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# Dynamics of Twointeracting Electronsinthree-Dimensional Lattice

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***Abstract:*** *The physical property of strongly correlated electrons on a three-dimensional (3D) 3 x 3 x 3 cluster of the simple cubic lattice is here presented.In the work we developed the unit step Hamiltonian as a solution to the single band Hubbard Hamiltonian for the case of two electrons interaction in a finite three dimensional 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. 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), thevariational parameters which describe the probability distribution of lattice electron system is the same. The spectra intensity for on-site electrons is zero for all values of the interaction strength.*

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

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## I. 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 (Domanski et al., 1996).In spite of the enormous successes of the approach (Rycerz and Spalek, 2001) based on the effective single particle wave equation for many 3-dimensional metals andsemiconductors, 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 (van Bemmel et al., 1994) 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.

The one-dimensional Hubbard Hamiltonianis a good prototype for an exactly solvable model of correlated electrons in narrow band systems (Vallejo et al., 2003), where at half-filling the ground state is found to be anti-ferromagnetic and insulating for a repulsive (positive) potential. The other exact solution for the Hubbard Hamiltonian is the case of an infinite dimensional lattice. The exact solutions have brought a very important progress in the understanding of strongly correlated systems.

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 then for the $t$ - $J$ model, (v) the model exhibits anti-ferromagnetism rather than ferromagnetism, (vi) the Hubbard Hamiltonian (Hubbard, 1963) becomes very cumbersome to handle when the size of the Hilbert space of a given dimensional lattice increases.

We have in this study extended the work of Chen and Mei (1989) which was limited to one-and two-dimensional (ID and 2D) lattice to three-dimensional (3D) lattice. We also devised a unit step Hamiltonian and simplified trial wavefunction for our variational calculation instead of the more complex Hubbard Hamiltonian and correlated trial wavefunction developed by Chen and Mei.

The organization of this paper is as follows.In section 1, we discussed the nature of superconductivity and the relevance of the single band Hubbard Hamiltonian and its limitation for solving correlated electrons system. In section 2 we provide the method of this study by giving a brief description of the single - band Hubbard Hamiltonian and thetrail wavefunction to be utilized. We also present in this section an analytical solution for the two particles interaction on a 3x3 x 3 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 andthis is immediately followed by an appendix and lists of references.

## II. Mathematical Theory

The single-band Hubbard Hamiltonian (Marsiglo, 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, $C^{+}_{i\sigma}(C_{j\sigma})$ is the creation (annihilation) operator with spin $\sigma = \uparrow or \downarrow$ at site $i$, and $n_{i\sigma} = C^{+}_{i\sigma} C_{i\sigma}$ is 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.

### 2.2 The correlated variational trial wave function (CVA)

The correlated variational trial wave function (CVA) given by Chen and Mei (1989) is of the form

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

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.

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 number of sites and number of particles.

With a careful application of the two equations above we can conveniently solve for the wave function and hence the groundstate 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)

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

The analytical geometry of the 3D 3 x 3 x 3 cluster is shown in the appendix. There are a total of five planar lattices. We have generally summarized the details of the two electrons interaction on the 3D 3 x 3 x 3 cluster of the simple cubic lattice in table 2.0.

**Table 2.0**The summary of the relevant information derived from the analytical geometry of the 3D 3X3X3 cluster on a simple cubic lattice.

| Lattice separation $l$ Between the two electrons and actual separation distance $d$ | | Pair wave function $\lvert\psi_l\rangle$ | Number of pair electronic states at lattice separation $l$ $\langle\psi_l\lvert\psi_l\rangle$ | Pair electronic states $\lvert i\uparrow, j\downarrow\rangle$ |
|---|---|---|---|---|
| $l$ | $d$ | | | |
| 0 | 0 | $\lvert\psi_0\rangle$ | 27 | $\lvert 111\uparrow,111\downarrow\rangle$,<br>$\ldots,\lvert 333\uparrow,333\downarrow\rangle$ |
| 1 | $a$ | $\lvert\psi_1\rangle$ | 162 | $\lvert 111\uparrow,211\downarrow\rangle$,<br>$\ldots,\lvert 332\uparrow,333\downarrow\rangle$ |
| 2 | $\sqrt{2}a$ | $\lvert\psi_2\rangle$ | 324 | $\lvert 111\uparrow,221\downarrow\rangle$,<br>$\ldots,\lvert 233\uparrow,332\downarrow\rangle$ |
| 3 | $2a$ | $\lvert\psi_3\rangle$ | 216 | $\lvert 111\uparrow,222\downarrow\rangle$,<br>$\ldots,\lvert 323\uparrow,232\downarrow\rangle$ |
| Total number of electronic states N=3; (N x N)$^3$ or (N x N x N)$^2$ | | | 729 | 729 |

