Journal of Astrophysics & Aerospace Technology
ISSN: 2329-6542

Obende, et al., J Astrophys Aerospace Technol 2015, 3:1
DOI: 10.4172/2329-6542.1000113

Review Article | Open Access

Correlation between Lanczos Method and Exact Diagonalisation Method in the Study of Highly Correlated Electrons System

Michael Obende[1]*, Okanigbuan OR[2] and Kolebaje Olusola[3]

[1]*Department of Physics, AfeBabalola University, Ado Ekiti, Nigeria*
[2]*Department of Physics, Ambrose Alli University Ekpoma, Edo State, Nigeria*
[3]*Department of Physics, Adeyemi College of Education, Ondo, Ondo State, Nigeria*

Abstract

The ground state energy and wave function of the single band hubbard model on the one dimensional lattice is computed using the Lanczos methods. It is shown that the ground state energies obtained for different values of the interaction strength it, compare nicely with that obtained using the method of exact calculation.

Keywords: Hubbard model; Lanczos method; Exact method

Introduction

The Hubbard model is an approximate model used to describe the transition between conducting and insulating systems. The Hubbard model, named after John Hubbard 1963, is the simplest model of interacting particles in lattices, with the only two tennis in the Hamiltonian; a kinetic term allowing for hopping of particles between soles of the lattice and a potential term consisting of an on sites interaction. The particles can either be fermions or bosons [1].

The Hubbard model is a good approximate for particles in a periodic potential at sufficiently low temperature that all the particles are in the lowest Bloch band, as long as any long-range interactions between the particles can be ignored. If interaction between particles on different sites of the lattice are included, the model is often referred to as the extended Hubbard model [2].

The model was originally proposed to describe electrons in solids and has since been the focus of particular interest as a model for high temperature super conductivity. For electron in a solid, the Hubbard model can be considered as an improvement on the tight-binding model, which includes only the hopping term for strong interaction, it can give qualitatively different behavior from the tight. Binding model, and correctly predicts the existence of so called mott insulators, which are prevented from becoming conducting by the strong repulsion between the particles [3,4].

The Hubbard model is based on the tight –binding approximation.

In the tight-binding approximation, electrons are viewed as occupying the standard orbital of their hopping between atoms, and then hopping between atoms, and then hopping between atoms during conduction. Mathematically, this is represented as hopping integral or transfer integral between neighboring atoms, which can be viewed as the physical principle that creates electrons bonds in crystalline materials [5-7].

The Hubbard Hamiltonian takes the form:

$$H = -+\sum_{(i,j)\sigma} C^{+}_{i\sigma} C_{j\sigma} + U\sum_{i=1}^{N} ni\uparrow nj\downarrow \tag{1.1}$$

Where $C^{+}_{i\sigma} C_{j\sigma}$ *and* ni are the creation, annihilation, and number operations, respectively, for an electron of spin σ in the wannier state on the on the ith lattice Fi, j means that only interest neighbor site hopping are allowed [8,9].

The Hubbard model has been extensively studied the single band Hubbard model in both one dimensional ring and two dimensional torus. By the exact calculation of the pair correlation function Fi, j defined as the possibility of finding an electron at site j when there has been an electron of opposite at site I, it is shown that for two electrons, the interaction is always repulsive in the ground state for any positive value of the on–site coulomb interaction u .

Enable and Idiodi studied the single –band tight-binding model with on-site repulsion u and nearest neighbor-exchange interaction *j* (the so called Hubbard Hirsch Hamiltonian) with the help of a correlated variational approach [10,11]. Two finite sized lattices with periodic boundary conditions were considered and the criteria for the occurrence of a transition from an anti-ferromagnetic phase to a ferromagnetic phase were discussed.

Theoretical Background

The Lanczos Tridiagonalization Method

The basic idea of the Lanczos method is that a special basis can be constructed where the Hamiltonian has a tridiagonal representation. This is carried out iteratively as shown below. First, it is necessary to select an arbitrary vector $\varnothing_0$ in the Hilbert space of the model being studied. If the Lanczos method is used to obtain the ground state energy of the model, then it is necessary that the overlap between the actual ground stat $|\not+_o\rangle$ e and the initial state $|\varnothing_o$ be non-zero [12,13]. If there is no priori information about the ground state is know, this requirement is usually satisfied by selecting an initial state with randomly satisfied by selecting an initial state randomly chosen co-efficient in the working basis that is being used. If some other information about the ground state is known, like it is convenient to initiate the iterations with a state already belonging to the subspace having those quantum numbers (and still with random coefficient within this subspace) [14,15].

