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GROUND STATE PROPERTIES OF THE ONE-DIMENSIONAL HUBBARD MODEL: A SYMMETRY PROJECTED VARIATIONAL WAVE FUNCTION APPROACH.

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Abstract

We use the C_{4v} symmetry group of the 4-site Hubbard model to construct a ground State variational wave function of two and four interacting electrons. In the limit $U \to 0$, ground state energies (E_g) of the two and four interacting electrons system is of the order $-4t$ .The variational wave function of the four interacting electrons obtained using the B_1 irreducible representation is valid for onsite coulomb repulsion (U), while the one obtained using the A_1 representation is valid for negative values of coulomb interaction. The system exhibit antiferromagnetic correlations.

1.1 INTRODUCTION

The Hubbard model is the simplest generic model for strongly correlated electrons This arose from the independent work of Hubbard [1], Gutzwiller [2] and kanamori [3]. One of the main motivations of studying the Hubbard model is that it is the simplest generalization beyond the band theory description of solids yet still appears to capture the gross features of many systems characterized by more general interaction parameters [4]. The Hubbard model has been used in attempts to describe:(i) the electronic properties of solids with narrow bands(ii) band magnetism in iron, cobalt and nickel(iii) Mott metal-insulator transition(iv)electronic properties of high-T_C cuprates in the normal state.

Despite its apparent simplicity, no fully consistent treatment of the Hubbard model is available in general[4]. A rigorous mathematical solution by Lieb and Wu exists in one dimension [5]. Using the formulation of Bethe Ansatz they reduced the problem of diagonalizing the Hamiltonian to solving a set of coupled nonlinear equations. They showed that the Hubbard model at half-filling is an insulator for all positive values of the interaction U. In more than one-dimension many important physical questions remain unresolved, despite the great number of different theoretical approaches that have been applied. In the absence of exact results reliable way to describe the properties of strongly correlated models is to resort to approximate analytical and numerical techniques. These techniques have proved to be very useful in dealing with finite size lattices [6,7].

The Hubbard Hamiltonian consists of two contributions,

$$H = \sum_{\langle i,j\rangle\sigma} t_{ij}\left(C^{\dagger}_{i,\sigma}C_{j,\sigma} + h.c\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} \qquad (1.1)$$

a kinetic term describing the motion of electrons between neighboring sites (th e hopping integral t_{ij} ,is usually restricted to nearest-neighbours, and is assumed translationally invariant, namely $t_{ij} = -t, t > 0$),and an on-site term, which approximates the interaction among electrons, whose strength is given by the parameter U. $U > 0$ corresponds to repulsive coulomb interaction, whereas $U < 0$ could eventually describe an effective attraction mediated by the ions. $\langle i, j\rangle$ denotes nearest neighbour sites of a D-dimensional lattice Λ , $\sigma = \uparrow, \downarrow$ denotes the spin and $C^{\dagger}_{i,\sigma}, C_{j,\sigma}$ are the electrons creation and destruction operators, with $n_{i\sigma} = C^{\dagger}_{i,\sigma}C_{i,\sigma}$.

The aim of this present study is to obtain the ground state properties of the one dimensional Hubbard model using the variational wave function approach [8]. The construction of the variational wave function is based on the space group

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symmetry of the Hamiltonian eqn (1.1). We consider the Hubbard model on a four site ring , with band fillings $\rho = \frac{1}{2}$ and $\rho = 1$.

The main motivation for this study is the work done using the variational approach [8] where the construction of the trial wave function was done without recourse to the space symmetry group of the Hamiltonian.

The remaining part of this paper is organized as follows: the methodology and computation of the ground state energy for the various band fillings are shown in Sec. 1.2.In Sec. 1.3 we compute the correlation functions (charge and spin correlations). In Sec.1.4 we present numerical results, while Sec.1.5 is devoted to discussion of results, and in Sec.1.6 we draw up conclusions.