It can be shown from the lattice symmetry that the central site for any odd 3D N x N x N lattices is $\left(\frac{N+1}{2},\frac{N+1}{2},\frac{N+1}{2}\right)$,from which for the 3D 3 x 3 x 3 it is (222).A lattice separation of $l = 0$, then means that both electrons are at the same site $(i,i,i)$. Whilea lattice separation of $l = 1$,then means that both electrons are on different sites at a separation distance of 1 and so on. Note that the actual separation distance $d$ comprises of both linear and diagonal lengths.Details of how to calculate the respective actual separation distance for various separation lengthsbetween the two interacting electrons, can be found in (Akpojotor et al, 2002) and (Enaibe, 2003).

## 2.3 The Unit Step Hamiltonian in 3D cluster of the simple 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 and redistribute 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. Also from the geometry of the 3D lattice we can recast (2.2) as

$$\lvert\Psi\rangle = \sum_{l=0}^{l} X_l \;\lvert\Psi_l\rangle \quad (2.5)$$

where$\lvert\Psi_l\rangle$ 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$\lvert(ijk)\uparrow,(lmn)\downarrow\rangle$. Then

$$\begin{aligned} H\lvert (ijk)\uparrow,(lmn)\downarrow\rangle = -t\Big\{ &\lvert (i\pm 1)\, jk\uparrow,(lmn)\downarrow\rangle + \lvert i\,(j\pm 1)\,k\uparrow,(lmn)\downarrow\rangle + \\ &\lvert ij\,(k\pm 1)\uparrow,(lmn)\downarrow\rangle + \lvert (ijk)\uparrow,(l\pm 1)\,mn\downarrow\rangle + \\ &\lvert (ijk)\uparrow, l(m\pm 1)n\downarrow\rangle + \lvert (ijk)\uparrow, lm\,(n\pm 1)\downarrow\rangle \Big\} \\ + U\lvert (iii)\uparrow,(iii)\downarrow\rangle \quad (2.6) \end{aligned}$$

$$
\begin{aligned}
&H \left|(ijk)\uparrow, (lmn)\downarrow\right\rangle = -t \Big\{ \left|(i+1)\,j\,k\uparrow,\ (lmn)\downarrow\right\rangle + \left|(i-1)\ j\ k\uparrow, (lmn)\downarrow\right\rangle + \\
&\left| i\,(j+1)\,k\uparrow, (lmn)\downarrow\right\rangle + \left| i\,(j-1)\,k\uparrow, (lmn)\downarrow\right\rangle + \\
&\left| ij\ (k+1)\uparrow,\ (lmn)\downarrow\right\rangle + \left| ij\ (k-1)\uparrow,\ (lmn)\downarrow\right\rangle + \\
&\left| (ijk)\uparrow,\ (l+1)\,mn\downarrow\right\rangle + \left| (ijk)\uparrow,\ (l-1)\,m\,n\downarrow\right\rangle + \\
&\left| (ijk)\uparrow,\ l\,(m+1)\,n\downarrow\right\rangle + \left| (ijk)\uparrow,\ l\,(m-1)\,n\downarrow\right\rangle + \\
&\left| (ijk)\uparrow,\ l\,m\,(n+1)\downarrow\right\rangle + \left| (ijk)\uparrow,\ l\,m\,(n-1)\downarrow\right\rangle \Big\} \\
&+\ U\ \left| (\,i\,i\,i\,)\uparrow, (\,i\,i\,i\,)\downarrow\right\rangle \qquad (2.7)
\end{aligned}
$$

## 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 3x3x3simple cubic lattice where there are a total of 729 pair electronic states; $H\left|\Psi_l\right\rangle :\ l = 1, 2, 3, \ldots, 729$. While for 3D 5 x 5 x 5 simple cubic lattice wherethere are a total of 15625 pair electronic states; then $H\left|\Psi_l\right\rangle :\ l = 1, 2, 3, \ldots, 15625$. This process as we all know is actually cumbersome and it will be very difficult to handle without error.