***Corresponding author:** Michael Obende, Department of Physics, AfeBabalola University, Ado Ekiti, Nigeria, E-mail: princeobende@yahoo.com

Received March 24, 2015; **Accepted** April 29, 2015; **Published** May 20, 2015

Citation: Obende M, Okanigbuan OR, Olusola K (2015) Correlation between Lanczos Method and Exact Diagonalisation Method in the Study of Highly Correlated Electrons System. J Astrophys Aerospace Technol 3: 113. doi:10.4172/2329-6542.1000113

After $|\varnothing_o$ is selected, we can define a new vector by applying Hamiltonian H to the initial state subtraction the projection over $|\varnothing_o$, we obtain.

$$|\varnothing_o = \hat{\mathrm{H}}|\varnothing_o - \frac{\varnothing_o\left|\hat{\mathrm{H}}\right|\varnothing_0}{\varnothing_o|\varnothing_o}|\varnothing_o \tag{2.1.0}$$

$Which\ satisfies\ \langle\varnothing_o|\varnothing_o\rangle = 0.$

Now we can construct a new state that is orthogonal to the previous two as:

$$\varnothing_2 = \hat{\mathrm{H}}|\varnothing_o - \frac{\varnothing_1\left|\hat{\mathrm{H}}\right|\varnothing_1}{\varnothing_1|\varnothing_1}|\varnothing_1 \tag{2.1.1}$$

$Where\ n = 0,1,2,------ and\ the\ co-efficient\ are\ given\ by:$

$$an = \frac{\varnothing_n\left|\hat{\mathrm{H}}\right|\varnothing_n}{\varnothing_n|\varnothing_n},\ b_{n=}^2 \frac{\varnothing_n|\varnothing_n}{\varnothing_{n-1}|\varnothing_{n-1}} \tag{2.1.2}$$

$Supplemented\ by\ b_o = 0, |\varnothing_{-1} = 0$

$In\ this\ basis, it\ can\ be\ shown\ that\ the\ Hamiltonian\ matrix\ becomes$

$$H = \begin{bmatrix} a_o & b_1 & O & O & . & . & . \\ b_1 & a_1 & b_2 & O & . & . & . \\ O & b_2 & a_2 & b_3 & . & . & . \\ O & O & b_3 & a_3 & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix} \tag{2.1.3}$$

i.e it is tridiagonal, as expected. Once in this form the matrix can be diagonalized easily using standard library subroutine. However, to diagonalise completely the model being studied on a smote cluster, a number of iterations to the size of the Hilbert space (or of the subspace under consideration) are needed [16].

However, one of the advantages of this technique is that accurate enough information about the ground state of the problem can be obtained after a small number of iterations /typically of the order of $\approx 100 or\ less$). Thus the method is suitable for the analysis of low temperature properties of the models of correlated electrons described.

Ground state energy of the two electrons on 2 sites of aid lattice using the lanczos method

In the Lanczos method, a special basis is constructed such that the Hamiltonian has a tridigonal representation [17], Firstly, we select an arbitrary vector $|\varnothing_o\rangle$ in the Hilbert space of the model being studied for a two site system containing 2 electrons, we have the following many body states;

$$|1\rangle = |1\uparrow 1\downarrow\rangle$$

$$|2\rangle = |1\uparrow 2\downarrow\rangle$$

$$|3\rangle = |1\uparrow 2\uparrow\rangle$$

$$|6\rangle = |1\uparrow 2\downarrow\rangle$$

$$|\ \ \rangle = |1\uparrow 2\downarrow\rangle$$

Let $|\varnothing_o\rangle = |1\rangle = |1\uparrow 1\downarrow\rangle$. We now define a new vector $|\varnothing_o\rangle$ by applying the Hubbard Hamiltonian $\hat{H}$ to the state $|\varnothing_o\rangle$ subtracting the projection over $|\varnothing_o\rangle$,we obtai

$$|\varnothing_1\rangle = \hat{H}|\varnothing_o \_\_ \frac{\varnothing_o\left|\hat{\mathrm{H}}\right|\varnothing_o\rangle}{\varnothing_o|\varnothing_o}|\varnothing_o\rangle$$

$Recall\ equation 1.1$

$$H = -+\left\{\sum_{i,j\sigma} C_{i\sigma}^{+}C_{j\sigma} + H.C\right\} + u\sum_i n_i\uparrow n_i\downarrow \tag{2.2.1}$$

$For\ two\ electrons\ on\ two\ sites$

$$H = -+\left\{C_{1\uparrow}^{+}C_{2\uparrow} + C_{2\uparrow}^{+}C_{1\uparrow} + C_{1\downarrow}^{+}C_{2\downarrow} + C_{2\downarrow}^{+}C_{1\downarrow}\right\} + u\left\{C_{1\uparrow}^{+}C_{1\uparrow}C_{1\downarrow}C_{1\downarrow} + C_{2\uparrow}^{+}C_{2}\right.$$

$$H|\varnothing_o\rangle = -\mathrm{t}\,C_{1\uparrow}^{+}C_{2\uparrow}|\varnothing_o|1\uparrow 1\downarrow + C^{+} -$$

$$tC_{2\uparrow}^{+}C_{1\uparrow}1\uparrow 1\downarrow\rangle - tC_{1\uparrow}^{+}C_{2\uparrow}|\varnothing_o|1\uparrow 1\downarrow\rangle - tC_{2\uparrow}^{+}C_{1\downarrow}|1\uparrow 1\downarrow\rangle + UC_{1\uparrow}^{+}C_{1\uparrow}C_{1\downarrow}^{+}C_{1\downarrow}|1\uparrow 1\downarrow\rangle + uC_{2\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}|1\uparrow 1\downarrow\rangle \tag{2.2.2}$$

