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

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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 i, j 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-site 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 can give qualitatively different behavior from the tight. Binding model, which includes only the hopping term for strong interaction, it can be considered as an improvement on the tight-binding model [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:

\[ H = \sum_{\langle i, j \rangle \sigma} C_{i\sigma} C_{j\sigma} + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} \]  

Where \( C_{i\sigma} \) and \( n_i \) are the creation, annihilation, and number operations, respectively, for an electron of spin \( \sigma \) in the wanner state on the on the \( i \)th lattice \( F_i, j \) 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 \( F_i, j \) 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 \( \varphi_0 \) 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 state \( |\psi> \) and the initial state \( |\varphi_0> \) 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].

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

$$|∅_n\rangle = \hat{H}|∅_n\rangle - \frac{\langle ∅_n | H | ∅_n \rangle}{\langle ∅_n | ∅_n \rangle} |∅_n\rangle$$  \hspace{1cm} (2.1.0)

Which satisfies $\langle ∅_n | ∅_n \rangle = 0$.

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

$$|∅_2\rangle = \hat{H}|∅_1\rangle - \frac{\langle ∅_1 | H | ∅_1 \rangle}{\langle ∅_1 | ∅_1 \rangle} |∅_1\rangle$$  \hspace{1cm} (2.1.1)

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

$$a_n = \frac{\langle ∅_n | H | ∅_1 \rangle}{\langle ∅_n | ∅_n \rangle}, \quad b_n = | ∅_{n-1} \rangle$$  \hspace{1cm} (2.1.2)

Supplemented by $b_n = 0, |∅_{-1}\rangle = 0$.

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

$$H = \begin{bmatrix}
    a_0 & b_1 & O & O & \cdots & \\
    b_1 & a_1 & b_2 & O & \cdots & \\
    O & b_2 & a_2 & b_3 & \cdots & \\
    O & O & b_3 & a_3 & \cdots & \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \ddots
\end{bmatrix}$$  \hspace{1cm} (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 smotere 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 $|∅_1\rangle$ in the Hilbert space of the model being studied for a two site system containing 2 electrons, we have the following many body states:

$$|1\rangle = |↑\downarrow\rangle$$  
$$|2\rangle = |↑\downarrow\rangle$$  
$$|3\rangle = |↑\uparrow\rangle$$  
$$|4\rangle = |↑\uparrow\rangle$$  
$$|5\rangle = |↑\downarrow\rangle$$  
$$|6\rangle = |↑\downarrow\rangle$$

Let $|∅_0\rangle = |↑\downarrow\rangle$. We now define a new vector $|∅_1\rangle$ by applying the Hubbard Hamiltonian $\hat{H}$ to the state $|∅_0\rangle$ subtracting the projection over $|∅_0\rangle$, we obtai

$$|∅_1\rangle = \hat{H}|∅_0\rangle - \frac{\langle ∅_0 | H | ∅_0 \rangle}{\langle ∅_0 | ∅_0 \rangle} |∅_0\rangle$$

Recall equation1.

$$H = -t \left( \sum_{i,j=\sigma} C_{i\sigma} C_{j\sigma} + H.C. \right) + t \sum_{i,j} n_i \downarrow n_j \downarrow$$  \hspace{1cm} (2.2.1)

For two electrons on two sites

$$H = -t \left( C_{1\uparrow} C_{2\uparrow} + C_{2\uparrow} C_{1\downarrow} + C_{1\downarrow} C_{2\uparrow} + C_{2\downarrow} C_{1\uparrow} \right) + \sum_{i,j=\sigma} u_i C_{i\sigma} C_{j\sigma}$$  \hspace{1cm} (2.2.2)

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

$$|∅_{n+1}\rangle = \hat{H}|∅_n\rangle - \frac{a_n |∅_n\rangle - b_n |∅_{n-1}\rangle}{|⟨∅_{n-1}|∅_n⟩|^2}$$  \hspace{1cm} (2.2.3)

Similarly,

$$H|∅_1\rangle = -2t |↑\downarrow\rangle + t |↑\uparrow\rangle - t |↑\downarrow\rangle$$

$$H|∅_1\rangle = -2t |↑\downarrow\rangle + 2t |↑\uparrow\rangle - 2t |↑\downarrow\rangle$$

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

$$|∅_{n+1}\rangle = \hat{H}|∅_n\rangle - a_n |∅_n\rangle - b_n |∅_{n-1}\rangle$$  \hspace{1cm} (2.3.4)

Where $n = 0, 1, 2, \ldots$ and the coefficients are given by
\[
\langle \hat{\mathcal{O}}_n | H | \hat{\mathcal{O}}_n \rangle - \langle \hat{\mathcal{O}}_n | H | \hat{\mathcal{O}}_n \rangle = \langle \hat{\mathcal{O}}_n | H | \hat{\mathcal{O}}_n \rangle - \langle \hat{\mathcal{O}}_n | H | \hat{\mathcal{O}}_{n-1} \rangle
\]