The advantage of theunit 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 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 $\left\langle\Psi\right|H\left|\Psi\right\rangle$ 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.

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

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 theeigen 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

$$
H\left|\ \Psi\ \right\rangle = H\sum X_l \left|\ \Psi_l\ \right\rangle = HX_l\left|\ \Psi_l\ \right\rangle = HX_0\left|\ \Psi_0\ \right\rangle + HX_1\left|\ \Psi_1\ \right\rangle + HX_2\left|\ \Psi_2\ \right\rangle + HX_3\left|\ \Psi_3\ \right\rangle \qquad (2.9)
$$

$$
\begin{aligned}
&H\left|\ \Psi_0\ \right\rangle = H\left|\ 111\uparrow,111\downarrow\ \right\rangle = -t\,X_0 \Big\{\left|\ 311\uparrow,111\downarrow\ \right\rangle + \left|\ 211\uparrow,111\downarrow\ \right\rangle + \left|\ 131\uparrow,111\downarrow\ \right\rangle + \\
&\left|\ 121\uparrow,111\downarrow\ \right\rangle + \left|\ 113\uparrow,111\downarrow\ \right\rangle + \left|\ 112\uparrow,111\downarrow\ \right\rangle + \left|\ 111\uparrow,211\downarrow\ \right\rangle + \left|\ 111\uparrow,311\downarrow\ \right\rangle + \\
&\left|\ 111\uparrow,131\downarrow\ \right\rangle + \left|\ 111\uparrow,121\downarrow\ \right\rangle + \left|\ 111\uparrow,113\downarrow\ \right\rangle + \left|\ 111\uparrow,112\downarrow\ \right\rangle\Big\} \quad + U\,X_0\left|\Psi_0\right\rangle \qquad (2.10)
\end{aligned}
$$

Note that in the process of applying this technique, for instance, if ( $i$ + 1 ) = 4 or ( $i$ - 1 ) = 0, since there is no 4 or 0 in the information providedby thelattice geometry in table 2.0, then 4 ( = 1) and 0 ( = 3 ) because of the requirements of the repeated boundary conditions. It is obvious from the parentheses of (2.10) that all the 12 new eigen states generated are ofthe same separation $l = 1$ and thereforehavingeigen state $|\psi_1\rangle$.

$$H|\Psi_0\rangle = -t\{12|\Psi_1\rangle\} + U X_0 |\Psi_0\rangle \qquad (2.11)$$

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

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

$$H|\Psi_0\rangle = -t X_0 \left(\frac{12 \times 27 \times |\Psi_1\rangle}{162}\right) + U X_0 |\Psi_0\rangle = -t X_0 \left(2|\Psi_1\rangle\right) + U X_0 |\Psi_0\rangle \quad (2.13)$$

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

$$H|\Psi_1\rangle = H|111\uparrow,211\downarrow\rangle = -t X_1 \Big\{ |211\uparrow,211\downarrow\rangle^0 + |311\uparrow,211\downarrow\rangle^1 + |121\uparrow,211\downarrow\rangle^2 +$$
$$|131\uparrow,211\downarrow\rangle^2 + |112\uparrow,211\downarrow\rangle^2 + |113\uparrow,211\downarrow\rangle^2 + |111\uparrow,311\downarrow\rangle^1 + |111\uparrow,111\downarrow\rangle^0 +$$
$$|111\uparrow,221\downarrow\rangle^2 + |111\uparrow,231\downarrow\rangle^2 + |111\uparrow,212\downarrow\rangle^2 + |111\uparrow,213\downarrow\rangle^2 \Big\} \qquad (2.14)$$

Where for clarity of purpose the superscripts only indicate the respective separations generated. We can now revert to (2.8) for the summation technique.