$$tC_{1\uparrow}^{+}C_{2\uparrow}|\varnothing_o|1\uparrow 1\downarrow\rangle - tC_{2\uparrow}^{+}C_{1\downarrow}|1\uparrow 1\downarrow\rangle + UC_{1\uparrow}^{+}C_{1\uparrow}C_{1\downarrow}^{+}C_{1\downarrow}|1\uparrow 1\downarrow\rangle + uC_{2\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}|1\uparrow 1\downarrow\rangle$$

$$= -t|2\uparrow 1\downarrow\rangle - tC_2^{+}|1\uparrow 1\downarrow\rangle - t|1\uparrow, 2\downarrow\rangle + u|1\downarrow 1\downarrow\rangle \tag{2.3.2}$$

$$H|\varnothing_o\rangle = -\mathrm{t}\left[|2\uparrow 1\downarrow\rangle + |1\uparrow 2\downarrow\right] + u|1\uparrow 1\downarrow\rangle$$

$$\langle\varnothing_o|\mathrm{H}|\varnothing\rangle_o = -\mathrm{t}\varnothing_o|2\uparrow 1\downarrow\rangle - \mathrm{t}|\varnothing_o|1\uparrow 2\downarrow\rangle + \mathrm{u}\varnothing_o|1\uparrow 1\downarrow\rangle$$

$$= -t\langle 1\uparrow 1\downarrow 1\uparrow 1\downarrow\rangle$$

$$= 0 - 0 + u(1)$$

$$= u$$

$$\langle\varnothing_o|\mathrm{H}|\varnothing_o\rangle = \mathrm{u}, \langle\varnothing_o|\mathrm{H}|\varnothing\rangle_o = \mathrm{u}, \langle\varnothing_o|\varnothing_o\rangle = 1$$

$$|\varnothing_o\rangle + \mathrm{t}1\uparrow 2\uparrow\rangle - |1\uparrow 2\downarrow\rangle + u|1\uparrow 1\downarrow\rangle - u|1\uparrow 1\downarrow\rangle$$

$$= t|1\uparrow 2\downarrow\rangle - t|1\uparrow 2\downarrow\rangle$$

$Similary,$

$$|\varnothing_2\rangle = H\left|\varnothing_1\rangle - \frac{\langle\varnothing_1|\mathrm{H}|\varnothing_1\rangle}{\langle\varnothing_1|\varnothing_1\rangle}|\varnothing_2\rangle - \frac{\langle\varnothing_1|\varnothing_1\rangle}{\langle\varnothing_o|\varnothing\rangle_o}|\varnothing_o\rangle\right. \tag{2.3.3}$$

$$\mathrm{H}|\varnothing_o\rangle = -\mathrm{t}^2|2\downarrow 2\uparrow\rangle + |1\downarrow 1\uparrow\rangle + \mathrm{t}^2|2\uparrow 2\downarrow\rangle + |1\uparrow 2\downarrow + |1\uparrow 1\downarrow\rangle$$

$$= 2t^2|2\uparrow 2\downarrow\rangle + 2t^2|1\uparrow 1\downarrow\rangle$$

$$= 2\mathrm{t}1\uparrow 1\downarrow + |2\uparrow 2\downarrow\rangle$$

$$\langle\varnothing_1|\mathrm{H}|\varnothing_1\rangle = 0$$

$$:\langle\varnothing_1|\mathrm{H}|\varnothing_1\rangle = 2\mathrm{t}^2, \langle\varnothing_o|\varnothing_o\rangle = 1$$

$$|\varnothing_2\rangle = 2\mathrm{t}^2|1\uparrow 1\downarrow\rangle + 2\mathrm{t}^2|2\uparrow 2\downarrow\rangle - 2\mathrm{t}^2|1\uparrow 1\downarrow\rangle$$

$$|\varnothing_2\rangle = 2\mathrm{t}^2|2\uparrow 2\downarrow\rangle$$

The procedure can be generalized by defining an orthogonal basis recursively as:

$$|\varnothing_{n+1}\rangle = \hat{H}|\varnothing_n\rangle - an|\varnothing_n\rangle - b_n^2|\varnothing_{n-1}\rangle \tag{2.3.4}$$

$Where\ n = 0,1,2,---- and\ the\ coefficients\ are\ given\ by$

$$an = \frac{\langle \varnothing_n | \hat{H} | \varnothing_n \rangle}{\langle \varnothing_n | \varnothing \rangle_n}, b_n = \frac{\langle \varnothing_n | \hat{H} | \varnothing_n \rangle}{\langle \varnothing_{n-1} | \varnothing_{n-1} \rangle}$$

Supplemented by $b_o = O, |\varnothing_{-1}\rangle = 0$. in this basis. We have the Hamiltonian matrix:

$$H = \begin{matrix} U & \sqrt{2t} & O & O & . & . & . \\ \sqrt{2t} & O & \sqrt{2t} & O & . & . & . \\ O & \sqrt{2t} & U & O & . & . & . \\ O & O & O & O & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{matrix} \quad (2.3.5)$$