1.2 METHODOLOGY

The Hubbard Hamiltonian Eqn. (1.1) admits C_{4v} symmetry [9]. The group C_{4v} is a group of symmetry operations when applied to a square produces an equivalent or an identical configuration [10]. The symmetry operations include rotation by $\frac{\pi}{2}$, π, $\frac{3\pi}{2}$, and 2π , then reflections in two planes of symmetry σ_v and σ_d. thus there are five classes and therefore five irreducible representations. $[A_1, A_2, B_1, B_2]$ are one – dimensional and E is two dimensional. For a given system size N and number of fermions n , the dimension of the Hilbert space is given by: $\dim = 2N_{C_n}$ We chose to work in the subspace $S_z = 0$, where the number of up spins ($n\uparrow$) equals the number of down spins ($n\downarrow$), and the dimension of Hilbert space becomes $\dim = \left(N_{C_{\frac{n}{2}}}\right)^2$. For a system of two interacting electrons that is $n = 2$, $\dim H = (4_{C_1})^2 = 16$. By making use of the projection operator

$$\hat{p}^{(j)} = \frac{l_j}{h}\sum_R \chi(R)^j \hat{R} \qquad (1.2)$$

of the j[th], irreducible representation of the group C_{4v}, we can project out symmetry invariant subspaces of the Hilbert space. For an arbitrary basis in the Hilbert space say $|1\rangle = |1\uparrow,1\downarrow\rangle$ and putting $j = A_1$ where A_1 is one of the four one dimensional representation of the group, Eqn. (1.2) becomes

$$P^{A_1} = \frac{l_A}{h}\sum_R \chi(R)^A \hat{R} \qquad (1.3)$$

where we have made use of the character table of the group C_{4v} for the irreducible representation A_1

$$P^{A_1}|1\uparrow 1\downarrow\rangle = \frac{1}{4}\left(|1\uparrow 1\downarrow\rangle + |2\uparrow,2\downarrow\rangle + |3\uparrow,3\downarrow\rangle + |4\uparrow,4\downarrow\rangle\right)$$

Similarly $P^{A_1}|1\uparrow,2\downarrow\rangle = \frac{1}{8}\left(|1\uparrow 2\downarrow\rangle - |1\downarrow,2\uparrow\rangle + |2\uparrow,3\downarrow\rangle - |2\downarrow,3\uparrow\rangle + |1\uparrow,4\downarrow\rangle - |1\downarrow,4\uparrow\rangle + |3\uparrow,4\downarrow\rangle - |3\downarrow,4\uparrow\rangle\right)$

And $P^{A_1}|1\uparrow,3\downarrow\rangle = \frac{1}{4}\left(|1\uparrow 3\downarrow\rangle - |1\downarrow,3\uparrow\rangle + |2\uparrow,4\downarrow\rangle - |2\downarrow,4\uparrow\rangle\right)$

Thus, we have a 3 dim. invariant subspace of the 16 dimensional Hilbert space, i.e.

$$|\alpha\rangle = \frac{1}{2}\left(|1\uparrow,1\downarrow\rangle + |2\uparrow,2\downarrow\rangle + |3\uparrow,3\downarrow\rangle + |4\uparrow,4\downarrow\rangle\right)$$

$$|\beta\rangle = \frac{1}{2\sqrt{2}}\left(|1\uparrow,2\downarrow\rangle - |1\downarrow,2\uparrow\rangle + |2\uparrow,3\downarrow\rangle - |2\downarrow,3\uparrow\rangle + |1\downarrow,4\uparrow\rangle - |1\downarrow,4\uparrow\rangle + |3\uparrow,4\downarrow\rangle - |3\downarrow,4\uparrow\rangle\right)$$

$$|\gamma\rangle = \frac{1}{2}\left(|1\uparrow,3\downarrow\rangle - |1\downarrow,3\uparrow\rangle + |2\uparrow,4\downarrow\rangle - |2\downarrow,4\uparrow\rangle\right)$$

Using the basis $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$ we construct a trial variational wave function of the form.

