 20]. It has only one type of electronic configurations of the basis states as shown in Fig. 5 starting with the basis state /2↑, 2↓,1↑,1↓,3↑, 3↓, 4↑>. The removal of only one electron means the number of electrons with spin in one direction will be more than the ones in the opposite direction. This immediately will affect the antiferromagnetic order. Thus the FER approach which can be achieved in real systems by doping is very appropriate to study the superconducting cuprates in which doping level determine the phase diagram [19, 20]. In the Hubbard model, doping is expected to destroy the long range antiferromagnetic order to pave way for the transition into the superconducting state [9, 16, 21].

Further, the inequality of the electronic spins in opposite direction will leads to no degeneracy of the groundstate energy of the triplet states because there are usually more new states for the spin direction with the addition spin than the spin with opposite direction.

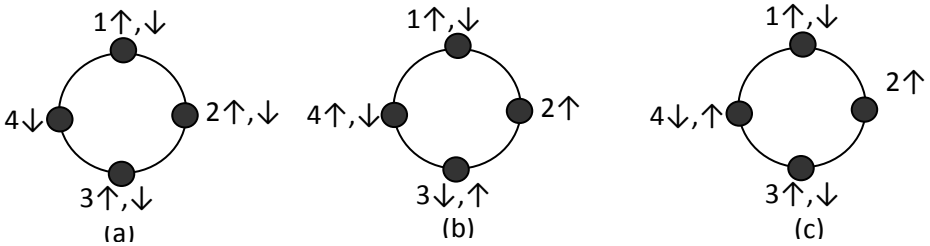

Fig. 5 The electronic configuration of the basis states for the various separation for $N_p = 7$ on N = 4 starting with the state /2↑, 2↓,1↑,1↓,3↑,4↓>.

Observe that the electronic configuration for the basis states with separations $L_c = 1$ and $L_c = 2$ appear similar but for their spins. Now there is difference between the outcome of the activation of these two basis states because of the differences in the number of electrons with spin-up and spin-down.

The activation of these basis states will yield

H_P /2↑, 2↓,1↑,1↓,3↑, 3↓, 4↑> = /2↑, 2↓,1↑,4↓,3↑, 3↓, 4↑>, /2↑, 2↓,1↑,1↓,3↑, 4↓, 4↑>

H_P /2↑, 3↓,1↑,1↓,3↑, 4↓, 4↑> = /2↑, 2↓,1↑,1↓,3↑, 4↓, 4↑>, /2↑, 3↓,1↑,2↓,3↑, 4↓, 4↑>

H_P /2↑, 4↓,1↑,1↓, 3↑, 3↓, 4↑> = /2↑, 4↓,1↑,2↓, 3↑, 3↓, 4↑>, /2↑, 4↓,1↑,1↓, 3↑, 2↓, 4↑>

The L_{CX}, L_X and $T_{L_{CX}L_X}$ are obtained and then taking into account Eq.(1), the matrix representation of the Hubbard interaction for $N_p = 7$ on N = 4 will be

$$\begin{bmatrix} E+4-4(U/4t) & 8 & 4 \\ 4 & 8 & 4 \\ 4 & 8 & 4 \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

Eq. (12) is solved numerically and the results depicted graphically showing the effect of increasing the U/4t from 0 to 20 on the variational parameters for Np = 7 on N = 4 as shown in Fig. 10.

4.0 Presentation and Discussion of Results

It is a common knowledge that at T = 0, there are two important terms that dominate the Hubbard model: the relative interaction strength U/4t and electron density hence the filling level. Therefore the results presented here is to simply consider the effect of the Coulomb interaction hence correlation on the electronic states for various fillings. This is achieved by first switching off the Coulombic interaction strength U/4t = 0 and then switching it on gradually till U/4t = 20. The effect of the role of the Coulomb interaction is monitored by the variational parameters. The first observation which is consistent with earlier studies of only two electron interaction on many sites in 1D – 3D is that for all fillings, the trend is that switching off the Coulombic interaction makes all the variational parameters to have the same values which means the same probability of being occupied [3-7]. The physical interpretation is that the electrons are not localized and therefore are free to move into any site. This simply means the kinetic part dominates. Then as U/4t is increased, the values of the on-site various parameters decrease at all fillings while the inter-site states increases as shown in Figs. 6-10. This observation which is also consistent with the aforementioned earlier studies means the electrons are gradually being localized due to increasing correlation effect to form the Mott insulator state. Now for the quarter filling and half filling, the numerical values of the variational parameters X_{L_1} and X_{L_2} are different meaning the electrons prefer to stay apart from each other, that is, localized on atomic different sites as shown in Figs. 6-8 This is also long range antiferromagnetic order. On the contrary, as shown in Figs. 9 and 10, increasing the density of electrons beyond half filling makes the other variational parameters beyond $L_c = 0$ to have the same numerical values ($X_{L_1} = X_{L_2}$) that is, they now have equal probability of being occupied. The implication is that the electrons are no longer localized in the inter-site states as the effect of correlation is now purely restricted to the on-site states. This clearly explain why the Mott insulator is observed in most studies [9, 10, 15, 16] at half filling for many electron Hubbard interaction. Since it is caused by the on-site Coulomb repulsion, this standard Hubbard Mott insulator is also known as intrasite Mott insulator. Thus it can be generalized by including inter-site Coulomb repulsion leading to generalized Mott insulator and such Hamiltonians become extended versions of the Hubbard model. The simplest of them is the t-U-V model [22, 23] where the V is the NN inter-site Coulombic interaction. A special case is when the V term is considered as the hybridization between different layers leading to the Periodic Anderson model (PAM) which has been demonstrated to be antiferromagnetic like the parent Hubbard model [24, 25]. The PAM has been used to obtain very useful information on heavy fermions [26, 27].