From equation 1.4

$$|\varnothing_3\rangle = \hat{H}|\varnothing_2\rangle - a_2|\varnothing_2\rangle - b_2^2|\varnothing_1\rangle$$

$$\hat{H}|\varnothing_2\rangle - \frac{\langle \varnothing_2 | \hat{H} | \varnothing_2 \rangle}{\langle \varnothing_2 | \varnothing_2 \rangle}|\varnothing_2\rangle - \frac{\langle \varnothing_2 | \varnothing_2 | \varnothing_1 \rangle}{\langle \varnothing_1 | \varnothing_1 \rangle}$$

$$= \hat{H}|\varnothing_2\rangle = -2t^3|1\uparrow 2\downarrow\rangle - 2t^3|2\uparrow 1\downarrow\rangle + +2ut^2|2\uparrow 2\downarrow\rangle$$

$$\langle \varnothing_2 | \hat{H} | \varnothing_2 \rangle = 4ut^4, \langle \varnothing_2 | \varnothing_2 = 4t^4 \rangle,$$

$$\therefore |\varnothing_3\rangle = -2t^3|2\uparrow 2\downarrow\rangle + 2ut^3|2\uparrow 2\downarrow\rangle - 2ut^2|2\uparrow 2\downarrow\rangle - 2t^3|1\downarrow 2\uparrow\rangle +$$
$$2t^3|1\uparrow 2\downarrow\rangle |\varnothing_3 = 0$$

$$|\varnothing_4\rangle = H|\varnothing_3\rangle - an|\varnothing_3\rangle - b_n^2|\varnothing_2\rangle$$

$$H|\varnothing_3\rangle - \frac{\langle \varnothing_3 | H | \varnothing_3 \rangle}{\langle \varnothing_3 | \varnothing_3 \rangle}\Big|\varnothing_3\rangle - \frac{\langle \varnothing_3 \varnothing_3 \rangle}{\langle \varnothing_2 | \varnothing_2 \rangle}|\varnothing_2\rangle$$

$$|\varnothing_3\rangle = 0$$

$$\textit{Recall that}: |\varnothing_1\rangle = t|1\downarrow 2\uparrow\rangle - t|1\uparrow 2\downarrow\rangle$$

$$t\left[1\downarrow 2\uparrow\rangle - t|1\downarrow 2\uparrow\rangle - t|1\uparrow 2\downarrow\rangle\right]$$

$a^2\langle \varnothing_1 | \varnothing_1 \rangle = 1$, a is the normalizing factor

$$a^2 t^2 [1+1] = 1$$

$$2a^2t^2 = 1$$

$$\therefore |\varnothing_1\rangle = \frac{1}{\sqrt{2}}\left[|1\downarrow 2\uparrow\rangle - |1\uparrow 2\downarrow\rangle\right]$$

Also recall that,

$$|\varnothing_2\rangle = 2t^2|2\uparrow 2\downarrow\rangle = 1, a \textit{ is the normalizing factor} 4t^4a^2 = 1$$

$$\therefore a^2 = \frac{1}{4t^4} \Rightarrow a = \frac{1}{2t^2}$$

$$\therefore |\varnothing_2\rangle = |2\uparrow 2\downarrow\rangle$$

$$\langle \varnothing_o | H | \varnothing_o \rangle = u, \langle \varnothing_o | H | \varnothing_2 \rangle = 0, \langle \varnothing_o | H | \varnothing_n \rangle = o,$$

Since $|\varnothing_n\rangle = o, \rangle n2$.

$$\langle \varnothing_o | H | \varnothing_1 \rangle = \sqrt{2t},$$

$$\langle \varnothing_o | H | \varnothing_1 \rangle = \sqrt{2t}, \langle \varnothing_o | H | \varnothing_2 \rangle = o, \langle \varnothing_1 | H | \varnothing_2 \rangle = \sqrt{2t}$$

$\langle \varnothing_1 | H | \varnothing_n \rangle = o$ for $n\rangle 2$.

$$\langle \varnothing_2 | H | \varnothing_o \rangle = o, \langle \varnothing_2 | H | \varnothing_1 \rangle = \sqrt{2t, \langle \varnothing_2 | H | \varnothing_2 \rangle} = u$$

In this basis, we generate the Hamiltonian matrix

$$H = \begin{matrix} U & \sqrt{2t} & O & O & . & . & . \\ \sqrt{2t} & O & \sqrt{2t} & O & . & . & . \\ O & \sqrt{2t} & U & O & . & . & . \\ O & O & O & O & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{matrix} \quad (2.3.6)$$

Similarly,

$$a_o = \frac{\langle \varnothing_o | H | \varnothing_o \rangle}{\langle \varnothing_o | \varnothing_o \rangle} = u$$

$$a_1 = \frac{\langle \varnothing_o | H | \varnothing_1 \rangle}{\langle \varnothing_1 | \varnothing_1 \rangle} = o$$

$$a_2 = \frac{\langle \varnothing_2 | H | \varnothing_2 \rangle}{\langle \varnothing_2 | \varnothing_2 \rangle} = \frac{4ut^4}{4t^4} = u$$

$$a_3 = \frac{\langle \varnothing_3 | H | \varnothing_3 \rangle}{\langle \varnothing_3 | \varnothing_3 \rangle} = o$$

$$b_o^2 = \frac{\langle \varnothing_o \varnothing_o \rangle}{\langle \varnothing_{-1} | \varnothing_{-1} \rangle} = \text{in determinate}$$

$$b_1^2 = \frac{\langle \varnothing_1 \varnothing_1 \rangle}{\langle \varnothing_o | \varnothing_o \rangle} = 2t^2$$