$|\psi\rangle = x_0|\alpha\rangle + x_1|\beta\rangle + x_2|\gamma\rangle$, where x_0 , x_1 and x_3 are variational parameters. The variational ground state energy is given by;

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \qquad (1.4)$$

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{Ux_0 - 4t\sqrt{2}x_0x_1 - 4t\sqrt{2}x_1x_2}{x_0^2 + x_1^2 + x_2^2}$$

Employing the energy minimization condition $\frac{\partial E}{\partial x_i} = 0$ for $i = 0,1,2$ we obtain the variational ground state energy matrix

$$A = \begin{pmatrix} U & -2t\sqrt{2} & 0 \\ -2t\sqrt{2} & 0 & -2t\sqrt{2} \\ 0 & -2t\sqrt{2} & 0 \end{pmatrix} \qquad (1.5)$$

The procedure used above for the 2 interacting electrons can be extended to a system of 4 interacting electrons, that is $(N=4, n=4)$. In the subspace $S_Z = 0$

$\dim(H) = (4_{C_2})^2 = 36$. Accordingly, we label the 4 electron basis in this Hilbert space as

$|1\rangle = |1\uparrow,1\downarrow,2\uparrow,2\downarrow\rangle$ $|2\rangle = |1\uparrow,1\downarrow,3\uparrow,3\downarrow\rangle$ $|3\rangle = |1\uparrow,1\downarrow,4\uparrow,4\downarrow\rangle$ $|4\rangle = |2\uparrow,2\downarrow,3\uparrow,3\downarrow\rangle$

$|5\rangle = |2\uparrow,2\downarrow,4\uparrow,4\downarrow\rangle$ $|6\rangle = |3\uparrow,3\downarrow,4\uparrow,4\downarrow\rangle$ $|7\rangle = |1\uparrow,1\downarrow,2\uparrow,3\downarrow\rangle$ $|8\rangle = |1\uparrow,1\downarrow,2\downarrow,3\uparrow\rangle$

$|9\rangle = |1\uparrow,1\downarrow,2\uparrow,4\downarrow\rangle$ $|10\rangle = |1\uparrow,1\downarrow,2\downarrow,4\uparrow\rangle$ $|11\rangle = |1\uparrow,1\downarrow,3\uparrow,4\downarrow\rangle$ $|12\rangle = |1\uparrow,1\downarrow,3\downarrow,4\uparrow\rangle$

$|13\rangle = |1\uparrow,2\uparrow,2\downarrow,3\downarrow\rangle$ $|14\rangle = |1\downarrow,2\uparrow,2\downarrow,3\uparrow\rangle$ $|15\rangle = |1\uparrow,2\uparrow,2\downarrow,4\downarrow\rangle$ $|16\rangle = |1\downarrow,2\uparrow,2\downarrow,4\uparrow\rangle$

$|17\rangle = |2\uparrow,2\downarrow,3\uparrow,4\downarrow\rangle$ $|18\rangle = |2\uparrow,2\downarrow,3\downarrow,4\uparrow\rangle$ $|19\rangle = |1\uparrow,3\uparrow,3\downarrow,4\downarrow\rangle$ $|20\rangle = |1\downarrow,3\uparrow,3\downarrow,4\uparrow\rangle$

$|21\rangle = |1\uparrow,2\downarrow,3\uparrow,3\downarrow\rangle$ $|22\rangle = |1\downarrow,2\uparrow,3\uparrow,3\downarrow\rangle$ $|23\rangle = |2\uparrow,3\uparrow,3\downarrow,4\downarrow\rangle$ $|24\rangle = |2\downarrow,3\uparrow,3\downarrow,4\uparrow\rangle$

$|25\rangle = |1\uparrow,2\downarrow,4\uparrow,4\downarrow\rangle$ $|25\rangle = |1\uparrow,2\downarrow,4\uparrow,4\downarrow\rangle$ $|26\rangle = |1\downarrow,2\uparrow,4\uparrow,4\downarrow\rangle$ $|27\rangle = |1\uparrow,3\downarrow,4\uparrow,4\downarrow\rangle$

$|28\rangle = |1\downarrow,3\uparrow,4\uparrow,4\downarrow\rangle$ $|29\rangle = |2\uparrow,3\downarrow,4\uparrow,4\downarrow\rangle$ $|29\rangle = |2\uparrow,3\downarrow,4\uparrow,4\downarrow\rangle$ $|30\rangle = |2\downarrow,3\uparrow,4\uparrow,4\downarrow\rangle$