$$H|\Psi_1\rangle = -t X_1 \{2|\Psi_0\rangle + 2|\Psi_1\rangle + 8|\Psi_2\rangle\} \qquad (2.15)$$

$$H|\Psi_1\rangle = -t X_1 \left(\frac{2 \times \langle\Psi_1|\Psi_1\rangle \times |\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} + \frac{2 \times \langle\Psi_1|\Psi_1\rangle \times |\Psi_1\rangle}{\langle\Psi_1|\Psi_1\rangle} + \frac{8 \times \langle\Psi_1|\Psi_1\rangle \times |\Psi_2\rangle}{\langle\Psi_2|\Psi_2\rangle}\right) \qquad (2.16)$$

$$H|\Psi_1\rangle = -t X_1 \left(\frac{2 \times 162 \times |\Psi_0\rangle}{27} + \frac{2 \times 162 \times |\Psi_1\rangle}{162} + \frac{8 \times 162 \times |\Psi_2\rangle}{324}\right) \qquad (2.17)$$

$$H|\Psi_1\rangle = -t X_1 \{12|\Psi_0\rangle + 2|\Psi_1\rangle + 4|\Psi_2\rangle\} \qquad (2.18)$$

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

$$H|\Psi_2\rangle = -t X_2 \{8|\Psi_1\rangle + 4|\Psi_2\rangle + 6|\Psi_3\rangle\} \qquad (2.19)$$

$$H|\Psi_3\rangle = -t X_3 \{4|\Psi_2\rangle + 6|\Psi_3\rangle\} \quad (2.20)$$

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.Hence in accordance with (2.8) and (2.9) we get

$$|\Psi\rangle = X_0|\Psi_0\rangle + X_1|\Psi_1\rangle + X_2|\Psi_2\rangle + X_3|\Psi_3\rangle \quad (2.21)$$

$$H|\Psi\rangle = -t\{2X_0|\Psi_1\rangle + 12X_1|\Psi_0\rangle + 2X_1|\Psi_1\rangle + 4X_1|\Psi_2\rangle + 8X_2|\Psi_1\rangle + 4X_2|\Psi_2\rangle + 6X_2|\Psi_3\rangle +$$
$$4X_3|\Psi_2\rangle + 6X_3|\Psi_3\rangle\} + UX_0|\Psi_0\rangle \quad (2.22)$$

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

$$\langle\Psi|\Psi\rangle = X_0^2\langle\Psi_0|\Psi_0\rangle + X_1^2\langle\Psi_1|\Psi_1\rangle + X_2^2\langle\Psi_2|\Psi_2\rangle + X_3^2\langle\Psi_3|\Psi_3\rangle \quad (2.23)$$

$$\langle\Psi|\Psi\rangle = 27\left(X_0^2 + 6X_1^2 + 12X_2^2 + 8X_3^2\right) \qquad (2.24)$$

$$\langle\Psi|H|\Psi\rangle = -(27)(4t)\left(6X_0X_1 + 24X_1X_2 + 24X_2X_3 + 3X_1^2 + 12X_2^2 + 12X_3^2 - (U/4t)X_0^2\right) \qquad (2.25)$$

### 2.5 The variational method

The variational method consists in evaluating the integral

$$E_g \langle \Psi | \Psi \rangle = \langle \Psi | H | \Psi \rangle = \langle \Psi | H_t + H_u | \Psi \rangle \qquad (2.26)$$

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.

$$\langle \Psi | \Psi \rangle \frac{\partial E_g}{\partial X_i} + E_g \frac{\partial}{\partial X_i} \langle \Psi | \Psi \rangle = \frac{\partial}{\partial X_i} \langle \Psi | H | \Psi \rangle \qquad (2.27)$$

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

$$\frac{\partial E_g}{\partial X_i} = 0 \qquad ; \quad \forall\, i = 0, 1, 2, 3 \qquad (2.28)$$

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

$$\left[ A - \lambda_l\, I \right] \vec{X}_l = 0 \, (2.29)$$

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.

$$\begin{pmatrix} E-4u & 12 & 0 & 0 \\ 2 & E+2 & 8 & 0 \\ 0 & 4 & E+4 & 4 \\ 0 & 0 & 6 & E+6 \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad (2.30)$$

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 Spectra density $\hat{f}(\omega)$ and spectra intensity $|\hat{f}(\omega)|^2$ of the two electrons.