In the basis $|\varnothing_1\rangle, |\varnothing_1\rangle$ *and* $|\varnothing_2\rangle$, *the* 3×3 *Hamiltonian matrix is constructed below.*

$$H = \begin{bmatrix} u & \sqrt{2t} & o \\ \sqrt{2t} & o & \sqrt{2t} \\ o & \sqrt{2t} & u \end{bmatrix} \quad (2.3.7)$$

Diagonalising equation (2.3.8), we solve the equation.

$$Dct(A - I\lambda) = o$$

$$A = \begin{bmatrix} u-\lambda & \sqrt{2t} & o \\ \sqrt{2t} & 0-\lambda & \sqrt{2t} \\ o & \sqrt{2t} & u-\lambda \end{bmatrix} = o$$

$$= (u-\lambda)\left\{-\lambda(u-\lambda) - 2t^2\right\} - \sqrt{2t}\left\{\sqrt{2t}(u-\lambda) - o\right\} + 0\{\} = 0$$

By expansions, we have that:

$$= -\lambda u^2 + \lambda^2 u - 2t^2 u + \lambda^2 u - \lambda^3 + 2t^\lambda - \sqrt{2t}\left\{\sqrt{2tu - \sqrt{2t}\ \lambda}\right\}$$

$$= -\lambda^3 + 2\lambda^2 u + \lambda u^2 + 4t^2 - 4t^2\lambda = 0$$

$$\lambda^3 - 2\lambda^2 u + \lambda u^2 + 4t^2 - 4t^2\lambda = 0$$

$$\lambda^3 - 2\lambda^2 u + \lambda u^2 - 4t^2\lambda + 4t^2 u = 0$$

$$\lambda^3 - 2\lambda^2 u + \lambda u^2 4t^2(\lambda - u) = 0$$

$$\textit{let } \lambda = u, \textit{so by inspection},$$

$$\lambda - u = 0 \quad \textit{is a factor}$$

Hence, by using polynomial division, we have that:

$$\lambda - u\overline{)\lambda^3 - 2\lambda^2 u + \lambda u^2 - 4t^2(\lambda - u)}$$
$$\lambda^3 - \lambda^2 u$$
$$-\lambda^2 u + \lambda u^2$$
$$-\lambda^2 u + \lambda u^2$$
$$-4t^2(\lambda - u)$$
$$-4t^2(\lambda - u)$$
$$\therefore (-4t^2(\lambda - u)\left(\lambda^2 - \lambda u - 4t^2\right) = 0$$
$$i.e\ \lambda_1 = u\ or\ \lambda^2 - \lambda u - 4t^2 = 0$$
$$For\ \lambda^2 - \lambda u - 4t^2 = 0$$

To determine the eigenvalue (x), we solve the above equation.

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$
$$Where\ a = 1, b = -u, C = -4t^2$$
$$\therefore = \frac{-(-u) \pm \sqrt{(-u) - 4 \times 1 \times -4t^2}}{2 \times 1}$$
$$\lambda = \frac{u \pm \sqrt{u^2 + 16t^2}}{2}$$
$$\lambda_2 = \frac{u + \sqrt{u^2 + 16t^2}}{2} or\ \lambda_3 = u\frac{\sqrt{u^2 + 16t^2}}{2}$$

Either:

$$\lambda_2 = \frac{u + \sqrt{u^2 + 16t^2}}{2} or\ \lambda_3 = u\frac{\sqrt{u^2 + 16t^2}}{2}$$

$$\frac{1}{2}\left[u + \sqrt{u^2 + 16t^2}\right] or \frac{1}{2}\left[u + \sqrt{u^2 - 16t^2}\right] \quad (2.3.8)$$

Hence equation (2.3.9) is the ground state energy.

$$Eg = \frac{1}{2}\left[u - \sqrt{u^2 + 16t^2}\right] \quad (2.3.9)$$

The Corresponding were function is given by:

$$\psi_{g.s} = X_1|\varnothing_2\rangle + X_2|\varnothing_1\rangle + X_3|\varnothing_3\rangle$$

Where:

