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Strongly Correlated Electron Systems in The Half Filled Band of The Hubbard Model

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Abstract

Strong correlation of interacting electrons has been widely studied under the single band Hubbard model with the aid of several techniques. These numerous studies have been carried out at different band filling. In this work, the ground state properties in the half filled band in one dimension are studied employing a simplified modification of the Lanczos technique with particular interest in the energies and the wave functions. Several interaction strengths are considered both in the positive u limit and negative u limit and the interesting case of no interaction.

1.0 Introduction

In contemporary high temperature superconductivity, the studies of the behavior of strongly correlated electronic systems remain a central problem. Years of intense studies has shown that the required theoretical skills and tools to deal effectively with strongly correlated electron systems are still lacking. This search for a theoretical explanation has generated an immense number of papers. There are some reviews which attempt to gather and put in perspective this large amount of work [1]. These reviews make it clear that there is still much work to be done, and reflect the generally inconclusive state of the research in this area. Despite a lack of overall explanation, a large amount of experimental information has been gathered.

The defining feature of all high-Tc superconductors is the presence of copper oxide planes, which are separated from each other by layers of other atoms. This common anti-ferromagnetic order is present at low temperature and low doping. Upon doping, long range spin order is destroyed, giving way first to a pseudo gap phase and eventually the superconducting phase. At higher temperatures than those that allow for superconductivity, a non-Fermi-liquid state appears. Eventually, at all temperatures, the system settles into a Fermi-liquid state.

For theoretical studies, physicists turn to model Hamiltonians which are defined to describe a system of fermions residing on a lattice. The Hamiltonian together with the lattice comprises a system which attempts to mimic the properties of the high-Tc superconductors. The lattice used is usually a simplified version of the structure of the material; for instance, since the copper oxide planes of the cuprates form a square lattice, a number of research works considers these lattices [2, 3, 4, 5]. The key property that most studies strive to explain is Cooper pairing, and the mechanism causing the pairs to form. Some reviews focusing on the question of the pairing mechanism can be found in [6, 7]. It was known prior to the discovery of high-T_c superconductor that singlet-pairing was enhanced in the strong on-site coupling limit of the Hubbard model [8] and that this led to an effective attractive interaction between anti-parallel spins on nearest neighbor sites. This effective attractive interaction is the key to the Cooper pairing problem [9].

In part and because of this, Anderson suggested the appropriate model to study the cuprates is the nearly half-filled two-dimensional Hubbard model, with moderately large on-site repulsion u, and anti-ferromagnetic exchange J [10]. Following this suggestion, extensive studies on the Hubbard and t−J models were carried out. Many of these studies focus on the large-u limit of the Hubbard model [11, 12, 13], where at half-filling it becomes equivalent to the Heisenberg model, a result that had been known for some time [8, 14].

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It is generally agreed that both the Hubbard and t − J models describe the normal state features of the cuprates [7]. For instance, anti-ferromagnetic order was also observed in the Heisenberg model [15, 16] using both Monte Carlo (MC) and renormalization group (RG) methods. The superconducting state, however, has not been described by these models; specifically, evidence of Cooper pair formation has not been conclusive. Several studies have approached the problem from different theoretical perspectives that find "conclusive" evidence of pairing, be it exact diagonalization [17, 18, 19, 20, 21], Monte Carlo [3, 22, 12, 21], or simply by direct analysis [23, 24]. However, there are other studies which either find no evidence of pair formation, or refute the claim that the t − J or Hubbard models superconduct at all [5, 2, 25].

Attempting to describe the interactions of many-electron systems is very complicated, and often theorists turn to simplified models which retain some of the important features of the system while ignoring other, hopefully less important features. Perhaps the simplest model of an interacting many-electron system is the Hubbard model [26]. The Hubbard model uses tight-binding arguments that exploit the fact that the electron density in a d-band transition metal is concentrated close to the nuclei and sparse in between. In effect, one can view the electrons as residing on a particular atom. The location of an atom in the material is referred to as a lattice site, or simply a site, where at most two electrons may occupy any single site provided they have opposite spin. The electrons may "hop" between nearest neighbour sites, contributing an off-diagonal element, −t, to the Hamiltonian. In addition, in the Hubbard model electrons interact only through Coulombic repulsion when residing on the same site. The hopping constitutes the kinetic energy part of the Hamiltonian. By itself it is sometimes called the "hopping term," which using occupation number formalism is given by

$$H_{HOP} = -t \sum_{<i,j>,\sigma} (C^{\dagger}_{i,\sigma} C_{j,\sigma} + C^{\dagger}_{j,\sigma} C_{i,\sigma}) \quad (1)$$

where i and j label the sites, and σ labels the spin. The brackets, <,>, indicate the sum is performed over nearest neighbour sites only, with each pair of sites only counted once. The Coulombic interaction between electrons comprises the potential energy of the Hamiltonian. In its most general form it is given by

$$Vee = u\sum_i n_{i,\uparrow} n_{i,\downarrow} + \sum_i V_{|i-j|} n_i n_j \quad (2)$$

where i and j run over the lattice sites. The first term, or u-term, considers only on-site interactions. The second term, or V -term, considers all other interactions, and, in general,