The spectra density $\hat{f}(\omega)$ defines the distribution of the probability of values of the momentum to the total energy $E$. The spectra density is defined as follows.

$$\hat{f}(\omega) = \frac{\lambda_l X_l^2}{\sqrt{2\pi}} \int_0^{\infty} f(x) e^{-i\omega x} dx \qquad (2.31)$$

But the kernel $f(x)$ in the integrand is simply $X^2$, this is because the variational parameters is the square of the lattice separation. Now suppose we evaluate (2.31) within the limits of the lattice spacing $l$ ($l$ =0, 1, 2, 3) then

$$\hat{f}(\omega) = \frac{\lambda_l X_l^2}{\sqrt{2\pi}} \int_0^{l} X^2 e^{-i\omega x} dx \qquad (2.32)$$

$$\hat{f}(\omega) = \frac{\lambda_l X_l^2}{\sqrt{2\pi}} \left\{ \frac{2}{\omega^2} \left( 1 + l\, e^{-i\omega l} - e^{-i\omega l} \right) \right\} + i \frac{\lambda_l X_l^2}{\sqrt{2\pi}} \left\{ \frac{l^2 e^{-i\omega l}}{\omega} \right\} \qquad (2.33)$$

The spectra intensity which is the absolute value of the spectra density is given by

$$\left|\hat{f}(\omega)\right|^2 = \left(\frac{\lambda_l X_l^2}{\sqrt{2\pi}}\right)^2 \left\{ \left(\frac{2}{\omega^2} + \frac{2l\,e^{\omega l}}{\omega^2} - \frac{2\,e^{\omega l}}{\omega^2}\right)^2 + \left(\frac{l^2\,e^{\omega l}}{\omega}\right)^2 \right\} \qquad (2.34)$$

Now because of the presence of the exponential function in (2.34) would make us to vary it logarithmically so that

$$l\,n\left|\hat{f}(\omega)\right|^2 = l\,n\left\{ \left(\frac{\lambda_l X_l^2}{\sqrt{2\pi}}\right)^2 \left( \left(\frac{2}{\omega^2} + \frac{2l\,e^{\omega l}}{\omega^2} - \frac{2\,e^{\omega l}}{\omega^2}\right)^2 + \left(\frac{l^2\,e^{\omega l}}{\omega}\right)^2 \right) \right\} \qquad (2.35)$$

After a careful arrangement we get that the spectra intensity is

$$\left|\hat{f}(\omega)\right|^2 = \left(\frac{\lambda_l\, X_l^2\, l^3}{\sqrt{2\pi}\,\omega^3}\right)^2 e^{1.39+2\omega l} \quad (2.36)$$

## III. Presentation of Results

**Table 3.0** 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=Eg/t | Variational parameters ( $X_l$ ) ( $l = 0, 1, 2, 3$) | | | |
|---|---|---|---|---|---|
| | | $X_0$ | $X_1$ | $X_2$ | $X_3$ |
| 50.00 | -11.5906 | 0.0278 | 0.4897 | 0.5941 | 0.6376 |
| 30.00 | -11.6394 | 0.0456 | 0.5008 | 0.5920 | 0.6298 |
| 20.00 | -11.6530 | 0.0659 | 0.5033 | 0.5908 | 0.6271 |
| 15.00 | -11.6656 | 0.0846 | 0.5055 | 0.5895 | 0.6243 |
| 10.00 | -11.6883 | 0.1181 | 0.5088 | 0.5867 | 0.6188 |
| 5.00 | -11.7415 | 0.1944 | 0.5142 | 0.5775 | 0.6035 |
| 1.00 | -11.8916 | 0.3871 | 0.5126 | 0.5370 | 0.5469 |
| 0.00 | -12.0000 | 0.5000 | 0.5000 | 0.5000 | 0.5000 |
| -1.00 | -12.2290 | 0.6700 | 0.4594 | 0.4200 | 0.4045 |
| -5.00 | -21.3825 | 0.9930 | 0.1144 | 0.0289 | 0.0113 |
| -10.00 | -40.6358 | 0.9986 | 0.0529 | 0.0059 | 0.0010 |
| -15.00 | -60.4149 | 0.9994 | 0.0346 | 0.0025 | 0.0003 |
| -20.00 | -80.3081 | 0.9997 | 0.0257 | 0.0014 | 0.0001 |
| -30.00 | -120.2035 | 0.9999 | 0.0170 | 0.0006 | 0.0000 |
| -50.00 | -200.1212 | 0.9999 | 0.0101 | 0.0002 | 0.0000 |

**Table 3.1** Shows the calculated values of the of the spectra intensity for various variational parameters and total energy with a fixed arbitrary value of the spatial frequency $\omega = 5 rad / m$.