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} is\ the\ eigenvector\ corresponding\ to$$

$$Eg = \frac{1}{2}\left[u - \sqrt{u^2 + 16t^2}\right] from\ 2.3.6,$$

$$\begin{bmatrix} \mathrm{u} - \frac{1}{2}(U - A) & \sqrt{2\mathrm{t}} & \mathrm{O} \\ \sqrt{2\mathrm{t}} & -\frac{1}{2}(U - A) & \sqrt{2\mathrm{t}} \\ \mathrm{O} & \sqrt{2\mathrm{t}} & \mathrm{u} - \frac{1}{2}(U - A) \end{bmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$Where\ A = \sqrt{u^2 + 16t^2}.$$

$$\begin{pmatrix} \frac{1}{2}(utA) & \sqrt{2t} & O \\ \sqrt{2t} & -\frac{1}{2}(U - A & \sqrt{2t} \\ O & \sqrt{2t} & \frac{1}{2}(U + A) \end{pmatrix} \begin{pmatrix} O \\ O \\ O \end{pmatrix} \backslash$$

$$\frac{1}{2}(U + A)X_1 + \sqrt{2t}\,X_2 = O \quad (1)$$

$$\sqrt{2t}X_1 + \frac{1}{2}(U + A)X_2 + \sqrt{2t}X_3 = O \quad (2)$$

$$\sqrt{2t}\lambda + \frac{1}{2}(U + A)X_3 =) \quad (3)$$

From equation (i)

$$\frac{1}{2}(U + A)X_1 = -\sqrt{2t}\,X_2$$

$$X_2 = -\frac{\frac{1}{2}(U + A)X_1}{\sqrt{2t}}$$

From equation (3)

$$\frac{1}{2}(U + A)X_3 = -\sqrt{2t}\,X_2$$

$$X_3 = \frac{\sqrt{2t}\,X_2}{\frac{1}{2}(U + A)}$$

$$X_3 = X_1$$

$$|X = \begin{bmatrix} X_1 \\ -\frac{\frac{1}{2}(U + A)}{\sqrt{2t}} \\ X_1 \end{bmatrix}$$

$$X_1^2 + \frac{\frac{1}{4}(U + A)^2}{2t^2}X_1^2 + X_1^2 = 1$$

$$2X_1^2 + \frac{\frac{1}{4}(U + A)^2}{2t^2}X_1^2 + X_1^2 = 1$$

$$X_1^2 + \left(\frac{2}{1} + \frac{(U + A)^2}{8t^2}\right) = 1$$

$$X_1^2 + \left(\frac{16t^2(U + A)^2}{8t^2}\right) = 1$$

$$\therefore X_1^2 \frac{8t^2}{16t^2(U + A)^2}$$

$$= \frac{8t^2}{2\left(A^2 + UA\right)}$$

$$\frac{2t}{\left(A^2 + UA\right)^{1/2}}$$

$$X_3 = \frac{2t}{\sqrt{U^2 + 16t^2 + U\sqrt{U^2 + 16t^2}}}$$

$$X_2 = \frac{-\frac{1}{2}(UtA)}{\sqrt{2t}} \times \frac{2t}{\left[A(Atu)\right]^{1/2}}$$

$$= -\frac{UtA}{\sqrt{2\left[(AtU)\right]^{1/2}}}$$

$$X_2 = \frac{(UtA)^{1/2}}{\sqrt{2}\,A^{1/2}}$$

$$X_2 = \frac{\sqrt{u + \sqrt{U^2 + 16t^2}}}{\sqrt{2}\left(\sqrt{U^2 + 16t^2}\right)}$$

Also,

$$X_2 = -\frac{1}{\sqrt{2}}\left[\frac{U + \sqrt{U^2 + 16t^2}}{\sqrt{U^2 + 16t}}\right]^{1/2}$$

$$X_1 = \frac{2t}{A^{1/2}(A+u)^{1/2}}$$

$$= \frac{2t(A-u)^{1/2}}{A^{1/2}(A+u)^{1/2}(A-u)^{1/2}}$$

$$\frac{2t\left[\sqrt{U^2 + 16t^2} - U\right]^{1/2}}{A^{1/2}\left[U^2 + 16t^2 - U^2\right]^{1/2}}$$

$$\frac{2t\left[\sqrt{U^2 + 16t^2} - U\right]^{1/2}}{A^{1/2} \times 4t^{1/2}}$$

$$\frac{\left[\sqrt{U^2 + 16t^2} - U\right]^{1/2}}{2\left[U^2 + 16t^2\right]^{1/2}}$$

$$\psi_{g.s} = X_1|\varnothing_o\rangle + X_2\frac{-1}{\sqrt{2}}\left[|1\uparrow 2\uparrow\rangle - |1\downarrow 2\uparrow\right] + X_3|2\uparrow 2\downarrow\rangle$$

$$X_1\left[|1\uparrow 1\downarrow\rangle + |2\uparrow 2\downarrow\right] - \frac{x_2}{\sqrt{2}}\left[|1\uparrow 2\downarrow\rangle - |1\downarrow 2\uparrow\rangle\right]$$

Ground state energy for two electrons on two sites (Exact Method)

Recall that:

$$H = -t\left[C_{1\uparrow}^{+}C_{2\uparrow} + C_{2\uparrow}^{+}C_{1} + C_{1\downarrow}^{+}C_{1\downarrow} + C_{2\downarrow}^{+}C_{1\downarrow}\right] +$$

$$U\left[C_{1\uparrow}^{+}C_{1\uparrow}C_{1\downarrow}^{+} + C_{2\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}C_{2\downarrow}\right]$$

For n electron on N sites, the number of many body states is given by

$$2N_{cn}, n = 2,\ N = 2$$

$$\Rightarrow \frac{4!}{(4-2)!2!} = \frac{4!}{2!2!} = 6$$

It has six states which are

$$|1\uparrow 1\downarrow\rangle,\quad |2\uparrow 2\downarrow\rangle,\quad |1\downarrow 1\uparrow,\quad and\ |1\downarrow 1\downarrow\rangle$$