$V_{|i-j|} \sim \frac{1}{|ri-rj|}$, where r_i is the position of the ith atom. u and V are energy scales which define the strength of the interaction. If u or V is positive (negative) the respective interaction is repulsive (attractive). The Hubbard model only considers repulsive, on-site interactions and so only the u-term is retained. Finally, the nearest neighbour-hopping Hubbard model is given by,

$$H_{Hub} = -t \sum_{<i,j>,\sigma} (C^{\dagger}_{i,\sigma} C_{j,\sigma} + C^{\dagger}_{j,\sigma} C_{i,\sigma}) + u\sum_i n_{i,\uparrow} n_{i,\downarrow} \quad (3)$$

Having made a choice of which electronic model to work with, the method or technique that should be applied to the study of this model becomes another challenge. If this is not properly chosen, it limits the extent of the work and the accuracy of results obtained. To check this, great effort was made in the review work of [1] to present several techniques that have been applied in the extensive study of highly correlated electron systems using the Hubbard model. One of the problems encountered is that there are no well controlled analytical techniques to analyze them. According to Dagotto's review paper, two methods were found to be self consistent these are the mean free theories and the variational approximations, but there were no standard ways to judge if they actually describe the properties of the ground state or if they converge to excited states. Of these aforementioned techniques, the exact method provide the exact solution, however, because of the exponential growth of the Hilbert space with the lattice size, exact calculation becomes inadequate to handle relatively large clusters. Even if some extrapolations were done, small size systems are inadequate in describing the phase transition region in the macroscopical limit. This fueled the need to look for an adequate approximation method that can produce near accurate results. It is in the light of this that a simple modification of the Lanczos algorithm was adopted to extract the desired information from the system operated on by the Hamiltonian. Hence for this research paper, a simplified modification of the Lanczos technique is employed. The simplified approach developed in this work reveals a clear cut formula for obtaining the improved ground state energy and wave function by every step of iteration taken. Values are inputted manually into the formula and results were obtained without heavy numerical involvement. In the modified Lanczos technique presented by Dagotto, two higher powers of <H> that is $<H^2>$ and $<H^3>$ must be obtained before the iteration to obtain the next improved ground state energy and wave function can be obtained. In the method presented here, just one power of <H>, that is $<H^2>$ is needed for the next iteration to be carried out. Result obtained from the iterations shows that there is easy access to obtaining some of the dynamical ground state properties like the correlation functions. Hence the aim of this research is to investigate to a high level of accuracy, the

low energy properties like the ground state energies and wave functions at half filling and at various interaction strengths in the large u (u>0) and small u (u<0) limit. Preliminary result for the four site problem has been presented by [27].

Generally, the plan of this research is as follows, the method is described in section II. In section III, it is applied to finite sized lattices in the half filled band of the one-dimensional Hubbard model and the results obtained are presented, discussed and extrapolated to the bulk limit per electron and comparison is made with existing results. Final comments and conclusions are made in section IV.

2.0 The Method

In this section, the modified Lanczos technique as applied in this work will be described. As in the standard Lanczos technique and the modified Lanczos method, the method requires the selection of an initial trial vector $|\phi_n\rangle$ (normalized to one) and n takes values from 0. If H acts on $|\phi_n\rangle$ the result can be written as

$$H\ |\phi_n\rangle = \frac{\langle\phi_n|H\ |\phi_n\rangle}{\langle\phi_n\ |\phi_n\rangle}|\phi_n\rangle + \ |\tilde{\phi}_n\rangle \tag{4}$$

Where $|\tilde{\phi}_n\rangle$ is a new state orthogonal to $|\phi_n\rangle$. Since $|\phi_n\rangle$ is normalized, Eqn. (4) becomes

$$|\tilde{\phi}_n\rangle = \frac{\left(H|\phi_n\rangle - \langle\phi_n|H|\phi_n\rangle|\phi_n\rangle\right)}{b_n} \tag{5}$$

The constant b_n ensures that $|\phi_n\rangle$ is normalized.

From Eqn. (5), it is observed that;

$$\langle\tilde{\phi}_n|\tilde{\phi}_n\rangle = \frac{\left[\langle\phi_n|H^2|\phi_n\rangle - \left(\langle\phi_n|H|\phi_n\rangle\right)^2\right]}{b_n^2} = 1 \tag{6}$$

Hence, Eqn. (6) gives

$$b_n = \left[\langle\phi_n|H^2|\phi_n\rangle - \left(\langle\phi_n|H|\phi_n\rangle\right)^2\right]^{1/2} \tag{7}$$

$$\left[\langle\phi_n|H^2|\phi_n\rangle\right] = \beta_n \tag{8}$$

$$\left[\langle\phi_n|H|\phi_n\rangle\right] = H_n \tag{9}$$

Having redefined the parameters used in Eqn (7), it can simply be put as

$$b_n = \left[\beta_n - (H_n)^2\right]^{1/2} \tag{10}$$

Also,

$$\langle\phi_n|H^3|\phi_n\rangle = \gamma_n \tag{11}$$

$$f_n = \frac{\gamma_n - 3H_n\beta_n + 2H_n^3}{2\left(\beta_n - H_n^2\right)^{3/2}} \tag{12}$$

$$\alpha_n = f_n - \left(f_n^2 + 1\right)^{1/2} \tag{13}$$

from Eqns. (9), (10) and (13) the improved energy can be obtained using Eqn. (14) below

$$\in_{n+1} = H_n + b_n\alpha_n \tag{14}$$

Where $\in_{n+1}$ is the improved ground state energy which is used for the next iteration.