$|31\rangle = |1\uparrow,2\downarrow,3\uparrow,4\downarrow\rangle$ $|32\rangle = |1\downarrow,2\uparrow,3\downarrow,4\uparrow\rangle$ $|33\rangle = |1\uparrow,2\uparrow,3\downarrow,4\uparrow\rangle$ $|34\rangle = |1\downarrow,2\downarrow,3\uparrow,4\uparrow\rangle$

$|35\rangle = |1\uparrow,2\downarrow,3\downarrow,4\uparrow\rangle$ $|35\rangle = |1\uparrow,2\downarrow,3\downarrow,4\uparrow\rangle$ $|36\rangle = |1\downarrow,2\uparrow,3\uparrow,4\downarrow\rangle$

By replacing j with B_1, one of the four one-dimensional representations of the group C_{4V}, together with an arbitrary basis, say $|1\rangle = |1\uparrow,1\downarrow,2\uparrow,2\downarrow\rangle$ we can project out symmetry invariant subspaces of the Hilbert space. That is;

$P^{(B_1)}|1\rangle = \frac{1}{4}[|1\rangle = |3\rangle - |4\rangle + |6\rangle]$

Similarly,

$P^{(B_1)}|1\rangle = \frac{1}{2}[|31\rangle + |32\rangle]$

$P^{(B_1)}|33\rangle = \frac{1}{2}[|35\rangle + |36\rangle + |34\rangle + |33\rangle]$ $P^{(B)}|7\rangle = \frac{1}{8}[|7\rangle - |25\rangle - |17\rangle - |20\rangle - |30\rangle + |15\rangle + |22\rangle + |12\rangle]$

$P^{(B_1)}|8\rangle = \frac{1}{8}[|8\rangle - |26\rangle - |18\rangle - |19\rangle - |29\rangle + |16\rangle + |21\rangle + |11\rangle]$ $P^{(B_1)}|2\rangle = 0$

$P^{(B_1)}|9\rangle = \frac{1}{8}[|9\rangle + |10\rangle + |13\rangle + |14\rangle - |23\rangle - |24\rangle - |27\rangle - |28\rangle]$

This leads us to the following new basis, that is

$|\psi_1\rangle = \frac{1}{2}[|1\rangle = |3\rangle - |4\rangle + |6\rangle]$

$|\psi_2\rangle = \frac{1}{4}[|7\rangle - |8\rangle + |15\rangle - |16\rangle + |19\rangle - |20\rangle + |29\rangle - |30\rangle + |12\rangle - |11\rangle + |26\rangle - |25\rangle + |22\rangle - |21\rangle + |18\rangle - |17\rangle]$

$|\psi_3\rangle = \frac{1}{2\sqrt{2}}[|9\rangle + |10\rangle + |13\rangle + |14\rangle - |23\rangle - |24\rangle - |27\rangle - |28\rangle]$

$|\psi_4\rangle = \frac{1}{2}[|35\rangle + |36\rangle + |34\rangle + |33\rangle]$

$|\psi_5\rangle = \frac{1}{\sqrt{2}}[|31\rangle + |32\rangle]$

The variational wave function becomes

$$\Psi = x_0|\psi_1\rangle + x_1|\psi_2\rangle + x_2|\psi_3\rangle + x_3|\psi_4\rangle + x_4|\psi_5\rangle \quad (1.6)$$

The ground state energy is obtained using the eqn.(1.3), that is

$$E = \frac{-4tx_0x_1 - 2txx_1x_3 - 2tx_3x_2 + 4t\sqrt{2}x_1x_4 + Ux_1^2 + Ux_2^2 + 2Ux_0^2}{x_0^2 + x_1^2 + x_2^2 + x_3^2 + x_4^2} \quad (1.7)$$

By employing the energy minimization condition $\frac{\partial E}{\partial x_i} = 0$ for $i = 0,1,2,3,4$, we obtain the variational ground state energy matrix.

$$B = \begin{pmatrix} 2U & -2t & 0 & 0 \\ -2t & U & -2t & 2\sqrt{2} \\ 0 & -2t & U & 0 \\ 0 & 2t\sqrt{2} & 0 & 0 \end{pmatrix} \quad (1.8)$$

A new basis, which constitutes five invariant subspaces of the Hilbert space, can be constructed using the irreducible representation A_1 of the symmetry group C_{4v} together with the projection operator eqn. (1.2).