With these Hamiltonian set up:

$$H = \begin{bmatrix} \langle 1|H|1\rangle\langle 1|H|2\rangle ----- & \langle 1|H|6\rangle \\ \langle 2|H|1\rangle\langle 2|H|2\rangle ----- & \langle 2|H|6\rangle \\ \langle 3|H|1\rangle\langle 3|H|2\rangle ----- & \langle 3|H|6\rangle \\ \langle 4|H|1\rangle\langle 4|H|2\rangle ----- & \langle 4|H|6\rangle \\ \langle 5|H|1\rangle\langle 5|H|2\rangle ----- & \langle 5|H|6\rangle \\ \langle 6|H|1\rangle\langle 6|H|2\rangle ----- & \langle 6|H|6\rangle \end{bmatrix}$$

$$H|1\rangle = -t\left[C_{1\uparrow}^{+}C_{2\uparrow} + C_{2\uparrow}^{+}C_{1\uparrow} + C_{1\downarrow}^{+}C_{2\downarrow} + C_{2\downarrow}^{+}C_{2\downarrow}\right] +$$

$$U\left[C_{1\uparrow}^{+}C_{1\uparrow} + C_{1\downarrow}^{+}C_{1\downarrow} + C_{2\uparrow}^{+}C_{2\uparrow} + C_{2\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle\right]$$

$$= -tC_{1\uparrow}^{+}C_{2\uparrow}|1\uparrow 1\downarrow\rangle tC_{2\uparrow}^{+}C_{1\uparrow}|1\uparrow 1\downarrow\rangle t\,C_{1\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle + tC_{2\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle$$

$$UC_{2\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle$$

$$= -tC_{1\uparrow}^{+}C_{2\uparrow}|1\uparrow 1\downarrow\rangle = 0$$

Here, $= -tC_{2\uparrow}^{+}C_{1\uparrow}|1\uparrow 1\downarrow\rangle = 0$

$$= -tC_{1\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle = 0$$

$$= UC_{1\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle = U|1\uparrow 1\downarrow\rangle$$

$$= UC_{1\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}C_{2\downarrow}|1\uparrow 1\downarrow\rangle = U|1\uparrow 1\downarrow\rangle$$

$$UC_{2\uparrow}^{+}C_{2\uparrow}C_{2\downarrow}^{+}|1\uparrow 1\downarrow\rangle = 0$$

$$H|1\rangle = -t|2\uparrow 1\downarrow\rangle - t|1\uparrow 2\downarrow\rangle + U|1\uparrow 1\downarrow\rangle$$

$$= t|1\uparrow 2\downarrow\rangle - t|1\uparrow 2\downarrow\rangle + U|1\uparrow 1\downarrow\rangle$$

$$t|4\rangle - t|3\rangle U|1\rangle$$

$$:\langle 1|\ H|1\rangle = t1|4\rangle - t1|3\rangle + U1|1\rangle \tag{2.4.0}$$

For

$$\langle 2|H|1\rangle = 0,\ \langle 3|H|1\rangle = -t, 4|H|1 = t,\quad \langle 5|H|1\rangle = 0,\quad and\,\langle 6|H|1\rangle = 0$$

Which gives

$$H_{ij} = \begin{matrix} u & o & -t & t & o & o \\ o & u & -t & t & o & o \\ -t & t & o & o & o & o \\ t & t & o & o & o & o \\ o & o & o & o & o & o \\ o & o & o & o & o & o \end{matrix}$$

$$H_{ij} = \begin{matrix} u & o & -t & t \\ o & u & -t & t \\ -t & t & o & o \\ t & t & o & o \end{matrix}$$

We now determine the eigenvalue, Where $A = (Hij)$ is a square matrix, X is a column matrix and λ is a scalar quantity [18-22].

Citation: Obende M, Okanigbuan OR, Olusola K (2015) Correlation between Lanczos Method and Exact Diagonalisation Method in the Study of Highly Correlated Electrons System. J Astrophys Aerospace Technol 3: 113. doi:10.4172/2329-6542.1000113

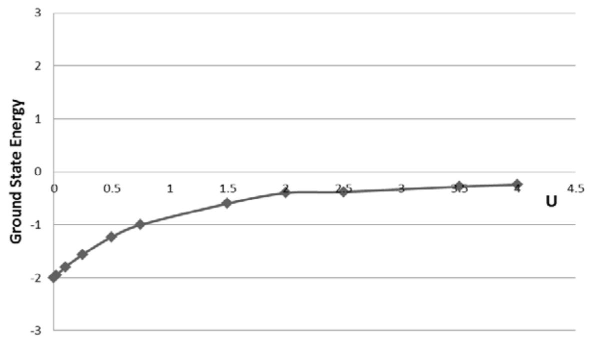

Figure 1: Ground state energy as a function of positive U for 2 electrons on 2 sites For Lanczos Result.