Also, using $|\varphi_n\rangle$, Equations (5) and (13), it can easily be shown that the new trial wave vector for the next iteration is

$$\left|\phi_{n+1}\right\rangle = \frac{1}{\left(1+\alpha_n^2\right)^{1/2}}\left|\phi_n\right\rangle + \frac{\alpha_n}{\left(1+\alpha_n^2\right)^{1/2}}\left|\tilde{\phi}_n\right\rangle \tag{15}$$

where

$$\frac{1}{\left(1+\alpha_n^2\right)^{1/2}} = \lambda_n \tag{16}$$

$$\frac{\alpha_n}{\left(1+\alpha_n^2\right)^{1/2}} = \mu_n \tag{17}$$

Eqn. (16) and (17) are the weights associated with the improved wave function $\left|\phi_{n+1}\right\rangle$

$$\therefore \left|\phi_{n+1}\right\rangle = \lambda_n\left|\phi_n\right\rangle + \mu_n\left|\tilde{\phi}_n\right\rangle \tag{18}$$

$\in_{n+1}$ and $\left|\phi_{n+1}\right\rangle$ are better approximations to E_0 (true ground state energy) and $\left|\Phi_0\right\rangle$ (true ground state wave function) than $\in_n$ and $\left|\phi_n\right\rangle$ respectively.

The method can be iterated by considering $\left|\phi_{n+1}\right\rangle$ as a new initial trial vector and repeating the steps from Eqn. (4) to (18). In each iteration, the orthogonal pairs ($\left|\phi\right\rangle, \left|\tilde{\phi}\right\rangle$), ($\left|\phi_i\right\rangle, \left|\tilde{\phi}_i\right\rangle$), etc are normalized.

3.0 (a) Two Electrons on Two Sites

In this section, the modified Lanczos algorithm is applied to the case of two electrons on two sites with periodic boundary condition. The relevant electronic states of this system are:

$$\left|1\right\rangle = \left|1\uparrow,1\downarrow\right\rangle, \left|2\right\rangle = \left|2\uparrow,2\downarrow\right\rangle, \left|3\right\rangle = \left|1\uparrow,2\downarrow\right\rangle, \left|4\right\rangle = \left|1\downarrow,2\uparrow\right\rangle \tag{19}$$

Consider the normalized initial trial vector $\left|\phi_0\right\rangle$ to be

$$\left|\phi_0\right\rangle = \frac{1}{\sqrt{2}}\left[\left|1\right\rangle + \left|2\right\rangle\right] = \left|1'\right\rangle \tag{20}$$

Eqn. (20) is the linear combination of translational invariant states.

When the Hubbard Hamiltonian given in Eqn. (3) acts on $\left|\phi_0\right\rangle$

$$H\left|\phi_0\right\rangle = \frac{1}{\sqrt{2}}\left[-2t\left|3\right\rangle + 2t\left|4\right\rangle + U\left|1\right\rangle + U\left|2\right\rangle\right] \tag{21}$$

When Eqns. (20) and (21) are combined, H_0 is obtained as given in Eqn. (22)

$$H_0 = \left\langle\phi_0\right|H\left|\phi_0\right\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}2U\right) = U \tag{22}$$

when the Hamiltonian acts on Eqn. (21), Eqn. (23) will be obtained as;

$$H^2\left|\phi_0\right\rangle = \frac{4t^2}{\sqrt{2}}\left[\left|1\right\rangle + \left|2\right\rangle\right] + \frac{U^2}{\sqrt{2}}\left[\left|1\right\rangle + \left|2\right\rangle\right] + \frac{2Ut}{\sqrt{2}}\left[\left|4\right\rangle - \left|3\right\rangle\right] \tag{23}$$

normalizing the result obtained in Eqn. (23) produces β_0 as given in Eqn. (24)

$$\beta_0 = \left\langle\phi_0\right|H^2\left|\phi_0\right\rangle = \frac{4t^2}{\sqrt{2}}\left(\frac{2}{\sqrt{2}}\right) + \frac{U^2}{\sqrt{2}}\left(\frac{2}{\sqrt{2}}\right) = 4t^2 + U^2 \tag{24}$$

From Eqn. (23) and (24), the normalizing factor is obtained as

$$b_0 = \left[4t^2 + U^2 - U^2\right]^{1/2} = 2t \tag{25}$$

using Eqns. (21), (22) and (25), the orthogonal state wave function is obtained as;

$$\left|\tilde{\phi}_0\right\rangle = \frac{1}{\sqrt{2}}\left[\left|4\right\rangle - \left|3\right\rangle\right] = \left|2'\right\rangle \tag{26}$$

Also, when the Hamiltonian acts on Eqn. (23), it becomes

$$H^3\left|\phi_0\right\rangle = \frac{8t^2U + U^3}{\sqrt{2}}\left[\left|1\right\rangle + \left|2\right\rangle\right] + \frac{8t^3 + 2U^2t}{\sqrt{2}}\left[\left|4\right\rangle - \left|3\right\rangle\right] \tag{27}$$