It is important to point out that as stated in the introduction, when the charge degree of freedom is localized, the spin and orbital degrees of freedom then combine to produce various ordering patterns. To account for the role of the spin degree of freedom, the NN superexchange interaction can be included to obtain the t-U-V-J_{ex} model. Now as it has been observed in previous studies, a two-electron system will always produce an antiferomagnetic order except we use the unrealistic configuration of the two electrons having the same spins to produce triplet basis states, /1↑, 2↑> and /1↓, 2↓>. The ground state energy of the triplet states is therefore degenerate. Now in the many electron HSCVA, the triplet basis states appear naturally: for example, in the starting basis state /2↑, 2↓, 1↑,3↓> for the half-filling case of $N_p = 4$ on N = 4, the natural triplet states are /2↑, 1↑> and /2↓, 3↓>. Since the activation of these states produce the same new states as the activation of /2↓, 1↓> and /2↑, 3↑>, the ground state energy will also be degenerate. Therefore the generalized HSCVA equation for both the singlet and triplet states of $N_p = 2$ on N = 2 [5] will also be applicable to the many electron interaction in a t-U-V-J_{ex} model which has vast application in spin ordering systems in 1D, 2D and 3D. Similarly, the HSCVA many electron interaction can also be used to study the strong coupling limit of the Hubbard model wherein $U \rightarrow \infty$ yielding the t-J model which has been extensively investigated for the high T_C superconductivity in the cuprates.

5.0 Conclusion

The effect of filling has been investigated in the many electron interaction HSCVA on four atomic sites since filling plays an important role in electronic correlations in a partially filled *d* electron band as often found in transition metal oxides including the high temperature superconducting copper oxides and the partially filled f electron in heavy fermionic systems. The Mott Insulator state is observed at half-filling while the quarter-filling provides the check on the formation of the HSCVA. The possibility of applying the HSCVA to the study of other models is also discussed. As it has been consistently pointed out [19], the beauty of the HSCVA is that one can start the investigation by obtaining the bandwidth of the non-interacting case. Thereafter one can introduce the desired interactions and monitor their effects. Thus the enhancement and extension of the study here to larger numbers of electrons and lattice sizes in all three dimensions as well as the application of the many electron interaction HSCVA to other models beyond the Hubbard model studied here are open challenges in making this approach a viable pedagogical but powerful mathematical tool for studying strongly correlated models and systems.

Table 2. A table showing the separation of the basis states, L_{CX}, separation of the new states from activation of the basis states, L_X and the number of new states new states with separation, $T_{L_{CX}L_X}$.

On-site interaction strength U/4t	Ground State Energy E_s	Variational parameters		
		X_0	X_1	X_2
0	-4.0000	0.5774	0.5774	0.5774
2	-3.2078	0.2179	0.6106	0.7614
4	-3.0462	0.1262	0.6010	0.7892
6	-2.9806	0.0882	0.5952	0.7987
8	-2.9452	0.0677	0.5915	0.8034
10	-2.9231	0.0549	0.5891	0.8062
12	-2.9081	0.0462	0.5874	0.8080
14	-2.8972	0.0398	0.5861	0.8092
16	-2.8889	0.0350	0.5851	0.8101
18	-2.8824	0.0312	0.5843	0.8109
20	-2.8771	0.0282	0.5837	0.8114

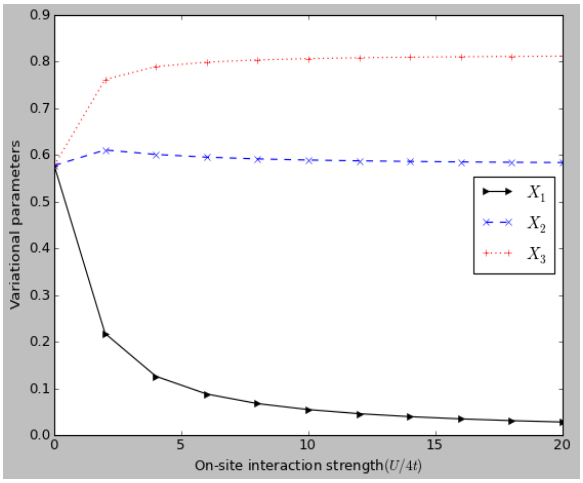

Fig. 6 (colour online): A graph showing the variation parameters as the on-site interaction strength, U/4t is increased from 0 to 20 for Np = 2 on N = 4.