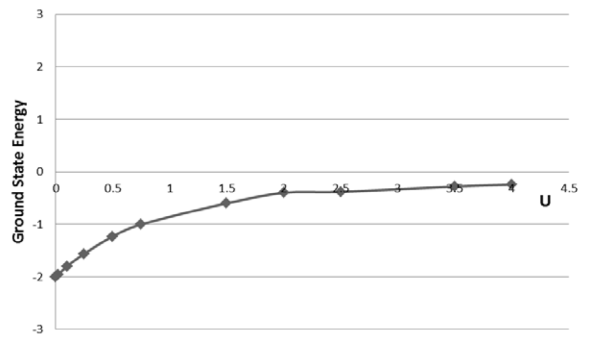

Figure 2: Ground state energy as a function of positive U for 2 electrons on 2 sites for Exact Result.

$U/_{4t}$	Lanczos	Exact
4	-0.24	-0.24
3.5	-0.28	-0.28
2.5	-0.38	-0.38
2	-0.4	-0.4
1.5	-0.6	-0.6
0.75	-1	-1
0.5	-1.23	-1.23
0.25	-1.56	-1.56
0.1	-1.8	-1.8
0.02	-1.96	-1.96
0.01	-1.98	-1.98
0	-2	-2
-0.01	-2.02	-2.02
-0.02	-2.04	-2.04
-0.1	-2.2	-2.2
-0.25	-2.56	-2.56
-1	-4.8	-4.8
-1.5	-6.6	-6.6
-2	-8.4	-8.4
-2.5	-10.4	-10.4
-3	-12.32	-12.32
-4	-16.24	-16.24

Table 1: Numerical Result Correlation Between Lanczos and Exact Method.

$$A\lambda = \lambda x$$

$$AX - \lambda x = 0$$

$$(A - \lambda I) \times = 0$$

Result and Discussion

Ground state energy for two electron system on two sites were analytically solved using 4× 4 matrix and the results obtained are presented in the figures and table below.

Figure 1 shows ground state energy as a function of positive U energy for 2 electrons on 2 sites for Lanczos method while Figure 2 shows ground state energy as a function of positive U for 2 electrons on 2 sites for exact method. Thus, the correlation between the two graphs are in perfect agreement.

Table 1 below shows the numerical results of Lanczos method and exact method which is in a good agreement with experimental values.

Conclusion

In this study, we have shown that Lanczos technique is a reliable numerical method in determining the ground state energy of a system described by the Hubbard Hamiltonian. Ground state energies obtained using the Lanczos method compare nicely with that obtained using exact method. The size of the Hamiltonian matrix to diagonalise is reduced from (4×4) matrix to a (3×3) matrix when Lanczos technique is applied.

Reference

1. Adrian cho "Second family of high temperature superconductors Discovered. science Now Daily New.
2. Bardeen J, Cooper LN, Schrieffer JR (1957) "Theory of superconductivity. Phys. Rev 108: 1175-1205.
3. Charles K (2004) Introduction to solid state Physics. New York.
4. Chen L, Mei C (1989) Exact calculation of the two electron interaction in the ground state of the Hubbard. Model Phys Rev B39: 9006.
5. Dagotto E (1994) correlated electrons in high temperature superconductors Rev mod Phys 66: 763-840.
6. Dagotto E, Moreo A (1984) Hamiltonian variational study of SU(2) lattice gauge theory Phys. Rev. D 29: 2350.
7. Dagotto E, Adriana Moreo (1985) Exact Diagonalization of Small System Phys. Rev. D 1: 865.
8. Dagotto E (1994) Correlated Electrons in High-Temperature superconductors. Reviews of Modern Physics 66: 763.
9. Doniach S, Sondhermer EH (1974) Green's Function for solid state physicists: 222-234.
10. Enaible AE, Idiodi JOA (2000) The two-electron problem studied within the t-j model and the Hubbard model. Proceedings of Nig Ass Math Phys 231-242.
11. Enabible AE, Idiodi JOA (2003) The two electron interaction in the ground state of the Hubbard-Hirsch Hamiltonian. J Nig Assoc Math Phys 275-280.
12. Feiner LF, Jefferson JH, Raimonddi R (1996) Effective single-band models for the high-Tc cuprates I. Coulomb interactions. Phys, Rev B 53: 8751.
13. Ginzburg VI, Landau ID (1950) "Microscopic derivation of the Ginzbury-Landau equations in the theory of superconductivity".
14. Hirsch JE (1989) Metallic ferromagnetism in a single-band model Phys. Rev 40: 2354.
15. Hubbard (1963) Electron Correlations in Narrow Energy Bands. J Proc Roy Soc London.
16. Hybertsen MS, Stechel EB, Schluter M Jennisons DR (1990) Phys Rev B41, P11068.

17. Lanczos C (1950) J Res Nat Bur Strand 45: 255.
18. Louis Eugene Felix (2001) Introduction of superconductivity.
19. Pettifor DG, Weaire DL (1985) The recursion method and its Applications, Springler series in solid-state sciences.
20. Richard MB (1951) Ferromagnetis.
21. Roomany, Wyld H (1980) Structural Elements in particle physics and statistical mechanics. Phys Rev D 21: 3341.
22. Tinkhams M (2004) Introduction to Superconductivity.