Hence on normalizing the result of Eqn. (27)

$$\gamma_0 = \left\langle\phi_0\left|H^3\right|\phi_0\right\rangle = 8t^2U + U^3 \tag{28}$$

but

$$f_0 = \frac{\gamma_0 - 3H_0\beta_0 + 2H_0^3}{2\left(\beta_0 - H_0^2\right)^{3/2}} \tag{29}$$

Hence, applying Eqns. (22), (24) and (28) in Eqn. (29) will yield

$$f_0 = \frac{-U}{4t} \tag{30}$$

using Eqn. (30), α_n is obtained to be

$$\alpha_0 = \frac{-U - \sqrt{16t^2 + U^2}}{4t} \tag{31}$$

from Eqns. (22), (25) and (31) in the relation

$$\in_{0+1} = H_0 + b_0\alpha_0$$

the improved ground state energy gives

$$\in_1 = \frac{1}{2}\left[U - \sqrt{U^2 + 16t^2}\right] \tag{32}$$

In the basis $\left|\phi_0\right\rangle$ and $\left|\tilde{\phi}_0\right\rangle$, the corresponding improved ground state wave function is

$$\left|\phi_1\right\rangle = \frac{\lambda_0}{\sqrt{2}}\left[\left|1\right\rangle + \left|2\right\rangle\right] + \frac{\mu_0}{\sqrt{2}}\left[\left|4\right\rangle - \left|3\right\rangle\right] \tag{33}$$

$$\lambda_0 = \frac{1}{\sqrt{2}}\left[\frac{\sqrt{16t^2 + U} - U}{\sqrt{16t^2 + U^2}}\right] \tag{34a}$$

$$\mu_0 = -\frac{1}{\sqrt{2}}\left[\frac{\sqrt{16t^2 + U} + U}{\sqrt{16t^2 + U^2}}\right] \tag{34b}$$

Eqns. (34a) and (34b) are obtained by putting Eqn. (31) into Eqns. (20) and (26) respectively. It is observed in this section that applying the linear combination of translational invariant states reduces the number of iterations required to obtain the ground state energy and wave function to one instead of the conventional four iterations corresponding to the number of states implying that the rate of convergence to the ground state is affected by the choice of initial trial wave vector.

(B) Four Electrons on Four Sites

As another example, the ground state energy and wave function will be obtained for four electrons on four sites. The antiferromagnetic states can be obtained using the formula;

$$\left(\frac{N!}{(N-\frac{n}{2})!\frac{n}{2}!}\right)^2 \tag{35}$$

therefore

$$\left(\frac{4!}{2!2!}\right)^2 = 36 \text{ states} \tag{36}$$

To obtain the new basis state vectors that will reduce the size of the Hilbert space from 36 states to three, we will proceed thus.

$$\begin{aligned} |2200\rangle &= |2200\rangle + |0220\rangle + |0022\rangle + |2002\rangle \\ |2020\rangle &= |2020\rangle + |0202\rangle \end{aligned} \tag{37}$$

Where **2** indicates that there are two electrons occupying that site and the four items in each bracket represents the four sites and the **0** shows the sites that are unoccupied. Doubly occupied sites account for 6 states out of the 36 states and this corresponds to one new basis state which is denoted by $|1'\rangle$ in Equation (40). When one site is doubly occupied and two other sites are singly occupied, the following are obtained

$$\begin{aligned} |2110\rangle &= |2110\rangle + |0211\rangle + |1021\rangle + |1102\rangle \\ |2011\rangle &= |2011\rangle + |1201\rangle + |1120\rangle + |0112\rangle \\ |2101\rangle &= |2101\rangle + |1210\rangle + |0121\rangle + |1012\rangle \end{aligned} \tag{38}$$

Also **2** indicate that a site is doubly occupied, **1** indicate that a site is singly occupied while **0** indicate that a site is empty. Taking the spin orientation into consideration, 24 states are accounted for and this corresponds to one new basis state denoted by $|2'\rangle$ in Equation (40). The last separation is when all sites are singly occupied and it is described by

$$|1111\rangle \tag{39}$$

When the spin orientations for the four electrons are taken into consideration, it accounts for 6 states and corresponds to one new basis state denoted by $|3'\rangle$ in Equation (40). Hence the 36 states have been adequately taken care of. Having understood the above explanation, the new basis states are

$$\begin{aligned} |1'\rangle &= |2200\rangle + |0220\rangle + |0022\rangle + |2002\rangle + |2020\rangle + |0202\rangle \\ |2'\rangle &= |2110\rangle + |0211\rangle + |1021\rangle + |1102\rangle + |2011\rangle + |1201\rangle \\ &+ |1120\rangle + |0112\rangle + |2101\rangle + |1210\rangle + |0121\rangle + |1012\rangle \\ |3'\rangle &= |1111\rangle \end{aligned} \tag{40}$$

When the Hubbard Hamiltonian given in Equation (3) is applied to these new basis states, the following are obtained

$$\begin{aligned} H|1'\rangle &= 2u|1'\rangle - 2t|2'\rangle \\ H|2'\rangle &= -8t|1'\rangle + (u-4t)|2'\rangle - 8t|3'\rangle \\ H|3'\rangle &= -2t|2'\rangle \end{aligned}$$