| Interaction strength U/4t | Total energy E=Eg/t | Spectra intensity $\left|\hat{f}(\omega)\right|^2$ | | | |
|---|---|---|---|---|---|
| | | $X_0$ | $X_1$ | $X_2$ | $X_3$ |
| 50.00 | -11.5906 | 0.0000 | 187.3164 | $5.72 \times 10^8$ | $1.90 \times 10^{14}$ |
| 30.00 | -11.6394 | 0.0000 | 206.6151 | $5.69 \times 10^8$ | $1.83 \times 10^{14}$ |
| 20.00 | -11.6530 | 0.0000 | 211.2646 | $5.65 \times 10^8$ | $1.80 \times 10^{14}$ |
| 15.00 | -11.6656 | 0.0000 | 215.4480 | $5.62 \times 10^8$ | $1.77 \times 10^{14}$ |
| 10.00 | -11.6883 | 0.0000 | 221.9907 | $5.53 \times 10^8$ | $1.72 \times 10^{14}$ |
| 5.00 | -11.7415 | 0.0000 | 233.6787 | $5.24 \times 10^8$ | $1.57 \times 10^{14}$ |
| 1.00 | -11.8916 | 0.0000 | 236.7220 | $4.02 \times 10^8$ | $1.08 \times 10^{14}$ |
| 0.00 | -12.0000 | 0.0000 | 218.2158 | $3.08 \times 10^8$ | $7.72 \times 10^{13}$ |
| -1.00 | -12.2290 | 0.0000 | 161.5063 | $1.59 \times 10^8$ | $3.43 \times 10^{13}$ |
| -5.00 | -21.3825 | 0.0000 | 1.8987 | $1.09 \times 10^4$ | $6.39 \times 10^7$ |
| -10.00 | -40.6358 | 0.0000 | 0.3135 | 68.3902 | $1.42 \times 10^4$ |
| -15.00 | -60.4149 | 0.0000 | 0.1268 | 4.8732 | 253.0000 |
| -20.00 | -80.3081 | 0.0000 | 0.0682 | 0.8468 | 5.5307 |
| -30.00 | -120.2035 | 0.0000 | 0.0293 | 0.0640 | 0.0000 |
| -50.00 | -200.1212 | 0.0000 | 0.0101 | 0.0022 | 0.0000 |

## IV. Discussion of Results

The total energies and the variational parameters for the 3D 3 x 3 x 3 simple cubic lattice obtained from the matrix (2.30) of section 2 is shown in table 3.0. The table shows that (i) the total energy 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$U/4t$ = 5.00 and then it starts to decrease as $U/4t$ is decreased, (iv) $X_2$and $X_3$ 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 $U/4t$ = 0, we observe a free electron system (the electrons are non-interacting). Since the electrons are not under the influence of any given potential they are free to hop to any preferable lattice site.

We infer from this result that when the interaction strength $U/4t$ 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 regime of $U/4t \to$ 20, the two electrons prefer to stay far apart as possible and the event is synonymous with ferromagnetism.

As indicated in table 3.1, 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 $U/4t$ =1.00 and thereafter it starts to decreasewhile $X_2$ and $X_3$decreases consistently to zero as the interaction strength is decreased. This implies that high values of positive interaction strength increase the intensity of the two electrons and they prefer to stay as far apart as possible. While high negative interaction strength decreases the intensity of the two electrons.

## V. Conclusion

This study demonstrates that for any positive on-site interaction strength ($U/4t$), the two electrons prefer to stay as far apart as possible in order to gain the lowest energy. 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. 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*. This study reveals that for free electron system (non-interacting), the probability distribution of lattice electron system is the same.