Supplemented by \( b_n = \mathbb{O} | \hat{\mathcal{O}}_{n+1} \rangle = 0 \). in this basis. We have the Hamiltonian matrix:

\[
H = \begin{bmatrix}
U & \sqrt{\mathcal{O}} & O & \ldots \\
\sqrt{\mathcal{O}} & O & \sqrt{\mathcal{O}} & \ldots \\
O & \sqrt{\mathcal{O}} & O & \ldots \\
O & O & O & \ldots
\end{bmatrix}
\]

(2.3.5)

Similarly,

\[
a_0 = \langle \hat{\mathcal{O}}_o | H | \hat{\mathcal{O}}_o \rangle = u
\]

\[
a_2 = \langle \hat{\mathcal{O}}_2 | H | \hat{\mathcal{O}}_2 \rangle = 4u^4 + 4u^4 = u
\]

\[
a_3 = \langle \hat{\mathcal{O}}_3 | H | \hat{\mathcal{O}}_3 \rangle = 0
\]

\[
b_2^2 = \langle \hat{\mathcal{O}}_2 | H | \hat{\mathcal{O}}_2 \rangle = 2t^2
\]

In this basis, we generate the Hamiltonian matrix

\[
H = \begin{bmatrix}
u & \sqrt{\mathcal{O}} & o & \ldots \\
\sqrt{\mathcal{O}} & o & \sqrt{\mathcal{O}} & \ldots \\
o & \sqrt{\mathcal{O}} & o & \ldots \\
o & o & o & \ldots
\end{bmatrix}
\]

(2.3.6)

Diagonalising equation (2.3.8), we solve the equation.

\[
\det(A - \lambda I) = 0
\]

\[
A = \begin{bmatrix}
u & \sqrt{\mathcal{O}} & o & \ldots \\
\sqrt{\mathcal{O}} & o & \sqrt{\mathcal{O}} & \ldots \\
o & \sqrt{\mathcal{O}} & o & \ldots \\
o & o & o & \ldots
\end{bmatrix}
\]

(2.3.7)

By expansions, we have that:

\[
\lambda = \sqrt{\mathcal{O}} \left( \sqrt{2} \mathcal{O} - \lambda - \sqrt{2} \right)
\]

let \( \lambda = u \), so by inspection, \( \lambda - u = 0 \) is a factor.
Hence, by using polynomial division, we have that:
\[
\lambda^2 - 2\lambda^2 u + \lambda^2 u^2 - 4r^2(\lambda - u) \\
= \lambda^2 - 2\lambda u + \lambda^2 u^2 \\
= -\lambda^2 u + \lambda u^2 \\
= -\lambda^2 u + \lambda u^2 \\
= -4r^2 (\lambda - u) \\
= -4r^2 (\lambda - u) \\
= (4r^2 (\lambda - u) (\lambda^2 - \lambda u - 4r^2)) = 0 \\
\]
\[i.e \lambda = u \text{ or } \lambda^2 - \lambda u - 4r^2 = 0 \\
\text{For } \lambda^2 - \lambda u - 4r^2 = 0 \]

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

\[\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \]
Where \(a = 1, b = -u, c = -4r^2 \)
\[\therefore = \frac{-(-u) \pm \sqrt{(-u) - 4 \times 1 \times (-4r^2)}}{2 \times 1} \]
\[\lambda = \frac{u \pm \sqrt{u^2 + 16r^2}}{2} \]
\[\lambda_2 = \frac{u + \sqrt{u^2 + 16r^2}}{2} \text{ or } \lambda_3 = \frac{u - \sqrt{u^2 + 16r^2}}{2} \]

Either:
\[\lambda_2 = \frac{u + \sqrt{u^2 + 16r^2}}{2} \] \(or\) \[\lambda_3 = \frac{u - \sqrt{u^2 + 16r^2}}{2} \]

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

Hence equation (2.3.9) is the ground state energy.
\[E_g = \frac{1}{2} \left[ u - \sqrt{u^2 + 16r^2} \right] \] \[
(2.3.9) \]

The Corresponding were function is given by:
\[\psi_g = X_1 |\psi_2\rangle + X_2 |\psi_1\rangle + X_3 |\psi_3\rangle \]

Where:
\[X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \text{ is the eigenvector corresponding to } \]
\[E_g \]
\[\]
\[\frac{1}{2} \left[ u - \sqrt{u^2 + 16r^2} \right] \text{ from 2.3.6,} \]
\[\]
\[\begin{pmatrix} u - \frac{1}{2} (U - A) & \sqrt{2t} & 0 \\ \sqrt{2t} & - \frac{1}{2} (U - A) & \sqrt{2t} \\ 0 & \sqrt{2t} & u - \frac{1}{2} (U - A) \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \]
\[\]
\[\begin{pmatrix} 1 \left[ u - \frac{1}{2} (U - A) \right] \text{ \ } \sqrt{2t} \text{ \ } 0 \\ \sqrt{2t} \text{ \ } - \frac{1}{2} (U - A) \text{ \ } \sqrt{2t} \\ 0 \text{ \ } \sqrt{2t} \text{ \ } u - \frac{1}{2} (U - A) \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \]