At this point, the modification of the Lanczos technique is applied and the iterations are carried out until the ground state energy is obtained. As an example, the first iteration will be thoroughly treated, let the initial normalized trial vector be

$$|\phi_0\rangle = \frac{1}{\sqrt{6}}|1'\rangle = A_1|1'\rangle \tag{41}$$

When the Hamiltonian acts on Eqn. (41) and the result normalized, H_0 is obtained in Eqn. (42) as

$$H_0 = 6A_1B_1 \tag{42}$$

the parameters generated are defined as

$B_1 = 2uA_1$, $B_2 = -2tA_1$

when the Hamiltonian acts twice on Eqn.(41) and normalized, β_0 is obtained as

$$\beta_0 = 6A_1C_1 \tag{43}$$

the parameters generated are defined as

Where $C_1 = 2uB_1 - 8tB_2$, $C_2 = -2tB_1 + (u-4t)B_2$

Using Eqns. (42) and (43), the normalizing factor the first iteration is defined in Eqn. (44)

$$b_0 = (\beta_0 - H_0{}^2)^{1/2} \tag{44}$$

Subtracting the normalized initial trial wave vector from the wave vector generated after the Hamiltonian has acted gives the new orthogonal states as Eqn. (45)

$$\left|\tilde{\phi}_0\right\rangle = D_1\left|1'\right\rangle + D_2\left|2'\right\rangle \tag{45}$$

the parameters generated are defined as

$$D_1 = \frac{B_1 - H_0A_1}{b_0}, D_2 = \frac{B_2}{b_0}$$

when the Hamiltonian acts the third time on Eqn. (41) and the result normalized, γ_0 will be obtained as given in Eqn. (46)

$$\gamma_0 = 6A_1(2uC_1 - 8tC_2) \tag{46}$$

with all the parameters for f_0 already defined, f_0 is simply written as

$$f_0 = \frac{\gamma_0 - 3H_0\beta_0 + 2H_0^3}{2\left(\beta_0 - H_0^2\right)^{3/2}} \tag{47}$$

from Eqn (47), α_0 is defined as

$$\alpha_0 = f_0 - \left(f_0^2 + 1\right)^{1/2} \tag{48}$$

using Eqns (42), (44) and (48), the improved energy comparing to the actual ground state energy is given in Eqn (49) as

$$\in_1 = H_0 + b_0\alpha_0 \tag{49}$$

the wave function corresponding to the energy obtained in Eqn. (49) is obtained by inserting Eqns. (41), (45) and (48) into Eqn. (15) given above yields;

$$\left|\phi_{0+1}\right\rangle = \left|\phi_1\right\rangle = \frac{A_1 + \alpha_0D_1}{\left(1+\alpha_0^2\right)^{1/2}}\left|1'\right\rangle + \frac{\alpha_0D_2}{\left(1+\alpha_0^2\right)^{1/2}}\left|2'\right\rangle \tag{50}$$

Equations (49) and (50) are better approximations to the true ground state energy and wave function than Eqns. (41) and (42). It is observed that after five iterations, the result obtained becomes repetitive showing that the lowest energy and wave function has been obtained and that the system has converged.

Results from the ground state energy equation obtained in Eqns. (32) and (49) for interaction strength of u = -5.00 – 5.00 is presented in Table 1 and 3 respectively. The second and the third column of Table 1 shows that the result accurately reproduces those obtained using exact method (column 2) and correlated variational approach (column 3) for two sites while the last column in Table 3 shows the converged ground state energy for four sites. It is observed that at exactly one electron per site, the energy change between the extreme strong u (u = 5.00) limit in this work and the extreme weak u (u = -5.00) limit in this work, is exactly $\Delta E/t$ = -5.00 for two sites and $\Delta E/t$ = -10.00 for four sites. It is also noteworthy that as the interaction strength changes per unit (5.00 to 4.00 …..), the ratio of energy change gradually increases as the u/t decreases and almost becomes a unit value between u/t = -4.00 and u/t = -5.00. This change in trend is even more evident in Fig. 1 (the graph of E/t versus u/t which was plotted from values obtained in Table 1). In this figure, it is noted that the space between the points are more clustered for u/t being positive than for u/t negative. This shows that the interaction energy at the ground state in the weak coupling regime (u/t < 0) reduces more rapidly than in the strong coupling limit (u/t > 0). Results in the strong coupling limit shows that anti-ferromagnetism is stable. The drop in energy value in Figs. 1 and 3 for negative u/t supports the proposition that the electrons prefer to stay together in the weak