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}[|2\rangle + |5\rangle]$$

$$|\psi_2\rangle = \frac{1}{2}[|1\rangle + |3\rangle + |4\rangle + |6\rangle]$$

$$|\psi_3\rangle = \frac{1}{4}[|7\rangle - |8\rangle + |11\rangle - |12\rangle + |15\rangle - |16\rangle + |17\rangle - |18\rangle + |19\rangle - |20\rangle + |21\rangle - |22\rangle + |25\rangle - |26\rangle + |29\rangle - |30\rangle]$$

$$|\psi_4\rangle = \frac{1}{2\sqrt{2}}[|9\rangle - |10\rangle + |13\rangle - |14\rangle + |23\rangle - |24\rangle + |27\rangle - |28\rangle]$$

$$|\psi_5\rangle = \frac{1}{2}[|3\rangle + |34\rangle - |35\rangle - |36\rangle]$$

and the trial variational wave function becomes

$$\Psi' = x_0|\psi_1\rangle + x_1|\psi_2\rangle + x_2|\psi_3\rangle + x_3|\psi_4\rangle + x_4|\psi_5\rangle \quad (1.9)$$

$x_i (i = 0,1,2,3,4)$ are variational parameters.

Using the same procedure, we obtain another form of the ground state energy matrix using the irreducible representation A_1 of the symmetry group C_{4v}.

The ground state energy matrix is thus given by

$$B = \begin{pmatrix} 2U & 0 & -2\sqrt{2}t & 0 \\ 0 & 2U & -2t & 0 \\ -2\sqrt{2}t & -2t & U & -2t \\ 0 & 0 & -2t & 0 \end{pmatrix} \quad (1.10)$$

1.3 CHARGE – CHARGE AND SPIN CORRELATION FUNCTIONS.

Correlation functions can be calculated from the wave function. Charge –charge correlation function is given by the formula

$$P(i,j) = \langle \Psi | C^{\dagger}_{i\uparrow} C_{i\uparrow} C^{\dagger}_{j\downarrow} C_{j\downarrow} | \Psi \rangle \quad (1.11)$$

$P(i,j)$ measures the probability of finding an electron onsite i when an electron of opposite spin is sitting on site j. For the two electron system, we obtain the following correlation functions.

$$P(i,j) = \frac{x_0^2}{4}, i = 1,2,\ldots 4 \quad (1.12)$$

and

$$P(i,j) = \frac{x_1^2}{8} \text{ for } |i-j| = 1 \quad (1.13)$$

$$P(i,j) = \frac{x_2^2}{4} \text{ for } |i-j| = 2 \quad (1.14)$$

The-spin correlation function is given by:

$$S(i,j) = \langle \Psi | \vec{S}_i . \vec{S}_j | \Psi \rangle. \quad (1.15)$$

With $S_i . S_j = \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right) + S_i^z S_j^z$

Negative values of $S(i,j)$ between sites denotes antiferromagnetic correlations.

$$S(i,j) = \frac{-3x_1^2}{16} \text{ for } |i-j| = 1 \quad (1.16)$$

and

$$S(i,j) = \frac{-3x_2^2}{8} \text{ for } |i-j| = 2 \quad (1.17)$$

Similarly for a system of four electrons, we have for positive values of the onsite repulsion U the following results.

$$P(i,i) = \frac{x_0^2}{2} + \frac{x_1^2}{4} \quad |i-j| = 0, \text{ and} \quad (1.18)$$

$$P(i,j)=\frac{x_0^{\,2}+x_1^{\,2}+x_3^{\,2}}{4}+\frac{x_4^{\,2}}{2}\quad,\quad |i-j|=1 \tag{1.19}$$

$$S(1,2)=\frac{-x_1^{\,2}}{4}-x_4^{\,2}$$

and . (1.20)

For negative U values, we have the following results.

$$P(i,i)=\frac{1}{2}\left(x_0^{\,2}+x_1^{\,2}\right)+\frac{x_2^{\,2}}{2}\quad,\quad |i-j|=0 \tag{1.21}$$

$$P(i,j)=\frac{1}{4}\left(x_1^{\,2}+x_2^{\,2}+x_4^{\,2}\right)$$

and $,|i-j|=1$ (1.22)

1.4 NUMERICAL RESULTS.

In this section we present numerical results of the ground state energies, correlation functions and variational parameters for values of the onsite coulomb repulsion (U)

Table 1.1 Ground state energy in unit of t and the corresponding variational parameters as a function of coulomb repulsion (U) for a system of 2 interacting electrons.