## Appendix

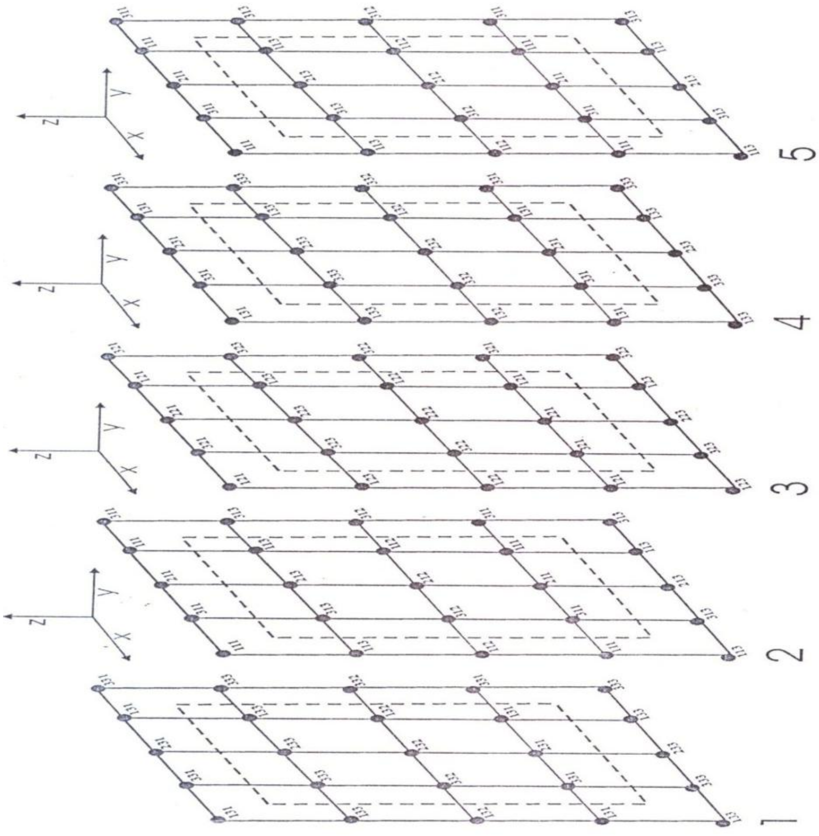

Fig. A3.1 THE 3D 3X3X3 SIMPLE CUBIC LATTICE WITH PERIODIC BOUNDARY CONDITIONS. THE NUMBERS REPRESENT COORDINATES OF A LATTICE SITE

### 2.7 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. 2.5, we can therefore summarize the details of the two electrons interaction in table 2.9 below.

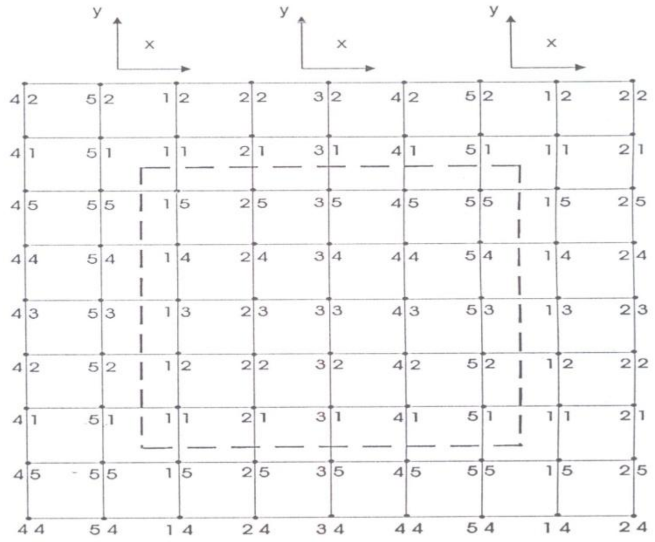

**FIG. 2.5. 2D 5 X 5 square lattice with periodic boundary conditions. The inner dashed lines map out the actual lattice size of our study. The numbers represent co-ordinates of lattice sites.**

The dotted square maps out the boundary of our interest in a given planar lattice. We consider the origin at(111). Now for lattice separation $l = 0$, for instance means the two electrons are on the same site and the lattice distance between them is $l \approx 0$, there are 27 of such possibility.

For lattice separation $l = 1$, nearest neighbour sites NN, we have a single linearlattice distance $d = a$, that means one electron is at lattice site (111) and the second one is at site (211) within the same plane or (121) in the second plane and there are 162 of the possibility of the two electrons to interact. Note that these two positions are also equivalent to (212) or (232) and (221) or (223).

For lattice separation $l = 2$, we have a diagonal lattice distance $d = \sqrt{2}a$ , that means one electron is at lattice site (111)and the second one is at site (212) within the same plane or (122) on the second plane and there are 324 of such possibility.

For lattice separation $l = 3$, we have a double lattice distance $l = 2a$ , that means one electron is at lattice site (111) and the second one is at site (113) within the same plane or (131) on the third plane and there are 216 of such possibility.

The total number of sites $n$ at a separation parameter $l$ from the origin (111); for $l = 0$, $n = 1; l = 1$, $n = 6$ (4 NN from one plane while 2 from either sides of the plane), $l = 2$, $n = 12$, $l = 3$, $n = 8$.

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