coupling limit. On the contrary, in the strong coupling limit (positive u/t), the drop in energy is a very slight parabola indicating that the electrons prefer to stay in their singly occupied sites. Figs. 2 and 4 which is the plot of the weights of the ground state wave function versus the interaction strength shows a very interesting trend, the two plots only intersect at the point where u/t = 0. The intersect in Figs. 2 and 4 and the value in Tables 2 and 4 for u = 0 tells us that the weights of the wave functions are the same both for the two and four electrons being on the same site and for the two and four electrons occupying separate sites showing that at half-filling, the electrons have equal probability of occupying any site. Using the two site result as a case study, the λ in Fig. 2 represented by the dotted line is the weight of the wave function for the two electrons on the same site and it is observed that at u = -5.00, the weight is at a peak of 0.6494 while at u = 5.00, the weight is 0.0326. The higher value shows a greater probability of finding the electron at that site. This clearly shows that at positive u the electrons prefer to stay apart. On the other hand, μ in Fig. 2 represents the case of one electron per site and for u = -5.00, the weight of the wave function is 0.1315 while at u = 5.00 it goes to a peak of 0. 7483 showing that the probability of finding the electron here is even higher. It is interesting to note that in Fig. 4, *series 2* representing two on site electrons and two inter-site electrons have a fairly stable and equal probability of being occupied both at u < 0 and u > 0 limit and it has its highest probability of occupation at u = 0. So for positive u, the electrons prefer to stay apart. It can be safely concluded from results before us that strongly correlated electron system is better discussed in the positive u/t regime. In Fig. 2, it is observed that as u/t increases or decreases, the change in the weight of the wave function stabilizes but this is not the case in Fig. 4 because the electrons have more sites to hop to hence expending more energy. This displays the limitation in the number of sites considered in this work. It is also noteworthy that when the weights of the wave function for both the on-site and the inter-site arrangement are added it gives a value of ~1 in Table 2 and adds up to ~ 0.5 in Table 4. When the result in this work is extrapolated to bulk limit at energy per site, the result stands at a value of 1.0000. This result agrees well with that obtained by [28] where they worked on the Heisenberg model in the half filled band for up to 24 sites using the modified Lanczos technique. It is observed from their work that as the number of sites increases, the energy per site stabilizes to an average value of about -0.8862.

Table 1 Ground-state energy E/t for two electrons on two sites as a function of u/t (at t=1).

Interaction strength (u/t)	Energy (E/t)		
	Modified Lanczos method (This work)	Exact method	Variational calculation
5.00	-0.7016	-0.7016	-0.7016
4.00	-0.8284	-0.8284	-0.8284
3.00	-1.0000	-1.0000	-1.0000
2.00	-1.2361	-1.2361	-1.2361
1.00	-1.5616	-1.5616	-1.5616
0.00	-2.0000	-2.0000	-2.0000
-1.00	-2.5616	-2.5616	-2.5616
-2.00	-3.2361	-3.2361	-3.2361
-3.00	-4.0000	-4.0000	-4.0000
-4.00	-4.8284	-4.8284	-4.8284
-5.00	-5.7016	-5.7016	-5.7016

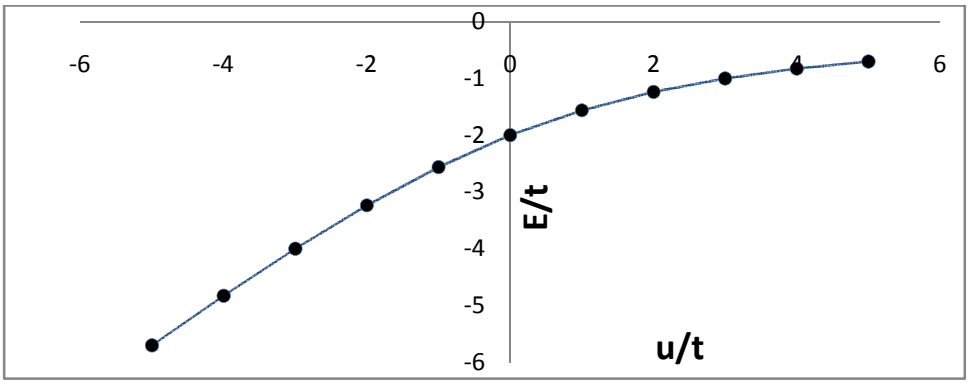

Figure 1: The ground state energy E/t versus the interaction strength u/t for two electrons on two sites

Table 2: Ground state wave function (ψ_G) for two electrons on two sites at u/t = -5.00 to 5.00 the ket notation is as defined on Eqn. 20 and 26)

INTERACTION STRENGTH u/t	**WAVE FUNCTIONS**	**WEIGHT DESCRIBING WAVE FUNCTION**
		1^{ST}
5.00	$\|1'\rangle$	0.0326
	$\|2'\rangle$	0.7483
4.00	$\|1'\rangle$	0.0417
	$\|2'\rangle$	0.7488
3.00	$\|1'\rangle$	0.1359
	$\|2'\rangle$	0.7359
2.00	$\|1'\rangle$	0.2507
	$\|2'\rangle$	0.6979
1.00	$\|1'\rangle$	0.3787
	$\|2'\rangle$	0.6213
0.00	$\|1'\rangle$	0.5000
	$\|2'\rangle$	0.5000
-1.00	$\|1'\rangle$	0.5909
	$\|2'\rangle$	0.3484
-2.00	$\|1'\rangle$	0.6419
	$\|2'\rangle$	0.1947
-3.00	$\|1'\rangle$	0.6606
	$\|2'\rangle$	0.0606
-4.00	$\|1'\rangle$	0.6597
	$\|2'\rangle$	0.0474
-5.00	$\|1'\rangle$	0.6494
	$\|2'\rangle$	0.1315