Where \(A = \sqrt{u^2 + 16r^2} \).
\[\begin{pmatrix} \frac{1}{2} (U + A) \text{ \ } \sqrt{2t} \text{ \ } 0 \\ \sqrt{2t} \text{ \ } - \frac{1}{2} (U - A) \text{ \ } \sqrt{2t} \\ 0 \text{ \ } \sqrt{2t} \text{ \ } \frac{1}{2} (U + A) \end{pmatrix} \begin{pmatrix} O \\ O \end{pmatrix} = \begin{pmatrix} O \\ O \end{pmatrix} \]

\[\frac{1}{2} (U + A)X_1 + \sqrt{2t}X_2 = O \]
(1)
\[\sqrt{2t}X_1 + \frac{1}{2} (U + A)X_2 + \sqrt{2t}X_3 = O \]
(2)
\[\sqrt{2t}X_2 + \frac{1}{2} (U + A)X_3 = 0 \]
(3)

From equation (i)
\[\frac{1}{2} (U + A)X_1 = -\sqrt{2t}X_2 \]
\[X_2 = -\frac{1}{2} (U + A)X_1 \]

From equation (3)
\[\frac{1}{2} (U + A)X_3 = -\sqrt{2t}X_2 \]
\[X_3 = \frac{\sqrt{2t}X_2}{\frac{1}{2} (U + A)} \]

\[X_3 = X_1 \]

\[X_1^2 + \frac{1}{4} (U + A)^2 \]
\[\]
\[2X_1^2 + \frac{1}{4} (U + A)^2 \]
\[X_1^2 + \frac{2}{U + A} \]
\[X_1^2 + \frac{\left( U + A \right)^2}{8r^2} \]
\[X_1^2 + \frac{16r^2 (U + A)^2}{16r^2 (U + A)^2} \]
\[X_1^2 \]
\[\vdots \]
\[
\begin{align*}
X_3 &= \frac{2t}{\sqrt{U^2 + 4U^2 + U^2 + 16^2}} \\
X_2 &= \frac{-1}{\sqrt{2}t} \times \left[ \frac{2t}{\sqrt{t^2 + 16^2}} \right]
\end{align*}
\]

Also,
\[
X_2 = -\left[ \frac{U^2 + 4U^2 + U^2 + 16^2}{\sqrt{2}t^2 + 16^2} \right]^{1/2}
\]

For \( n \) electron on \( N \) sites, the number of many body states is given by
\[
2 \times \frac{n!}{(4-2)!} = \frac{4!}{2!} = 6
\]

It has six states which are
\[
\begin{align*}
| \uparrow \downarrow \rangle, \quad | \uparrow \uparrow \rangle, \quad | \downarrow \uparrow \rangle, \quad | \downarrow \downarrow \rangle, \quad \text{and} \quad | \downarrow \downarrow \rangle
\end{align*}
\]

With these Hamiltonian set up:
\[
H = \begin{bmatrix}
(1|1\rangle\langle 1|1\rangle) & \cdots & (1|1\rangle\langle 1|1\rangle)
\end{bmatrix}
\]

\[
\begin{align*}
U \left[ C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 \right]
\end{align*}
\]

\[
\begin{align*}
H | \psi \rangle &= -\{C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 + C_{11}^2 C_{22}^4 \} | \uparrow \downarrow \rangle
\end{align*}
\]

\[
\begin{align*}
= -iC_{11}^2 C_{22}^4 | \uparrow \downarrow \rangle = 0
\end{align*}
\]

For \( \langle 2|H|1 \rangle = 0, \langle 3|H|1 \rangle = -4|e|f|1 \rangle = t, \langle 5|H|1 \rangle = 0, \text{ and } \langle 6|H|1 \rangle = 0 \)

Which gives
\[
\begin{align*}
u & \quad o & -t & t & o & o & o \\
o & -t & t & o & o & o & o \\
H_{ij} &= -t & t & o & o & o & o & o \\
o & o & -t & t & o & o & o \\
o & o & o & -t & t & o & o \\
o & o & o & o & -t & t & o \\
o & o & o & o & o & -t & t
\end{align*}
\]

We now determine the eigenvalue, Where \( A = \{H_{ij}\} \) is a square matrix, \( X \) is a column matrix and \( \lambda \) is a scalar quantity [18-22].
\[ A\lambda = \lambda x \]
\[ AX - \lambda x = 0 \]
\[ (A - \lambda I)x = 0 \]

**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.

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