U	E_g	x_0	x_1	x_2
0	-4.0000	-0.5000	-0.7071	-0.5000
2	-3.6272	-0.3685	-0.7331	-0.5717
4	-3.4186	-0.2818	-0.7392	-0.6116
6	-3.2915	-0.2550	-0.7390	-0.6350
8	-3.2078	-0.1860	-0.7370	-0.6498
10	-3.1489	-0.1580	-0.7346	-0.6598
12	-3.1056	-0.1371	-0.7323	-0.6670
-2	-4.6858	-0.6696	-0.6359	-0.3838
-4	-5.8064	-0.8152	-0.5207	-0.2536
-6	-7.2915	-0.8981	-0.4101	-0.1591
-8	-8.9879	-0.9390	-0.3280	-0.1032
-10	-10.7957	-0.9602	-0.2701	-0.0708
-12	-12.6648	-0.9722	-0.2285	-0.0510

Table 1.2 Pair correlation function and Spin correlation function versus onsite coulomb repulsion (U) for a system of 2 interacting electrons.

U	P(i,i)	P(i,j) $\lvert i-j\rvert=1$	P(i,j) $\lvert i-j\rvert=2$	S(i,j) $\lvert i-j\rvert=1$	S(i,j) $\lvert i-j\rvert=2$
0	0.0625	0.0625	0.0625	-0.0937	-0.0938
2	0.0339	0.0672	0.0817	-0.1008	-0.1226
4	0.0199	0.0683	0.0935	-0.1025	-0.1403
6	0.0163	0.0683	0.1008	-0.1024	-0.1512
8	0.0086	0.0679	0.1056	-0.1018	-0.1583
10	0.0062	0.0675	0.1088	-0.1012	-0.1633
12	0.0047	0.0670	0.1112	-0.1019	-0.1668
-2	0.1121	0.0505	0.0368	-0.0758	-0,0552
-4	0.1661	0.0339	0.0161	-0.0508	-0.0241
-6	0.2016	0.0210	0.0063	-0.0315	-0.0095
-8	0.2204	0.0134	0.0027	-0.0202	-0.0040
-10	0.2305	0.00912	0.0013	-0.0137	-0.0019
-12	0.2363	0.00653	0.0007	-0.0098	-0.0010

Table 1.3 Ground state energies in unit of t and variational parameters as a function of positive values of the onsite coulomb repulsion (U) for a system of 4 interacting electrons.

U	E_g	x_0	x_1	x_2	x_3	x_4
0	--4.0000	-0.3536	-0.7071	0.0000	0.3536	-0.5000
0.5	-3.6490	-0 .2978	-0.6923	0.0000	0.3795	-0.5366
1.0	-3.3408	-0.2516	-0.6719	0.0000	0.4022	-0.5688
1.5	-3.0691	-0.2135	-0.6479	0.0000	0.4222	-0.5971
2.0	-2.8284	-0.1821	-0.6219	0.0000	0.4397	-0.6219
2.5	-2.6147	-0.1563	-0.5950	0.0000	0.4552	-0.6437
3.0	-2.4244	-0.1349	-0.5682	0.0000	0.4687	- 0.6628
3.5	-2.2546	-0.1171	-0.5417	0.0000	0.4806	-0.6796
4.0	-2.1027	-0.1022	-0.5162	0.0000	0.4910	-0.6943

Table 1.4 Ground state energies in unit of t and variational parameters as a function of negative values of the onsite coulomb repulsion (U) for a system of 4 interacting electrons.