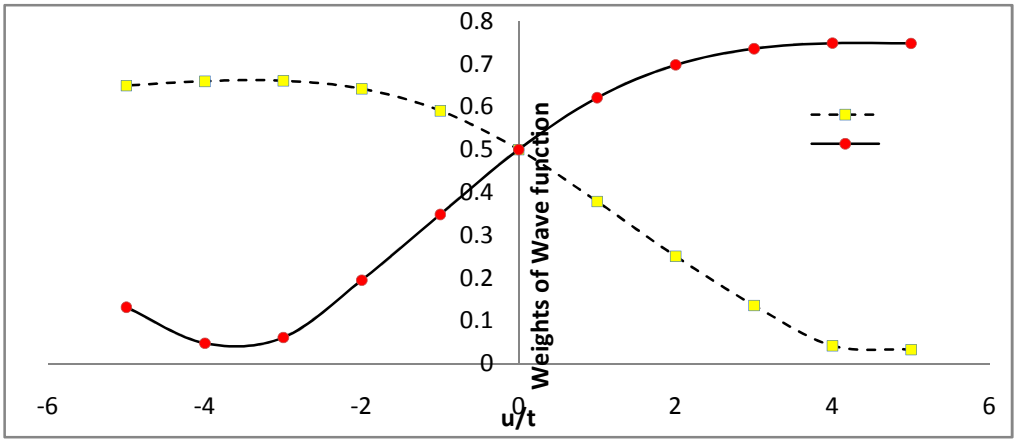

Figure 2: Weight of ground state wave function (ψ_G) versus the interaction strength u/t for two electrons on two sites

Table 3: Ground state energy (E/t) for four electrons on four sites as a function u/t (at t=1).

u/t	**ENERGY (E/t)**				
	ITERATIONS				
	1^{ST}	2^{ND}	3^{RD}	4TH	5^{TH}
5.00	-0.5208	-4.0083	-4.0682	-4.0692	-4.0692
4.00	-1.6568	-4.6157	-4.6795	-4.6803	-4.6804
3.00	-2.8151	-5.3126	-5.3765	-5.3788	-5.3800
2.00	-4.0000	-6.0988	-6.1661	-6.1677	-6.1677
1.00	-5.2170	-6.9725	-7.0397	-7.0417	-7.0417
0.00	-6.4721	-7.9318	-7.9974	-8.0000	-8.0000
-1.00	-7.7720	-8.9762	-9.0388	-9.0416	-9.0417
-2.00	-9.1231	-10.1066	-10.1645	-10.1676	-10.1677
-3.00	-10.5311	-11.3251	-11.3757	-11.3798	-11.3800
-4.00	-12.0000	-12.6332	-12.6773	-12.6801	-12.6803
-5.00	-13.5311	-14.0306	-14.0665	-14.0690	-14.0692

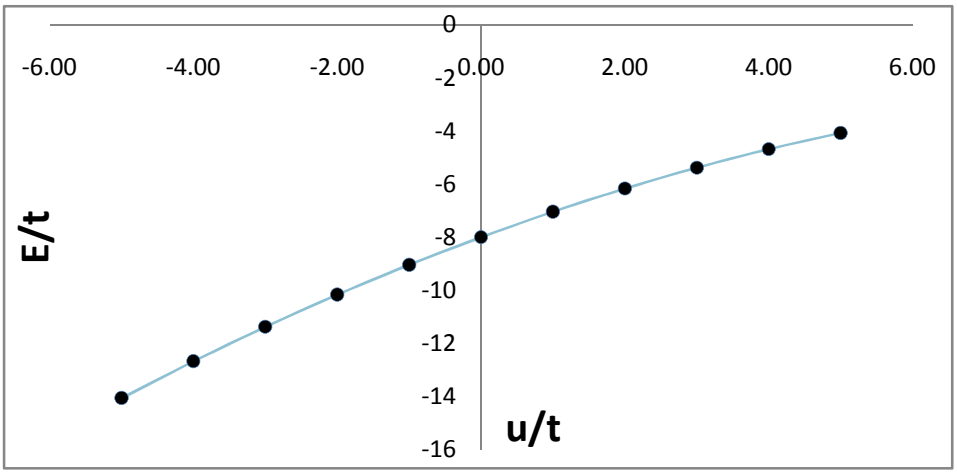

Figure 3: The ground state energy E/t versus the interaction strength u/t for four electrons on four sites

Table 4: Ground state wave function for four electrons on four sites at u/t = -5.00 to 5.00 (the ket notation is as defined in Eqn. (40))