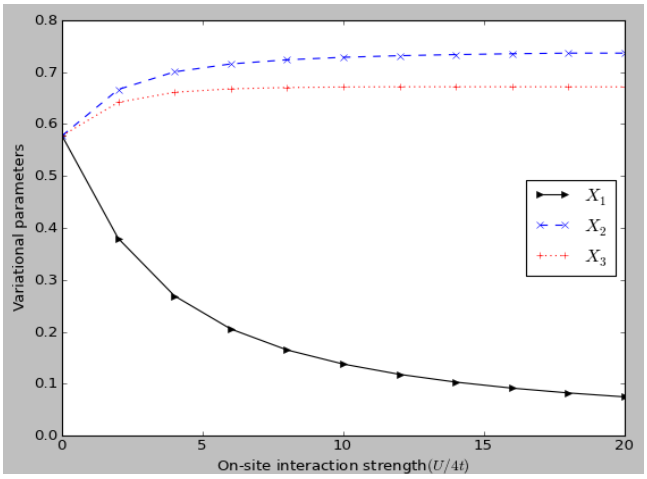

Fig. 7 (colour online): A graph showing the variation parameters as the on-site interaction strength, U/4t is increased from 0 to 20 for Np = 4 on N = 4 starting with basis state /2↑,2↓,1↑,3↓>.

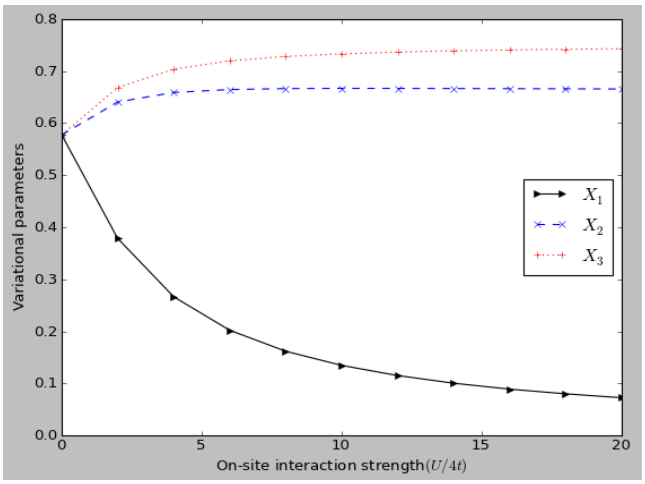

Fig. 8 (colour online): A graph showing the variation parameters as the on-site interaction strength, U/4t is increased from 0 to 20 for Np = 4 on N = 4 starting with basis state /2↑,2↓,1↑,4↓>.

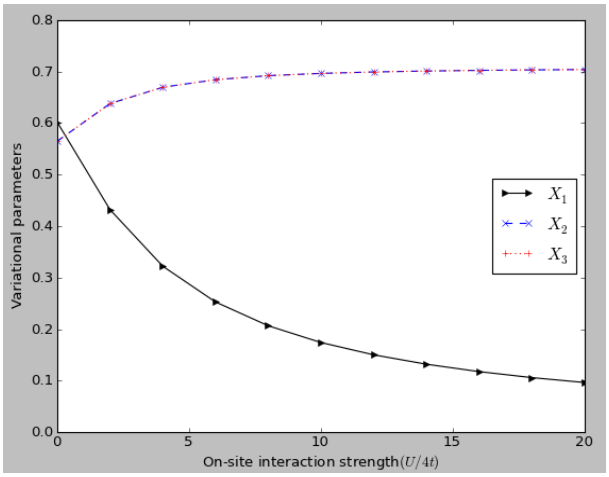

Fig. 9 (colour online): A graph showing the variation parameters as the on-site interaction strength, U/4t is increased from 0 to 20 for Np = 6 on N = 4

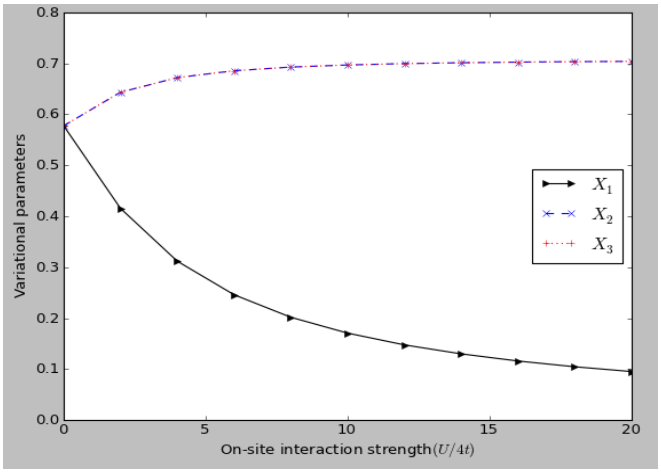

Fig. 10 (colour online): A graph showing the variation parameters as the on-site interaction strength, U/4t is increased from 0 to 20 for Np = 7 on N = 4

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