U	E_g	x_0	x_1	x_2	x_3	x_4
0	--4.0000	0. 5000	-0.3536	0.7071	0.0000	0.3536
-0.5	-4.6490	0 .5366	-0.3795	0.6923	0.0000	-0.2978
-1.0	-5.3408	-0.5688	-0.4022	-0.6719	0.0000	-0.2516
-1.5	-6.0691	0.5971	-0.4222	0.6479	0.0000	0.2135
-2.0	-6.8284	-0.6219	-0.4397	-0.6219	0.0000	-0.1821
-2.5	-7.6147	-0.6437	-0.4552	-0.5950	0.0000	-0.1563
-3.0	-8.4244	0.6628	-0.4687	- 0.5682	0.0000	0.1349
-3.5	-9.2546	0.6796	-0.4806	-0.5417	0.0000	0.1171
-4.0	-10.1027	-0.6943	-0.4910	-0.5162	0.0000	-0.1022

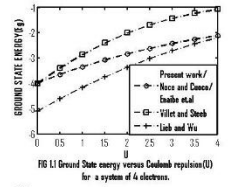

FIG 1.1 Ground State energy versus Coulomb repulsion(U) for a system of 4 electrons.

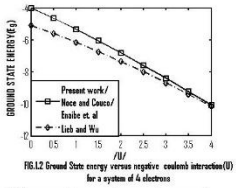

FIG.1.2 Ground State energy versus negative coulomb interaction(U) for a system of 4 electrons

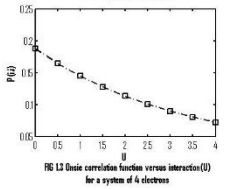

FIG 1.3 Onsite correlation function versus interaction(U) for a system of 4 electrons

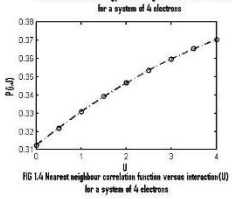

FIG 1.4 Nearest neighbour correlation function versus interaction(U) for a system of 4 electrons

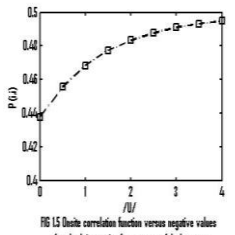

FIG 1.5 Onsite correlation function versus negative values of coulomb interaction for a system of 4 electrons.

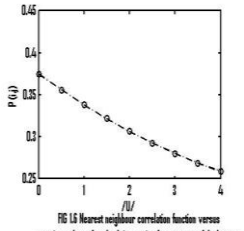

FIG 1.6 Nearest neighbour correlation function versus negative values of coulomb interaction for a system of 4 electrons

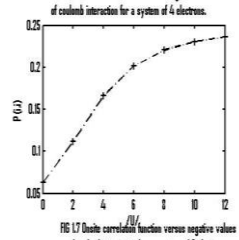

FIG 1.7 Onsite correlation function versus negative values of coulomb interaction for a sysytem of 2 electrons.

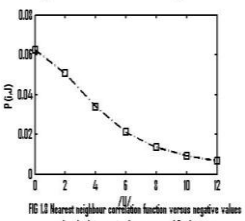

FIG 1.8 Nearest neighbour correlation function versus negative values of coulomb interaction for a system of 2 electrons

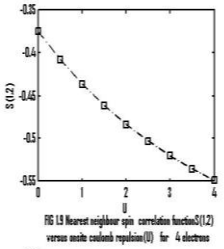

FIG 1.9 Nearest neighbour spin correlation function S(1,2) versus onsite coulomb repulsion(U) for 4 electrons

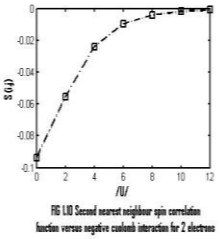

FIG 1.10 Second nearest neighbour spin correlation function versus negative coulomb interaction for 2 electrons

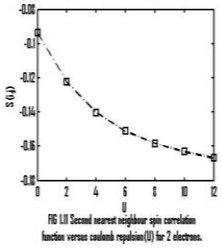

FIG 1.11 Second nearest neighbour spin correlation function versus coulomb repulsion(U) for 2 electrons.