INTERACTION STRENGTH u/t	**WAVE FUNCTION**	**WEIGHTS OF WAVE FUNCTION**					
		1ST	**2ND**	**3RD**	**4TH**	**5TH**	**6TH**
5.00	$\|1'\rangle$	0.1451	0.1061	0.0822	0.0814	0.0811	0.0812
	$\|2'\rangle$	0.1908	0.1395	0.1438	0.1426	0.1427	0.1427
	$\|3'\rangle$		0.2785	0.2779	0.2805	0.2805	0.2805
4.00	$\|1'\rangle$	0.1562	0.1220	0.0966	0.0956	0.0952	0.0952
	$\|2'\rangle$	0.1886	0.1472	0.1521	0.1506	0.1509	0.1509
	$\|3'\rangle$		0.2552	0.2546	0.2579	0.2579	0.2579
3.00	$\|1'\rangle$	0.1687	0.1391	0.1125	0.1113	0.1109	0.1108
	$\|2'\rangle$	0.1859	0.1533	0.1589	0.1576	0.1577	0.1577
	$\|3'\rangle$		0.2309	0.2303	0.2344	0.2344	0.2344
2.00	$\|1'\rangle$	0.1828	0.1575	0.1300	0.1287	0.1280	0.1280
	$\|2'\rangle$	0.1828	0.1575	0.1638	0.1625	0.1627	0.1626
	$\|3'\rangle$		0.2066	0.2060	0.2109	0.2108	0.2109
1.00	$\|1'\rangle$	0.1979	0.1769	0.1489	0.1475	0.1466	0.1466
	$\|2'\rangle$	0.1785	0.1596	0.1667	0.1655	0.1657	0.1657
	$\|3'\rangle$		0.1831	0.1826	0.1881	0.1880	0.1882
0.00	$\|1'\rangle$	0.2146	0.1973	0.1692	0.1678	0.1668	0.1667
	$\|2'\rangle$	0.1736	0.1596	0.1676	0.1664	0.1667	0.1667
	$\|3'\rangle$		0.1610	0.1605	0.1665	0.1664	0.1667
-1.00	$\|1'\rangle$	0.2325	0.2184	0.1909	0.1896	0.1883	0.1883
	$\|2'\rangle$	0.1678	0.1575	0.1663	0.1653	0.1657	0.1656
	$\|3'\rangle$		0.1404	0.1400	0.1463	0.1463	0.1466
-2.00	$\|1'\rangle$	0.2512	0.2398	0.2138	0.2125	0.2111	0.2110
	$\|2'\rangle$	0.1609	0.1536	0.1630	0.1622	0.1627	0.1626

	$\|3'\rangle$		0.1216	0.1212	0.1277	0.1276	0.1279
-3.00	$\|1'\rangle$	0.2702	0.2612	0.2372	0.2361	0.2346	0.2345
	$\|2'\rangle$	0.1530	0.1479	0.1578	0.1571	0.1577	0.1576
	$\|3'\rangle$		0.1045	0.1042	0.1105	0.1104	0.1108
-4.00	$\|1'\rangle$	0.2887	0.2817	0.2605	0.2595	0.2581	0.2580
	$\|2'\rangle$	0.1443	0.1409	0.1508	0.1503	0.1509	0.1509
	$\|3'\rangle$		0.0892	0.0890	0.0948	0.0948	0.0952
-5.00	$\|1'\rangle$	0.3061	0.3008	0.2827	0.2819	0.2806	0.2806
	$\|2'\rangle$	0.1351	0.1328	0.1424	0.1420	0.1425	0.1426
	$\|3'\rangle$		0.0757	0.0755	0.0808	0.0807	0.0811

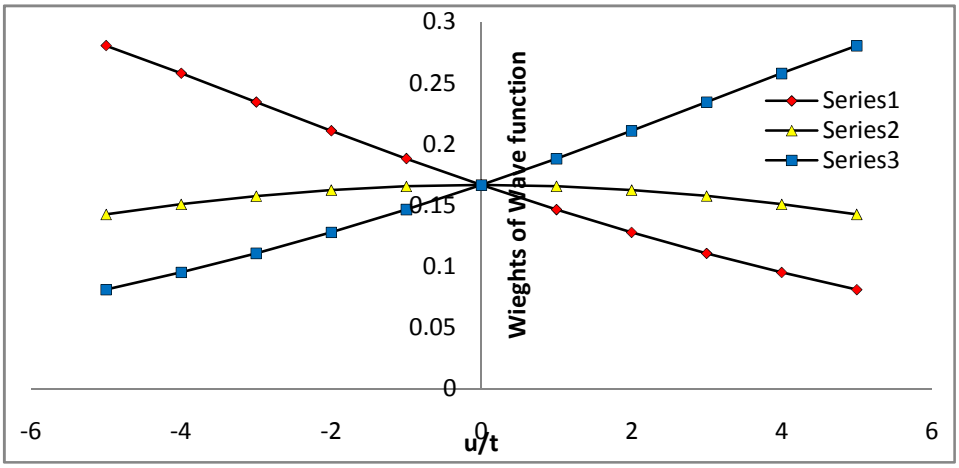

Figure 4 **Weights of the ground state wave function (ψ_G) versus the interaction strength u/t for four electrons on four sites at u/t = -5.00 to 5.00**

Conclusion

In this paper, the single band Hubbard model has been analyzed at half filling using a simplified modification of the Lanczos technique. Accurate results were obtained for precisely two and four site problems. Regarding the ground state energy and wave function, as far as was analyzed in this work, there is no evidence of an anomalous behavior. Based on the variational theory that says the lower the energy the better the wavefunction, the result obtained as the ground state energy for four sites in this work is a better energy than that obtained by (27).

Again, the number of iteration required to obtain the ground state properties treated was greatly reduced by using the linear combination of translational invariant states and this reduced the number of iterations by a factor of approximately four. The method presented here converges faster than the usual Lanczos technique and requires less numerical calculation.

It is hoped that this work will be extended to larger and more realistic sites based on the explicit and foundational work that has been presented here. We also hope to treat the effect of energy gap and correlation functions in the half-filled band in future work.

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