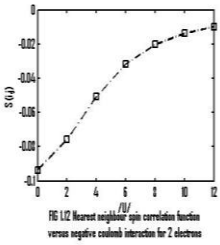

FIG 1.12 Nearest neighbour spin correlation function versus negative coulomb interaction for 2 electrons

1.5 Discussion of Results

Let us begin our discussion with the non-half filled case that is a system of two interacting electrons. In table 1.1 the ground state energy increases as the coulomb repulsion (U) increases, and decreases when the interaction becomes negative (attractive).This is expected to happen since the coulomb interaction is measured in units of the hopping integral t. In fact ground state energies obtained in Table 1.1 for the two interacting electrons is exactly the same as the one's obtained using the correlated variational wavefunction approach[11]. In table 1.2, computed values of pair correlation functions and spin correlation functions are presented for two electron systems. It is observed that the onsite or double occupancy correlation function decreases as the repulsive coulomb repulsion increases. Of particular interest is the first nearest neighbor correlation function which increases up to $U = 4t$, for $U > 4t$, it starts to decrease. This behavior is similar to the result obtained by Hirsh [12] for two electrons on 4sites using the Monte Carlo method. In Fig 1.7 onsite pair correlation function increases for negative values of coulomb interaction (U), whereas Fig 1.8 shows a decrease for first nearest neighbour correlation function.

The overall behavior of pair correlation function $p(i, j)$ can be explained as follows; when an electron with an up-spin sits at a site, and the coulomb repulsion is switched on, a down spin electron will be pushed away from that place. The probability of finding down-spin electrons has to increase in the neighbourhood of the studied place, to guarantee the conservation of down-spin electrons. Negative values of spin correlation functions between sites characterize antiferromagnetic correlations and extend along the lattice; it decreases for repulsive values of U and increases for negative values of U as shown in Fig. 1.11 and 1.12 respectively.

Let us now conclude our discussion by looking at a half-filled system; that is a system of 4 interaction electrons. In tables 1.7 and 1.8, we have computed ground state energies for values of coulomb interaction (U). It is observed in the limit $U \to 0$, $E_g = -4.0000\ t$ and this reproduces the well known result of $E_o = -tL$ of Dongen and Vollhardt[13] obtained at half filling. Computed values of the ground state energies of four interacting electrons are in excellent agreement with the results obtained by Enaibe et al.[8] ,Nonce and Cuoco[6] as shown in Fig 1.1 and Fig 1.2 repectively.Our results also compare nicely with the values obtained by Salerno[14,15] and Leprevost et al.[16] In the large U limit ,say $U = 4t$, $E_g = -2.1027\ t$, while the famous result of Lieb and Wu[5] gives $E_g = 2.1810\ t$. Our result also show a significant improvement when compared with result obtained by Villet and Steeb[9] who took account of the C_{4v} space group symmetry in diagonalizing the half-filled 4-site Hubbard model. In fact for $U = 4t$, we obtained $-2.1027\ t$ while Villet and Steeb[9] got $-1.0681\ t$ .The dependence of correlation functions on coulomb interaction (U) for 4 electrons is similar to the non-half filled case of 2 interacting electrons.

Finally, we have used the two different one-dimensional representations of the C_{4v} group, that is B_1 and A_1 to construct two different variational wave function of four interacting electrons. The ground state energy matrix Eqn (1.8) obtained using B_1 is valid for coulomb repulsion (U), while the ground state energy matrix Eqn (1.10) obtained using A_1 is valid for negative values of a U (attractive interaction).These are shown in Fig 1.1 and Fig 1.2 respectively.

1.6 Conclusion

In closing this paper we have presented a method to compute the ground state properties of the 4-site Hubbard model at half-filling and away from half filling using the space symmetry group C_{4v} of the Hamiltonian Eqn.(1.1). We have also derived a scheme to construct a variational wavefunction that will enable us to determine ground state properties of interacting electrons other than ground state energies. The variational wavefunction constructed using this approach shows significant improvement when compared with the correlated variational wavefunction approach of Enaibe et al.[8] , where the largest matrix block to be diagonalized is (9×9). In our present scheme, the largest block is a (4×4) matrix.

This scheme can also be easily applied to other strongly correlated models such as $t - J$, Heisenberg and Anderson models.

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